Quantum Mechanics and Geometry

(preliminary draft updated Jan 2025)

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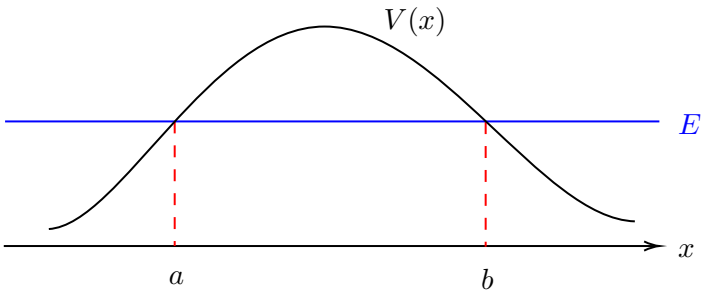
量子隧穿的启示[1]：无惧虚度时间，逾越高山险阻。



$$\underbrace{-i\int_a^b \sqrt{\frac{m}{2(V(x)-E)}}\,dx}$$

imaginary time (虚时间) for quantum tunneling

Thanks very much for your support of this note! Comments and suggestions are greatly appreciated. You can contact me at sili@mail.tsinghua.edu.cn. The draft will be updated on my homepage:

https://sili-math.github.io/

[1] See Section 2.7.3

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Preface

In April 2021, Qiuzhen College (求真书院) was newly established at Tsinghua University under the leadership of Professor Shing-Tung Yau. It homes the distinguished elite mathematics program in China starting in 2021: the "Yau Mathematical Sciences Leaders Program" (丘成桐数学科学领军人才培养计划). This program puts strong emphasis on basic sciences related to mathematics in a broad sense. Though majored in mathematics, students in this program are required to study fundamental theoretical physics such as classical mechanics, electromagnetism, quantum mechanics, and statistical mechanics, in order to understand global perspectives of theoretical sciences. It is an exciting challenge both for students and for instructors.

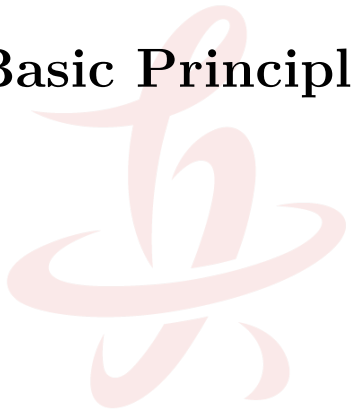
This preliminary note is intended for the course "Quantum Mechanics" that I lectured at Tsinghua University in 2023 and 2024. It is a continuation of [36, 37] in this series. The first part of the note is physics-oriented and aims to elucidate the fundamentals of quantum mechanics. Chapter 1 explains the foundational principles of traditional Hilbert space and operator approach to quantum mechanics. This formalism establishes a framework for describing the evolution of quantum systems in terms of unitary transformations and measurements. Chapter 2 explains the path integral approach to quantum mechanics, which characterizes quantum dynamics of particles in terms of probabilistic paths. This formalism provides a powerful tool for calculating transition amplitudes and understanding quantum phenomena, and has been widely generalized and developed within modern quantum field theory. These two equivalent formalisms are deeply intertwined and illustrate different faces of the exciting development of quantum mechanics.

The second part of the note is mathematics-oriented with emphasis on modern geometric and algebraic formulations of quantization. Chapter 3 explains the phase-space formalism of quantum mechanics as well as the theory of geometric quantization and perturbative approach to path integrals in phase space. Chapter 4 is focused on the algebraic theory of deformation quantization which deals with the operator of quantum observables as a formal deformation of classical observables. In this theory, the Planck's constant $\hbar$ is treated as a formal variable parametrizing a family of quantum algebras.

Two parts of the note are closed related and we explain the bridge along the way. Some useful resources that we consulted are listed at the end of this note.

Part I

Basic Principles



Chapter 1 Hilbert Space Formalism

In this chapter, we explain the foundational principles of Hilbert space and operator approach to quantum mechanics. This formalism establishes a framework for describing the evolution of quantum systems in terms of unitary transformations and measurements.

1.1 State Space

1.1.1 Classical State

One fundamental difference between classical mechanics and quantum mechanics is how a state of the system is described. Recall that in classical mechanics, the state of a particle is usually described by a point in the phase space M, whose geometry is described by a symplectic manifold. For most cases of our interest, M is parametrized by $\{x^i, p_i\}$, where

$$\begin{cases} x^i = \text{(generalized) position,} \\ p_i = \text{(generalized) momentum conjugate to } x^i. \end{cases}$$

The time evolution of the state is described by a trajectory parametrized by the time:

$$\{x^i(t), p_i(t)\} : \qquad \text{state at time } t.$$

In the Hamiltonian formalism, this classical evolution is described by Hamilton's equations

$$\begin{cases} \dfrac{dx^i}{dt} = \dfrac{\partial \mathscr{H}}{\partial p_i}, \\ \dfrac{dp_i}{dt} = -\dfrac{\partial \mathscr{H}}{\partial x^i}. \end{cases}$$

Here $\mathscr{H}$ is a function on the phase space, called the *Hamiltonian function*. The system of Hamilton's equations determines the evolution of the state.

1.1.2 Quantum State

In quantum mechanics, the state of the particle is represented by a vector in a *Hilbert space* $\mathbb{V}$. We will always assume that the Hilbert space $\mathbb{V}$ is separable.

Definition 1.1.1. A Hilbert space is a $\mathbb{C}$-linear vector space equipped with a positive definite Hermitian inner product such that the space is complete with respect to the induced norm.

One can also talk about $\mathbb{R}$-linear Hilbert spaces, but we will focus on the $\mathbb{C}$-linear case. As we will see, the angular phase factor will play an important role in quantum mechanics.

Let $\mathbb{V}$ be a Hilbert space. The Hermitian inner product is a sesquilinear pairing

$$\langle -|- \rangle : \mathbb{V} \times \mathbb{V} \longrightarrow \mathbb{C}$$

which is conjugate linear in the first argument and linear in the second:

$$\begin{cases} \langle \lambda\psi|\varphi\rangle = \overline{\lambda}\langle\psi|\varphi\rangle \\ \langle \psi|\lambda\varphi\rangle = \lambda\langle\psi|\varphi\rangle \end{cases} \qquad \forall \lambda \in \mathbb{C},\ \psi, \varphi \in \mathbb{V}.$$

The Hermitian property says

$$\overline{\langle\psi|\varphi\rangle} = \langle\varphi|\psi\rangle \qquad \forall \psi, \varphi \in \mathbb{V}.$$

The positive definite property says

$$\begin{cases} \langle\psi|\psi\rangle \geq 0 & \forall \psi \in \mathbb{V} \\ \langle\psi|\psi\rangle = 0 & \text{if and only if } \ \psi = 0. \end{cases}$$

The induced norm on $\mathbb{V}$ is given by

$$\|\psi\| := \sqrt{\langle\psi|\psi\rangle}, \qquad \psi \in \mathbb{V}.$$

Being a Hilbert space, $\mathbb{V}$ has to be complete with respect to the norm $\|\cdot\|$.

Example 1.1.2. $\mathbb{V} = \mathbb{C}^n$. *A vector $u \in \mathbb{V}$ is represented by*

$$u = \begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix}, \qquad z_i \in \mathbb{C}.$$

We can define the standard Hermitian inner product by

$$\langle u|v\rangle = \sum_i \overline{z}_i w_i$$

for $u = \begin{pmatrix} z_1 & \cdots & z_n \end{pmatrix}^T$, $v = \begin{pmatrix} w_1 & \cdots & w_n \end{pmatrix}^T$. Then $\mathbb{C}^n$ is a finite dimensional Hilbert space.

Example 1.1.3. $\mathbb{V} = L^2(\mathbb{R})$. *For any $f, g \in L^2(\mathbb{R})$, define*

$$\langle f|g\rangle = \int_{\mathbb{R}} \overline{f}(x) g(x) dx.$$

This defines an infinite dimensional Hilbert space.

Remark 1.1.4. We will use Dirac's bra-ket notation and write a vector $\psi \in \mathbb{V}$ as a "ket"

$$|\psi\rangle \in \mathbb{V}.$$

A "bra" $\langle\varphi|$ for $\varphi \in \mathbb{V}$ represents the linear form

$$\begin{aligned} \langle\varphi| : \mathbb{V} &\longrightarrow \mathbb{C} \\ |\psi\rangle &\longmapsto \langle\varphi|\psi\rangle. \end{aligned}$$

In other words, the "bra" is related to the "ket" in terms of Hermitian conjugate.

For example of $\mathbb{V} = \mathbb{C}^n$, given

$$u = \begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix}, \qquad v = \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix} \qquad \in \mathbb{V},$$

we can represent

① "ket": $|v\rangle = \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix}$

② "bra": $\langle u| = \begin{pmatrix} \overline{z}_1 & \cdots & \overline{z}_n \end{pmatrix}$.

Then the Hermitian inner product is

$$\langle u|v\rangle = \begin{pmatrix} \overline{z}_1 & \cdots & \overline{z}_n \end{pmatrix} \cdot \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix}.$$

So what is the essential change for the description of state from classical to quantum?

Classical State	Quantum State
Set	Vector space

The algebraic structure on the space of states has been enhanced from a set to a vector space! This in particular implies that we can take a linear superposition of two quantum states $|\psi_1\rangle, |\psi_2\rangle \in \mathbb{V}$ to form another quantum state

$$\lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle \qquad \in \mathbb{V}$$

where $\lambda_1, \lambda_2 \in \mathbb{C}$. This linear operation is not allowed on the set of classical states. As we will see later in this note, many interesting quantum phenomena come out of this linear structure.

To get a first impression, consider a quantum system described by a two dimensional Hilbert space spanned by

$$|\uparrow\rangle, \qquad |\downarrow\rangle.$$

For example, this could be a spin system, where $|\uparrow\rangle$ indicates a state with "spin up", and $|\downarrow\rangle$ indicates a state with "spin down". Then we can take a combination to obtain a state

$$\frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{1}{\sqrt{2}}|\downarrow\rangle.$$

This is a new state. But what is its spin? You should keep this simple question in mind along the way. It is as good as the state $|\uparrow\rangle$ or the state $|\downarrow\rangle$.

As another example for illustration, let us consider how to describe the state for two particles. In the classical case, if the set of states for particle i is M_i, $i = 1, 2$, then the state space for the total is

$$M_1 \times M_2.$$

In the quantum case, if the state space for particle i is $\mathbb{V}_i$, then the naive set-theoretical product $\mathbb{V}_1 \times \mathbb{V}_2$ does not work. This is simply because $\mathbb{V}_1 \times \mathbb{V}_2$ is not a linear vector space. Instead, we have to consider its linearization and arrive at the tensor product

$$\mathbb{V}_1 \otimes \mathbb{V}_2.$$

A main difference between $M_1 \times M_2$ and $\mathbb{V}_1 \otimes \mathbb{V}_2$ is that a point in $M_1 \times M_2$ is of the form

$$m_1 \times m_2 \qquad \text{where } m_1 \in M_1,\ m_2 \in M_2$$

while a vector in $\mathbb{V}_1 \otimes \mathbb{V}_2$ could be of the form

$$\sum_{i=1}^{k} \psi_i \otimes \varphi_i \qquad \text{where } \psi_i \in \mathbb{V}_1,\ \varphi_i \in \mathbb{V}_2.$$

For example, this tensor structure is the origin of quantum entanglement.

1.1.3 Schrödinger Equation

We next discuss the law governing the time evolution of quantum states.

Definition 1.1.5. Let A be a linear operator on the Hilbert space $\mathbb{V}$ with a dense domain $\mathrm{Dom}(A) \subset \mathbb{V}$. The adjoint operator A^* of A is defined by

$$A^* : \mathrm{Dom}(A^*) \longrightarrow \mathbb{V}$$

where the domain of A^* is

$$\mathrm{Dom}(A^*) = \left\{ \psi \in \mathbb{V} \,\middle|\, \exists \tilde{\psi} \in \mathbb{V} : \langle \psi | A\varphi \rangle = \left\langle \tilde{\psi} \middle| \varphi \right\rangle, \quad \forall \varphi \in \mathrm{Dom}(A) \right\}.$$

Here, for $\psi \in \mathrm{Dom}(A^*)$ and $\tilde{\psi}$ as above,

$$A^*\psi = \tilde{\psi}.$$

Symbolically, the defining relation for the adjoint is

$$\langle A^*\psi | \varphi \rangle = \langle \psi | A\varphi \rangle$$

for $\varphi \in \mathrm{Dom}(A)$, $\psi \in \mathrm{Dom}(A^*)$.

Definition 1.1.6. If $A = A^*$, then A is called *self-adjoint*.

Remark 1.1.7. When $\mathbb{V}$ is finite dimensional and A is represented by a matrix, A^* is given by the conjugate transpose. There a self-adjoint operator is the same as a Hermitian matrix. When $\mathbb{V}$ is infinite dimensional, which is of our interest in quantum mechanics, self-adjoint operators are much more delicate and we have to work with densely defined domain. Nevertheless, interested readers can refer to standard context in functional analysis to clarify related statements.

In quantum mechanics, the time evolution of quantum state $|\psi(t)\rangle$ obeys the

$$\textit{Schrödinger equation}: \qquad i\hbar\frac{d}{dt}|\psi(t)\rangle = \widehat{\mathrm{H}}\,|\psi(t)\rangle.$$

Here $\widehat{\mathrm{H}}$ is a self-adjoint operator, called the *Hamiltonian operator*. The positive number $\hbar$ is called the *Planck constant*, which is one of the fundamental constants in physics.

Assume $\widehat{\mathrm{H}}$ is time-independent, then the Schrödinger equation can be formally solved by

$$|\psi(t)\rangle = e^{-i\,\widehat{\mathrm{H}}\,t/\hbar}|\psi(0)\rangle.$$

The operator $e^{-i\,\widehat{\mathrm{H}}\,t/\hbar}$ (which can be defined using functional calculus) is a one-parameter family of unitary operators on $\mathbb{V}$, known as the time-evolution operators. Conversely, a strongly continuous one-parameter family of unitary transformations is generated infinitesimally by a self-adjoint operator. This is known as Stone's Theorem.

1.2 Observables

1.2.1 Classical Observables

In classical mechanics, observables are represented by functions on the phase space M

$$\mathrm{Obs}^{cl} = \mathcal{O}(M).$$

Here $\mathcal{O}(M)$ means (appropriate) space of functions on M. We will not specify the class of functions to avoid technical discussions unnecessary for our purpose. You can safely work with smooth functions here.

Since M is a symplectic manifold, the space of functions $\mathcal{O}(M)$ on it naturally carries a structure of Poisson bracket

$$\{-,-\} : \mathcal{O}(M)\times\mathcal{O}(M) \longrightarrow \mathcal{O}(M).$$

It is a bilinear map and satisfies the following properties

- Skew-symmetry: $\{f,g\} = -\{g,f\}$.
- Leibniz rule: $\{f,gh\} = \{f,g\}h + g\{f,h\}$.
- Jacobi identity: $\{\{f,g\},h\} + \{\{g,h\},f\} + \{\{h,f\},g\} = 0$.

For example, assume the phase space M is parametrized by $\{x^i\}$ and their conjugates $\{p_i\}$, such that the symplectic structure takes the form

$$\sum_i dx^i \wedge dp_i.$$

Then a classical observable is a function $f(x,p)$ of $\{x^i, p_i\}$. The Poisson bracket takes the form

$$\{f,g\} = \sum_i \left(\frac{\partial f}{\partial x^i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial x^i} \right).$$

1.2.2 Quantum Observables

In quantum mechanics, quantum observables consist of self-adjoint linear operators on the Hilbert space $\mathbb{V}$ of the system. We have seen one such quantum observable, the Hamiltonian $\widehat{\mathrm{H}}$, which governs the dynamical evolution of the system via the Schrödinger equation.

Let Obs^q denote the space of quantum observables. Let A, B be two self-adjoint operators

$$A = A^*, \qquad B = B^*.$$

We consider their commutator

$$[A,B] := AB - BA.$$

Its adjoint is

$$\begin{aligned}[A,B]^* &= B^*A^* - A^*B^* = [B^*, A^*] \\ &= [B,A] = -[A,B].\end{aligned}$$

Therefore $i[A,B]$ is again self-adjoint. The combination

$$[-,-]_\hbar := -\frac{i}{\hbar}[-,-] : \mathrm{Obs}^q \times \mathrm{Obs}^q \longrightarrow \mathrm{Obs}^q$$

defines the *quantum bracket* on quantum observables. Here the positive number $\hbar$ is the Planck constant. The quantum bracket is again skew-symmetric

$$[A,B]_\hbar = -[B,A]_\hbar$$

and satisfies the Jacobi identity

$$[A,[B,C]_\hbar]_\hbar + [B,[C,A]_\hbar]_\hbar + [C,[A,B]_\hbar]_\hbar = 0.$$

These properties follow from the associativity of the composition of operators.

The algebraic relation between classical and quantum observables can be summarized by

$$\begin{array}{ccc} \mathrm{Obs}^{cl} & & \mathrm{Obs}^q \\ \\ \text{Poisson algebra} & \xrightarrow{\text{quantization}} & \text{Associative algebra} \\ \\ (\cdot, \{-,-\}) & \xleftarrow{\text{classical limit}} & (*_\hbar, [-,-]_\hbar) \end{array}$$

The classical Poisson bracket $\{-,-\}$ measures the leading order noncommutativity of quantum operators. Strictly speaking, we have extended Obs^q to contain linear operators that are not self-adjoint, in order to perform compositions to form an associative algebra. The study of such algebraic correspondence is the main subject of deformation quantization. We will discuss in details about this in Chapter 4.

1.2.3 Expectation

Let $\mathbb{V}$ be the Hilbert space of a quantum system. Let $\mathcal{O}$ be a quantum observable, which is a self-adjoint operator on $\mathbb{V}$. Assume the system is at the state $|\psi\rangle \in \mathbb{V}$. The expectation value of $\mathcal{O}$ of the system is defined to be

$$\langle \mathcal{O} \rangle_\psi := \frac{\langle \psi | \mathcal{O} | \psi \rangle}{\langle \psi | \psi \rangle}.$$

Here $\mathcal{O}|\psi\rangle = |\mathcal{O}\psi\rangle$ is the action of $\mathcal{O}$ on the state $|\psi\rangle$. It would be convenient to normalize the state such that

$$\|\psi\| = \sqrt{\langle \psi | \psi \rangle} = 1.$$

In many contexts, states of quantum system are referred to normalized vectors in the Hilbert space. Then in the normalized case

$$\langle \mathcal{O} \rangle_\psi = \langle \psi | \mathcal{O} | \psi \rangle.$$

Note that the expectation values of quantum observables are real numbers. In fact,

$$\langle \psi | \mathcal{O} | \psi \rangle = \langle \psi | \mathcal{O}\psi \rangle = \langle \mathcal{O}^* \psi | \psi \rangle \overset{\mathcal{O}^* = \mathcal{O}}{=\!=} \langle \mathcal{O}\psi | \psi \rangle = \overline{\langle \psi | \mathcal{O}\psi \rangle} = \overline{\langle \psi | \mathcal{O} | \psi \rangle}$$

$$\Longrightarrow \qquad \langle \psi | \mathcal{O} | \psi \rangle \in \mathbb{R}.$$

Here we have used the self-adjoint property of $\mathcal{O}$. This implies that eigenvalues of $\mathcal{O}$ are real.

Assume $|\psi\rangle$ is a normalized eigenvector of A with eigenvalue λ. By our discussion above, λ has to be a real number. As we will discuss soon later, eigenvalues are the outcomes of physical measurement for quantum observables.

1.3 Measurement

1.3.1 Born Rule

We have discussed two basic postulates of quantum mechanics:

- *a quantum state is a vector in a Hilbert space* $\mathbb{V}$.
- *a quantum observable is a self-adjoint operator on* $\mathbb{V}$.

Now we turn to the interpretation of measurement for a quantum observable in a given quantum state. The first statement is

- *possible outcomes of quantum measurements are eigenvalues of quantum observables.*

Let $\mathcal{O}$ be a quantum observable, which is a self-adjoint operator on $\mathbb{V}$. As we have seen, self-adjointness implies that eigenvalues of $\mathcal{O}$ are all real numbers. The above postulate says that these real numbers are the possible outcomes of measurements of $\mathcal{O}$.

Assume the system is now at a state $|\psi\rangle \in \mathbb{V}$. How come to obtain an eigenvalue of $\mathcal{O}$ out of the quantum state $|\psi\rangle$ under a measurement?

Firstly, assume $|\psi\rangle$ is an eigenvector of $\mathcal{O}$ with eigenvalue λ

$$\mathcal{O}|\psi\rangle = \lambda|\psi\rangle.$$

Then it is natural to expect that the measurement of $\mathcal{O}$ in the state $|\psi\rangle$ is λ. This is indeed the case. However, in general $|\psi\rangle$ may not be an eigenvector of $\mathcal{O}$, What do we get? The answer is probabilistic, known as the *Born rule*.

Let us first mention that two vectors in $\mathbb{V}$, which are proportional by a nonzero complex number, represent the same physical states. In other words, each physical state is represented by a "ray" in the Hilbert space $\mathbb{V}$. For example, the expectation value of the quantum observable $\mathcal{O}$ in a state $|\psi\rangle$

$$\langle\mathcal{O}\rangle_\psi = \frac{\langle\psi|\mathcal{O}|\psi\rangle}{\langle\psi|\psi\rangle}$$

is the same if you replace $|\psi\rangle$ by $a|\psi\rangle$ for any complex number $a \in \mathbb{C}^*$. Therefore we usually normalize the state and represent a physical state by a vector of length 1

$$\langle\psi|\psi\rangle = 1.$$

We will call such vector of unit length a *normalized state*.

Let $\mathcal{O}$ be a given quantum observable. Assume $|\psi_1\rangle$ and $|\psi_2\rangle$ are eigenvectors

$$\mathcal{O}|\psi_1\rangle = \lambda_1|\psi_1\rangle, \qquad \mathcal{O}|\psi_2\rangle = \lambda_2|\psi_2\rangle$$

with different eigenvalues $\lambda_1 \neq \lambda_2$. Then these two vectors $|\psi_1\rangle$ and $|\psi_2\rangle$ must be orthogonal

$$\langle\psi_1|\psi_2\rangle = 0.$$

This follows from the self-adjointness of $\mathcal{O}$

$$\lambda_2\langle\psi_1|\psi_2\rangle = \langle\psi_1|\mathcal{O}\psi_2\rangle = \langle\mathcal{O}\psi_1|\psi_2\rangle = \lambda_1\langle\psi_1|\psi_2\rangle$$

$$\Longrightarrow \qquad \langle\psi_1|\psi_2\rangle = 0.$$

If $|\psi_1\rangle$ and $|\psi_2\rangle$ have the same eigenvalue $\lambda_1 = \lambda_2$, then they may not be orthogonal. Nevertheless, we can apply the Gram-Schmidt procedure to rearrange them to be orthogonal.

Let us assume that the quantum state $|\psi\rangle$ of the system under measurement can be decomposed in terms of orthonormal eigenstates of the quantum observable $\mathcal{O}$

$$|\psi\rangle = \sum_\alpha c_\alpha|\psi_\alpha\rangle, \qquad c_\alpha \in \mathbb{C}.$$

Here $\mathcal{O}|\psi_\alpha\rangle = \lambda_\alpha|\psi_\alpha\rangle$ for eigenvalues λ_α, and $|\psi_\alpha\rangle$'s are normalized vectors and orthogonal with each other for different α's. Things could be complicated in general where some λ_α's could be the same (so with degenerate eigenspace) or eigenvalue spectrum could be continuous (see Section 1.8 for one example). Let us not worry about these issues at the moment.

Assume $|\psi\rangle$ is normalized. The normalization condition $\langle\psi|\psi\rangle = 1$ implies (using the orthonormal property of $|\psi_\alpha\rangle$'s)

$$\sum_\alpha |c_\alpha|^2 = 1.$$

One interprets this formula as probability.

Born rule: the result of measurement of a quantum observable $\mathcal{O}$ in the quantum state $|\psi\rangle$ is probabilistic: the probability of the measurement with answer λ is

$$P(\lambda) = \sum_{\lambda_\alpha=\lambda} |c_\alpha|^2.$$

Using the orthonormal property, the complex number c_α can be obtained by

$$c_\alpha = \langle\psi_\alpha|\psi\rangle$$

which is called the *probability amplitude*. Thus the Born rule can be stated as

$$\text{Probability} = |\text{Amplitude}|^2$$

Remark 1.3.1. In the case of continuous spectrum, we need to invoke spectral theorem to give probability measure.

1.3.2 Collapse of the State Vector

The experiment for measurement in quantum mechanics involves the composite systems essentially. Said in another way, any measurement of a quantum system (with an external apparatus) will disturb the state. In fact, it is even more mysterious. After measurement of a quantum observable $\mathcal{O}$, with outcome of an eigenvalue λ, the state will change into an eigenstate of the corresponding eigenvalue λ. This phenomenon is called the

"*collapse of the state vector*".

Since the state becomes an eigenvector after the measurement, if there is no other disturbance of the system, then the further repeated measurement of $\mathcal{O}$ will always produce λ.

There are a collection of views about the meaning of quantum mechanics, including the above Born rule and collapse of the state vector. It coins the term "*Copenhagen interpretation*". It is not entirely satisfactory, and leads to many confusions and debates in the history. Concerning the collapse, there is also the "*many-worlds interpretation*" by Hugh Everett, which assumes that the state vector does not collapse, but all possible outcomes of quantum measurements are realized in some parallel worlds. We will not go further into these issues here.

Nevertheless, quantum mechanics works, and has been one of the most successful framework in physics. Many people take practical viewpoints. Here is a famous quote by David Mermin:

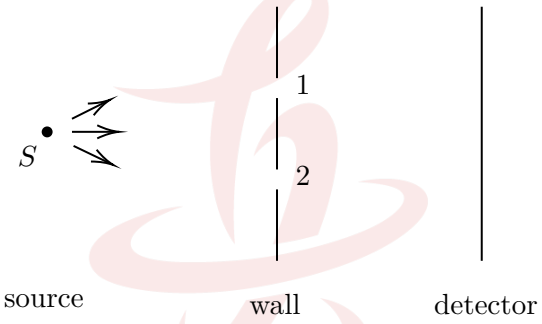
"*If I were forced to sum up in one sentence what the Copenhagen interpretation says to me, it would be 'Shut up and Calculate!'* "

So we see that even though the evolution of the state is deterministic, captured by the Schrödinger equation, the prediction for the measurement is probabilistic. Furthermore, the measurement will change the state. Then how do we test quantum mechanics?

To test such probabilistic prediction, we need to prepare a quantum ensemble consisting of a large number of particles in the same state. Then we do the same measurement for each particle. The outcome of each measurement ends up with some eigenvalue, which may differ in a repeated measurement for another particle in the same state. Then we can collect the statistical result of these measurement to check with the probabilistic prediction.

1.3.3 The Double Slit Experiment

Consider the following experiment set-up: there is a source S on the left which is able to emit particles in all directions; there is a wall in the middle with two small holes on it; there is a screen on the right which is a detector that can record each particle when it arrives.



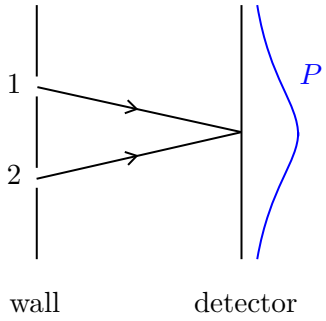
We are looking for the outcome distribution of particle counts on the detector.

In the classical picture, if we close the hole 2, we find a distribution of particle counts on the detector that come from the hole 1 only. Let us call this P_1. Similarly, if we close the hole 1 and leave the hole 2 open, we find a distribution P_2 that counts particles that come from the hole 2. Now if we open both holes, we shall see the distribution on the detector as the sum of the above two

$$P = P_1 + P_2.$$

The resulting distribution P would look like

Classical Picture:



In the quantum case, we have a superposition of the above two situations. From the linear relation

$$\langle\phi|\psi_1+\psi_2\rangle=\langle\phi|\psi_1\rangle+\langle\phi|\psi_2\rangle$$

we see that it is the probability amplitude that is summed over from each case

$$\mathcal{A}=\mathcal{A}_1+\mathcal{A}_2.$$

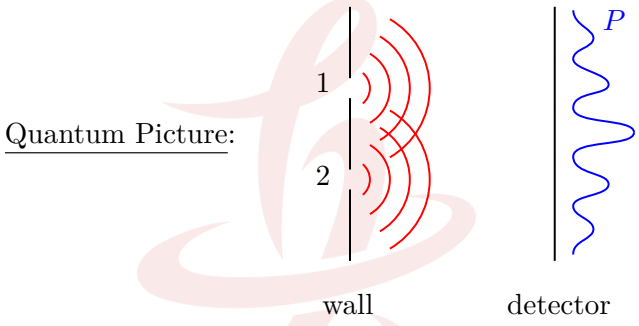
As we have seen, the probability distribution of the measurement is the square of the amplitude

$$P_1=|\mathcal{A}_1|^2,\qquad P_2=|\mathcal{A}_2|^2,$$
$$P=|\mathcal{A}|^2=|\mathcal{A}_1+\mathcal{A}_2|^2.$$

Since the amplitudes are complex numbers,

$$P\neq P_1+P_2,$$

we will observe interference pattern like that for light waves.



Now this can be tested for a beam of quantum particles, say electrons. The outcome indeed exhibits the interference pattern of the quantum picture.

This is surprising. One can try to set up another apparatus near the hole to tell us each time which hole each particle passes through the wall. To measure this, you will necessarily disturb the state of the particle. For example, you may try to achieve this by using photons to detect the electron at the hole. Such measurement will collapse the state vector. As a result, you will find the interference pattern disappears, and we arrive at the classical picture. Quantum particles behave as both waves and particles! This is the concept of wave-particle duality.

The double slit experiment was originally designed to demonstrate the wave behavior of light. It was de Broglie who made the brave postulation that all matters have wave properties. This prediction was soon verified for electrons.

1.4 Uncertainty Principle

1.4.1 Commutator and Uncertainty

Measurement of a quantum observable $\mathcal{O}$ will produce an eigenvalue of $\mathcal{O}$ and collapses the state into an eigenvector of $\mathcal{O}$. It is natural to ask whether we can measure two quantum

observables simultaneously. For example, we would like to measure the position and the momentum. This is not a problem in classical mechanics. However, we will run into trouble in quantum mechanics.

Let A, B be two quantum observables. Our postulate on measurement asks for common eigenvectors of A and B under a simultaneous measurement of them. As we have learned in linear algebra, common eigenvectors may not exist if A and B do not commute. For example, assume the case when A and B satisfy

$$[A, B] = iI$$

where I is the identity operator. Assume $|\psi\rangle$ is a common eigenvector of A and B

$$A|\psi\rangle = \lambda_1|\psi\rangle, \qquad B|\psi\rangle = \lambda_2|\psi\rangle.$$

Then

$$i|\psi\rangle = [A, B]|\psi\rangle = (AB - BA)|\psi\rangle = (\lambda_1\lambda_2 - \lambda_2\lambda_1)|\psi\rangle = 0.$$

Thus the problem of simultaneous measurement is related to the commutator of quantum observables. Let us first introduce the notion of uncertainty of a quantum observable in a state.

Definition 1.4.1. The uncertainty of $\mathcal{O}$ in a quantum state $|\psi\rangle$ is defined to be

$$(\Delta_\psi \mathcal{O})^2 := \left\langle \left(\mathcal{O} - \langle \mathcal{O} \rangle_\psi\right)^2 \right\rangle_\psi .$$

Explicitly, let $|\psi\rangle$ be a normalized state. Since $\langle \mathcal{O} \rangle_\psi \in \mathbb{R}$, we have

$$(\Delta_\psi \mathcal{O})^2 = \left\langle \left(\mathcal{O} - \langle \mathcal{O} \rangle_\psi\right) \psi \middle| \left(\mathcal{O} - \langle \mathcal{O} \rangle_\psi\right) \psi \right\rangle.$$

In particular, $\Delta_\psi \mathcal{O} = 0$ if and only if

$$\mathcal{O}|\psi\rangle = \langle \mathcal{O} \rangle_\psi |\psi\rangle,$$

i.e. when $|\psi\rangle$ is an eigenvector of $\mathcal{O}$. In this case, the measurement of $\mathcal{O}$ is certain, given by the corresponding eigenvalue. In general, the uncertainty measures the average fluctuation around the expectation. In probability, the uncertainty is also called the standard derivation. Note that we also have

$$(\Delta_\psi \mathcal{O})^2 = \left\langle \mathcal{O}^2 - 2\langle \mathcal{O} \rangle_\psi \mathcal{O} + \langle \mathcal{O} \rangle_\psi^2 \right\rangle_\psi = \langle \mathcal{O}^2 \rangle_\psi - \langle \mathcal{O} \rangle_\psi^2 .$$

A precise form of the uncertain principle is the following statement.

Proposition 1.4.2. *Consider two quantum observables A, B in a quantum state $|\psi\rangle$. Then*

$$(\Delta_\psi A)^2 (\Delta_\psi B)^2 \geq \frac{1}{4} \left| \langle [A, B] \rangle_\psi \right|^2 .$$

Proof: If one of $\Delta_\psi A$ or $\Delta_\psi B$ is zero, say $\Delta_\psi A = 0$. Then ψ is an eigenstate of A, and

$$\langle [A, B] \rangle_\psi = \langle A\psi | B\psi \rangle - \langle B\psi | A\psi \rangle = \langle A \rangle_\psi \left(\langle \psi | B\psi \rangle - \langle B\psi | \psi \rangle \right) = 0.$$

Thus we only need to consider the case when both $\Delta_\psi A$ and $\Delta_\psi B$ are nonzero.

Let $\overline{A} = A - \langle A \rangle_\psi I$ and $\overline{B} = B - \langle B \rangle_\psi I$. Then we have $\left\langle \overline{A} \right\rangle_\psi = \left\langle \overline{B} \right\rangle_\psi = 0$ and

$$\Delta_\psi \overline{A} = \Delta_\psi A, \qquad \Delta_\psi \overline{B} = \Delta_\psi B, \qquad \left[\overline{A}, \overline{B} \right] = [A, B].$$

Therefore we can assume $\langle A \rangle_\psi = \langle B \rangle_\psi = 0$ without lost of generality.

Let $|\psi\rangle$ be normalized. Then

$$\begin{cases} (\Delta_\psi A)^2 = \left\langle A^2 \right\rangle_\psi = \langle \psi | A^2 | \psi \rangle \\ (\Delta_\psi B)^2 = \left\langle B^2 \right\rangle_\psi = \langle \psi | B^2 | \psi \rangle \end{cases}$$

Since A, B are self-adjoint, the following quantities

$$\left\langle A^2 \right\rangle_\psi, \qquad \left\langle B^2 \right\rangle_\psi, \qquad i \langle [A, B] \rangle_\psi$$

are all real numbers. Let γ_1, γ_2 be two arbitrary real numbers. Then

$$\begin{aligned} 0 &\leq \| (\gamma_1 A + i\gamma_2 B) \psi \|^2 \\ &= \langle (\gamma_1 A + i\gamma_2 B) \psi | (\gamma_1 A + i\gamma_2 B) \psi \rangle \\ &= \langle \psi | (\gamma_1 A - i\gamma_2 B) (\gamma_1 A + i\gamma_2 B) | \psi \rangle \\ &= (\Delta_\psi A)^2 \gamma_1^2 + i \langle [A, B] \rangle_\psi \gamma_1 \gamma_2 + (\Delta_\psi B)^2 \gamma_2^2. \end{aligned}$$

Since this holds for arbitrary real values of γ_1, γ_2, we have

$$(\Delta_\psi A)^2 (\Delta_\psi B)^2 \geq \frac{1}{4} \left| \langle [A, B] \rangle_\psi \right|^2.$$

□

Remark 1.4.3. From the above proof, it is not hard to see that the equality in the above proposition holds if and only if there exists real numbers $(\gamma_1, \gamma_2) \neq (0, 0)$ such that $|\psi\rangle$ is an eigenvector of $\gamma_1 A + i\gamma_2 B$.

Proposition 1.4.2 states that if $\langle [A, B] \rangle_\psi \neq 0$, then there is a lower bound on the product of the uncertainties of A and B. For readers who are careful about linear operators on Hilbert spaces, you may worry about the domain for the operators in Proposition 1.4.2. There is indeed such mathematical subtleties. We will briefly comment shortly in the next subsection.

Example 1.4.4. *As we will discuss extensively later, the position operator $\hat{x}$ and momentum $\hat{p}$ in quantum mechanics satisfy the following commutation relation*

$$[\hat{x}, \hat{p}] = i\hbar.$$

Then the uncertainty inequality implies

$$(\Delta_\psi \hat{x}) (\Delta_\psi \hat{p}) \geq \frac{\hbar}{2}.$$

This is the celebrated *Heisenberg uncertainty relation.* It says that in any quantum system, we can not make precise measurement for both the position and momentum simultaneously.

1.4.2 Some Mathematical Subtleties

In quantum mechanics, we will often encounter a pair of quantum observables satisfying

$$[A, B] = i\hbar.$$

This is called the "*canonical commutation relation*". They arise naturally from the quantum observables associated to canonical conjugate quantities. The position $\hat{x}$ and momentum $\hat{p}$ is such an example.

For canonical commutation relation to hold, the Hilbert space $\mathbb{V}$ is necessarily infinite dimensional. In fact, assume $\dim_{\mathbb{C}} \mathbb{V} < \infty$, and A, B are two linear operators on $\mathbb{V}$ satisfying the canonical commutation relation. Then

$$0 = \mathrm{Tr}[A, B] = \mathrm{Tr}(i\hbar) = i\hbar \dim_{\mathbb{C}} \mathbb{V}.$$

This is a contradiction.

Let us now assume $\mathbb{V}$ is an infinite dimensional Hilbert space. We know that bounded and unbounded linear operators behave very differently. For examples, bounded linear operators can be defined on the whole $\mathbb{V}$, while unbounded linear operators can only be defined on dense subspaces of $\mathbb{V}$. The domains for relevant operators become a subtle issue, and we have to live with that. For example, the Hamiltonian operator $\widehat{\mathrm{H}}$, which captures the dynamical evolution of quantum states, is usually an unbounded operator. The next proposition reveals another essential appearance of unbounded operators.

Proposition 1.4.5. *Assume A, B are two self-adjoint operators on $\mathbb{V}$ that satisfy the canonical commutation relation*

$$[A, B] = i\hbar.$$

Then at least one of A, B is unbounded.

Proof: Let $\hbar = 1$ for simplicity. Assume both A and B are bounded, so their operator norms $\|A\| < \infty$, $\|B\| < \infty$. Since B is self-adjoint, we have $\|B^n\| = \|B\|^n$.

Inductively, one can show

$$[A, B^k] = i\ kB^{k-1}, \qquad k \geq 1.$$

Then

$$k\,\|B\|^{k-1} = \left\| i\ kB^{k-1} \right\| = \left\| [A, B^k] \right\| \leq 2\,\|A\| \left\| B^k \right\|,$$

which implies that

$$\|A\|\,\|B\| \geq \frac{k}{2}, \qquad \forall k \geq 1.$$

This is a contradiction. □

Let $\mathrm{Dom}(A)$ denote the domain of A. A mathematical precise statement of Proposition 1.4.2 is that

$$(\Delta_\psi A)^2\,(\Delta_\psi B)^2 \geq \frac{1}{4}\left|\langle [A, B] \rangle_\psi\right|^2$$

holds for a state ψ belonging to the common domain of AB and BA, i.e., for

$$\psi \in \mathrm{Dom}(AB) \cap \mathrm{Dom}(BA).$$

This indeed could lead to some mathematical subtleties. Here is one example.

Example 1.4.6. *Consider the Hilbert space*

$$\mathbb{V} = L^2([0,1]).$$

A state $\psi \in \mathbb{V}$ is a function $\psi(x)$ on $x \in [0,1]$ which is square integrable.

We define the position operator $\hat{x}$ by multiplication with x

$$(\hat{x}\psi)(x) := x\psi(x).$$

$\hat{x}$ is a bounded operator since $x \in [0,1]$.

We define the momentum operator $\hat{p}$ by the differential operator

$$\hat{p} := -i\hbar\frac{d}{dx}.$$

It is clear that the canonical commutation relation holds

$$[\hat{x}, \hat{p}] = i\hbar.$$

This implies that $\hat{p}$ must be unbounded, and so only densely defined.

For example, we can define $\hat{p}$ on continuously differentiable functions on $[0,1]$ that satisfy the periodic boundary condition

$$\psi(0) = \psi(1).$$

We can verify that for two such functions, the adjoint property holds:

$$\begin{aligned}\langle\psi_1|\hat{p}\psi_2\rangle &= \int_0^1 \overline{\psi}_1(x)\left(-i\hbar\frac{d}{dx}\psi_2(x)\right)dx \\ &= -i\hbar\overline{\psi}_1(x)\psi_2(x)\big|_0^1 + \int_0^1 \overline{-i\hbar\frac{d}{dx}\psi_1(x)}\psi_2(x)dx \\ &= 0 + \langle\hat{p}\psi_1|\psi_2\rangle = \langle\hat{p}\psi_1|\psi_2\rangle.\end{aligned}$$

One can further show that we can extend such defined $\hat{p}$ to a self-adjoint operator.

Now consider the following normalized state

$$\psi(x) = e^{2\pi i x}.$$

This is an eigenstate of $\hat{p}$ since $\hat{p}\psi = 2\pi\hbar\psi$. Thus $\Delta_\psi\hat{p} = 0$. It is also straight-forward to compute $\Delta_\psi\hat{x} = \frac{1}{\sqrt{12}}$. On the other hand,

$$\langle[\hat{x}, \hat{p}]\rangle_\psi = i\hbar \neq 0.$$

In this case, we find

$$(\Delta_\psi\hat{x})^2(\Delta_\psi\hat{p})^2 = 0$$

while

$$\frac{1}{4}\left\|\langle[\hat{x},\hat{p}]\rangle_\psi\right\|^2=\frac{1}{4}\hbar^2.$$

The uncertainty inequality of Proposition 1.4.2 fails in this case. The issue is about the domain. $\hat{x}\psi$ is no longer periodic and does not lie in the domain of $\hat{p}$.

In practice, we will work with nice state vectors in appropriate domain for relevant examples in physics, so that the uncertainty inequality does hold. We will not check this subtlety all the time. Careful readers can keep this in mind.

1.5 Wave Function

We now focus on studying quantum particles in the space $\mathbb{R}^n$. Main examples will be focused on one-dimensional case ($n=1$) and three dimensional case ($n=3$). We will use

$$\mathbf{x}=(x^1,x^2,\cdots,x^n)$$

to parametrize positions in $\mathbb{R}^n$.

1.5.1 Hilbert Space of Quantum Particle

The relevant Hilbert space that realizes the scalar quantum particle in $\mathbb{R}^n$ is

$$\mathbb{V}=L^2(\mathbb{R}^n).$$

An element $f\in\mathbb{V}$ is a complex valued measurable function that is square integrable

$$\int_{\mathbb{R}^n}d^n\mathbf{x}\;|f(\mathbf{x})|^2<+\infty.$$

Here $d^n\mathbf{x}:=dx^1dx^2\cdots dx^n$ is the standard measure on $\mathbb{R}^n$. The Hermitian inner product is

$$\langle g|f\rangle:=\int_{\mathbb{R}^n}d^n\mathbf{x}\,\overline{g(\mathbf{x})}f(\mathbf{x}).$$

In particular, the norm of f is

$$\|f\|=\sqrt{\int_{\mathbb{R}^n}d^n\mathbf{x}\;|f(\mathbf{x})|^2}.$$

Thus a function $f\in L^2(\mathbb{R}^n)$ will be also called *normalizable*. Otherwise, a function which is not square integrable will be called *non-normalizable*.

As we have discussed before, physical states are represented by normalizable functions. Nevertheless, non-normalizable functions will also play an important role. For example, given any $\mathbf{p}=(p_1,\cdots,p_n)\in\mathbb{R}^n$, the following function

$$e^{i\mathbf{p}\cdot\mathbf{x}/\hbar},\qquad\text{where}\quad\mathbf{p}\cdot\mathbf{x}=\sum_i p_ix^i$$

is non-normalizable since

$$\left|e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}\right|^2=1\qquad\text{everywhere.}$$

However, any normalizable function f can be expressed as a superposition

$$f(\mathbf{x}) = \frac{1}{(2\pi\hbar)^{n/2}} \int_{\mathbb{R}^n} d^n\mathbf{p}\, e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} \hat{f}(\mathbf{p}).$$

This is the celebrated *Fourier transform*. The corresponding Fourier modes $\hat{f}(\mathbf{p})$ can be also obtained via the inverse Fourier transform

$$\hat{f}(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{n/2}} \int_{\mathbb{R}^n} d^n\mathbf{x}\, e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar} f(\mathbf{x}).$$

1.5.2 Wave Function

Quantum mechanics describes a moving particle by a path (parametrized by the time t) in the Hilbert space. Explicitly, this is realized by a complex valued function

$$\Psi(\mathbf{x}, t)$$

such that $\Psi(\mathbf{x}, t)$ is normalizable at any fixed time t. This is called the *wave function* of the quantum particle. The evolution of the wave function obeys the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \widehat{\mathrm{H}}\, \Psi.$$

Here $\widehat{\mathrm{H}}$ is the Hamiltonian operator, which is a self-adjoint operator on the Hilbert space. We will discuss the form of $\widehat{\mathrm{H}}$ shortly.

First, we observe that the Schrödinger equation implies the invariance of norm under time evolution. In fact,

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \langle \Psi | \Psi \rangle &= \left\langle -i\hbar \frac{\partial}{\partial t} \Psi \middle| \Psi \right\rangle + \left\langle \Psi \middle| i\hbar \frac{\partial}{\partial t} \Psi \right\rangle \\ &= \left\langle -\widehat{\mathrm{H}}\, \Psi \middle| \Psi \right\rangle + \left\langle \Psi \middle| \widehat{\mathrm{H}}\, \Psi \right\rangle \\ &= 0 \qquad \text{(using self-adjointness of } \widehat{\mathrm{H}}) \end{aligned}$$

i.e., $\langle \Psi | \Psi \rangle$ does not depend on time t. Therefore we will assume the wave function is normalized by $\langle \Psi | \Psi \rangle = 1$ at any time, i.e.,

$$\int_{\mathbb{R}^n} d^n\mathbf{x}\, |\Psi(\mathbf{x}, t)|^2 = 1.$$

In the beginning, Schrödinger interpreted the wave function $\Psi(\mathbf{x}, t)$ as representing a particle that could spread out and disintegrate. There the magnitude of $|\Psi(\mathbf{x}, t)|^2$ would represent the fraction density of the particle to be found at position $\mathbf{x}$ and time t. However, this turns out to be inconsistent with experiments. Born figured out the solution and proposed the probabilistic interpretation:

$$\int_V d^n\mathbf{x}\, |\Psi(\mathbf{x}, t)|^2 = \text{probability of finding the particle in the region } V \subset \mathbb{R}^n \text{ at time } t.$$

This is precisely the Born rule. The magnitude of $|\Psi(\mathbf{x}, t)|^2$ is the probability density at $\mathbf{x} \in \mathbb{R}^n$. The total probability over the whole space $\mathbb{R}^n$ is 1, as promised by the normalization condition. Thus this probability interpretation is compatible with the quantum dynamics.

1.5.3 Position and Momentum

The quantum operator $\hat{x}^i$ associated to the i-th position is defined to be multiplying by x^i

$$\left(\hat{x}^i f\right)(\mathbf{x}) := x^i f(\mathbf{x}).$$

In order to understand the quantum operator $\hat{p}_j$ associated to the corresponding conjugate momentum, we recall that conjugate variables are related by Fourier transform. If we go to the momentum space

$$f(\mathbf{x}) \quad \longleftrightarrow \quad \hat{f}(\mathbf{p})$$

then the effect of $\hat{p}_j$ should correspond to multiplying by p_j in the Fourier dual

$$\left(\hat{p}_j f\right)(\mathbf{x}) \quad \longleftrightarrow \quad p_j \hat{f}(\mathbf{p})$$

Implementing this relation into the Fourier transform

$$f(\mathbf{x}) = \frac{1}{(2\pi\hbar)^{n/2}} \int_{\mathbb{R}^n} d^n\mathbf{p}\, e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} \hat{f}(\mathbf{p})$$

we find

$$\left(\hat{p}_j f\right)(\mathbf{x}) = -i\hbar \frac{\partial}{\partial x^j} f(\mathbf{x}).$$

In other words, $\hat{p}_j$ is represented by the differential operator

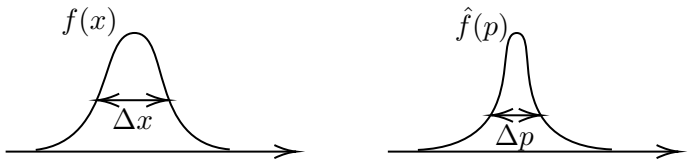
$$\hat{p}_j = -i\hbar \frac{\partial}{\partial x^j}.$$

It is now clear that the position operators and momentum operators satisfy the canonical commutation relation

$$\left[\hat{x}^k, \hat{p}_j\right] = i\hbar\delta^k_j.$$

Here δ^k_j is the Kronecker delta symbol. In particular, Heisenberg uncertainty relation holds

$$\Delta\hat{x}^k \Delta\hat{p}_k \geq \frac{\hbar}{2}.$$



1.5.4 Hamiltonian Operator

We consider a particle of mass m moving in the potential $V(\mathbf{x}, t)$. Classically, the dynamics is described by the Hamiltonian function $\mathscr{H}(\mathbf{x}, \mathbf{p})$ in the phase space

$$\mathscr{H} = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}, t).$$

Here $\frac{\mathbf{p}^2}{2m}$ is the kinetic energy, and V is the potential energy which is real valued.

In quantum mechanics, the Hamiltonian function will be quantized to a self-adjoint Hamiltonian operator. The natural candidate is to replace

$$x^i \to \hat{x}^i, \qquad p_i \to \hat{p}_i.$$

In this way we find the Hamiltonian operator

$$\widehat{\mathrm{H}} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}, t),$$

where $\nabla^2 = \sum_i \frac{\partial}{\partial x^i}\frac{\partial}{\partial x^i}$ is the Laplacian operator.

We will mainly study the Hamiltonian operator of the above form in this chapter. The corresponding Schrödinger equation now takes the explicit form

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x}, t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}, t)\right)\Psi(\mathbf{x}, t).$$

The fact that the Hamiltonian operator $\widehat{\mathrm{H}}$ is a differential operator also leads to a local form of the conservation of probability. Let

$$\rho(\mathbf{x}, t) = |\Psi(\mathbf{x}, t)|^2$$

denote the probability density. As we have seen, the Schrödinger equation implies the conservation of total probability

$$\frac{d}{dt}\int d^n\mathbf{x}\,\rho(\mathbf{x}, t) = 0.$$

This conservation law can be promoted to a standard local form

$$\frac{\partial}{\partial t}\rho + \nabla\cdot\vec{j} = 0$$

for a current vector field $\vec{j}$. Indeed, using the Schrödinger equation and reality of V,

$$\begin{aligned}
\frac{\partial}{\partial t}\rho &= \overline{\frac{\partial\Psi}{\partial t}}\Psi + \overline{\Psi}\frac{\partial\Psi}{\partial t} \\
&= \frac{i}{\hbar}\overline{\left(\widehat{\mathrm{H}}\,\Psi\right)}\Psi - \frac{i}{\hbar}\overline{\Psi}\left(\widehat{\mathrm{H}}\,\Psi\right) \\
&= \frac{i}{\hbar}\left[-\frac{\hbar^2}{2m}\left(\nabla^2\overline{\Psi}\right)\Psi + V\overline{\Psi}\Psi + \frac{\hbar^2}{2m}\overline{\Psi}\nabla^2\Psi - V\overline{\Psi}\Psi\right] \\
&= -\frac{i\hbar}{2m}\nabla\cdot\left[\left(\nabla\overline{\Psi}\right)\Psi - \overline{\Psi}\nabla\Psi\right] \\
\Longrightarrow \qquad \vec{j} &= \frac{i\hbar}{2m}\left[\left(\nabla\overline{\Psi}\right)\Psi - \overline{\Psi}\nabla\Psi\right] = \frac{\hbar}{m}\,\mathrm{Im}\left(\overline{\Psi}\nabla\Psi\right).
\end{aligned}$$

Here $\nabla = (\partial_{x^1}, \cdots, \partial_{x^n})$ is the gradient operator. Thus

$$\vec{j} = \frac{\hbar}{m}\,\mathrm{Im}\left(\overline{\Psi}\nabla\Psi\right)$$

which is called the *probability current*. For any fixed region $V \subset \mathbb{R}^n$, we have

$$\frac{d}{dt}\int_V d^n\mathbf{x}\,\rho(\mathbf{x}, t) = \int_V d^n\mathbf{x}\,\partial_t\rho \quad = -\int_V d^n\mathbf{x}\,\nabla\cdot\vec{j} = -\int_{\partial V} d\vec{\sigma}\cdot\vec{j}.$$

Here $d\vec{\sigma}$ is the vector surface element on ∂V. This says that the probability of finding the particle inside V changes by the flow of the probability current out of the boundary ∂V.

1.5.5 Stationary States

We consider the quantum particle moving in a potential V that only depends on the position $\mathbf{x} \in \mathbb{R}^n$ but not on the time: $V = V(\mathbf{x})$. In this case, the Hamiltonian operator $\widehat{\mathrm{H}}$ is time-independent

$$\widehat{\mathrm{H}} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}).$$

We look for special solutions of the Schrödinger equation of the form

$$\Psi(\mathbf{x}, t) = e^{-i\omega t}\psi(\mathbf{x}).$$

Inserting this expression into the Schrödinger equation, we find

$$\widehat{\mathrm{H}}\,\psi(\mathbf{x}) = E\psi(\mathbf{x}) \qquad (*)$$

where $E = \hbar\omega$. In other words, $\psi(\mathbf{x})$ is an eigenstate of the Hamiltonian $\widehat{\mathrm{H}}$. Based on our discussion on measurement, the eigenvalue E is naturally understood as the energy of the state ψ. Equation (*) is called the *time-independent Schrödinger equation*. Since $\widehat{\mathrm{H}}$ is self-adjoint, E must be real.

Solutions of the form

$$\Psi(\mathbf{x}, t) = e^{-iEt/\hbar}\psi(\mathbf{x}) \qquad \text{with} \qquad \widehat{\mathrm{H}}\,\psi = E\psi$$

are also called *stationary states*. The probability density

$$|\Psi(\mathbf{x}, t)|^2 = |\psi(\mathbf{x})|^2$$

does not depend on time t. These states are eigenstates of the Hamiltonian $\widehat{\mathrm{H}}$ at any time

$$\widehat{\mathrm{H}}\,\Psi(\mathbf{x}, t) = E\Psi(\mathbf{x}, t).$$

In particular, the expectation of $\widehat{\mathrm{H}}$ in the state Ψ is

$$\left\langle \widehat{\mathrm{H}} \right\rangle_{\Psi} = E$$

and the uncertainty of $\widehat{\mathrm{H}}$ in the state Ψ vanishes

$$\Delta_{\Psi}\,\widehat{\mathrm{H}} = 0.$$

Once we have found all the stationary states ψ_α with energy E_α, then a general solution of the Schrödinger equation can be constructed as a superposition

$$\sum_{\alpha} c_\alpha e^{-iE_\alpha t/\hbar}\psi_\alpha(\mathbf{x}).$$

Thus it is fundamental to understand stationary states first, i.e., to study the time-independent Schrödinger equation. In general, $\widehat{\mathrm{H}}$ could have discrete spectrum and continuous spectrum. For the continuous spectrum, the above sum $\sum_\alpha$ has to be replaced by an appropriate integral.

Both the discrete spectrum and the continuous spectrum have specific physical meanings. We will illustrate by a few examples of different spectrum types in subsequence sections.

1.6 Free Particle: Example of Continuous Spectrum

1.6.1 Wave Packet

Let us consider a free quantum particle where the potential $V = 0$. The Hamiltonian is

$$\widehat{\mathrm{H}} = -\frac{\hbar^2}{2m}\nabla^2.$$

The free Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x},t)$$

admits plane wave solutions by

$$\psi_{\mathbf{k}}(\mathbf{x},t) = e^{i(\mathbf{k}\cdot\mathbf{x}-\omega(\mathbf{k})t)}.$$

Here the wave vector $\mathbf{k}$ and the angular frequency ω are determined by the momentum $\mathbf{p}$ and the energy E by

$$\mathbf{p} = \hbar\mathbf{k}, \qquad E = \hbar\omega.$$

These are called the *de Broglie relations*, which work for general matter waves.

Using $\widehat{\mathrm{H}} = -\frac{\hbar^2}{2m}\nabla^2$, we find $E = \frac{\mathbf{p}^2}{2m}$, or

$$\omega(\mathbf{k}) = \frac{\hbar\mathbf{k}^2}{2m}.$$

This gives the dispersion relation in this case.

However, the plane wave solution $\Psi_{\mathbf{k}}$ is non-normalizable

$$|\Psi_{\mathbf{k}}|^2 = 1 \qquad \text{at any } \mathbf{x} \text{ and } t.$$

The integral of $|\Psi_{\mathbf{k}}|^2$ over space will be infinity. So $\Psi_{\mathbf{k}}$ does not give a physical state.

Nevertheless, a general solution can be obtained as a wave packet in terms of superposition of plane waves

$$\Psi(\mathbf{x},t) = \frac{1}{(2\pi\hbar)^{n/2}}\int d^n\mathbf{p}\,\hat{\psi}_0(\mathbf{p})e^{i(\mathbf{p}\cdot\mathbf{x}-E(\mathbf{p})t)/\hbar}.$$

Clearly, let $\psi_0(\mathbf{x})$ denote the wave function at $t = 0$

$$\psi_0(\mathbf{x}) = \Psi(\mathbf{x},0).$$

Then $\hat{\psi}_0(\mathbf{p})$ is the Fourier transform of $\psi_0(\mathbf{x})$ to the momentum space. This gives the explicit solution of the wave function from specified initial condition at $t = 0$.

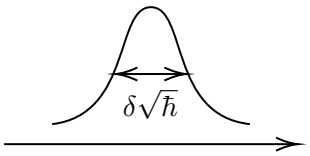
Example 1.6.1 (Gaussian Packet)**.** *Consider the one-dimensional case $n = 1$. Let us give the initial wave function at $t = 0$ by*

$$\psi_0(x) = e^{ip_0x/\hbar}\frac{e^{-x^2/4\delta^2\hbar}}{(2\pi\delta^2\hbar)^{1/4}}, \qquad \delta > 0.$$

The coefficient is chosen such that the normalization condition holds

$$\int_{\mathbb{R}} dx\ |\psi_0(x)|^2 = \frac{1}{\sqrt{2\pi\hbar}\delta}\int_{\mathbb{R}} dx\, e^{-x^2/2\delta^2\hbar} = 1.$$

The magnitude of $|\psi_0(x)|^2 = \frac{e^{-x^2/2\delta^2\hbar}}{\sqrt{2\pi\hbar}\delta}$ is Gaussian.



The parameter δ is related to the uncertainty of $\hat{x}$

$$\Delta_{\psi_0}\hat{x} = \left(\int_{\mathbb{R}} dx\, x^2 |\psi_0(x)|^2\right)^{1/2} = \delta\sqrt{\hbar}.$$

The Fourier transform of $\psi_0(x)$ is

$$\begin{aligned}\hat{\psi}_0(p) &= \int_{\mathbb{R}} dx\, e^{-ipx/\hbar}\psi_0(x) \\ &= \int_{\mathbb{R}} dx\, e^{-i(p-p_0)x/\hbar}\frac{e^{-x^2/4\delta^2\hbar}}{(2\pi\hbar\delta^2)^{1/4}} \\ &= \frac{e^{-(p-p_0)^2\delta^2/\hbar}}{((2\pi\hbar)^{-1}(2\delta)^{-2})^{1/4}}.\end{aligned}$$

The uncertainty of the momentum operator $\hat{p}$ can be computed via $\hat{\psi}_0$

$$\Delta_{\psi_0}\hat{p} = \frac{\sqrt{\hbar}}{2\delta}.$$

In this case, we find the Heisenberg uncertainty

$$\Delta_{\psi_0}\hat{x}\cdot\Delta_{\psi_0}\hat{p} = \frac{\hbar}{2}.$$

The wave function at any time t is therefore solved by

$$\begin{aligned}\Psi(x,t) &= \frac{1}{2\pi\hbar}\int_{\mathbb{R}} dp\,\hat{\psi}_0(p)e^{i\left(px-p^2t/2m\right)/\hbar} \\ &= \frac{1}{2\pi\hbar}\int_{\mathbb{R}} dp\,\frac{e^{-(p-p_0)^2\delta^2/\hbar}}{((2\pi\hbar)^{-1}(2\delta)^{-2})^{1/4}}e^{i\left(px-p^2t/2m\right)/\hbar} \\ &= \frac{1}{\left(\sqrt{2\pi\hbar}\left(\delta+\frac{it}{2m\delta}\right)\right)^{1/2}}e^{\frac{ip_0}{\hbar}\left(x-\frac{p_0t}{2m}\right)}\exp\left(-\frac{\left(x-\frac{p_0t}{m}\right)^2}{4\left(\delta^2+\frac{it}{2m}\right)\hbar}\right).\end{aligned}$$

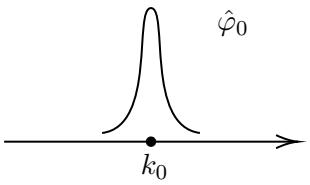
1.6.2 Group Velocity

We would like to understand how a localized wave packet moves in the space. Let us start with a general one-dimensional wave packet of the form

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int dk\,\hat{\varphi}_0(k)e^{i(kx-\omega(k)t)}.$$

Here we have used the wave vector k instead of the momentum $p = \hbar k$ for the Fourier transform. $\omega(k)$ is a function of k, describing the dispersion relation.

Assume $\hat{\varphi}_0(k)$ is concentrated near $k = k_0$, so only when $k \sim k_0$ is important.



We ask for which value of x and t such that the magnitude of the wave packet $\Psi(x,t)$ takes the largest value. For $k \sim k_0$, we can approximate

$$\omega(k) \simeq \omega(k_0) + \omega'(k_0)(k - k_0).$$

Substituting this into the wave packet, we have

$$\begin{aligned}\Psi(x,t) &= \frac{1}{\sqrt{2\pi}} \int dk\, \hat{\varphi}_0(k) e^{i(kx - \omega(k)t)} \\ &\simeq \frac{1}{\sqrt{2\pi}} e^{-i\omega(k_0)t + ik_0\omega'(k_0)t} \int dk\, \hat{\varphi}_0(k) e^{ik(x - \omega'(k_0)t)} \\ &= e^{-i\omega(k_0)t + ik_0\omega'(k_0)t} \Psi(x - \omega'(k_0)t, 0).\end{aligned}$$

Assume the peak of the magnitude of the initial wave function $\Psi(x,0)$ is at $x = x_0$. The above calculation shows that the peak of the magnitude of $\Psi(x,t)$ at time t appears approximately at

$$x = \omega'(k_0)t + x_0.$$

In other words, the peak of the wave packet moves at the velocity $\omega'(k_0)$. This is called the *group velocity*

$$\text{group velocity} = \left.\frac{d\omega}{dk}\right|_{k=k_0}.$$

It describes the approximate speed at which the wave packet propagates.

In contrast, there is another notion called the *phase velocity* defined by

$$\text{phase velocity} = \left.\frac{\omega}{k}\right|_{k=k_0}.$$

It describes the speed at which the pure plane wave $e^{i(k_0 x - \omega(k_0)t)}$ propagates.

For linear dispersion relation

$$\omega(k) = \alpha k \qquad \text{where} \qquad \alpha = \text{const},$$

the group velocity and the phase velocity coincide, both equal to α. Electromagnetic waves in the vacuum are such examples.

In general, group velocity is different from the phase velocity. Let us consider the example of one-dimensional free quantum particles. The de Brogile relations

$$p = \hbar k, \qquad E = \hbar\omega$$

and $E = p^2/2m$ lead to the dispersion relation

$$\omega(k) = \frac{\hbar k^2}{2m}.$$

For a wave packet whose momentum is concentrated at $p_0 = \hbar k_0$, the group velocity is

$$\left.\frac{d\omega}{dk}\right|_{k=k_0} = \frac{\hbar k_0}{m} = \frac{p_0}{m}.$$

This is the expected velocity for a free particle with momentum p_0 and mass m. As a comparison, the phase velocity is

$$\left.\frac{\omega}{k}\right|_{k=k_0} = \frac{\hbar k_0}{2m} = \frac{p_0}{2m}.$$

In the Gaussian packet example 1.6.1,

$$\Psi(x,t) = \frac{1}{\left(\sqrt{2\pi\hbar}\left(\delta + \frac{it}{2m\delta}\right)\right)^{1/2}} e^{\frac{ip_0}{\hbar}\left(x - \frac{p_0 t}{2m}\right)} \exp\left(-\frac{\left(x - \frac{p_0 t}{m}\right)^2}{4\left(\delta^2 + \frac{it}{2m}\right)\hbar}\right).$$

The momentum mode $\hat{\psi}_0(p)$ is concentrated around p_0 for small $\hbar$. We see clearly that the peak of $\Psi(x,t)$ travels at the group velocity p_0/m.

1.7 Harmonic Oscillator: Example of Discrete Spectrum

In this section we study the exactly solvable example of harmonic oscillator, which is one of the most important model in quantum physics.

For simplicity, we focus on the one-dimensional case. The classical Hamiltonian is

$$\mathscr{H} = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

where m is the particle's mass, $k > 0$ is a constant. The potential $V = \frac{1}{2}kx^2$ is quadratic in x and time-independent.

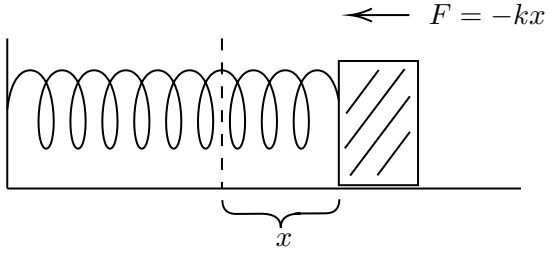
Classically, the particle's motion obeys the Hamilton's equations

$$\begin{cases} \dot{x} = \dfrac{\partial \mathscr{H}}{\partial p} = \dfrac{p}{m} \\ \dot{p} = -\dfrac{\partial \mathscr{H}}{\partial x} = -kx \end{cases}$$

The equation of motion in x is

$$m\ddot{x} = -kx.$$

The force that is applied to the particle is governed by Hooke's law $F = -kx$.



The equation of motion is solved by

$$x(t) = A\cos\omega t + B\sin\omega t,$$

where A, B are constants, and

$$\omega = \sqrt{\frac{k}{m}}$$

is the angular frequency of oscillation.

Quantum mechanically, the Hamiltonian operator is

$$\widehat{\mathrm{H}} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2.$$

It suffices to solve the time-independent Schrödinger equation for a stationary $\psi(x)$

$$\widehat{\mathrm{H}}\,\psi(x) = E\psi(x).$$

The corresponding wave function will then be given by $\psi(x,t) = \psi(x)e^{-iEt/\hbar}$.

1.7.1 Ladder Operators

Remarkably, the time-independent Schrödinger equation for harmonic oscillator can be exactly solved by a simple algebraic method. Let us write

$$\widehat{\mathrm{H}} = \frac{\hat{p}^2}{2m} + \frac{k}{2}\hat{x}^2 = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2,$$

where $\hat{x}$ is the position operator, and $\hat{p} = -i\hbar\frac{d}{dx}$ is the momentum operator. $\hat{x}$ and $\hat{p}$ satisfy the canonical commutation relation

$$[\hat{x}, \hat{p}] = i\hbar.$$

We can rewrite the Hamiltonian operator as

$$\begin{aligned}
\widehat{\mathrm{H}} &= \frac{1}{2m}\left(\hat{p}^2 + m^2\omega^2\hat{x}^2\right) \\
&= \frac{1}{2m}\left[(m\omega\hat{x} - i\hat{p})\,(m\omega\hat{x} + i\hat{p}) - im\omega\,(\hat{x}\hat{p} - \hat{p}\hat{x})\right] \\
&= \frac{1}{2m}\,(m\omega\hat{x} - i\hat{p})\,(m\omega\hat{x} + i\hat{p}) + \frac{1}{2}\hbar\omega \\
&= \hbar\omega\left[\frac{1}{2m\hbar\omega}\,(m\omega\hat{x} - i\hat{p})\,(m\omega\hat{x} + i\hat{p}) + \frac{1}{2}\right] \\
&= \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)
\end{aligned}$$

where we have introduced two operators

$$a^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}\,(m\omega\hat{x} - i\hat{p})\,, \qquad a = \frac{1}{\sqrt{2m\hbar\omega}}\,(m\omega\hat{x} + i\hat{p})\,.$$

They are called *ladder operators*. The reason for the names will be clear soon. As the symbol suggests, the two operators $a^\dagger$ and a are adjoint of each other.

Firstly we observe that the ladder operators satisfy the commutation relation

$$\left[a, a^\dagger\right] = 1.$$

This leads to the following commutation relations

$$[\widehat{\mathrm{H}}, a^\dagger] = \hbar\omega a^\dagger, \qquad [\widehat{\mathrm{H}}, a] = -\hbar\omega a.$$

The key is the following statement.

Proposition 1.7.1. *If ψ solves the time-independent Schrödinger equation with energy E, then $a^\dagger\psi$ (or $a\psi$) solves the time-independent Schrödinger equation with energy $E+\hbar\omega$ (or $E-\hbar\omega$).*

Proof: Assume ψ satisfies $\widehat{\mathrm{H}}\,\psi = E\psi$. Then

$$\begin{aligned}\widehat{\mathrm{H}}\left(a^\dagger\psi\right) &= [\widehat{\mathrm{H}}, a^\dagger]\psi + a^\dagger\,\widehat{\mathrm{H}}\,\psi \\ &= \hbar\omega a^\dagger\psi + Ea^\dagger\psi \\ &= (E+\hbar\omega)\,a^\dagger\psi.\end{aligned}$$

The calculation for $a\psi$ is similar. □

For this reason, the ladder operators $a^\dagger, a$ allow us to climb up and down in energy. We also call $a^\dagger$ the *raising operator* and a the *lowering operator*.

1.7.2 Ground State

The second crucial statement is the following.

Proposition 1.7.2. *The energy E of a stationary state is nonnegative.*

Proof: For the normalized stationary state ψ with energy E,

$$\begin{aligned}E = \langle\psi|\,\widehat{\mathrm{H}}\,|\psi\rangle &= \int_{\mathbb{R}} dx\,\overline{\psi}(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2\right)\psi(x) \\ &= \int_{\mathbb{R}} dx\,\frac{\hbar^2}{2m}\left|\frac{d}{dx}\psi(x)\right|^2 + \frac{1}{2}kx^2|\psi(x)|^2 \geq 0.\end{aligned}$$

Here we have cheated a bit by assuming without proof that ψ is differentiable with appropriate decay condition at space infinity. We leave it to more careful readers. □

Now given a stationary state ψ with energy E, we can use the lowering operator a to lower the energy. Since the energy of a nonzero state is nonnegative, $a^m\psi = 0$ for m sufficiently large.

Let $E_0 \geq 0$ be the smallest possible energy. States with the lowest energy are called *ground states*. Let ψ_0 be one ground state with energy E_0. We will soon see that ground state is unique (up to a normalization) in this case. For ψ_0 being a ground state, we must have

$$a\psi_0 = 0$$

which is the same as the differential equation

$$\left(\hbar\frac{d}{dx}+m\omega x\right)\psi_0(x)=0.$$

Up to a normalization, there is a unique solution given by

$$\psi_0(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}e^{-\frac{m\omega}{2\hbar}x^2}.$$

The coefficient is chosen such that

$$\int_{\mathbb{R}}dx\,|\psi_0(x)|^2=1.$$

The corresponding energy is

$$\widehat{\mathrm{H}}\,\psi_0=\hbar\omega\left(a^\dagger a+\frac{1}{2}\right)\psi_0=\frac{1}{2}\hbar\omega\psi_0$$

$$\Longrightarrow\qquad E_0=\frac{1}{2}\hbar\omega.$$

Note that classical mechanically, the smallest possible energy for harmonic oscillator is zero (for example, the energy for a static particle sitting at $x=0$). Quantum mechanically, the smallest energy is $E_0=\frac{1}{2}\hbar\omega$! This lift of ground state energy is purely a quantum effect.

1.7.3 Excited States

Starting from the ground state, we obtain higher energy states simply by applying the raising operator

$$\psi_n(x)=A_n(a^\dagger)^n\psi_0(x)\qquad\text{with}\qquad E_n=\left(n+\frac{1}{2}\right)\hbar\omega,$$

where A_n is the normalization constant. To calculate A_n, we use the fact that $a^\dagger$ and a are adjoint of each other. Therefore

$$\langle\psi_n|\psi_n\rangle=|A_n|^2\Big\langle(a^\dagger)^n\psi_0\Big|(a^\dagger)^n\psi_0\Big\rangle=|A_n|^2\langle\psi_0|a^n(a^\dagger)^n|\psi_0\rangle.$$

Using $a\psi_0=0$ and $\left[a,a^\dagger\right]=1$, we find

$$a^n(a^\dagger)^n|\psi_0\rangle=na^{n-1}(a^\dagger)^{n-1}|\psi_0\rangle=\cdots=n!|\psi_0\rangle.$$

Thus

$$\langle\psi_n|\psi_n\rangle=|A_n|^2n!\langle\psi_0|\psi_0\rangle.$$

The normalization condition $\langle\psi_n|\psi_n\rangle=1$ gives $A_n=\frac{1}{\sqrt{n!}}$. So

$$\psi_n=\frac{1}{\sqrt{n!}}(a^\dagger)^n\psi_0.$$

Finally we show that ψ_n's are all the stationary states.

Proposition 1.7.3. *Let ψ be a stationary state with energy E. Then ψ must be of the form ψ_n (up to a normalization) for some n and $E = \left(n + \frac{1}{2}\right)\hbar\omega$.*

Proof: Since the energies are bounded from below, there exists $n \geq 0$ such that

$$a^n\psi \neq 0, \qquad a^{n+1}\psi = 0.$$

Then $a(a^n\psi) = 0$. By the uniqueness of the ground state, we must have

$$a^n\psi = \alpha\psi_0 \qquad \text{for some } \alpha \neq 0.$$

Comparing both sides, this readily shows

$$E - n\hbar\omega = E_0 \qquad \Longrightarrow \qquad E = E_n = \left(n + \frac{1}{2}\right)\hbar\omega.$$

Assume ψ and ψ_n are linearly independent. Applying the Gram-Schmidt orthogonalization, we can assume that

$$\langle\psi_n|\psi\rangle = 0.$$

On the other hand, using the fact that $a, a^\dagger$ are adjoint of each other,

$$\langle\psi_n|\psi\rangle \propto \left\langle (a^\dagger)^n\psi_0 \middle| \psi \right\rangle = \langle\psi_0|a^n\psi\rangle = \alpha\langle\psi_0|\psi_0\rangle = \alpha \neq 0.$$

This is a contradiction. So up to a normalization, ψ is the same as ψ_n. □

Thus we have found all stationary states. The states ψ_n for $n > 0$ are called *excited states*, which are created from the ground states ψ_0 by applying $a^\dagger$. Note that unlike the classical picture, the energies in the quantum case are discrete. They are quantized! Moreover, these states $\{\psi_n\}_{n\geq 0}$ form an orthonormal basis of the Hilbert space $L^2(\mathbb{R})$.

The ground state is explicitly given by the Gaussian function

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}.$$

The excited states ψ_n can be explicitly expressed in terms of Hermite polynomials.

For convenience, let us redefine the variable by

$$y = \sqrt{\frac{m\omega}{\hbar}}x.$$

Then the ground state is

$$\psi_0(x) = c_0 e^{-y^2/2}, \qquad c_0 := \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}.$$

The ladder operators are

$$\begin{cases} a^\dagger = \dfrac{1}{\sqrt{2m\hbar\omega}}\left(m\omega x - \hbar\dfrac{d}{dx}\right) = \dfrac{1}{\sqrt{2}}\left(y - \dfrac{d}{dy}\right) \\ a = \dfrac{1}{\sqrt{2m\hbar\omega}}\left(m\omega x + \hbar\dfrac{d}{dx}\right) = \dfrac{1}{\sqrt{2}}\left(y + \dfrac{d}{dy}\right) \end{cases}$$

We can rewrite the raising operator as the composition of three operators

$$a^\dagger = \frac{1}{\sqrt{2}} e^{\hat{y}^2/2} \cdot \left(-\frac{d}{dy}\right) \cdot e^{-\hat{y}^2/2}$$

where $e^{\hat{y}^2/2}$ means the operator by multiplying the function $e^{y^2/2}$. Then

$$\begin{aligned}
\psi_n(x) &= \frac{1}{\sqrt{n!}} (a^\dagger)^n \psi_0 \\
&= \frac{c_0}{\sqrt{n!}} \frac{1}{(\sqrt{2})^n} e^{\hat{y}^2/2} \cdot \left(-\frac{d}{dy}\right)^n \cdot e^{-\hat{y}^2/2} e^{-y^2/2} \\
&= \frac{c_0}{\sqrt{n! 2^n/2}} e^{-y^2/2} \left[e^{y^2} \left(-\frac{d}{dy}\right)^n e^{-y^2} \right] \\
&= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(y) e^{-y^2/2}.
\end{aligned}$$

Here

$$H_n(y) := (-1)^n e^{y^2} \frac{d^n}{dy^n} \left(e^{-y^2}\right)$$

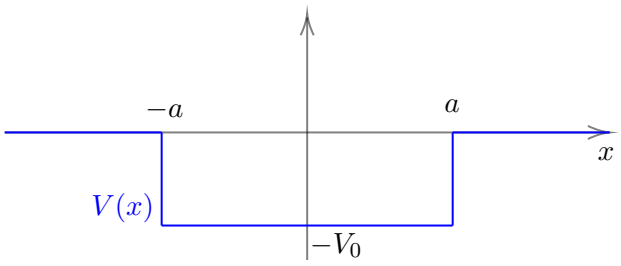
are the *Hermite polynomials*. The first a few look like

$$\begin{aligned}
H_0(y) &= 1 \\
H_1(y) &= 2y \\
H_2(y) &= 4y^2 - 2 \\
H_3(y) &= 8y^3 - 12y \\
H_4(y) &= 16y^4 - 48y^2 + 12 \\
&\vdots
\end{aligned}$$

1.8 Square Well: Example of Mixed Spectrum

We have seen an example where the Schrödinger operator $\widehat{\mathrm{H}}$ has a pure continuous spectrum (free particle) and an example where $\widehat{\mathrm{H}}$ has a pure discrete spectrum (harmonic oscillator). We now discuss an example where both the continuous and the discrete spectrum are present. It is about the finite square well potential of depth $V_0 > 0$ and width $2a$ in dimension one

$$V(x) = \begin{cases} -V_0 & -a \le x \le a \\ 0 & |x| > a \end{cases}$$



1.8.1 Matching Condition

We consider the time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\psi(x)=E\psi(x).$$

① In the region $|x|>a$, the equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)=E\psi,$$

which has two linearly independent solutions given by

$$e^{\pm\sqrt{-2mE}x/\hbar}.$$

The solution ψ can be rewritten as a linear combination

$$\psi=c_1e^{\sqrt{-2mE}x/\hbar}+c_2e^{-\sqrt{-2mE}x/\hbar}.$$

The coefficients c_1,c_2 are to be determined. The solution ψ is smooth in the region $|x|>a$.

② In the region $|x|<a$, the equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi=(E+V_0)\,\psi.$$

Again, ψ can be expressed as a linear combination of the two independent solutions

$$e^{\pm\sqrt{-2m(E+V_0)}x/\hbar}.$$

ψ is also smooth in the region $|x|<a$.

By ①②, we see that the only possible place where the smoothness of ψ fails is when $x=\pm a$. The natural boundary condition to be imposed at $x=\pm a$ is

$$\psi \text{ and } \psi' \text{ are continuous at } x=\pm a. \qquad (*)$$

Otherwise, ψ'' will have a δ-function contribution at $x=\pm a$, breaking the Schrödinger equation. We will call this boundary condition (*) the "*matching condition*".

1.8.2 Bound States

We first consider the case when the solution ψ is normalizable. Such energy eigenstate is called a *bound state*.

In the region $|x|>a$, $\psi(x)$ is a linear combination of

$$e^{\pm\sqrt{-2mE}x/\hbar}.$$

For such ψ to be normalizable, it is necessary to have $E<0$ and such that

$$\psi(x)=\begin{cases}\alpha e^{\sqrt{-2mE}x/\hbar} & x<-a\\ \beta e^{-\sqrt{-2mE}x/\hbar} & x>a\end{cases}$$

for some constants α, β.

On the other hand, the equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi$$

implies

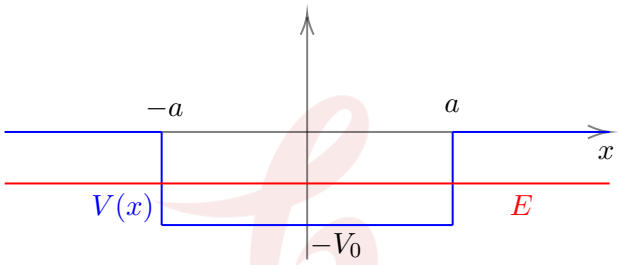
$$\left\langle \psi \middle| -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi \right\rangle = \langle \psi | (E - V(x))\psi \rangle,$$

i.e.,

$$\int dx\, (E - V(x))|\psi(x)|^2 = \frac{\hbar^2}{2m}\int dx\, |\psi'(x)|^2.$$

To obtain a nontrivial solution ψ, it is necessary to have $E > \inf_x V(x) = -V_0$. So the bound state appears only for energy satisfying

$$-V_0 < E < 0.$$



Assume this holds. Then for $|x| < a$ inside the well, ψ is a linear combination of

$$\cos\left(\frac{\sqrt{2m(E+V_0)}x}{\hbar}\right) \quad \text{and} \quad \sin\left(\frac{\sqrt{2m(E+V_0)}x}{\hbar}\right).$$

To simplify notations, let

$$\lambda = \frac{\sqrt{-2mE}}{\hbar}, \qquad \mu = \frac{\sqrt{2m(E+V_0)}}{\hbar}.$$

A further simplification comes from the observation that the potential is an even function

$$V(x) = V(-x).$$

If $\psi(x)$ is a solution, then $\psi(-x)$ is also a solution. Therefore any solution can be written as a sum of an even solution and an odd solution

$$\psi(x) = \frac{1}{2}\left(\psi(x) + \psi(-x)\right) + \frac{1}{2}\left(\psi(x) - \psi(-x)\right).$$

Without loss of generality, we can assume ψ is either even or odd.

Let us first consider ψ being an even function. Then

$$\psi(x) = \begin{cases} \alpha e^{-\lambda x} & x > a \\ \beta \cos \mu x & |x| < a \\ \alpha e^{\lambda x} & x < -a \end{cases} \qquad \alpha, \beta \text{ are constants.}$$

Now we apply the matching condition. We only need to consider $x = a$ since $\psi(x)$ is even.

$$\begin{cases} \lim\limits_{x\to a^-} \psi(x) = \lim\limits_{x\to a^+} \psi(x) \\ \lim\limits_{x\to a^-} \psi'(x) = \lim\limits_{x\to a^+} \psi'(x) \end{cases}$$

leads to

$$\begin{cases} \beta \cos \mu a = \alpha e^{-\lambda a} \\ -\beta\mu \sin \mu a = -\alpha\lambda e^{-\lambda a} \end{cases}$$

Dividing these two equations, we get

$$\lambda = \mu \tan \mu a \tag{**}$$

Recall $\lambda = \sqrt{-2mE}/\hbar$, $\mu = \sqrt{2m(E+V_0)}/\hbar$. The above relation gives the allowed energies. Given E satisfying relation (**), we can solve for $\psi(x)$ which is unique up to a normalization. Thus it gives a unique physical state with the corresponding energy E.

To understand solutions to (**), let us redefine

$$\begin{cases} u = \mu a = \dfrac{\sqrt{2m(E+V_0)}a}{\hbar} \\ u_0 = \dfrac{\sqrt{2mV_0}a}{\hbar} \end{cases}$$

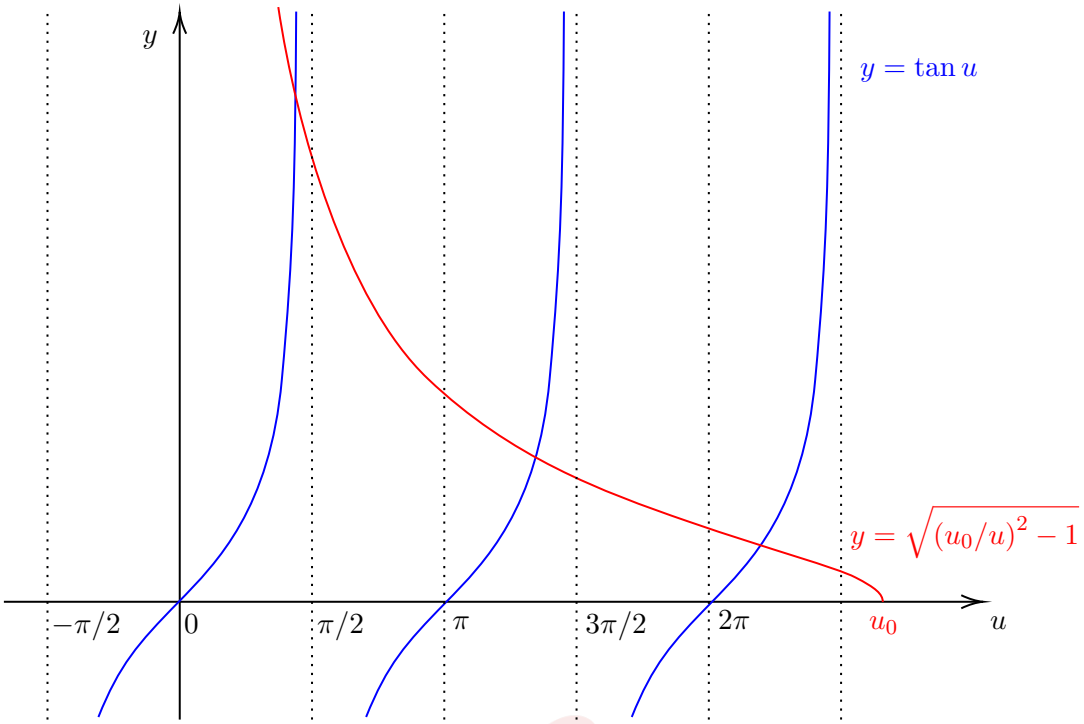
We can express λ, μ in terms of u, u_0

$$\begin{cases} \mu = \dfrac{u}{a} \\ \lambda = \sqrt{\left(\dfrac{u_0}{a}\right)^2 - \mu^2} = \dfrac{\sqrt{u_0^2 - u^2}}{a} \end{cases}$$

Then equation (**) becomes

$$\sqrt{\left(\frac{u_0}{u}\right)^2 - 1} = \tan u.$$

Solutions are given by the intersections of the curve $y = \sqrt{(u_0/u)^2 - 1}$ with the curve $y = \tan u$ for $0 < u < u_0$.



In particular, the figure shows that there are a finite number of intersections, i.e., a finite number of allowed energies. The number depends on the value of u_0. For larger u_0, which means wider and deeper well, we have more bound states. Nevertheless, it is clear that we have at least one solution, no matter how small u_0 is.

We next briefly discuss the case for ψ being an odd function. Then

$$\psi(x) = \begin{cases} \alpha e^{-\lambda x} & x > a \\ \beta \sin \mu x & |x| < a \\ -\alpha e^{\lambda x} & x < -a \end{cases}$$

The matching condition at $x = a$ gives

$$\begin{cases} \beta \sin \mu a = \alpha e^{-\lambda a} \\ \beta \mu \cos \mu a = -\alpha \lambda e^{-\lambda a} \end{cases}$$

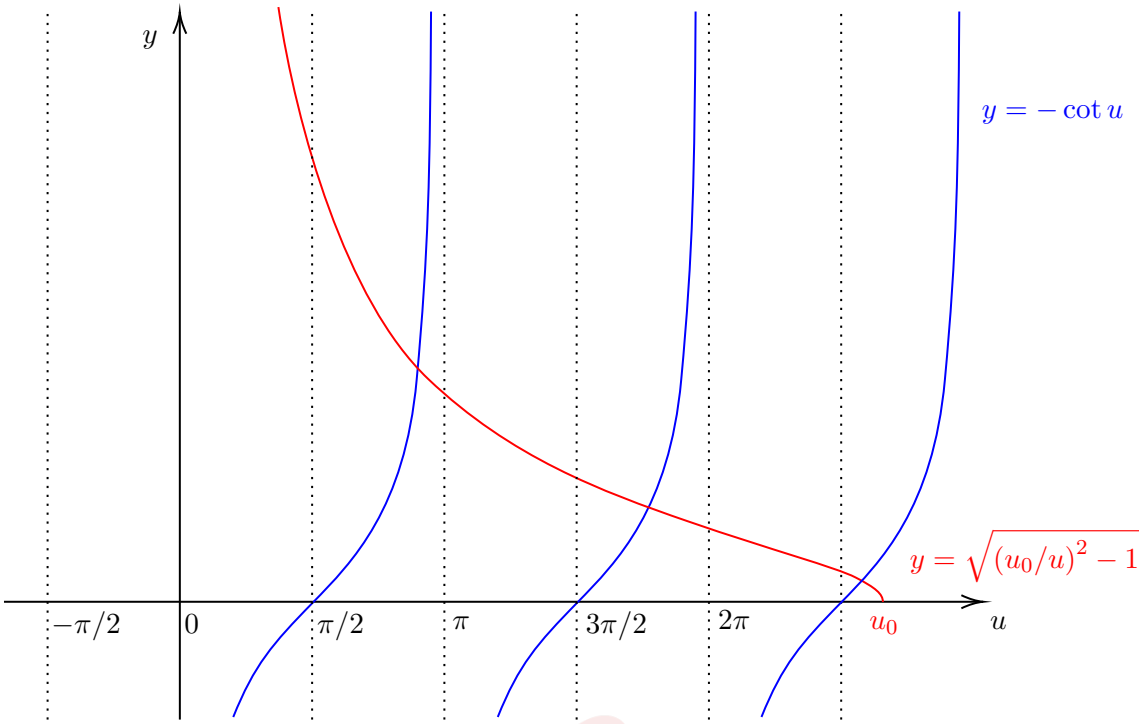
from which we find required relation for E

$$\mu \cot \mu a = -\lambda.$$

Using the same variables u and u_0 as above, this is

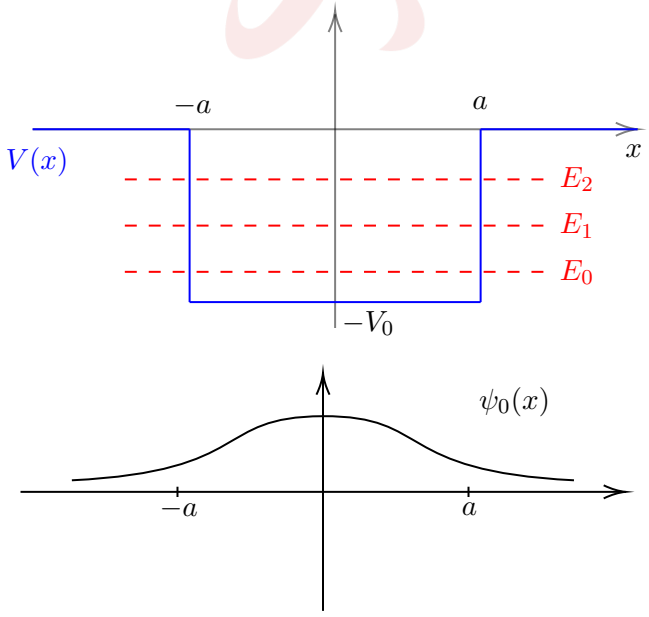
$$\sqrt{\left(\frac{u_0}{u}\right)^2 - 1} = -\cot u.$$

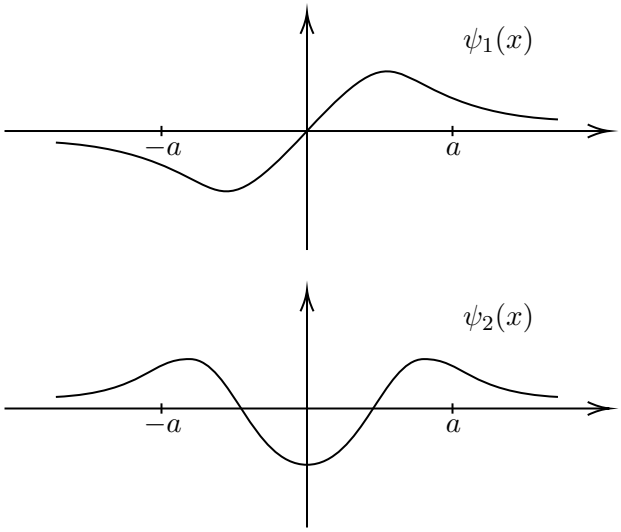
We plot the corresponding curves for $0 < u < u_0$



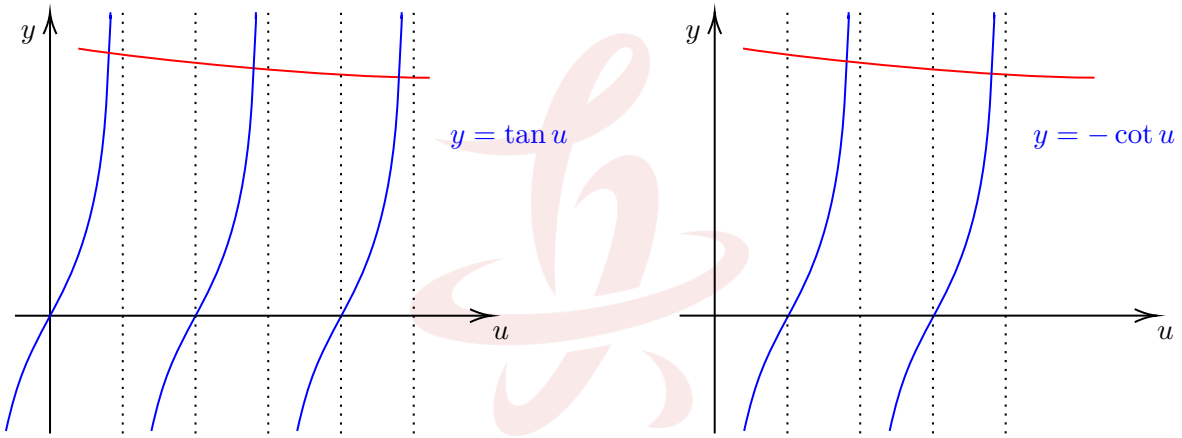
Again, we find only a finite number of intersections. The number of odd bound state is bigger for larger u_0, i.e., for wider and deeper well. However, for u_0 sufficiently small, say $u_0 < \pi/2$, there will be no odd bound state.

In summary, we have found a finite number of energies $-V_0 < E_0 < E_1 < \cdots < E_N < 0$ where each E_i has exactly one bound state $\psi_i(x)$. The wave function $\psi_i(x)$ is even/odd if i is even/odd. The ground state ψ_0 is even, and it always exists.





Let us briefly discuss the limit case $V_0 \to +\infty$. This corresponds to $u_0 \to +\infty$.



even case

odd case

In this deep well limit, the intersections approximately happen when u is an integer multiple of $\pi/2$. It follows that

$$\sqrt{2m(E_n + V_0)}\frac{a}{\hbar} \simeq \frac{(n+1)\pi}{2}$$

$$\Longrightarrow \qquad E_n + V_0 \simeq \frac{(n+1)^2\pi^2\hbar^2}{2m(2a)^2}, \qquad n = 0, 1, 2, \cdots$$

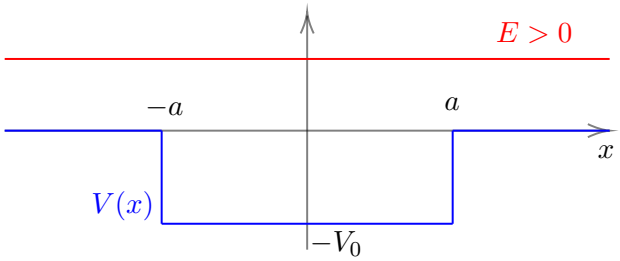
Surprisingly, we will find this formula reappearing for the resonant transmission in the scattering problem as we discuss next.

1.8.3 Scattering States

We have seen that the square well admits a finite number of bound states. The bound state energies correspond to the discrete spectrum of the Hamiltonian $\widehat{\mathrm{H}}$. Unlike the harmonic oscillator where the bound states form a basis of the Hilbert space, the space of bound states of square well is finite dimensional and so can not span the whole Hilbert space. There will

also exist the continuous spectrum of $\widehat{\mathrm{H}}$ like in the free particle case. In fact, when x is far away, the potential is zero and the particle behaves like a free particle there. This suggests non-normalizable solutions of the time-independent Schrödinger equation which behave like plane waves of free particle in the far away region. As we will see shortly, this is indeed the case. These solutions are called *scattering states*. The reason for the name will be explained in Section 1.9.

The scattering states appear for $E > 0$.



The time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi$$

can be solved in each region in the same way as we did for bound state.

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -a \\ C\sin\mu x + D\cos\mu x & -a < x < a \\ Fe^{ikx} + Ge^{-ikx} & x > a \end{cases}$$

Here A, B, C, D, F, G are constants, and

$$k = \frac{\sqrt{2mE}}{\hbar} > 0, \qquad \mu = \frac{\sqrt{2m(E+V_0)}}{\hbar} > 0.$$

At $x = \pm a$, we again impose the matching condition.

Since $E > 0$, the wave function $\psi(x)$ is oscillating instead of decaying when $x \to \infty$, hence is non-normalizable. However, such solutions will be the building blocks for scattering process as we will discuss in Section 1.9. Let us first illustrate the basic idea. Let

$$\psi(x,t) = \psi(x)e^{-iEt/\hbar}$$

be the corresponding solution of the time-dependent Schrödinger equation. Let us consider the region $x < -a$ where

$$\psi(x,t) = Ae^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} + Be^{-i\left(kx + \frac{\hbar k^2}{2m}t\right)}.$$

The first term $Ae^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}$ is a plane wave moving to the right at phase velocity $\frac{\hbar k}{2m}$. The second term $Be^{-i\left(kx+\frac{\hbar k^2}{2m}t\right)}$ is a plane wave moving to the left at the same phase velocity.

With the above interpretation, let us consider the stationary solution $\psi(x)$ of the form

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -a \\ C\sin\mu x + D\cos\mu x & -a < x < a \\ Fe^{ikx} & x > a \end{cases}$$

This wave function represents the following process: A wave of amplitude A is incident from the left at $x = -\infty$, and meets the square well; then a wave of amplitude B is reflected back to the left, while a wave of amplitude F is transmitted through the square well and moves to the right at $x = +\infty$.

A: incident wave amplitude
B: reflected wave amplitude
F: transmitted wave amplitude

We define

$$\text{reflection coefficient:} \quad R = \frac{|B|^2}{|A|^2}$$
$$\text{transmission coefficient:} \quad T = \frac{|F|^2}{|A|^2}$$

R represents the probability of reflection, and T represents the probability of transmission. From this physical interpretation, we should expect

$$T + R = 1.$$

One way to see this is to use the local form of probability conservation. Recall the probability current in Section 1.5.4

$$j(x) = \frac{\hbar}{m}\,\mathrm{Im}\left(\overline{\psi}\frac{d}{dx}\psi\right).$$

Substituting into the above ψ, we find

$$j(x) = \begin{cases} \dfrac{\hbar k}{m}\left(|A|^2 - |B|^2\right) & x < -a \\ \dfrac{\hbar k}{m}|F|^2 & x > a \end{cases}$$

For stationary solutions, the probability density ρ is time-independent. The conservation equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} j(x) = 0$$

implies that $j(x)$ must be x-independent: accumulation of probability can not happen at any region of space. It follows that

$$|A|^2 = |B|^2 + |F|^2 \qquad \Longrightarrow \qquad T + R = 1.$$

Now we move on to solve $\psi(x)$ via the matching condition

$$x = -a: \quad \begin{cases} Ae^{-ika} + Be^{ika} = -C\sin\mu a + D\cos\mu a \\ ik\left(Ae^{-ika} - Be^{ika}\right) = \mu\left(C\cos\mu a + D\sin\mu a\right) \end{cases}$$

$$x = \ a: \quad \begin{cases} C\sin\mu a + D\cos\mu a = Fe^{ika} \\ \mu\left(C\cos\mu a - D\sin\mu a\right) = ikFe^{ika} \end{cases}$$

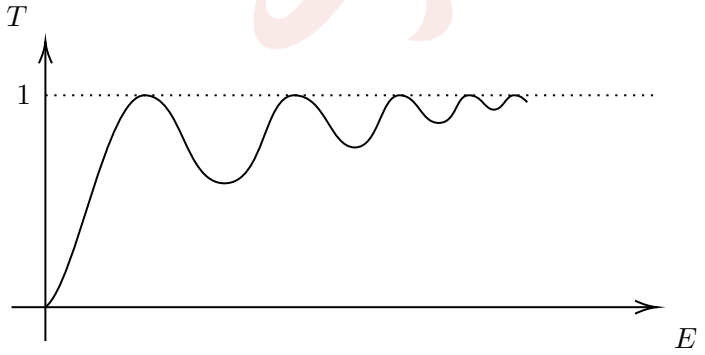
These four equations uniquely determine the five constants A, B, C, D, F up to a total normalization. After a laborious calculation, we find

$$\begin{cases} \dfrac{F}{A} = \dfrac{e^{-2ika}}{\cos 2\mu a - i\frac{\sin 2\mu a}{2k\mu}\left(k^2+\mu^2\right)} \\ \dfrac{B}{F} = i\dfrac{\sin 2\mu a}{2k\mu}\left(\mu^2 - k^2\right) \end{cases}$$

We can compute the reflection coefficient R, the transmission coefficient T and check $T + R = 1$ as promised. Explicitly, the transmission probability is

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \frac{V_0^2}{4E(E+V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)}.$$

The plot of T as a function of E looks like



Note that there are certain values of E making $T = 1$. In this case we have the full transmission as no waves are reflected: the well becomes transparent! From the above formula of T, the full transmission happens when

$$E_n + V_0 = \frac{(n+1)^2\pi^2\hbar^2}{2m(2a)^2}, \qquad n \in \mathbb{Z} \quad \text{such that} \quad E_n > 0.$$

Surprisingly, E_n corresponds to the bound state energies of the infinite square well that we find previously. For the energy E_n, the wavelength of ψ inside the well is

$$\frac{2\pi}{\mu} = \frac{2\pi\hbar}{\sqrt{2m(E_n+V_0)}} = \frac{4a}{n+1}.$$

So the well width $2a$ fits an integer number of half wavelength. This phenomenon is called *resonant transmission.*

We can also consider wave incidents from the right, and look for solutions of the form

$$\psi(x) = \begin{cases} Be^{-ikx} & x < -a \\ C\sin\mu x + D\cos\mu x & -a < x < a \\ Fe^{ikx} + Ge^{-ikx} & x > a \end{cases}$$

The interpretation is similar. The reflection and transmission coefficients are

$$R = \frac{|F|^2}{|G|^2}, \qquad T = \frac{|B|^2}{|G|^2}.$$

In general, we could have waves incident from both sides

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -a \\ C\sin\mu x + D\cos\mu x & -a < x < a \\ Fe^{ikx} + Ge^{-ikx} & x > a \end{cases}$$

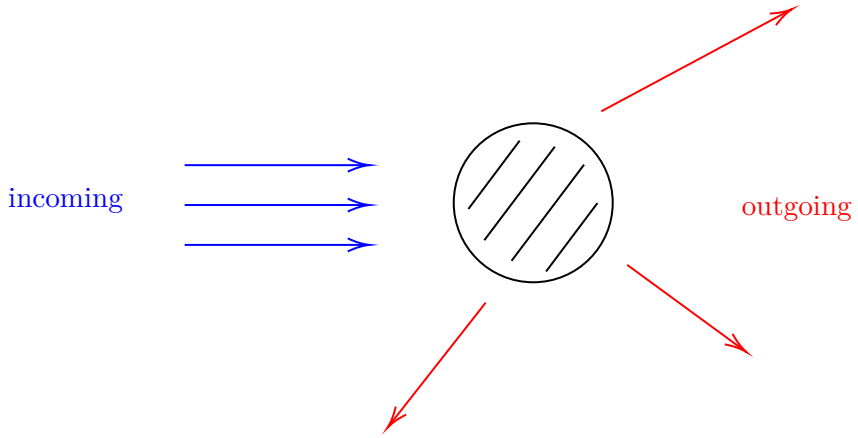
Then A, G represent incoming waves and B, F represent outgoing waves.

1.9 Scattering

In this section we discuss the basic idea of scattering process in the case of one-dimensional particles. We explain how this is related to the continuous spectrum of the Schrödinger operator.

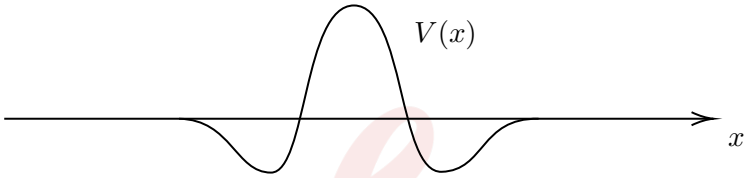
1.9.1 Wave Packet Scattering

In the study of scattering problem, we consider particles that come from far away and scatter against some potential produced by localized interaction.



We consider one-dimensional particles scattering in a compactly supported potential $V(x)$

$$V(x) = 0 \qquad \text{for } |x| \geq R.$$



Assume a particle comes from $x = -\infty$. Quantum mechanically, such a particle is represented by a wave packet

before the interaction

When the particle enters the region of V, it interacts with the potential. Afterwards, it will be transmitted through the potential toward $x = +\infty$, or be reflected back toward $x = -\infty$, with certain probability.

after the interaction

Explicitly, let us represent an incoming free particle by a localized wave packet

$$\psi_{\text{in}}(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} dk\, \alpha(k) e^{i(kx - \omega(k)t)}, \qquad \omega(k) = \hbar k^2/2m.$$

Here $\alpha(k)$ is nonzero only in a small neighborhood of $k_0 > 0$, so the wave packet will travel forward with group velocity $\hbar k_0/m$. We assume

$$\int_{\mathbb{R}} dk\, |\alpha(k)|^2 = 1,$$

so that the wave function is normalized

$$\int_{\mathbb{R}} dx\, |\psi_{\text{in}}(x,t)|^2 = 1.$$

To describe the scattering process, we observe that the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\psi = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi$$

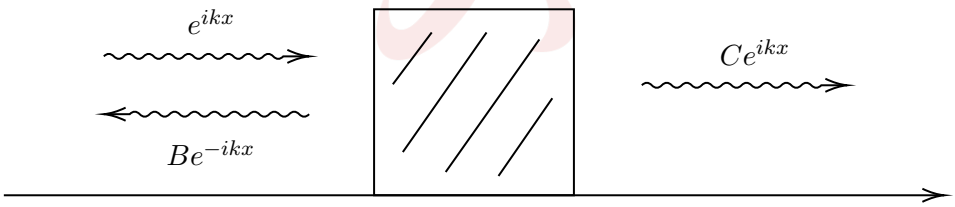
is linear in ψ. This linearity leads to the following strategy. We first look for solutions which are plane waves far away. Then we take the superposition of these asymptotic plane wave solutions with respect to the coefficient $\alpha(k)$ to obtain the physical solution for the scattering.

Precisely, let us consider the time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi, \quad \text{where} \quad E = \frac{(\hbar k)^2}{2m} > 0.$$

In the region $|x| >> 0$, the potential $V(x) = 0$ and so the wave function is given by linear combinations of $e^{\pm ikx}$. We look for the solution ψ_k of the form

$$\psi_k(x) = \begin{cases} e^{ikx} + B(k)e^{-ikx} & x \to -\infty \\ C(k)e^{ikx} & x \to +\infty \end{cases}$$



Here $B(k), C(k)$ are constants that depend on k, which are determined by solving the time-independent Schrödinger equation. Such a solution ψ_k is non-normalizable, but lies in the continuous spectrum with energy $E_k = \frac{(\hbar k)^2}{2m}$.

Assume we have found ψ_k's. Then we obtain a solution of the Schrödinger equation by

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} dk\, \alpha(k)\psi_k(x)e^{-i\frac{\hbar k^2}{2m}t}.$$

In the region $x \to -\infty$, we have

$$\psi(x,t) = \psi_{\text{in}}(x,t) + \psi_R(x,t),$$

where $\psi_{\text{in}}(x,t)$ is our prepared incoming wave packet above, and

$$\psi_R(x,t) = \frac{1}{\sqrt{2\pi}}\int dk\, \alpha(k)B(k)e^{-i\left(kx+\frac{\hbar k^2}{2m}t\right)}$$

represents the reflected wave packet.

In the region $x \to +\infty$, we have

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int dk\, \alpha(k) C(k) e^{i\left(kx - \frac{\hbar k^2}{2m} t\right)}$$

which represents the transmitted wave packet. Thus this wave function $\psi(x,t)$ contains the quantum information about the scattering of incoming particle ψ_{in} with the potential $V(x)$.

1.9.2 S-matrix

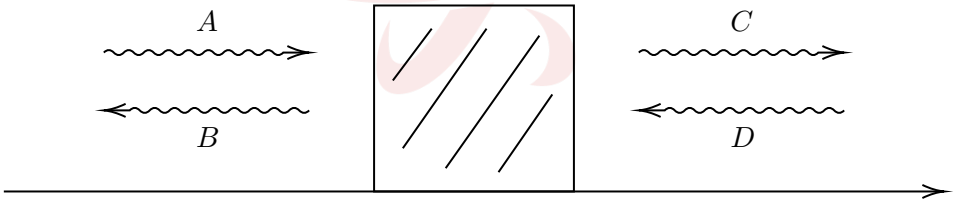
The S-matrix, or the scattering matrix, is about the relation for particle states before and after a scattering process. We illustrate the S-matrix in the one-dimensional scattering process.

We consider a localized one-dimensional potential $V(x)$ which is compactly supported. As we have discussed above, the scattering process is completely determined by solutions of the Schrödinger equation which are plane waves at $|x| \to \pm\infty$ outside the potential barrier. We look for solutions of the time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x), \qquad E = \frac{(\hbar k)^2}{2m},$$

which have the asymptotic plane wave behaviors by

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x \to -\infty \\ Ce^{ikx} + De^{-ikx} & x \to +\infty \end{cases}$$



- The case $D = 0$ represents a scattering process for an incident wave of amplitude A coming from the left. Then C is the amplitude for the transmitted wave and B is the amplitude for the reflected wave.
- The case $A = 0$ represents a scattering process for an incident wave of amplitude D coming from the right. Then B is the amplitude for the transmitted wave and C is the amplitude for the reflected wave.

In general, we could have both left and right incident waves. Let us represent the amplitudes of the incoming waves by a column vector

$$\Psi_{\text{in}} = \begin{pmatrix} A \\ D \end{pmatrix}$$

and represent the amplitudes of the outgoing waves by a column vector

$$\Psi_{\text{out}} = \begin{pmatrix} B \\ C \end{pmatrix}.$$

Since the Schrödinger equation is linear, Ψ_{out} is related to Ψ_{in} by a linear relation

$$\Psi_{\text{out}} = S\Psi_{\text{in}}$$

or explicitly

$$\begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix}.$$

The matrix for the transition

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$$

is called the *S-matrix*. The matrix entries S_{ij} are functions of the wave vector k, and these functions are completely determined by the localized potential $V(x)$.

To see the meaning of the entries of S, consider setting $D = 0$ and we have

$$S \begin{pmatrix} A \\ 0 \end{pmatrix} = \begin{pmatrix} S_{11}A \\ S_{21}A \end{pmatrix}.$$

This says that S_{11} is the reflection amplitude and S_{21} is the transmission amplitude for incident wave from the left. Similarly, setting $A = 0$

$$S \begin{pmatrix} 0 \\ D \end{pmatrix} = \begin{pmatrix} S_{12}D \\ S_{22}D \end{pmatrix}.$$

This says that S_{12} is the transmission amplitude and S_{22} is the reflection amplitude for incident wave from the right.

If we take the absolute value square of the transmission and reflection amplitudes, we find the corresponding transmission and reflection coefficients.

1.9.3 Unitarity

The S-matrix is in fact unitary. To see this, consider the probability current of ψ

$$j(x) = \frac{\hbar}{m} \operatorname{Im}\left(\overline{\psi}\frac{d}{dx}\psi\right).$$

For the stationary state, the probability density $\rho = |\psi|^2$ is time-independent. Then the local conservation of probability (which follows from Schrödinger equation for ψ)

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} j = 0$$

implies $\frac{d}{dx} j(x) = 0$. So $j(x)$ must be constant.

From the asymptotic behavior of $\psi(x)$, we have

$$j(x) = \begin{cases} \dfrac{\hbar k}{m}\left(|A|^2 - |B|^2\right) & x \to -\infty \\ \dfrac{\hbar k}{m}\left(|C|^2 - |D|^2\right) & x \to +\infty \end{cases}$$

Thus

$$|A|^2 - |B|^2 = |C|^2 - |D|^2 \qquad \Longrightarrow \qquad |A|^2 + |D|^2 = |B|^2 + |C|^2.$$

In other words,

$$\overline{\Psi}^t_{\text{out}} \Psi_{\text{out}} = \overline{\Psi}^t_{\text{in}} \Psi_{\text{in}}.$$

So the linear transformation S preserves the Hermitian inner product, i.e., S is unitary

$$S^* S = 1.$$

Here $S^* := \overline{S}^t$.

1.9.4 Time Reversal Symmetry

Assume the potential $V = V(x)$ is time-independent. Then the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\psi = \widehat{\mathrm{H}}\,\psi$$

has a time reversal symmetry: if $\psi(x,t)$ is a solution, then $\overline{\psi}(x,-t)$ is also a solution with the time direction reversed. For time-independent Schrödinger equation, if $\psi(x)$ solves

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x),$$

then $\overline{\psi}(x)$ also gives a solution.

Now given $\psi(x)$ with

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x \to -\infty \\ Ce^{ikx} + De^{-ikx} & x \to +\infty \end{cases}$$

the time-reversed solution $\overline{\psi}(x)$ satisfies

$$\overline{\psi}(x) = \begin{cases} \overline{B}e^{ikx} + \overline{A}e^{-ikx} & x \to -\infty \\ \overline{D}e^{ikx} + \overline{C}e^{-ikx} & x \to +\infty \end{cases}$$

In this presentation, $\overline{\Psi}_{\text{in}} = \begin{pmatrix} \overline{B} \\ \overline{C} \end{pmatrix}$, $\Psi_{\text{out}} = \begin{pmatrix} \overline{A} \\ \overline{D} \end{pmatrix}$. Therefore

$$\begin{pmatrix} \overline{A} \\ \overline{D} \end{pmatrix} = S \begin{pmatrix} \overline{B} \\ \overline{C} \end{pmatrix} \qquad \Longrightarrow \qquad \begin{pmatrix} B \\ C \end{pmatrix} = \overline{S}^{-1} \begin{pmatrix} A \\ D \end{pmatrix}.$$

It follows that

$$S = \bar{S}^{-1} \qquad \xrightarrow{\text{unitarity of } S} \qquad S = S^t.$$

So time reversal symmetry implies the S-matrix is symmetric.

1.10 WKB Approximation

The WKB method, named after Gregor Wentzel, Hendrik Kramers, and Léon Brillouin, provides approximate solutions for linear differential equations with spatially slow-varying coefficients. In applications to quantum mechanics, this is also called *semi-classical approximation*.

1.10.1 Approximation Scheme

Consider the one-dimensional time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\psi = E\psi.$$

We will analyze the solution ψ in three different regions.

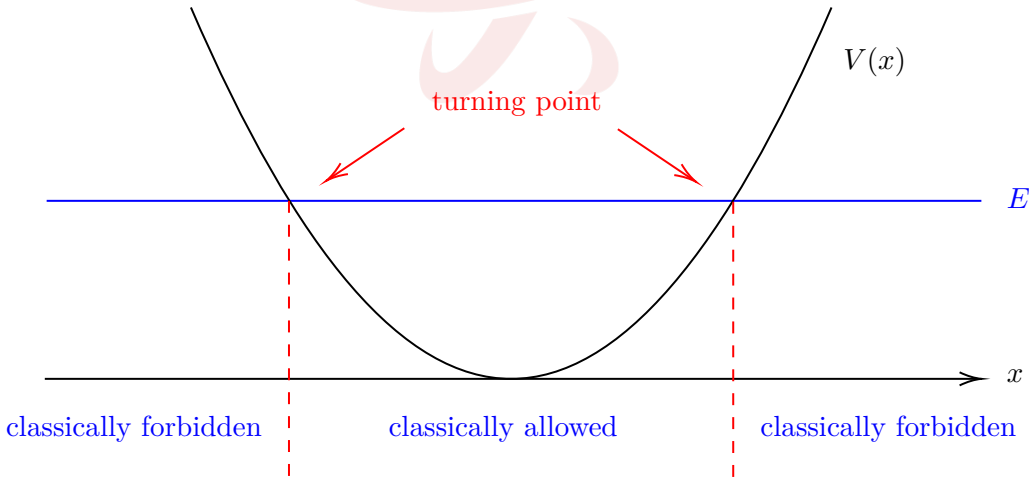
① Classically allowed region. This corresponds to positions where $V(x) < E$. Classically, the energy of motion is

$$E = \frac{p^2}{2m} + V(x).$$

So the classical particle can only move in this region.

② Classically forbidden region. This corresponds to positions where $V(x) > E$. Classical particles can not enter this region. However, as we have seen in previous examples of harmonic oscillator and square well bound states, quantum particles can penetrate into this region with certain probability.

③ Turning points. This corresponds to positions where $V(x) = E$.



The WKB approximation scheme looks for solutions of the stationary wave function of the exponential form (notation clarification: $S(x)$ here is not the S-matrix)

$$\psi(x) = e^{\frac{i}{\hbar}S(x)}, \qquad S(x) \in \mathbb{C}.$$

Plugging into the Schrödinger equation,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - (E - V(x))\right) e^{\frac{i}{\hbar}S(x)} = 0$$

$$\Longrightarrow \qquad \big(S'(x)\big)^2 - i\hbar S''(x) = 2m(E - V(x)).$$

Treating $\hbar$ as very small, this non-linear equation can be solved in order of $\hbar$ by setting

$$S(x) = \sum_{n=0}^{\infty} \hbar^n S_n(x).$$

Equating two sides of

$$\left(\sum_{n=0}^{\infty} \hbar^n S_n'(x)\right)^2 - i\hbar \sum_{n=0}^{\infty} \hbar^n S_n''(x) = 2m(E - V(x)),$$

we find

$$\begin{cases} S_0'(x)^2 = 2m(E - V(x)) \\ 2S_0'(x)S_1'(x) = iS_0''(x) \\ \qquad\qquad \vdots \\ 2S_0'(x)S_n'(x) = iS_{n-1}''(x) - \sum_{i=1}^{n-1} S_i'(x)S_{n-i}'(x) \\ \qquad\qquad \vdots \end{cases}$$

The semi-classical approximation looks for the solution up to order $\hbar^1$ and neglects terms of order $\hbar^2$ or higher. Thus we look for

$$S(x) = S_0(x) + \hbar S_1(x) + O(\hbar^2).$$

This can be solved by the above recursive relation

$$S_0(x) = \pm \int^x \sqrt{2m(E - V(y))}\, dy$$

$$S_1(x) = \frac{i}{2} \ln \sqrt{2m(E - V(x))} + C_1$$

where C_1 is some constant. Therefore

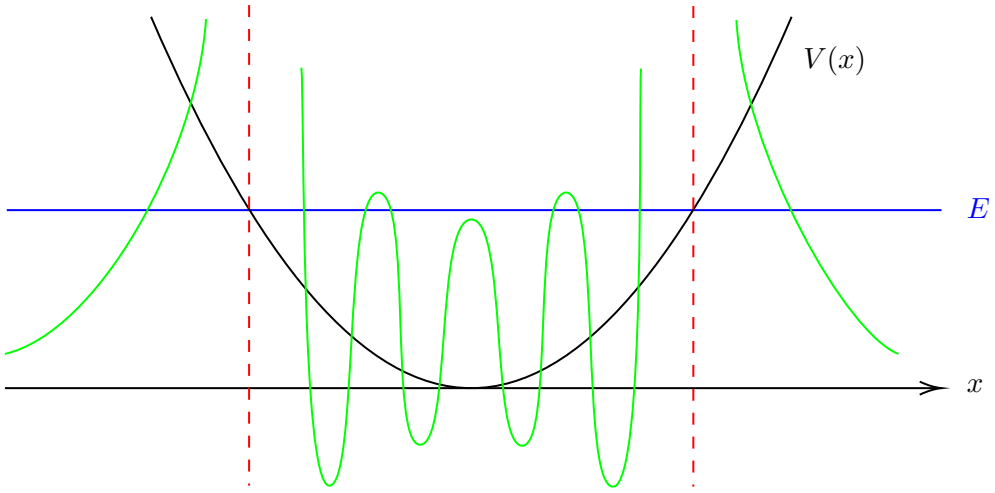
$$\begin{aligned} \psi(x) &= \exp\left(\frac{i}{\hbar}\left(S_0(x) + \hbar S_1(x) + O(\hbar^2)\right)\right) \\ &\simeq e^{\frac{i}{\hbar} S_0(x)} e^{iS_1(x)} \\ &= \frac{A}{(2m(E - V(x)))^{\frac{1}{4}}} e^{\pm \frac{i}{\hbar} \int^x \sqrt{2m(E - V(y))}\, dy} \end{aligned}$$

where A is some constant. The two expressions

$$\psi_{\pm} = \frac{A}{(2m(E - V(x)))^{\frac{1}{4}}} e^{\pm \frac{i}{\hbar} \int^x \sqrt{2m(E - V(y))}\, dy}$$

are the basic forms of the WKB approximation.

Note that this WKB form will blow up at the turning points where $E = V(x)$. This suggests that the WKB approximation is not good near turning points. There need some special treatments there and we will come back to this shortly.



WKB approximated solution. Amplitude blows up near the turning points.

In the classically allowed region $E > V(x)$, let us write

$$E - V(x) = \frac{\hbar^2 k(x)^2}{2m} \quad \text{with} \quad k(x) > 0.$$

Then the WKB approximated solution takes the form (A, B are some constants)

$$\psi(x) \simeq \frac{A}{\sqrt{k(x)}} e^{i\int^x k(y)dy} + \frac{B}{\sqrt{k(x)}} e^{-i\int^x k(y)dy}.$$

The first term with coefficient A represents a wave moving to the right, and the second term represents a wave moving to the left. This function is oscillating in this region.

In the classically forbidden region $E < V(x)$, let us write

$$E - V(x) = -\frac{\hbar^2 \lambda(x)^2}{2m} \quad \text{with} \quad \lambda(x) > 0.$$

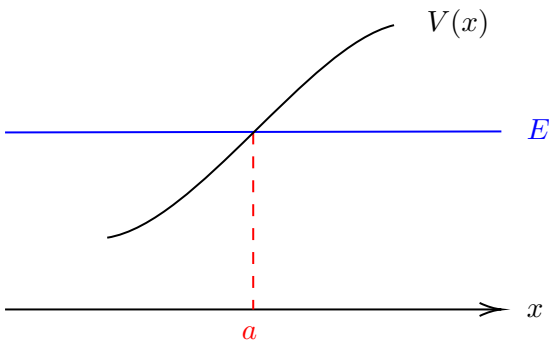
Then the WKB approximated solution takes the form

$$\psi(x) \simeq \frac{A}{\sqrt{\lambda(x)}} e^{\int^x \lambda(y)dy} + \frac{B}{\sqrt{\lambda(x)}} e^{-\int^x \lambda(y)dy}.$$

This function is essentially exponential growing or decaying in this region.

1.10.2 Turning Points and Airy Functions

Now we consider the region near a turning point $x = a$. We look for a suitable approximation near this turning point that connects the oscillating WKB approximation on one side and the exponential WKB approximation on the other side



We can approximate $V(x)$ locally around $x = a$ by a linear function

$$V(x) \simeq E + (x - a)V'(a).$$

This leads to the approximate equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + (x - a)V'(a)\psi = 0.$$

If we make a change of variable

$$z = \left(\frac{2mV'(a)}{\hbar^2}\right)^{1/3}(x - a),$$

then the above approximate equation becomes

$$\frac{d^2\psi}{dz^2} - z\psi = 0.$$

This is the *Airy equation*.

The Airy equation has two linearly independent solutions, denoted by $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$. They are called Airy functions and are given by

$$\mathrm{Ai}(z) = \frac{1}{\pi}\int_0^\infty \cos\left(\frac{t^3}{3} + zt\right) dt$$
$$\mathrm{Bi}(z) = \frac{1}{\pi}\int_0^\infty \left[\exp\left(-\frac{t^3}{3} + zt\right) + \sin\left(\frac{t^3}{3} + zt\right)\right] dt.$$

The Airy functions $\mathrm{Ai}(z), \mathrm{Bi}(z)$ have the approximate asymptotic behaviors

$$\mathrm{Ai}(z) \simeq \begin{cases} \frac{1}{2}\frac{1}{\sqrt{\pi}}|z|^{-\frac{1}{4}}\exp\left(-\frac{2}{3}|z|^{\frac{3}{2}}\right) & z \to +\infty \\ \frac{1}{\sqrt{\pi}}|z|^{-\frac{1}{4}}\cos\left(\frac{2}{3}|z|^{\frac{3}{2}} - \frac{\pi}{4}\right) & z \to -\infty \end{cases}$$

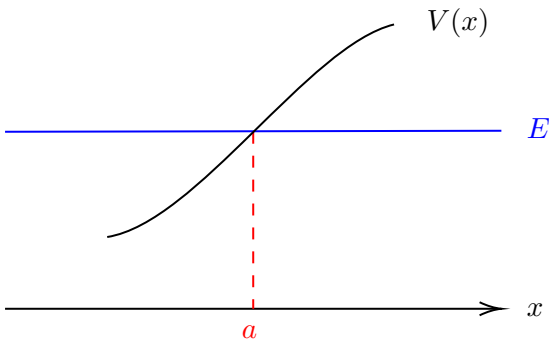
$$\mathrm{Bi}(z) \simeq \begin{cases} \frac{1}{\sqrt{\pi}}|z|^{-\frac{1}{4}}\exp\left(\frac{2}{3}|z|^{\frac{3}{2}}\right) & z \to +\infty \\ -\frac{1}{\sqrt{\pi}}|z|^{-\frac{1}{4}}\sin\left(\frac{2}{3}|z|^{\frac{3}{2}} - \frac{\pi}{4}\right) & z \to -\infty \end{cases}$$

The key observation is that these approximate behaviors connect precisely the WKB solutions on two sides of the turning point.

1.10.3 Connection Formula

Let us use the Airy functions to derive the connection condition for WKB solutions near the turning point $x = a$.

① Let us first consider the case $V'(a) > 0$.



The linear approximation of V near $x = a$ is

$$V(x) \simeq E + V'(a)(x - a).$$

In the classically allowed region $x < a$ near the turning point, we have approximately

$$k(x) = \frac{\sqrt{2m(E - V(x))}}{\hbar} \simeq \left(\frac{2mV'(a)}{\hbar^2}\right)^{1/2} \sqrt{a - x}$$

and

$$\int_a^x k(y)\, dy \simeq \left(\frac{2mV'(a)}{\hbar^2}\right)^{1/2} \int_a^x \sqrt{a - y}\, dy = -\frac{2}{3}|z|^{3/2}.$$

In the classically forbidden region $x > a$ near the turning point, we have approximately

$$\lambda(x) = \frac{\sqrt{2m(V(x) - E)}}{\hbar} \simeq \left(\frac{2mV'(a)}{\hbar^2}\right)^{1/2} \sqrt{x - a}$$

and

$$\int_a^x \lambda(y)\, dy \simeq \left(\frac{2mV'(a)}{\hbar^2}\right)^{1/2} \int_a^x \sqrt{y - a}\, dy = \frac{2}{3}|z|^{3/2}.$$

Assume the wave function has the leading behavior by a decaying exponential in the classically forbidden region, then the WKB solution must be the form

$$\psi(x) \simeq \frac{A}{\sqrt{\lambda(x)}} \exp\left(-\int_a^x \lambda(y)\, dy\right), \qquad x > a.$$

In other words, the growing exponential term $\frac{1}{\sqrt{\lambda(x)}} \exp\left(\int_a^x \lambda(y)\, dy\right)$ can not appear.

Remark 1.10.1. Note that if $\psi(x)$ has a leading behavior by a growing exponential, we can not exclude the possible appearance of the decaying exponential term since this is dominated by the growing exponential term and hence invisible in the leading behavior.

Comparing with the leading behavior of the Airy functions, we find that it can only be connected by $\mathrm{Ai}(z)$ and

$$\psi(x) \simeq \frac{2A}{\sqrt{k(x)}} \cos\left(\int_x^a k(y)\, dy - \frac{\pi}{4}\right), \qquad x < a.$$

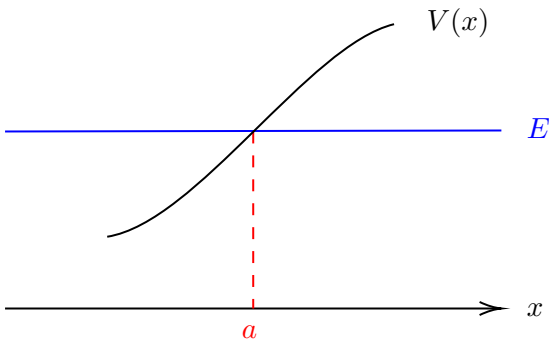
Similarly, if we find the approximate wave function

$$\psi(x) \simeq \frac{B}{\sqrt{k(x)}} \sin\left(\int_x^a k(y)\, dy - \frac{\pi}{4}\right), \qquad x < a$$

to the left of the turning point, then the leading behavior of $\mathrm{Bi}(z)$ implies

$$\psi(x) \simeq -\frac{B}{\sqrt{\lambda(x)}} \exp\left(\int_a^x \lambda(y)\, dy\right).$$

In summary, we have found the following connection condition for WKB solutions near the turning point $x = a$ with $V'(a) > 0$.

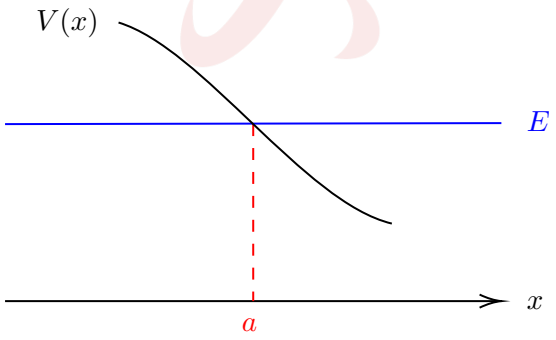


$$\frac{2A}{\sqrt{k(x)}} \cos\left(\int_x^a k(y)\, dy - \frac{\pi}{4}\right) \quad \Longleftarrow \quad \frac{A}{\sqrt{\lambda(x)}} \exp\left(-\int_a^x \lambda(y)\, dy\right)$$

$$\frac{B}{\sqrt{k(x)}} \sin\left(\int_x^a k(y)\, dy - \frac{\pi}{4}\right) \quad \Longrightarrow \quad -\frac{B}{\sqrt{\lambda(x)}} \exp\left(\int_a^x \lambda(y)\, dy\right)$$

The arrow is the implication direction.

② Let us then consider the case $V'(a) < 0$. The discussion is similar. We find the connection condition for WKB solutions near the turning point.



$$\frac{A}{\sqrt{\lambda(x)}} \exp\left(-\int_x^a \lambda(y)\, dy\right) \quad \Longrightarrow \quad \frac{2A}{\sqrt{k(x)}} \cos\left(\int_a^x k(y)\, dy - \frac{\pi}{4}\right)$$

$$-\frac{B}{\sqrt{\lambda(x)}} \exp\left(\int_x^a \lambda(y)\, dy\right) \quad \Longleftarrow \quad \frac{B}{\sqrt{k(x)}} \sin\left(\int_a^x k(y)\, dy - \frac{\pi}{4}\right)$$

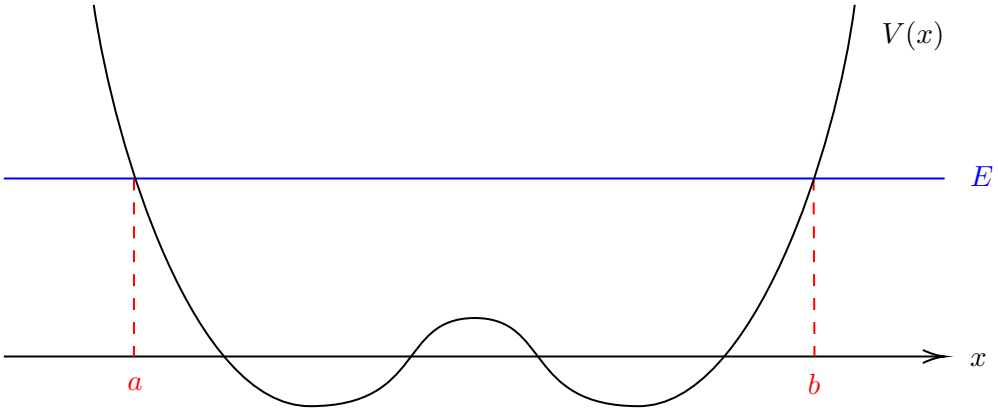
1.10.4 Semi-classical Quantization Rule

Let us consider a potential $V(x)$ such that

$$V(x) \to \infty \qquad \text{as } x \to \pm\infty.$$

We look for a bound state with energy E. By our experience with the harmonic oscillator, we expect that the allowed energies should be discrete.

Assume also that there exist exactly two turning points $x = a$ and $x = b$ with $a < b$.



For a bound state $\psi(x)$ which is normalizable, $\psi(x)$ should decay as $x \to \pm\infty$ in the forbidden region. The WKB approximation thus takes the form

$$\psi(x) = \begin{cases} \dfrac{A}{\sqrt{\lambda(x)}} \exp\left(-\displaystyle\int_x^a \lambda(y)\,dy\right) & x < a \\ \dfrac{B}{\sqrt{\lambda(x)}} \exp\left(-\displaystyle\int_b^x \lambda(y)\,dy\right) & x > b \end{cases}$$

By the connection formula, both these two behaviors will determine the behavior in the classically allowed region in between. Then the consistency condition gives

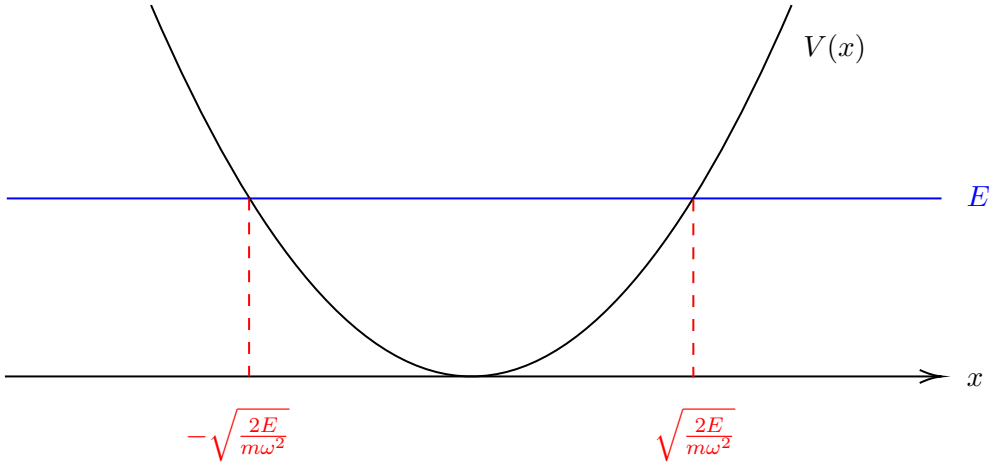
$$\int_a^x k(y)\,dy - \frac{\pi}{4} = -\left(\int_x^b k(y)\,dy - \frac{\pi}{4}\right) + n\pi$$

$$\implies \qquad \int_a^b k(y)\,dy = \pi\left(n + \frac{1}{2}\right) \qquad \text{for} \quad n \in \mathbb{Z}.$$

This is known as the *Einstein-Brillouin-Keller* (EBK) semi-classical quantization condition (or *Keller-Maslov* quantization condition), which improves the *Bohr-Sommerfeld quantization condition* via the Maslov index correction ($\frac{1}{2}$ here).

Example 1.10.2. *As an illustration, we consider the Harmonic oscillator with the potential*

$$V(x) = \frac{1}{2}m\omega^2 x^2.$$



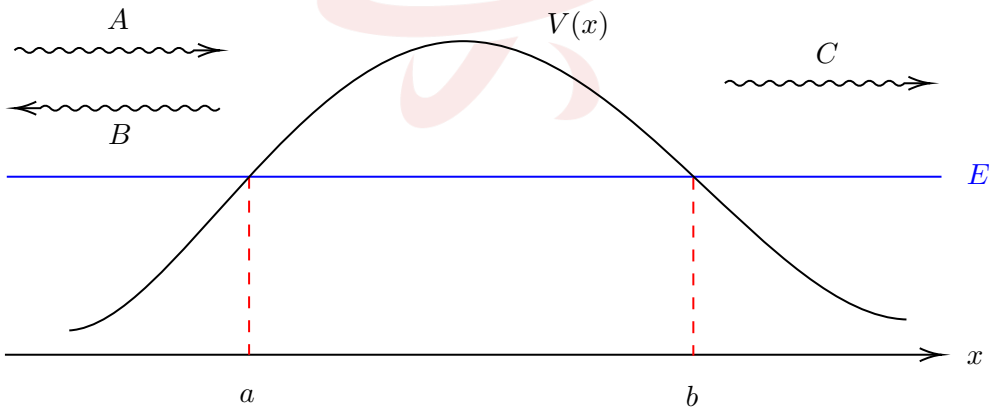
The EBK semi-classical quantization condition asks

$$\frac{\sqrt{2m}}{\hbar}\int_{-\sqrt{\frac{2E}{m\omega^2}}}^{\sqrt{\frac{2E}{m\omega^2}}}\sqrt{E-\frac{1}{2}m\omega^2x^2}\,dx=\pi\left(n+\frac{1}{2}\right)\qquad\Longrightarrow\qquad E=\left(n+\frac{1}{2}\right)\hbar\omega.$$

These are precisely the allowed energies of harmonic oscillators that we found before.

1.10.5 Quantum Tunneling

Consider a particle in the potential $V(x)$ with energy E. Classically, the particle can only move in the region $V(x)\le E$. Quantum mechanically, the particle has a chance to pass through a potential barrier which is classically forbidden. This phenomenon is called *quantum tunneling*.



Consider the potential as above, with $V(x)\to 0$ as $x\to\pm\infty$. Assume the energy $E>0$ which is smaller than the height of the potential. We consider the scattering problem with a wave incident from the left. Quantum mechanically, it has a chance to pass through the potential barrier. The tunnelling probability is the transmitted coefficient T as we discussed in Section 1.8.3. We will give an approximate formula for T via the WKB method.

Let us represent the WKB solution for the transmitted wave by

$$\begin{aligned}\psi(x)&\simeq\frac{C}{\sqrt{k(x)}}\exp\left(i\int_b^x k(y)\,dy-\frac{\pi}{4}i\right),\qquad x\gg b\\&=\frac{C}{\sqrt{k(x)}}\cos\left(\int_b^x k(y)\,dy-\frac{\pi}{4}\right)+\frac{iC}{\sqrt{k(x)}}\sin\left(\int_b^x k(y)\,dy-\frac{\pi}{4}\right).\end{aligned}$$

By the connection formula, the second term will match to an exponential that grows as we move to the left from $x = b$.

$$\begin{aligned} & -\frac{iC}{\sqrt{\lambda(x)}} \exp\left(\int_x^b \lambda(y)\,dy\right) \qquad\qquad a < x < b \\ = & -\frac{iC}{\sqrt{\lambda(x)}} \exp\left(-\int_a^x \lambda(y)\,dy\right) \exp\left(\int_a^b \lambda(y)\,dy\right). \end{aligned}$$

This in turn will match to the left of $x = a$ by

$$-\frac{2iC}{\sqrt{k(x)}} \exp\left(\int_a^b \lambda(y)\,dy\right) \cos\left(\int_x^a k(y)\,dy - \frac{\pi}{4}\right).$$

Decomposing this into left-moving and right-moving waves, the corresponding component for the right-moving wave is

$$-\frac{iC}{\sqrt{k(x)}} \exp\left(\int_a^b \lambda(y)\,dy\right) \exp\left(-i\int_x^a k(y)\,dy + \frac{\pi}{4}i\right).$$

This leads to the approximate relation

$$|A| = |C| \exp\left(\int_a^b \lambda(y)\,dy\right).$$

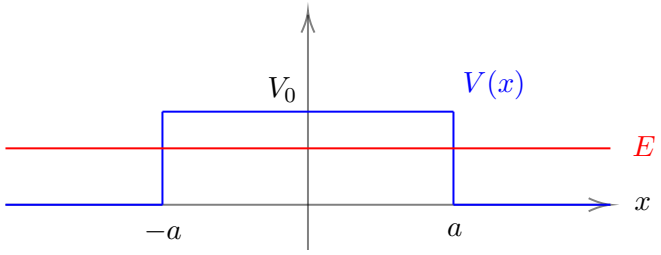
The WKB approximated transmission coefficient is

$$T \simeq \frac{|C|^2}{|A|^2} = \exp\left(-2\int_a^b \lambda(y)\,dy\right) = \exp\left(-\frac{2}{\hbar}\int_a^b \sqrt{2m(V(x)-E)}\,dx\right).$$

Remark 1.10.3. We will revisit this WKB formula of transmission coefficient via path integral method in Section 2.7.3. There the quantum tunneling is realized by a path in imaginary time.

Example 1.10.4. *Consider the potential of a square barrier*

$$V(x) = \begin{cases} V_0 & |x| < a \\ 0 & \textit{else} \end{cases}$$



The WKB approximated transmission coefficient is

$$T \simeq \exp\left(-\frac{2}{\hbar}\int_{-a}^{a} \sqrt{2m(V(x)-E)}\,dx\right) = \exp\left(-\frac{4a}{\hbar}\sqrt{2m(V_0-E)}\right).$$

1.11 Quantum Kepler Problem

In this section we study quantum particles in $\mathbb{R}^3$ under a potential of the form

$$V(\vec{r}) = -\frac{Z}{r}, \qquad Z > 0 \ \text{ constant.}$$

Here $\vec{r} = (x_1, x_2, x_3)$ are linear coordinates on $\mathbb{R}^3$ and

$$r = \sqrt{x_1^2 + x_2^2 + x_3^2}$$

is the length of $\vec{r}$. The corresponding force is

$$\vec{F} = -\nabla V = -\frac{Z}{r^2}\frac{\vec{r}}{r}.$$

In our assumption for $Z > 0$, this force is attractive via the inverse square law. For example, gravitational force and attractive electrostatic force are of this type. The problem with inverse square law is usually called the *Kepler problem*.

Classically, the Kepler problem exhibits rich symmetry and is completely integrable. Quantum mechanically, we will see that the bound state spectrum can be also exactly solved by symmetry. As an application, this allows us to compute the Hydrogen atom spectrum.

1.11.1 Angular Momentum

The angular momentum of the classical particle motion in $\mathbb{R}^3$ is

$$\vec{J} = \vec{r} \times \vec{p}$$

where $\vec{p}$ is the classical momentum. In components,

$$J_i = \sum_{j,k} \epsilon_{ijk} x_j p_k \quad \text{or explicitly} \quad \begin{cases} J_1 = x_2 p_3 - x_3 p_2 \\ J_2 = x_3 p_1 - x_1 p_3 \\ J_3 = x_1 p_2 - x_2 p_1 \end{cases}$$

Here ϵ_{ijk} is the Levi-Civita symbol with $\epsilon_{123} = 1$. Their Poisson bracket relations are

$$\{J_i, J_j\} = \sum_k \epsilon_{ijk} J_k.$$

In the quantum case, the angular momentums become the self-adjoint operators

$$\hat{J}_i = \sum_{j,k} \epsilon_{ijk} \hat{x}_j \hat{p}_k \quad \text{or explicitly} \quad \begin{cases} \hat{J}_1 = \hat{x}_2 \hat{p}_3 - \hat{x}_3 \hat{p}_2 \\ \hat{J}_2 = \hat{x}_3 \hat{p}_1 - \hat{x}_1 \hat{p}_3 \\ \hat{J}_3 = \hat{x}_1 \hat{p}_2 - \hat{x}_2 \hat{p}_1 \end{cases}$$

The canonical commutation relations

$$[\hat{x}_k, \hat{p}_j] = i\hbar \delta_{kj}$$

imply

$$\left[\hat{J}_k, \hat{J}_j\right] = i\hbar \sum_m \epsilon_{kjm} \hat{J}_m$$
$$\left[\hat{J}_k, \hat{x}_j\right] = i\hbar \sum_m \epsilon_{kjm} \hat{x}_m$$
$$\left[\hat{J}_k, \hat{p}_j\right] = i\hbar \sum_m \epsilon_{kjm} \hat{p}_m$$

Geometrically, these operators act on the Hilbert space $L^2(\mathbb{R}^3)$ with $p_k = -i\hbar \frac{\partial}{\partial x_k}$. Then

$$\begin{cases} \frac{i}{\hbar}\hat{J}_1 = x_2 \frac{\partial}{\partial x_3} - x_3 \frac{\partial}{\partial x_2} \\ \frac{i}{\hbar}\hat{J}_2 = x_3 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_3} \\ \frac{i}{\hbar}\hat{J}_3 = x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1} \end{cases}$$

They generate rotations in the x_2x_3-plane, x_3x_1-plane, x_1x_2-plane, respectively. Let

$$\hat{J}^2 := \hat{J} \cdot \hat{J} = \hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2.$$

Then it is direct to check that $\hat{J}^2$ commutes with $\hat{J}_1, \hat{J}_2, \hat{J}_3$

$$\left[\hat{J}^2, \hat{J}_1\right] = \left[\hat{J}^2, \hat{J}_2\right] = \left[\hat{J}^2, \hat{J}_3\right] = 0.$$

$\hat{J}^2$ is called the *Casimir element*.

The Hamiltonian operator of the Kepler problem

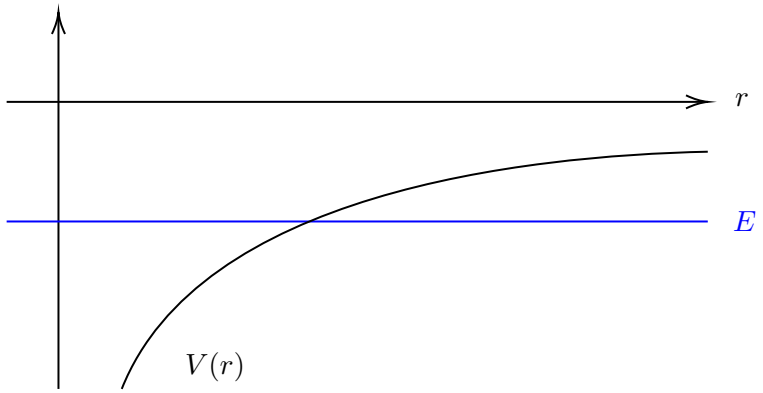
$$\widehat{\mathrm{H}} = \frac{\hat{p}^2}{2m} - \frac{Z}{r}$$

is clearly rotationally invariant. Therefore

$$\left[\widehat{\mathrm{H}}, \hat{J}_k\right] = 0, \qquad k = 1, 2, 3.$$

This can be also checked directly.

We are interested in bound states, which are normalizable solutions of the time-independent Schrödinger equation. The energy E of such bound state has to be negative in this case.



For $E < 0$, let us denote

$$B_E = \{\text{stationary states of energy } E\}\,.$$

Our goal is to find the allowed bound state energy E with non-trivial energy eigenspace B_E.

Since the angular momentum $\hat{J}_i$'s commute with $\widehat{\mathrm{H}}$, they actually act on the space B_E. Thus B_E forms a representation of SO(3), the three dimensional rotations. This puts important constraints on B_E, but is not enough to determine E since generators of these symmetries do not involve the Hamiltonian $\widehat{\mathrm{H}}$.

On the other hand, the Kepler problem of inverse square law has an enhanced symmetry

$$\mathrm{SO}(3) \longrightarrow \mathrm{SO}(4)$$

whose generators do involve the Hamiltonian. This will enable us to compute the bound state energy spectrum. We discuss next this enhanced symmetry.

1.11.2 Enhanced Symmetry

Classical Laplace-Runge-Lenz Vector

Consider a particle of mass m in the potential $V = -\frac{Z}{r}$. The classical Hamiltonian is

$$\mathscr{H} = \frac{p^2}{2m} - \frac{Z}{r}.$$

In the Kepler problem of inverse square force law, there exists an additional conserved quantity called the *Laplace-Runge-Lenz vector*. The classical Laplace-Runge-Lenz vector is

$$\vec{A} = \frac{\vec{p} \times \vec{J}}{mZ} - \frac{\vec{r}}{r}.$$

The classical conservation of $\vec{A} = (A_1, A_2, A_3)$ follows from the Poisson bracket relations

$$\{\mathscr{H}, A_k\} = 0, \qquad k = 1, 2, 3$$

which can be verified directly. This allows us to solve the classical motion as follows.

Consider the inner product

$$\vec{A} \cdot \vec{r} = \frac{\left(\vec{p} \times \vec{J}\right) \cdot \vec{r}}{mZ} - r = \frac{(\vec{r} \times \vec{p}) \cdot \vec{J}}{mZ} - r = \frac{J^2}{mZ} - r.$$

Let us write $\vec{A} \cdot \vec{r} = Ar\cos\theta$, where A is the length of $\vec{A}$ and θ is the angle between $\vec{A}$ and $\vec{r}$. Since both A and J^2 are conserved and hence are constants of motion, we find

$$r = \frac{J^2}{mZ} \frac{1}{1 + A\cos\theta}.$$

This immediately implies that the orbit in the classical Kepler problem must be an ellipse ($A < 1$), parabola ($A = 1$) or hyperbola ($A > 1$).

Classically, direct computation shows the following Poisson bracket relations

$$\{A_k, A_j\} = -\frac{2}{mZ^2}\sum_l \epsilon_{kjl} A_l \mathscr{H}.$$

Moreover, we have

$$\vec{A}\cdot\vec{J} = 0$$
$$A^2 = \vec{A}\cdot\vec{A} = 1 + \frac{2\mathscr{H}}{mZ^2}J^2.$$

Assume the classical energy is negative $\mathscr{H} < 0$. Then $A < 1$ and the orbits are ellipses. These are the classical analogues of bound states. Let us redefine two conserved vectors

$$\vec{I} = \frac{\vec{J} + \sqrt{\frac{mZ^2}{2|\mathscr{H}|}}\vec{A}}{2}, \qquad \vec{K} = \frac{\vec{J} - \sqrt{\frac{mZ^2}{2|\mathscr{H}|}}\vec{A}}{2}.$$

Then they satisfy the following Poisson bracket relations

$$\{I_i, I_j\} = \sum_l \epsilon_{ijl} I_l$$
$$\{K_i, K_j\} = \sum_l \epsilon_{ijl} K_l$$
$$\{I_i, K_j\} = 0$$

Thus $\{I_i, K_i\}$ form the Lie algebra $\mathrm{so}(3)\oplus\mathrm{so}(3)$, which is the same as the Lie algebra so(4). Since $\vec{I}, \vec{K}$ are conserved (they Poisson commute with $\mathscr{H}$), we conclude that the classical Kepler problem has enhanced SO(4) symmetry.

Quantum Laplace-Runge-Lenz Vector

Now we extend the above discussion to the quantum case. Define the quantum Laplace-Runge-Lenz vector by

$$\hat{A} = \frac{1}{2mZ}\left(\hat{p}\times\hat{J} - \hat{J}\times\hat{p}\right) - \frac{\vec{r}}{r}.$$

In the quantum case

$$\hat{p}\times\hat{J} \neq -\hat{J}\times\hat{p}$$

since entries of $\hat{p}$ and $\hat{J}$ do not commute. In components, we have

$$\begin{cases} \hat{A}_1 = \frac{1}{2mZ}\left[\left(\hat{p}_2\hat{J}_3 - \hat{p}_3\hat{J}_2\right) - \left(\hat{J}_2\hat{p}_3 - \hat{J}_3\hat{p}_2\right)\right] - \frac{\hat{x}_1}{r} \\ \hat{A}_2 = \frac{1}{2mZ}\left[\left(\hat{p}_3\hat{J}_1 - \hat{p}_1\hat{J}_3\right) - \left(\hat{J}_3\hat{p}_1 - \hat{J}_1\hat{p}_3\right)\right] - \frac{\hat{x}_2}{r} \\ \hat{A}_3 = \frac{1}{2mZ}\left[\left(\hat{p}_1\hat{J}_2 - \hat{p}_2\hat{J}_1\right) - \left(\hat{J}_1\hat{p}_2 - \hat{J}_2\hat{p}_1\right)\right] - \frac{\hat{x}_3}{r} \end{cases}$$

Using the commutation relations $\left[\hat{J}_k, \hat{p}_j\right] = i\hbar\sum_m \epsilon_{kjm}\hat{p}_m$, we find

$$\hat{J}\times\hat{p} = -\hat{p}\times\hat{J} + 2i\hbar\hat{p}.$$

Therefore we can equivalently write

$$\hat{A} = \frac{1}{mZ}\left(\hat{p} \times \hat{J} - i\hbar\hat{p}\right) - \frac{\vec{r}}{r}.$$

We also have

$$\hat{A} \cdot \hat{J} = \hat{J} \cdot \hat{A} = 0$$
$$\hat{A} \cdot \hat{A} = 1 + \frac{2\,\widehat{\mathrm{H}}}{mZ^2}\left(\hat{J} \cdot \hat{J} + \hbar^2\right).$$

This last quantum relation differs from the classical one by a quantum correction $\hbar^2$.

In the quantum case, we have the commutation relations (Exercise. See also [30] for a detailed presentation)

$$\left[\widehat{\mathrm{H}}, \hat{A}_i\right] = \left[\widehat{\mathrm{H}}, \hat{J}_i\right] = 0$$
$$\left[\hat{A}_k, \hat{A}_j\right] = -i\hbar\frac{2}{mZ^2}\sum_l \epsilon_{kjl}\hat{J}_l\,\widehat{\mathrm{H}}$$
$$\left[\hat{J}_k, \hat{A}_j\right] = i\hbar\sum_l \epsilon_{kjl}\hat{A}_l$$
$$\left[\hat{J}_k, \hat{J}_j\right] = i\hbar\sum_l \epsilon_{kjl}\hat{J}_l$$

Since $\hat{A}, \hat{J}$ commute with $\widehat{\mathrm{H}}$, they preserve the eigenspace B_E ($E < 0$)

$$\hat{A}_i, \hat{J}_i : B_E \longrightarrow B_E.$$

Restricting to this subspace B_E, we have

$$\left[\hat{A}_k, \hat{A}_j\right] = -i\hbar\frac{2}{mZ^2}\sum_l \epsilon_{kjl}E\hat{J}_l.$$

Now we can perform the same construction as in the classical case and redefine

$$\hat{I} = \frac{\hat{J} + \sqrt{\frac{mz^2}{2|E|}}\hat{A}}{2}, \qquad \hat{K} = \frac{\hat{J} - \sqrt{\frac{mz^2}{2|E|}}\hat{A}}{2} \qquad \text{on the subspace } B_E.$$

Their commutation relations again obey the Lie algebra of $\mathrm{so}(3) \oplus \mathrm{so}(3)$

$$\left[\hat{I}_j, \hat{I}_m\right] = i\hbar\sum_l \epsilon_{jml}\hat{I}_l$$
$$\left[\hat{K}_j, \hat{K}_m\right] = i\hbar\sum_l \epsilon_{jml}\hat{K}_l$$
$$\left[\hat{I}_j, \hat{K}_m\right] = 0$$

So we have quantum so(4) symmetry. The corresponding Casimir elements satisfy

$$\hat{I} \cdot \hat{I} = \hat{K} \cdot \hat{K} = \frac{mZ^2}{8|E|} - \frac{\hbar^2}{4} \qquad \text{on the subspace } B_E.$$

It is this relation that allows us to compute the bound state energies of quantum Kepler problem.

1.11.3 Representations of so(3)

We review some basic facts about representations of the Lie algebra so(3)

$$\mathrm{so}(3) = \big\{ A : 3 \times 3 \text{ real matrix} \,\big|\, A^T = -A \big\}.$$

This Lie algebra is three-dimensional with a basis by

$$t_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad t_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \qquad t_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Their commutation relations are

$$[t_i, t_j] = \sum_k \epsilon_{ijk} t_k.$$

To study the representation, it is convenient to redefine the following complexified basis

$$\begin{cases} L_+ := it_1 - t_2 \\ L_- := it_1 + t_2 \\ L_3 := it_3 \end{cases}$$

They satisfy the commutation relations

$$\begin{aligned} [L_3, L_+] &= L_+ \\ [L_3, L_-] &= -L_- \\ [L_+, L_-] &= 2L_3 \end{aligned}$$

Moreover, L_3 is Hermitian $L_3 = L_3^*$ and L_+, L_- are Hermitian adjoint of each other $L_+^* = L_-$.

A representation of so(3) is a vector space V together with a Lie algebra morphism

$$\rho : \mathrm{so}(3) \longrightarrow \mathrm{gl}(V).$$

We are interested in finite dimensional complex representations. Irreducible complex representations of so(3) are classified: for each non-negative half-integer $l = 0, \frac{1}{2}, 1, \frac{3}{2}, \cdots$, there exists precisely one isomorphic class of irreducible representation V_l of $\dim_{\mathbb{C}} V_l = 2l + 1$.

Let $\rho_l : \mathrm{so}(3) \to \mathrm{gl}(V_l)$ denote the corresponding representation. Then on each V_l, the element L_3 can be diagonalized by

$$\rho_l(L_3) = \begin{pmatrix} -l & & & & & & & \\ & -l+1 & & & & & & \\ & & -l+2 & & & & & \\ & & & \ddots & & & & \\ & & & & l-2 & & & \\ & & & & & l-1 & & \\ & & & & & & l & \end{pmatrix}.$$

The commutation relation

$$[L_3, L_\pm] = \pm L_\pm$$

says that the action of L_+ (L_-) will raise (lower) the eigenvalue of L_3 by one. So the actions of $L_3, L_\pm$ on the representation space V_l look like

Another way to distinguish these representations is to consider the Casimir element

$$\hat{C} = t_1^2 + t_2^2 + t_3^2 = -L_3^2 - \frac{1}{2}\left(L_+L_- + L_-L_+\right).$$

The Casimir element $\hat{C}$ commutes with all t_i's, hence becomes a constant when it acts on an irreducible representation. The crucial result is that on the irreducible representation V_l

$$\rho_l(\hat{C}) = -l(l+1).$$

We can generalize the above discussion to the representation of the Lie algebra $\mathrm{so}(4) = \mathrm{so}(3) \oplus \mathrm{so}(3)$. There the finite dimensional irreducible representations are classified by

$$V_k \otimes V_l, \qquad k, l = 0, \frac{1}{2}, 1, \frac{3}{2}, \cdots.$$

One copy of so(3) acts on the V_k-factor via the representation ρ_k and acts on the V_l factor as the identity. The other copy of so(3) acts on the V_l-factor via the representation ρ_l and acts on the V_k-factor as the identity. There are two Casimir elements $\hat{C}_1, \hat{C}_2$ corresponding to the two copies of so(3). In the representation $V_k \otimes V_l$, we have

$$\hat{C}_1 = -k(k+1), \quad \hat{C}_2 = -l(l+1) \qquad \text{on} \quad V_k \otimes V_l.$$

1.11.4 Energy Spectrum

Now we apply the so(3)-representation theory to analyze the quantum Kepler problem. We consider the eigenspace B_E of the Hamiltonian operator $\widehat{\mathrm{H}}$ with energy $E < 0$. This corresponds to bound states. A general spectral theory implies that B_E is finite dimensional.

We have operators

$$\hat{I}_i, \hat{K}_i : B_E \longrightarrow B_E$$

acting on B_E. Thus B_E forms a complex representation of the Lie algebra $\mathrm{so}(4) = \mathrm{so}(3) \oplus \mathrm{so}(3)$.

$$\left[\hat{I}_j, \hat{I}_m\right] = i\hbar \sum_l \epsilon_{jml} \hat{I}_l$$

$$\left[\hat{K}_j, \hat{K}_m\right] = i\hbar \sum_l \epsilon_{jml} \hat{K}_l$$

$$\left[\hat{I}_j, \hat{K}_m\right] = 0$$

Comparing with our conventions in Section 1.11.3, the Casimir element $\hat{C}_1$ for the so(3)-copy of $\{I_i\}$ and the Casimir element $\hat{C}_2$ for the so(3)-copy of $\{K_i\}$ are

$$\hat{C}_1 = -\frac{\hat{I}^2}{\hbar^2}, \qquad \hat{C}_2 = -\frac{\hat{K}^2}{\hbar^2}.$$

The algebraic relation on B_E

$$\hat{I} \cdot \hat{I} = \hat{K} \cdot \hat{K} = \frac{mZ^2}{8|E|} - \frac{\hbar^2}{4}$$

implies $\hat{C}_1 = \hat{C}_2$ on B_E. Thus B_E consists of copies of $V_k \otimes V_k$ for some k. Then

$$\hat{C}_1 = \hat{C}_2 = -k(k+1) \qquad \Longrightarrow \qquad |E| = \frac{mZ^2}{8\left(k+\frac{1}{2}\right)^2\hbar^2}.$$

Let $n = 2k+1$ which is a positive integer. Then the possible bound state energies are

$$E_n = -\frac{mZ^2}{2\hbar^2 n^2}, \qquad n = 1, 2, \cdots.$$

It turns out (via some further analysis) that each E_n does appear in the discrete spectrum and each $V_k \otimes V_k$ appears precisely once

$$B_{E_n} = V_{\frac{n-1}{2}} \otimes V_{\frac{n-1}{2}}.$$

In particular, the dimension of E_n-eigenstates is

$$\dim B_{E_n} = \left(\dim V_{\frac{n-1}{2}}\right)^2 = n^2.$$

1.11.5 Hydrogen Atom

The Hydrogen atom consists of a proton and an electron in dimension three. This can be viewed as a two-body quantum mechanical problem.

Let $\{\vec{x}_p, \vec{p}_p\}$ denote the position and momentum of the proton, and $\{\vec{x}_e, \vec{p}_e\}$ denote the position and momentum of the electron. The corresponding quantum operators satisfy the canonical commutation relations

$$\left[(\hat{x}_p)_i, (\hat{p}_p)_j\right] = i\hbar\delta_{ij}$$
$$\left[(\hat{x}_e)_i, (\hat{p}_e)_j\right] = i\hbar\delta_{ij}$$
$$[\hat{x}_p \text{ or } \hat{p}_p, \hat{x}_e \text{ or } \hat{p}_e] = 0.$$

The quantum Hamiltonian of the Hydrogen atom is

$$\widehat{\mathrm{H}} = \frac{\hat{p}_p^2}{2m_p} + \frac{\hat{p}_e^2}{2m_e} + V\left(|\vec{x}_e - \vec{x}_p|\right)$$

where m_p is the proton mass and m_e is the electron mass. V is the central Coulomb potential

$$V(r) = -\frac{e^2}{r},$$

where e is the elementary electric charge.

We can simplify this problem by introducing the center-of-mass coordinates. Precisely, let us define the center-of-mass position and momentum operators by

$$\hat{x}_c = \frac{m_e \hat{x}_e + m_p \hat{x}_p}{m_e + m_p}, \qquad \hat{p}_c = \hat{p}_p + \hat{p}_e.$$

Define the relative position and momentum operators by

$$\hat{x}_R = \hat{x}_e - \hat{x}_p, \qquad \hat{p}_R = \frac{m_p \hat{p}_e - m_e \hat{p}_p}{m_e + m_p}.$$

Then we can check that they still satisfy the canonical commutation relation

$$\begin{aligned} \left[(\hat{x}_c)_i, (\hat{p}_c)_j\right] &= i\hbar\delta_{ij} \\ \left[(\hat{x}_R)_i, (\hat{p}_R)_j\right] &= i\hbar\delta_{ij} \\ [\hat{x}_c \text{ or } \hat{p}_c, \hat{x}_R \text{ or } \hat{p}_R] &= 0. \end{aligned}$$

We can work with $\hat{x}_c, \hat{p}_c, \hat{x}_R, \hat{p}_R$ instead. The Hamiltonian operator now becomes

$$\widehat{\mathrm{H}} = \frac{\hat{p}_c^2}{2M_c} + \frac{\hat{p}_R^2}{2M_R} + V\left(|\vec{x}_R|\right)$$

where

$$M_c = m_e + m_p, \qquad M_R = \frac{m_e m_p}{m_e + m_p}.$$

We can solve the time-independent Schrödinger equation by using separation of variables

$$\psi(x_c, x_R) = \psi_c(x_c)\psi_R(x_R)$$

where $\psi_c(x_c)$ and $\psi_R(x_R)$ solve separately

$$\frac{\hat{p}_c^2}{2M_c}\psi_c = E_c\psi_c$$

$$\left(\frac{\hat{p}_R^2}{2M_R} + V\left(|\vec{x}_R|\right)\right)\psi_R = E_R\psi_R.$$

The total energy is

$$E = E_c + E_R.$$

The equation for ψ_c says that the center of mass moves as a free particle of mass M_c. The equation for ψ_R says that the relative motion between the proton and the electron is a quantum Kepler problem. By our result in Section 1.11.4, the energies E_R for bound states are quantized

$$E_{R,n} = -\frac{M_R e^4}{2\hbar^2 n^2}, \qquad n = 1, 2, \cdots.$$

The number of bound states with energy $E_{R,n}$ is n^2.

This formula explains precisely the emission spectrum of atomic hydrogen which occurs when an electron transits, or jumps, from a higher energy state to a lower energy state. The observed spectral lines match with the energy difference between two energy levels as above.

Chapter 2 Path Integral Formalism

In this chapter, we explain the path integral approach to quantum mechanics, which characterizes quantum dynamics of particles in terms of probabilistic paths. This formalism provides a powerful tool for calculating transition amplitudes and understanding quantum phenomena. It has been widely generalized and developed within modern quantum field theory. The presentation in this chapter will focus on intuition and examples to elucidate the basic idea.

2.1 Path Integral: Introduction

2.1.1 Quantum Evolution and Feynman Kernel

We have discussed the state space of quantum mechanics by wave functions ψ (vectors in a Hilbert space) and the law of quantum time evolution by the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi = \widehat{\mathrm{H}}\,\psi.$$

Here $\widehat{\mathrm{H}}$ is the Hamiltonian operator (also called Schrödinger operator), which is a differential operator that quantizes the classical Hamiltonian function $\mathscr{H}$.

We focus on time-independent $\widehat{\mathrm{H}}$ in this chapter. Viewing $\widehat{\mathrm{H}}$ as a self-adjoint operator on the Hilbert space of states, the time evolution of states via Schrödinger equation is solved by

$$\big|\psi(t'')\big\rangle = e^{-i\,\widehat{\mathrm{H}}(t''-t')/\hbar}\big|\psi(t')\big\rangle, \qquad t' < t''.$$

Thus the time evolution in quantum mechanics is completely encoded in the one-parameter family of unitary operators $e^{-i\,\widehat{\mathrm{H}}\,t/\hbar}$ on the Hilbert space.

As we will see, the operator $e^{-i\,\widehat{\mathrm{H}}\,t/\hbar}$ can be represented by an integral kernel. This means that the evolution of the wave function $\psi(\mathbf{x},t)$ can be expressed by the integral relation

$$\psi(\mathbf{x}'',t'') = \int d\mathbf{x}'\, K(\mathbf{x}'',t'';\mathbf{x}',t')\psi(\mathbf{x}',t').$$

This integral kernel K plays the major role in a different formulation of quantum mechanics: the "*path integral*" approach.

In classical mechanics, the principle of least action plays a primary role. The classical system is usually described by an action functional

$$S\left[\mathbf{x}(t)\right] = \int dt\,\mathscr{L}\left(\mathbf{x}(t),\dot{\mathbf{x}}(t)\right)$$

where $\mathscr{L}$ is called the *Lagrangian*. The trajectories of classical particles are stationary points of the action S, which can be described by the Euler-Lagrange equation

$$\frac{\partial \mathscr{L}}{\partial x_i} - \frac{d}{dt}\left(\frac{\partial \mathscr{L}}{\partial \dot{x}_i}\right) = 0.$$

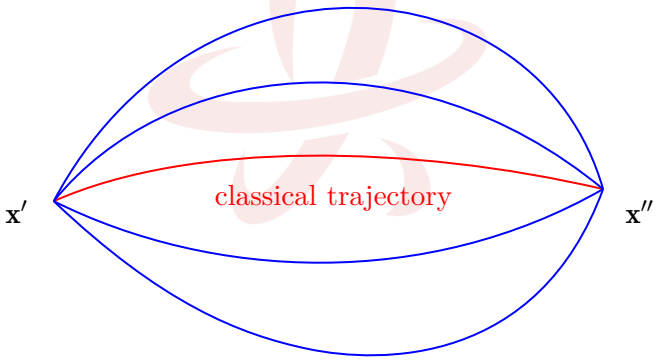
This Lagrangian formulation of classical mechanics is related to the Hamiltonian formulation by the Legendre transform

$$\mathscr{H}(\mathbf{x}, \mathbf{p}) = \mathbf{p} \cdot \dot{\mathbf{x}} - \mathscr{L}(\mathbf{x}, \dot{\mathbf{x}}).$$

Here $p_i = \frac{\partial \mathscr{L}}{\partial \dot{x}_i}$ is the Legendre transform from $\dot{\mathbf{x}}$, which is called the conjugate momentum of x_i.

Remarkably, the study of this integral kernel K leads directly to the Lagrangian formulation! This was first observed by Dirac in his study of canonical transformation of conjugate variables in quantum mechanics. This viewpoint was not essentially used until Feynman who developed the complete story of the "path integral approach to quantum mechanics". In this story, the integral kernel K has the interpretation as an "integration" over the space of paths

$$K(\mathbf{x}'', t''; \mathbf{x}', t') = \int_{\mathbf{x}(t')=x'}^{\mathbf{x}(t'')=x''} [D\mathbf{x}(t)]\, e^{\frac{i}{\hbar} S[\mathbf{x}(t)]}.$$



Here $[D\mathbf{x}(t)]$ is expected to be certain measure over the space of paths

$$\mathbf{x} : [t', t''] \longrightarrow \text{Space}$$

with endpoints $\mathbf{x}(t') = \mathbf{x}'$, $\mathbf{x}(t'') = \mathbf{x}''$.

One essential feature is that all paths will contribute to the integral kernel K through the action functional S. This expression provides a direct relation between classical and quantum mechanics. In the classical limit when $\hbar \to 0$, the method of stationary phase suggests that the above path integral will have dominate contributions from the stationary paths, which are precisely the classical trajectories! This clean and intuitive interpretation has been generalized and applied to many quantum physics and now become standard in textbooks.

Unfortunately, the path space is very big and infinite dimensional. In many quantum mechanical cases of our interest at hand, this can be related to Markovian evolution and Brownian

motion, thus the Wiener's measure is available. For general path integral in quantum field theory, the rigorous mathematical construction of the corresponding measure is yet unknown. This has been one of the major foundational challenges for modern quantum theory.

Nevertheless, the path integral approach offers a deep insight into many quantum problems. Even without a general rigorous measure available, we can still do many concrete calculations in physics. Actually, one major motivation of Feynman in developing the path integral formulation is to apply this to study quantum electrodynamics. One reason for the calculation power of path integral lies in the formalism itself. For the usual finite dimensional integral

$$\int f$$

we almost never compute it by definition of Riemann integral or Lebesgue integral. Instead, we usually compute it by symmetry and differential equations that can be derived from certain formal and natural properties provided by the integration. This is usually the situation how we manipulate path integrals in physics. Assuming some natural elementary properties of the path integral that we borrow from the ordinary integral, we can do many concrete calculations.

The above story of path integral is also called the *Feynman path integral*. The integral kernel K is usually called the *Feynman kernel* in the literature.

2.1.2 Position and Momentum Representation

We will mainly focus on the Hilbert space

$$L^2(\mathbb{R}^n).$$

A state $\psi(\mathbf{x}) \in L^2(\mathbb{R}^n)$ is a square integrable measurable function

$$\int d^n\mathbf{x}\, |\psi(\mathbf{x})|^2 < \infty.$$

The inner product is

$$\langle \psi_1 | \psi_2 \rangle = \int d^n\mathbf{x}\, \overline{\psi_1(\mathbf{x})} \psi_2(\mathbf{x}).$$

It would be convenient to introduce the eigenvector $|\mathbf{x}'\rangle$ of the position operator $\hat{x}$ by

$$\hat{x}_i \big|\mathbf{x}'\big\rangle = x_i' \big|\mathbf{x}'\big\rangle.$$

Strictly speaking, $|\mathbf{x}'\rangle$ does not lie in the Hilbert space and corresponds to the continuous spectra of the self-adjoint operator $\hat{x}$. The wave function of $|\mathbf{x}'\rangle$ is the δ-function

$$\big|\mathbf{x}'\big\rangle \quad \rightsquigarrow \quad \delta(\mathbf{x} - \mathbf{x}')$$

which is non-normalizable. This state lies in the space of tempered distributions. Nevertheless, we can formally work with such states to simplify many presentations. For example, we can treat all eigenvectors of the position operator as a "basis" with normalized inner product by

$$\big\langle \mathbf{x}'' \big| \mathbf{x}' \big\rangle = \delta(\mathbf{x}'' - \mathbf{x}').$$

Any state $|\psi\rangle$ can be expanded in this basis by

$$|\psi\rangle = \int d^n\mathbf{x}\, \psi(\mathbf{x})|\mathbf{x}\rangle.$$

Thus the wave function has the interpretation as the coefficients in terms of such a basis of position eigenvectors. Equivalently, we can write

$$\psi(\mathbf{x}) = \langle\mathbf{x}|\psi\rangle.$$

This can be justified by

$$\langle\mathbf{x}|\psi\rangle = \langle\mathbf{x}|\int d^n\mathbf{x}'\, \psi(\mathbf{x}')\big|\mathbf{x}'\big\rangle = \int d^n\mathbf{x}'\, \psi(\mathbf{x}')\big\langle\mathbf{x}\big|\mathbf{x}'\big\rangle = \int d^n\mathbf{x}'\, \psi(\mathbf{x}')\delta(\mathbf{x}-\mathbf{x}') = \psi(\mathbf{x}).$$

We can also rewrite the formula

$$|\psi\rangle = \int d^n\mathbf{x}\, \langle\mathbf{x}|\psi\rangle|\mathbf{x}\rangle = \int d^n\mathbf{x}\, |\mathbf{x}\rangle\langle\mathbf{x}|\psi\rangle$$

as the completeness relation

$$\int d^n\mathbf{x}\, |\mathbf{x}\rangle\langle\mathbf{x}| = 1$$

where 1 represents the identity operator.

Similarly, we can introduce the eigenvectors $|\mathbf{p}'\rangle$ of the momentum operator $\hat{p}$ by

$$\hat{p}_i\big|\mathbf{p}'\big\rangle = p_i'\big|\mathbf{p}'\big\rangle.$$

In our convention, we will normalize them by

$$\big\langle\mathbf{p}''\big|\mathbf{p}'\big\rangle = (2\pi\hbar)^n\delta(\mathbf{p}''-\mathbf{p}').$$

Thus the completeness relation reads

$$\frac{1}{(2\pi\hbar)^n}\int d^n\mathbf{p}\, |\mathbf{p}\rangle\langle\mathbf{p}| = 1.$$

The position and momentum eigenvectors are related by Fourier transform

$$|\mathbf{p}\rangle = \int d^n\mathbf{x}\, e^{i\mathbf{x}\cdot\mathbf{p}/\hbar}|\mathbf{x}\rangle$$

or equivalently

$$\langle\mathbf{x}|\mathbf{p}\rangle = e^{i\mathbf{x}\cdot\mathbf{p}/\hbar}.$$

Its complex conjugate gives

$$\langle\mathbf{p}|\mathbf{x}\rangle = e^{-i\mathbf{x}\cdot\mathbf{p}/\hbar}.$$

A state $|\psi\rangle$ can be either expanded by the position eigenvectors to get

$$\psi(\mathbf{x}) = \langle\mathbf{x}|\psi\rangle$$

or expanded by the momentum eigenvectors to get

$$\hat{\psi}(\mathbf{p}) = \langle\mathbf{p}|\psi\rangle.$$

They are related by

$$\psi(\mathbf{x}) = \langle \mathbf{x}|\psi\rangle = \langle \mathbf{x}| \frac{1}{(2\pi\hbar)^n} \int d^n\mathbf{p}\, |\mathbf{p}\rangle\langle \mathbf{p}|\psi\rangle = \frac{1}{(2\pi\hbar)^n} \int d^n\mathbf{p}\, e^{i\mathbf{x}\cdot\mathbf{p}/\hbar} \hat{\psi}(\mathbf{p})$$

$$\hat{\psi}(\mathbf{p}) = \langle \mathbf{p}|\psi\rangle = \langle \mathbf{p}| \int d^n\mathbf{x}\, |\mathbf{x}\rangle\langle \mathbf{x}|\psi\rangle = \int d^n\mathbf{x}\, e^{-i\mathbf{x}\cdot\mathbf{p}/\hbar} \psi(\mathbf{x})$$

which are precisely the Fourier transform formula.

We can use the above representation to express the integral kernel K. Let $|\psi\rangle$ be an initial state at $t = 0$. Let $|\psi, t\rangle$ denote the state at time t hence $|\psi\rangle = |\psi, 0\rangle$. Then

$$|\psi, t\rangle = e^{-i\,\widehat{\mathrm{H}}\,t/\hbar}|\psi\rangle.$$

The corresponding wave function is

$$\psi(\mathbf{x}, t) = \langle \mathbf{x}|\psi, t\rangle = \langle \mathbf{x}|e^{-i\,\widehat{\mathrm{H}}\,t/\hbar}|\psi\rangle.$$

If we compare at two different times t' and t'',

$$\begin{aligned}
\psi(\mathbf{x}'', t'') &= \big\langle \mathbf{x}''\big|e^{-i\,\widehat{\mathrm{H}}\,t''/\hbar}|\psi\rangle = \big\langle \mathbf{x}''\big|e^{-i\,\widehat{\mathrm{H}}(t''-t')/\hbar} e^{-i\,\widehat{\mathrm{H}}\,t'/\hbar}|\psi\rangle \\
&= \big\langle \mathbf{x}''\big|e^{-i\,\widehat{\mathrm{H}}(t''-t')/\hbar} \left(\int d^n\mathbf{x}'\, \big|\mathbf{x}'\big\rangle\big\langle \mathbf{x}'\big| \right) e^{-i\,\widehat{\mathrm{H}}\,t'/\hbar}|\psi\rangle \\
&= \int d^n\mathbf{x}'\, \big\langle \mathbf{x}''\big|e^{-i\,\widehat{\mathrm{H}}(t''-t')/\hbar}\big|\mathbf{x}'\big\rangle \psi(\mathbf{x}', t')
\end{aligned}$$

we find the following expression for the Feynman kernel K

$$K(\mathbf{x}'', t''; \mathbf{x}', t') = \big\langle \mathbf{x}''\big|e^{-i\,\widehat{\mathrm{H}}(t''-t')/\hbar}\big|\mathbf{x}'\big\rangle.$$

In summary, we can view $K(\mathbf{x}'', t''; \mathbf{x}', t')$ as the matrix entries of the evolution operator $e^{-i\,\widehat{\mathrm{H}}(t''-t')/\hbar}$ represented in the basis of the position eigenvectors.

2.2 Path Integral via Time Slicing

2.2.1 Free Particle

We start the study of the Feynman kernel K from the example of the free particle. The Hamiltonian is

$$\widehat{\mathrm{H}}_0 = \frac{\hat{p}^2}{2m}, \qquad m = \text{mass}.$$

We denote the Feynman kernel of the free particle by K_0

$$K_0(\mathbf{x}'', t''; \mathbf{x}', t') = \big\langle \mathbf{x}''\big|e^{-i\,\widehat{\mathrm{H}}_0(t''-t')/\hbar}\big|\mathbf{x}'\big\rangle.$$

To describe this kernel, we can first compute

$$\langle \mathbf{p}|e^{-i\,\widehat{\mathrm{H}}_0\,t/\hbar}|\mathbf{x}\rangle = \langle \mathbf{p}|e^{-i\,\frac{\hat{p}^2 t}{2m\hbar}}|\mathbf{x}\rangle \underset{\langle \mathbf{p}|\hat{p}_i = p_i\langle \mathbf{p}|}{\overset{\text{using}}{=\!=\!=}} e^{-i\,\frac{\mathbf{p}^2 t}{2m\hbar}} \langle \mathbf{p}|\mathbf{x}\rangle = e^{-i\,\frac{\mathbf{p}^2 t}{2m\hbar}} e^{-i\mathbf{x}\cdot\mathbf{p}/\hbar}.$$

It follows that

$$\begin{aligned}\langle \mathbf{x}'' | e^{-i\,\widehat{\mathrm{H}}_0(t''-t')/\hbar} | \mathbf{x}' \rangle &= \frac{1}{(2\pi\hbar)^n} \int d^n\mathbf{p}\, \langle \mathbf{x}'' | \mathbf{p} \rangle \langle \mathbf{p} | e^{-i\,\widehat{\mathrm{H}}_0(t''-t')/\hbar} | \mathbf{x}' \rangle \\ &= \frac{1}{(2\pi\hbar)^n} \int d^n\mathbf{p}\, e^{-i\frac{\mathbf{p}^2(t''-t')}{2m\hbar}} e^{i(\mathbf{x}''-\mathbf{x}')\cdot\mathbf{p}/\hbar}.\end{aligned}$$

Using the Gaussian integral formula

$$\int du\, e^{-au^2+bu} = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}},$$

the above integral is (strictly speaking we need to do analytic continuation. See Section 2.5.2)

$$K_0(\mathbf{x}'', t''; \mathbf{x}', t') = \left(\frac{m}{2\pi\hbar i(t''-t')}\right)^{\frac{n}{2}} e^{\frac{i}{\hbar}\frac{m(\mathbf{x}''-\mathbf{x}')^2}{2(t''-t')}}.$$

This gives an explicit formula for the integral kernel of the free particle.

Remark 2.2.1. Note that when the time is purely imaginary with

$$i(t''-t') = \tau > 0$$

and when $m = \frac{\hbar}{2}$, the kernel K becomes

$$\frac{1}{(4\pi\tau)^{n/2}} e^{-\frac{(\mathbf{x}''-\mathbf{x}')^2}{4\tau}},$$

which is precisely the kernel for the heat operator $e^{\tau\nabla^2}$ on $\mathbb{R}^n$. This is the expected result since in this case $\widehat{\mathrm{H}}_0 = -\frac{\hbar^2}{2m}\nabla^2 = -\hbar\nabla^2$ and

$$\langle \mathbf{x}'' | e^{\tau\nabla^2} | \mathbf{x}' \rangle = \langle \mathbf{x}'' | e^{-\widehat{\mathrm{H}}_0\,\tau/\hbar} | \mathbf{x}' \rangle = \frac{1}{(4\pi\tau)^{n/2}} e^{-\frac{(\mathbf{x}''-\mathbf{x}')^2}{4\tau}}.$$

We will come back to the discussion of imaginary time in Section 2.2.5.

2.2.2 Infinitesimal Time

We next consider the Feynman kernel for the general Hamiltonian operator

$$\widehat{\mathrm{H}} = \frac{\hat{p}^2}{2m} + V(\mathbf{x})$$

with the evolution in an infinitesinally small amount of time δt

$$K(\mathbf{x}'', t+\delta t; \mathbf{x}', t) = \langle \mathbf{x}'' | e^{-i\,\widehat{\mathrm{H}}\,\delta t/\hbar} | \mathbf{x}' \rangle.$$

Keeping the first order in δt, we have approximately

$$e^{-i\,\widehat{\mathrm{H}}\,\delta t/\hbar} \simeq e^{-i\frac{\hat{p}^2\delta t}{2m\hbar}} e^{-i\frac{V(\hat{\mathbf{x}})\delta t}{\hbar}}.$$

Using the previous result on the free Feynman kernel, we find

$$\begin{aligned}K(\mathbf{x}'', t+\delta t; \mathbf{x}', t) &\simeq \langle \mathbf{x}'' | e^{-i\frac{\hat{p}^2\delta t}{2m\hbar}} e^{-i\frac{V(\hat{\mathbf{x}})\delta t}{\hbar}} | \mathbf{x}' \rangle \\ &= \langle \mathbf{x}'' | e^{-i\frac{\hat{p}^2\delta t}{2m\hbar}} | \mathbf{x}' \rangle e^{-i\frac{V(\mathbf{x}')\delta t}{\hbar}} \\ &= \left(\frac{m}{2\pi\hbar i\delta t}\right)^{\frac{n}{2}} e^{i\frac{m(\mathbf{x}''-\mathbf{x}')^2}{2\hbar\delta t} - i\frac{V(\mathbf{x}')\delta t}{\hbar}} \\ &= \left(\frac{m}{2\pi\hbar i\delta t}\right)^{\frac{n}{2}} e^{\frac{i}{\hbar}\left[\frac{m}{2}\left(\frac{\mathbf{x}''-\mathbf{x}'}{\delta t}\right)^2 - V(\mathbf{x}')\right]\delta t}.\end{aligned}$$

Note that the Lagrangian of the classical system emerges naturally. In a small amount of time, the quantity $\frac{m}{2}\left(\frac{\mathbf{x}''-\mathbf{x}'}{\delta t}\right)^2$ is approximately the kinetic energy. Thus the expression

$$\frac{m}{2}\left(\frac{\mathbf{x}''-\mathbf{x}'}{\delta t}\right)^2 - V(\mathbf{x}')$$

approximates precisely the kinetic energy minus the potential energy, i.e., the Lagrangian.

2.2.3 Composition Law

The quantum evolution fulfills the semi-group property

$$e^{-i\,\widehat{\mathrm{H}}(t'''-t')/\hbar} = e^{-i\,\widehat{\mathrm{H}}(t'''-t'')/\hbar} e^{-i\,\widehat{\mathrm{H}}(t''-t')/\hbar}, \qquad t' < t'' < t'''.$$

In terms of the integral kernel, this becomes

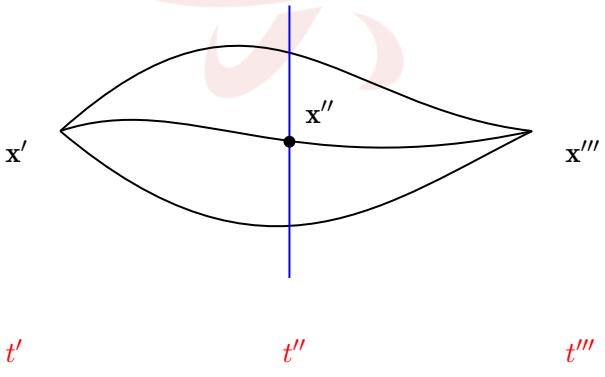
$$\begin{aligned}\left\langle \mathbf{x}'''\middle| e^{-i\,\widehat{\mathrm{H}}(t'''-t')/\hbar}\middle|\mathbf{x}'\right\rangle &= \left\langle \mathbf{x}'''\middle| e^{-i\,\widehat{\mathrm{H}}(t'''-t'')/\hbar} e^{-i\,\widehat{\mathrm{H}}(t''-t')/\hbar}\middle|\mathbf{x}'\right\rangle \\ &= \int d^n\mathbf{x}''\, \left\langle \mathbf{x}'''\middle| e^{-i\,\widehat{\mathrm{H}}(t'''-t'')/\hbar}\middle|\mathbf{x}''\right\rangle \left\langle \mathbf{x}''\middle| e^{-i\,\widehat{\mathrm{H}}(t''-t')/\hbar}\middle|\mathbf{x}'\right\rangle,\end{aligned}$$

i.e.,

$$K(\mathbf{x}''', t'''; \mathbf{x}', t') = \int d^n\mathbf{x}''\, K(\mathbf{x}''', t'''; \mathbf{x}'', t'') K(\mathbf{x}'', t''; \mathbf{x}', t').$$

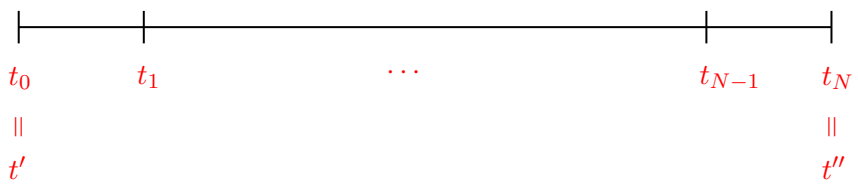
This is the *composition law* for the Feynman kernel K.

Geometrically, this composition law can be illustrated by



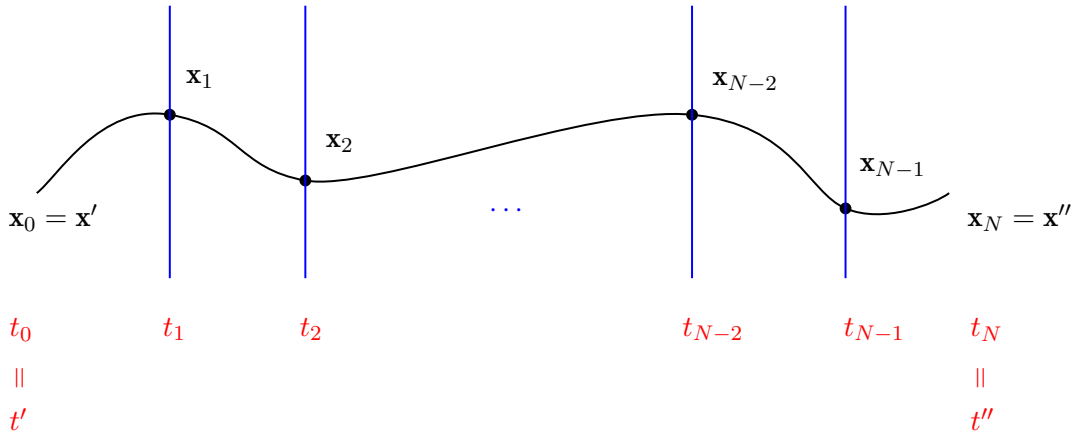
Thinking about $K(\mathbf{x}''', t'''; \mathbf{x}', t')$ as a transition amplitude from $\mathbf{x}'$ at time t' to $\mathbf{x}'''$ at time t''', the composition law says that this transition amplitude is the same as summing over all the transitions at the intermediate time t'' for all possible $\mathbf{x}''$.

We can further subdivide the time interval for $t_0 = t' < t_1 < t_2 < \cdots < t_{N-1} < t_N = t''$.



Then the same consideration leads to the composition law

$$K(\mathbf{x}'',t'';\mathbf{x}',t') = \int d^n\mathbf{x}_1 \int d^n\mathbf{x}_2 \cdots \int d^n\mathbf{x}_{N-1}$$
$$K(\mathbf{x}'',t'';\mathbf{x}_{N-1},t_{N-1})K(\mathbf{x}_{N-1},t_{N-1};\mathbf{x}_{N-2},t_{N-2})\cdots K(\mathbf{x}_1,t_1;\mathbf{x}',t').$$



This is again interpreted as summing over all possible intermediate transitions at time $t_1, t_2, \cdots, t_{N-1}$.

2.2.4 Path Integral

Now we can subdivide the time interval $[t', t'']$ into small intervals for sufficiently large N

$$t_0 = t' < t_1 < t_2 < \cdots < t_{N-1} < t_N = t'',$$

where

$$t_j = t' + j\epsilon, \qquad \epsilon = \frac{t''-t'}{N}.$$

The composition law gives

$$K(\mathbf{x}'',t'';\mathbf{x}',t') = \int \prod_{j=1}^{N-1} d^n\mathbf{x}_j \prod_{j=0}^{N-1} K(\mathbf{x}_{j+1},t_{j+1};\mathbf{x}_j,t_j), \qquad \mathbf{x}_0 = \mathbf{x}',\ \mathbf{x}_N = \mathbf{x}''.$$

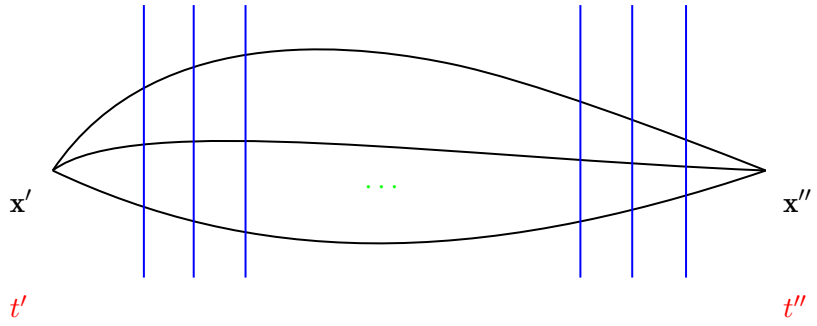
Applying our result for the integral kernel over small time interval, this is approximated by

$$\simeq \left(\frac{m}{2\pi\hbar i\epsilon}\right)^{Nn/2} \int \prod_{j=1}^{N-1} d^n\mathbf{x}_j \, e^{\frac{i}{\hbar}\sum_{j=0}^{N-1}\left[\frac{m}{2}\left(\frac{\mathbf{x}_{j+1}-\mathbf{x}_j}{\epsilon}\right)^2 - V(\mathbf{x}_j)\right]\epsilon}.$$

In the limit $N \to \infty$ or $\epsilon \to 0$, this integral is expected to reach the following form of Feynman path integral

$$K(\mathbf{x}'',t'';\mathbf{x}',t') = \int_{\mathbf{x}(t')=\mathbf{x}'}^{\mathbf{x}(t'')=\mathbf{x}''} [D\mathbf{x}(t)]\, e^{\frac{i}{\hbar}\int_{t'}^{t''}\left(\frac{m}{2}\dot{\mathbf{x}}^2 - V(\mathbf{x})\right)dt}$$

for some suitable measure on the space of paths going from $\mathbf{x}'$ at time t' to $\mathbf{x}''$ at time t''.



Note that

$$S\left[\mathbf{x}(t)\right] = \int_{t'}^{t''} \left(\frac{m}{2}\dot{\mathbf{x}}^2 - V(\mathbf{x})\right) dt$$

is precisely the classical action functional. So the integral kernel K can be also written as

$$K(\mathbf{x}'', t''; \mathbf{x}', t') = \int_{\mathbf{x}(t')=\mathbf{x}'}^{\mathbf{x}(t'')=\mathbf{x}''} [D\mathbf{x}(t)]\, e^{\frac{i}{\hbar}S[\mathbf{x}(t)]}.$$

We will illustrate how to analyze this path integral in a suitable sense in subsequence sections.

It light of this above formula, Feynman's path integral can be understood as a *Lagrangian formulation of quantum mechanics*, providing an alternative viewpoint compared to the traditional Hamiltonian operator approach.

2.2.5 Imaginary Time

A more convenient way to obtain a mathematically better behaved path integral is to make an analytic continuation in time to

$$t = -i\tau, \qquad \tau \in \mathbb{R}.$$

This analytic continuation is called *Wick rotation*. The corresponding path integral is called the *Euclidean path integral*. We denote the integral kernel in imaginary time by

$$\begin{aligned} K_E(\mathbf{x}'', \tau''; \mathbf{x}', \tau') &:= K(\mathbf{x}'', -i\tau''; \mathbf{x}', -i\tau') = \left\langle \mathbf{x}'' \middle| e^{-\widehat{\mathrm{H}}(\tau''-\tau')/\hbar} \middle| \mathbf{x}' \right\rangle \\ &= \int_{\mathbf{x}(\tau')=\mathbf{x}'}^{\mathbf{x}(\tau'')=\mathbf{x}''} [D_E\mathbf{x}(\tau)]\, e^{-\frac{1}{\hbar}\int_{\tau'}^{\tau''}\left(\frac{m}{2}\dot{\mathbf{x}}^2 + V(\mathbf{x})\right)d\tau}. \end{aligned}$$

At this point we can use the conditional Wiener measure to define $[D_E\mathbf{x}(\tau)]$. In the mathematical literature, this above path integral representation for the Euclidean Feynman path integral is established as the *Feynman-Kac formula*.

We will also denote the Euclidean action by

$$S_E\left[\mathbf{x}(\tau)\right] = \int \left(\frac{m}{2}\dot{\mathbf{x}}^2 + V(\mathbf{x})\right) d\tau.$$

The Euclidean path integral becomes

$$K_E(\mathbf{x}'', \tau''; \mathbf{x}', \tau') = \int_{\mathbf{x}(\tau')=\mathbf{x}'}^{\mathbf{x}(\tau'')=\mathbf{x}''} [D_E\mathbf{x}(\tau)]\, e^{-\frac{1}{\hbar}S_E[\mathbf{x}(\tau)]}.$$

The physical meaning of imaginary time is that the Euclidean kernel

$$\rho(\mathbf{x}'', \mathbf{x}'; \beta) := \left\langle \mathbf{x}'' \middle| e^{-\beta\,\widehat{\mathrm{H}}} \middle| \mathbf{x}' \right\rangle$$

becomes the density matrix in statistical mechanics.

2.3 Gaussian Path Integral

2.3.1 Gaussian Integral

Recall the Gaussian integral formula

$$\int_{\mathbb{R}} dx\, e^{-ax^2} = \sqrt{\frac{\pi}{a}}, \qquad a > 0.$$

This Gaussian integral can be extended to the imaginary phase $a = -i\lambda$ via analytic continuation (see Example 2.5.2). It picks up the branch of $\sqrt{\frac{\pi}{a}} = \sqrt{\frac{i\pi}{\lambda}}$ by

$$\int_{\mathbb{R}} dx\, e^{i\lambda x^2} = \sqrt{\frac{i\pi}{\lambda}} = e^{\frac{i\pi}{4}\operatorname{sign}\lambda}\sqrt{\frac{\pi}{|\lambda|}}, \qquad \lambda \in \mathbb{R} - \{0\}.$$

This can be generalized to n-dimensional case as follows.

Proposition 2.3.1. *Let $A = (a_{ij})$ be a symmetric positive definite real matrix. Then*

$$\int_{\mathbb{R}^n} d^n\mathbf{x}\, e^{-\mathbf{x}^t A\mathbf{x}} = \frac{\pi^{n/2}}{\sqrt{\det A}}. \tag{*}$$

Here $\mathbf{x}^t A\mathbf{x} = \sum_{i,j=1}^{n} a_{ij}x_i x_j$. More generally, we have

$$\int_{\mathbb{R}^n} d^n\mathbf{x}\, e^{-\mathbf{x}^t A\mathbf{x}+\mathbf{J}^t\cdot\mathbf{x}} = \frac{\pi^{n/2}}{\sqrt{\det A}} e^{\frac{1}{4}\mathbf{J}^t A^{-1}\mathbf{J}}.$$

Proof: Let $A = P\begin{pmatrix}\lambda_1 & & \\ & \ddots & \\ & & \lambda_n\end{pmatrix}P^{-1}$ where $P \in SO(n)$. We consider the change of variables

$$\mathbf{x} = P\mathbf{y}.$$

Since $P \in SO(n)$, this change of variables has trivial Jacobian $d^n\mathbf{x} = d^n\mathbf{y}$. Moreover

$$\mathbf{x}^t A\mathbf{x} = \mathbf{y}^t P^t AP\mathbf{y} = \mathbf{y}^t P^{-1}AP\mathbf{y} = \mathbf{y}^t\begin{pmatrix}\lambda_1 & & \\ & \ddots & \\ & & \lambda_n\end{pmatrix}\mathbf{y} = \lambda_1 y_1^2 + \lambda_2 y_2^2 + \cdots + \lambda_n y_n^2.$$

Therefore

$$\int_{\mathbb{R}^n} d^n\mathbf{x}\, e^{-\mathbf{x}^t A\mathbf{x}} = \int_{\mathbb{R}^n} d^n\mathbf{y}\, e^{-\sum_{i=1}^{n}\lambda_i y_i^2} = \prod_{i=1}^{n}\sqrt{\frac{\pi}{\lambda_i}} = \frac{\pi^{n/2}}{\sqrt{\det A}}.$$

The case with a linear term $\mathbf{J}^t\cdot\mathbf{x}$ follows by completing the square. □

Remark 2.3.2. This result can be analytically continued to the imaginary case $A = -i\Lambda$ and

$$\int_{\mathbb{R}^n} d^n\mathbf{x}\, e^{i\mathbf{x}^t\Lambda\mathbf{x}} = \frac{\pi^{n/2}}{\sqrt{\det(-i\Lambda)}} = e^{\frac{i\pi}{4}(n_+ - n_-)}\frac{\pi^{n/2}}{\sqrt{|\det\Lambda|}}$$

where n_+ and n_- are respectively the numbers of positive and negative eigenvalues of Λ.

2.3.2 Zeta Function Regularization

Let us apply the idea of Gaussian integral to path integrals. To illustrate the basic idea, we start with the simplest example of one-dimensional free particle to compute the kernel

$$K_0(x'', T; x', 0) = \int_{x(0)=x'}^{x(T)=x''} [Dx(t)]\, e^{\frac{i}{\hbar}\int_0^T \left(\frac{m}{2}\dot{x}^2\right) dt}.$$

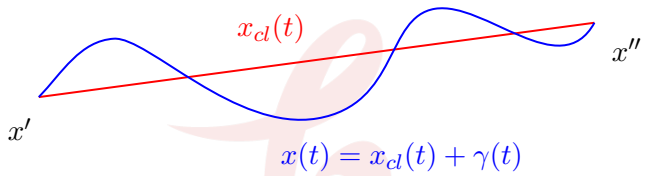
Let $x_{cl}(t)$ denote the classical trajectory from x' at time $t = 0$ to x'' at time $t = T$

$$x_{cl}(t) = x' + \frac{t}{T}(x'' - x').$$

Any path $x(t)$ with $x(0) = x'$, $x(T) = x''$ can be written as

$$x(t) = x_{cl}(t) + \gamma(t),$$

where the path $\gamma(t)$ satisfies $\gamma(0) = \gamma(T) = 0$. We can view $\gamma(t)$ as the quantum fluctuations around the classical trajectory $x_{cl}(t)$.



Since the classical trajectory $x_{cl}(t)$ is a stationary point of the action, the action functional $S[x] = S[x_{cl} + \gamma]$ has no linear dependence in γ. Thus

$$S[x] = \int_0^T \frac{m}{2}(\dot{x}_{cl} + \dot{\gamma})^2\, dt = \int_0^T \frac{m}{2}\dot{x}_{cl}{}^2\, dt + \int_0^T \frac{m}{2}\dot{\gamma}^2\, dt = S[x_{cl}] + \int_0^T \frac{m}{2}\dot{\gamma}^2\, dt.$$

This can be also checked directly. We can write the second term via integration by part as

$$\int_0^T \frac{m}{2}\dot{\gamma}^2\, dt = -\frac{m}{2}\int_0^T \gamma\left(\frac{d^2}{dt^2}\right)\gamma\, dt.$$

Thus the path integral becomes

$$K(x'', T; x', 0) = e^{\frac{i}{\hbar}S[x_{cl}]} \int_{\gamma(0)=0}^{\gamma(T)=0} [D\gamma(t)]\, e^{\frac{im}{2\hbar}\int_0^T \gamma\left(-\frac{d^2}{dt^2}\right)\gamma\, dt}.$$

Observe that the path integral in $\gamma(t)$ becomes the form of Gaussian integral, though in the infinite dimensional space of paths $\gamma(t)$ with the Dirichlet boundary conditions $\gamma(0) = \gamma(t) = 0$. The analogy with the finite dimensional Gaussian integral is

$$\begin{aligned} i &\quad\longleftrightarrow\quad t \\ x_i &\quad\longleftrightarrow\quad \gamma(t) \\ \sum_i &\quad\longleftrightarrow\quad \int dt \\ \int \prod_i dx_i &\quad\longleftrightarrow\quad \int [D\gamma(t)] \end{aligned}$$

Let us denote the elliptic operator

$$A = -\frac{d^2}{dt^2}.$$

Comparing with the finite dimensional Gaussian integral, we would expect a result of the form

$$\int_{\gamma(0)=0}^{\gamma(T)=0} [D\gamma(t)]\, e^{\frac{im}{2\hbar}\int_0^T \gamma\left(-\frac{d^2}{dt^2}\right)\gamma\, dt} = N\,(\det A)^{-\frac{1}{2}}\,,$$

where N is some normalization constant to be determined.

We need to give a meaning to the determinant of the operator A. We consider the eigenvalue problem for A with Dirichlet boundary conditions

$$A\gamma_m(t) = \lambda_m \gamma_m(t), \qquad \gamma_m(0) = \gamma_m(T) = 0.$$

We know from the general theory of eigenvalue problem that

$$0 < \lambda_1 \le \lambda_2 \le \cdots \le \lambda_m \le \cdots\,, \qquad \lambda_m \to \infty \quad \text{as } m \to +\infty$$

and $\{\gamma_m(t)\}$ form an orthonormal basis of the Hilbert space of square integrable functions $\gamma(t)$ with $\gamma(0) = \gamma(T) = 0$. Then the naive definition of $\det A$ would be

$$\det A \stackrel{?}{=} \prod_{m=1}^{\infty} \lambda_m.$$

However, this naive product is divergent since $\lambda_m \to \infty$ as $m \to \infty$.

Fortunately, there is a way out using analytic continuation. Let us define the zeta function associated to the elliptic operator A by

$$\zeta_A(s) := \sum_{m=1}^{\infty} \frac{1}{\lambda_m^s}, \qquad s \in \mathbb{C}.$$

It is known that the series for $\zeta_A(s)$ is well-defined for $\operatorname{Re} s$ sufficiently large, and can be analytically continued to the origin $s = 0$. Thus

$$\zeta_A'(0) \text{ is well defined.}$$

Intuitively, the derivative formula

$$\zeta_A'(s) = \sum_{m=1}^{\infty} \frac{-\ln \lambda_m}{\lambda_m^s}, \qquad \operatorname{Re} s \gg 0$$

suggests that the naive product $\prod_{m=1}^{\infty} \lambda_m$ should be defined by the analytic continuation

$$\text{“}\prod_{m=1}^{\infty} \lambda_m\text{”} := e^{-\zeta_A'(0)}.$$

Then we can define the functional determinant of the operator A by

$$\det A := e^{-\zeta_A'(0)}.$$

Let us see how this works. The eigenfunctions and eigenvalues of A are easily found

$$\begin{cases} \gamma_m(t) = c_m \sin\left(\dfrac{m\pi t}{T}\right), & c_m \text{ some constant} \\ \lambda_m = \left(\dfrac{\pi m}{T}\right)^2. \end{cases}$$

Thus the zeta function $\zeta_A(s)$ is

$$\zeta_A(s) = \sum_{m=1}^{\infty} \left(\frac{T}{\pi m}\right)^{2s} = \left(\frac{T}{\pi}\right)^{2s} \zeta(2s),$$

where

$$\zeta(s) = \sum_{m=1}^{\infty} \frac{1}{m^s}$$

is the Riemann zeta function. Using the known result

$$\zeta(0) = -\frac{1}{2}, \qquad \zeta'(0) = -\frac{1}{2}\ln 2\pi,$$

we compute

$$\zeta_A'(0) = 2\ln\left(\frac{T}{\pi}\right)\zeta(0) + 2\zeta'(0) = -\ln\left(\frac{T}{\pi}\right) - \ln 2\pi = -\ln 2T.$$

Thus

$$\det A = e^{-\zeta_A'(0)} = 2T.$$

Plugging this into the path integral, we arrive at

$$K_0(x'', T; x', 0) = \frac{N}{\sqrt{2T}} e^{\frac{i}{\hbar}S[x_{cl}]} = \frac{N}{\sqrt{2T}} e^{\frac{im(x''-x')^2}{2\hbar T}}.$$

This is consistent with our previous result for free particle, with the normalization constant

$$N = \left(\frac{m}{\pi i\hbar}\right)^{\frac{1}{2}}.$$

This result suggests that for general elliptic operator A in dimension one, we have the Gaussian path integral

$$\int_{\gamma(0)}^{\gamma(T)} [D\gamma(t)]\, e^{\frac{im}{2\hbar}\int_0^T \gamma A\gamma\, dt} = \left(\frac{m}{\pi i\hbar}\right)^{\frac{1}{2}} (\det A)^{-\frac{1}{2}}$$

where $\det A$ is defined via the analytic continuation through the zeta function $\zeta_A(s)$

$$\det A := e^{-\zeta_A'(0)}.$$

This method is called *zeta function regularization*.

2.4 Harmonic Oscillator

2.4.1 Integral Kernel

As an illustration of the path integral method, we revisit the example of one-dimensional harmonic oscillator. The Hamiltonian operator is

$$\widehat{\mathrm{H}} = \frac{1}{2m}\hat{p}^2 + \frac{m}{2}\omega^2\hat{x}^2.$$

We calculate the integral kernel

$$K(x'', T; x', 0) = \left\langle x'' \middle| e^{-i\,\widehat{\mathrm{H}}\,T/\hbar} \middle| x' \right\rangle = \int_{x(0)=x'}^{x(T)=x''} [Dx(t)]\, e^{\frac{i}{\hbar}\int_0^T \left(\frac{m}{2}\dot{x}^2 - \frac{m}{2}\omega^2 x^2\right) dt}.$$

The action functional is

$$S\left[x(t)\right] = \int_0^T \left(\frac{m}{2}\dot{x}^2 - \frac{m}{2}\omega^2 x^2\right) dt.$$

Let $x_{cl}(t)$ be the classical trajectory which satisfies the classical equation of motion

$$\ddot{x}_{cl}(t) = -\omega^2 x_{cl}(t)$$

with specified boundary condition $x_{cl}(0) = x'$ and $x_{cl}(T) = x''$. This is solved by

$$x_{cl}(t) = \frac{\sin\omega(T-t)}{\sin\omega T}x' + \frac{\sin\omega t}{\sin\omega T}x''.$$

We can decompose any path $x(t)$ with $x(0) = x'$ and $x(T) = x''$ by

$$x(t) = x_{cl}(t) + \gamma(t),$$

where $\gamma(t)$ is an arbitrary path with boundary condition

$$\gamma(0) = \gamma(T) = 0.$$

The action becomes

$$\begin{aligned} S\left[x(t)\right] &= S\left[x_{cl}(t) + \gamma(t)\right] \\ &= S\left[x_{cl}(t)\right] + \int_0^T \left(\frac{m}{2}\dot{\gamma}^2 - \frac{m}{2}\omega^2\gamma^2\right) dt \\ &= S\left[x_{cl}(t)\right] + \frac{m}{2}\int_0^T \gamma\left(-\frac{d^2}{dt^2} - \omega^2\right)\gamma\, dt \\ &= S\left[x_{cl}(t)\right] + \frac{m}{2}\int_0^T \gamma A\gamma\, dt. \end{aligned}$$

Here A is the elliptic operator

$$A = -\frac{d^2}{dt^2} - \omega^2.$$

The path integral is Gaussian and therefore

$$K(x'', T; x', 0) = e^{\frac{i}{\hbar}S[x_{cl}(t)]} \int_{\gamma(0)=0}^{\gamma(T)=0} [D\gamma(t)]\, e^{\frac{im}{2\hbar}\int_0^T \gamma A\gamma\, dt} = \left(\frac{m}{\pi i\hbar}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S[x_{cl}(t)]} \left(\det A\right)^{-\frac{1}{2}}.$$

We compute $\det A$ via the zeta function regularization as in Section 2.3.2. The eigenfunctions and eigenvalues are

$$\begin{cases} \gamma_m(t) = c_m \sin\left(\dfrac{m\pi t}{T}\right), & c_m \text{ some constant} \\ \lambda_m = \left(\dfrac{\pi m}{T}\right)^2 - \omega^2 = \left(\dfrac{\pi m}{T}\right)^2 \left[1 - \left(\dfrac{\omega T}{\pi m}\right)^2\right] \end{cases}$$

Then naively we find

$$\det A = \prod_{m=1}^{\infty} \left[\left(\frac{\pi m}{T}\right)^2 \left(1 - \left(\frac{\omega T}{\pi m}\right)^2\right)\right] = \prod_{m=1}^{\infty} \left(\frac{\pi m}{T}\right)^2 \prod_{m=1}^{\infty} \left[1 - \left(\frac{\omega T}{\pi m}\right)^2\right].$$

The first term is regularized by Riemann zeta function, which is computed in Section 2.3.2

$$\prod_{m=1}^{\infty} \left(\frac{\pi m}{T}\right)^2 = 2T.$$

The second term is convergent. In fact, using

$$\prod_{m=1}^{\infty} \left[1 - \left(\frac{z}{\pi m}\right)^2\right] = \frac{\sin z}{z},$$

we have

$$\prod_{m=1}^{\infty} \left[1 - \left(\frac{\omega T}{\pi m}\right)^2\right] = \frac{\sin \omega T}{\omega T}.$$

Therefore

$$\det A = (2T)\left(\frac{\sin \omega T}{\omega T}\right) = \frac{2 \sin \omega T}{\omega}.$$

The Feynman kernel K becomes

$$K(x'', T; x', 0) = \left(\frac{m\omega}{2\pi i\hbar \sin \omega T}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar} S[x_{cl}(t)]}.$$

The action of the classical trajectory is

$$\begin{aligned} S\left[x_{cl}(t)\right] &= \frac{m}{2} \int_0^T \left(\dot{x_{cl}}^2 - \omega^2 x_{cl}^2\right) dt \\ &= \frac{m}{2} x_{cl} \dot{x}_{cl} \Big|_0^T - \frac{m}{2} \int_0^T \left(x_{cl} \ddot{x}_{cl} + \omega^2 x_{cl}^2\right) dt \\ &= \frac{m}{2} \left(x_{cl}(T) \dot{x}_{cl}(T) - x_{cl}(0) \dot{x}_{cl}(0)\right) \\ &= \frac{m}{2} \left(-\frac{\omega}{\sin \omega T} x' + \omega \frac{\cos \omega T}{\sin \omega T} x''\right) x'' - \frac{m}{2} \left(-\omega \frac{\cos \omega T}{\sin \omega T} x' + \frac{\omega}{\sin \omega T} x''\right) x' \\ &= \frac{m\omega}{2 \sin \omega T} \left[\left((x')^2 + (x'')^2\right) \cos \omega T - 2x'x''\right]. \end{aligned}$$

We arrive at the final result for the integral kernel of the quantum harmonic oscillator

$$K(x'', T; x', 0) = \left(\frac{m\omega}{2\pi i\hbar \sin \omega T}\right)^{\frac{1}{2}} e^{\frac{im\omega}{2\hbar} \left[\left((x')^2 + (x'')^2\right) \cot \omega T - \frac{2x'x''}{\sin \omega T}\right]}.$$

2.4.2 Partition Function

We would like to compare the Feynman kernel of the harmonic oscillator with previous result on the energy spectrum in Section 1.7. The link is the partition function defined by

$$\operatorname{Tr} e^{-\beta \hat{\mathrm{H}}}.$$

We will compute this partition function in two different ways.

The first way is to compute the partition function through the energy spectrum

$$\operatorname{Tr} e^{-\beta \hat{\mathrm{H}}} = \sum_{n=0}^{\infty} e^{-\beta E_n} = \sum_{n=0}^{\infty} e^{-\beta\left(n+\frac{1}{2}\right)\hbar\omega} = \frac{e^{-\frac{1}{2}\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}} = \frac{1}{2\sinh\left(\beta\hbar\omega/2\right)}.$$

The second way of computing the partition function is to use the Feynman kernel. Let us consider the imaginary time

$$T = -i\tau$$

and the Euclidean integral kernel

$$K_E(x'', \tau; x', 0) = K(x'', -i\tau; x', 0) = \left\langle x'' \middle| e^{-\hat{\mathrm{H}}\tau/\hbar} \middle| x' \right\rangle.$$

The partition function as a trace can be also expressed by

$$\operatorname{Tr} e^{-\beta \hat{\mathrm{H}}} = \int dx \, \langle x | e^{-\beta \hat{\mathrm{H}}} | x \rangle = \int dx \, K_E(x, \beta\hbar; x, 0) = \int dx \, K(x, -i\beta\hbar; x, 0).$$

Plugging our explicit result for the Feynman kernel,

$$\begin{aligned}
\operatorname{Tr} e^{-\beta \hat{\mathrm{H}}} &= \int_{\mathbb{R}} dx \left(\frac{m\omega}{2\pi\hbar\sinh(\beta\omega\hbar)}\right)^{\frac{1}{2}} e^{-\frac{2m\omega\sinh^2(\beta\omega\hbar/2)}{\hbar\sinh(\beta\omega\hbar)}x^2} \\
&= \left(\frac{m\omega}{2\pi\hbar\sinh(\beta\omega\hbar)}\frac{\pi\hbar\sinh(\beta\omega\hbar)}{2m\omega\sinh^2(\beta\omega\hbar/2)}\right)^{\frac{1}{2}} \\
&= \frac{1}{2\sinh(\beta\omega\hbar/2)}.
\end{aligned}$$

This is the same result as the energy spectrum calculation in a nontrivial way. Physics works!

2.5 Asymptotic Method

In this section, we review some basic tools for asymptotic analysis of the oscillatory integrals. This will help us tackle path integrals in later sections to obtain semi-classical results in quantum mechanics. The subject is rather classical, but could run easily into very technical discussion. Instead, we choose the intuitive approach and illustrate the basic idea via examples, aiming at motivating our later path integral manipulations.

2.5.1 Laplace's Method

We start with Laplace's method for analyzing integrals of the form

$$\int_a^b e^{-\lambda f(x)}\, dx$$

which provides the leading asymptotic approximation as $\lambda \to +\infty$. For simplicity, we assume

- $[a, b]$ is a finite interval. The discussion can be generalized to the case when $a = -\infty$ or $b = +\infty$ (or both) under further mild assumption of f near the infinity endpoint.
- f is a twice continuously differentiable function on $[a, b]$ with a unique global minimum at an interior point $x_0 \in (a, b)$ and

$$f''(x_0) > 0.$$

Under these assumptions, Laplace' method shows

$$\lim_{\lambda\to\infty} \frac{\int_a^b e^{-\lambda f(x)}\, dx}{e^{-\lambda f(x_0)}\sqrt{\frac{2\pi}{\lambda f''(x_0)}}} = 1. \tag{*}$$

We will usually write this as an asymptotic approximation

$$\int_a^b e^{-\lambda f(x)}\, dx \simeq e^{-\lambda f(x_0)}\sqrt{\frac{2\pi}{\lambda f''(x_0)}} \quad \text{as } \lambda \to +\infty.$$

The idea of the approximation formula (*) via Laplace's method is that in the limit $\lambda \to +\infty$, the integral is dominated by

$$\int_{x_0-\varepsilon}^{x_0+\varepsilon} e^{-\lambda f(x)}\, dx$$

in a small neighborhood of the global minimum x_0. If we do Taylor series expansion around x_0 (note that $f'(x_0) = 0$)

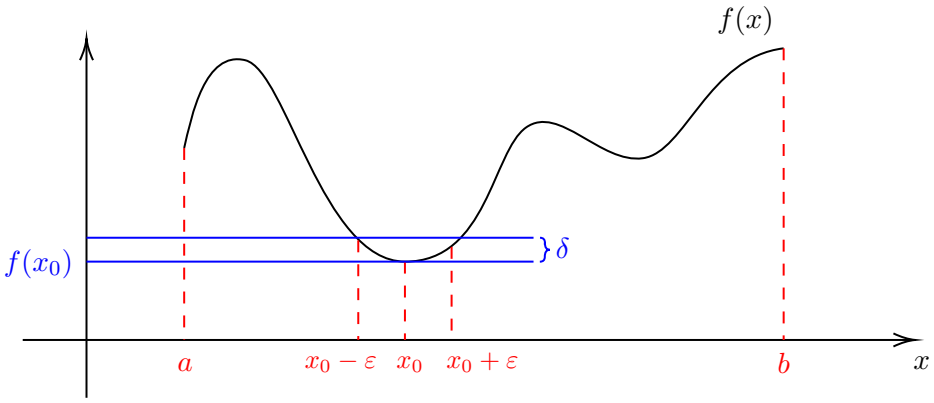
$$f(x) = f(x_0) + \frac{f''(x_0)}{2}(x - x_0)^2 + O((x - x_0)^3)$$

and perform a change of variable

$$x = x_0 + \frac{y}{\sqrt{\lambda}},$$

then

$$\begin{aligned}
\int_{x_0-\varepsilon}^{x_0+\varepsilon} e^{-\lambda f(x)}\, dx &= \frac{e^{-\lambda f(x_0)}}{\sqrt{\lambda}} \int_{-\sqrt{\lambda}\varepsilon}^{\sqrt{\lambda}\varepsilon} e^{-\frac{f''(x_0)}{2}y^2 + O\left(\frac{1}{\sqrt{\lambda}}\right)}\, dy \\
&\simeq \frac{e^{-\lambda f(x_0)}}{\sqrt{\lambda}} \int_{-\infty}^{+\infty} e^{-\frac{f''(x_0)}{2}y^2}\, dy \qquad \text{as} \quad \lambda \to +\infty \\
&= e^{-\lambda f(x_0)}\sqrt{\frac{2\pi}{\lambda f''(x_0)}}.
\end{aligned}$$



Outside $[x_0-\varepsilon, x_0+\varepsilon]$, $e^{-\lambda f(x)} = e^{-\lambda f(x_0)} O(e^{-\lambda\delta})$

The proof of (*) is basically to realize the above idea via a careful analysis of the error. This asymptotic formula can be generalized to the case when $a = -\infty$ or $b = +\infty$ (or both) under some further mild assumption of f near the infinity endpoint.

We can also generalize the above discussion to

$$\int_a^b g(x) e^{-\lambda f(x)}\, dx$$

where $g(x)$ is positive. Then

$$\int_a^b g(x) e^{-\lambda f(x)}\, dx \simeq g(x_0) e^{-\lambda f(x_0)} \sqrt{\frac{2\pi}{\lambda f''(x_0)}} \qquad \text{as} \quad \lambda \to +\infty.$$

Example 2.5.1. *Consider the* Γ*-function*

$$\Gamma(s) = \int_0^{+\infty} dx\, x^{s-1} e^{-x}.$$

We consider its asymptotic behavior as $s \to +\infty$*. The above discussion generalizes to this case.*

Let us rewrite it as

$$\Gamma(s) = (s-1)^s \int_0^{+\infty} dx\, e^{-(x-\ln x)\lambda}\,, \qquad \lambda = s-1$$

thus $f(x) = x - \ln x$ *in this case. The minimum is at the point*

$$f'(x_0) = 1 - \frac{1}{x_0} = 0 \qquad \Longrightarrow \qquad x_0 = 1.$$

It follows that we have an asymptotic approximation

$$\begin{aligned}
\Gamma(s) &\simeq (s-1)^s \sqrt{\frac{2\pi}{\lambda f''(x_0)}} e^{-\lambda f(x_0)} \\
&= \sqrt{2\pi} (s-1)^{s-1/2} e^{1-s} \\
&= \sqrt{\frac{2\pi}{s}} \frac{\sqrt{s}}{\sqrt{s-1}} s^s \left(1 - \frac{1}{s}\right)^s e^{1-s} \\
&\simeq \sqrt{\frac{2\pi}{s}} \left(\frac{s}{e}\right)^s \qquad \text{as} \quad s \to +\infty.
\end{aligned}$$

This is known as the Stirling's formula.

The above discussion can be generalized to the n-dimensional case

$$\int_\Gamma e^{-\lambda f(\mathbf{x})}\, d^n\mathbf{x}, \qquad \mathbf{x} = (x^1, \cdots, x^n).$$

Assume $f(\mathbf{x})$ has a unique global minimum $\mathbf{x}_0$ in the interior of the domain for integration, and the Hessian matrix $H_f = (\partial_{x^i}\partial_{x^j} f)$ is positive definite at $\mathbf{x}_0$

$$H_f(\mathbf{x}_0) > 0.$$

By a similar consideration, in the limit $\lambda \to +\infty$, the dominate contribution comes from the near neighborhood of $\mathbf{x}_0$ and the leading approximation is given by the Gaussian integral

$$e^{-\lambda f(\mathbf{x}_0)} \int_{\mathbb{R}^n} d^n\mathbf{x}\, e^{-\frac{\lambda}{2}\mathbf{x}^t H_f(\mathbf{x}_0)\mathbf{x}} = \left(\frac{2\pi}{\lambda}\right)^{n/2} \frac{1}{\sqrt{\det(H_f(\mathbf{x}_0))}} e^{-\lambda f(\mathbf{x}_0)}.$$

Thus Laplace's method leads to

$$\int d^n\mathbf{x}\, g(\mathbf{x}) e^{-\lambda f(\mathbf{x})} \simeq \left(\frac{2\pi}{\lambda}\right)^{n/2} \frac{g(\mathbf{x}_0)}{\sqrt{\det(H_f(\mathbf{x}_0))}} e^{-\lambda f(\mathbf{x}_0)} \qquad \text{as} \quad \lambda \to +\infty.$$

2.5.2 Method of Steepest Descent

Laplace's method can be extended to the complex oscillatory integrals of the form

$$I(\lambda) = \int_C dz\, g(z) e^{-\lambda f(z)}$$

where $f(z)$ and $g(z)$ are analytic functions of z. By Cauchy integral formula, this complex integral is invariant under continuous deformations of C (with appropriate boundary condition at infinity boundary of C). This will allow us to perform analytic continuation and asymptotic analysis by deforming the contour suitably.

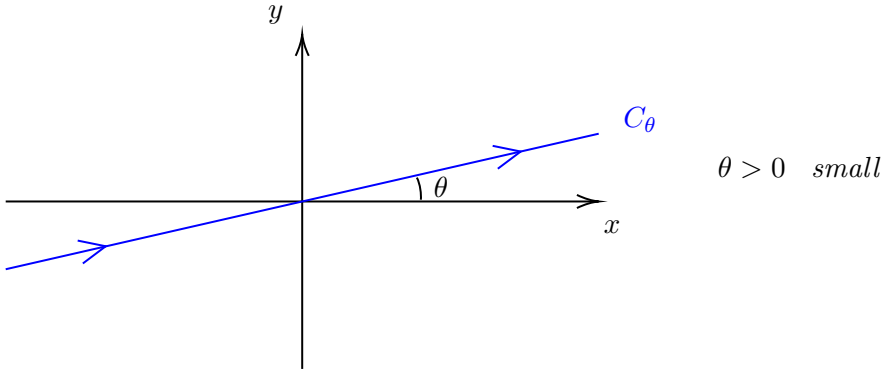
Example 2.5.2. *Consider the following integral*

$$\int_C e^{ix^2}\, dx.$$

It can be viewed as an analytic continuation of the standard Gaussian integral

$$\int_{\mathbb{R}} e^{-\lambda x^2}\, dx, \qquad \lambda > 0.$$

The analytic continuation from $\lambda > 0$ to $\lambda = -i$ can be realized by choosing the contour:



Then

$$I(\lambda) = \int_{C_\theta} e^{-\lambda z^2}\, dz$$

is convergent for $\operatorname{Re}\lambda \geq 0$, $\operatorname{Im}\lambda \leq 0$, $\lambda \neq 0$. *Thus* $I(\lambda)$ *gives the analytic continuation from* $\lambda \in \mathbb{R}_{>0}$ *to* $\lambda \in i\mathbb{R}_{<0}$. *In particular*

$$I(-i) = \int_{C_\theta} e^{iz^2}\, dz = \int_{C_{\frac{\pi}{4}}} e^{iz^2}\, dz = e^{\frac{\pi}{4}i} \int_{-\infty}^{+\infty} e^{-u^2}\, du = e^{\frac{\pi}{4}i}\sqrt{\pi}.$$

Similarly, if we deform the contour clock-wise, then we obtain an analytic continuation from $\lambda > 0$ *to* $\lambda = i$

$$\int_{C_{-\frac{\pi}{4}}} e^{-iz^2}\, dz = e^{-\frac{\pi}{4}i}\sqrt{\pi}.$$

This explains our discussion on Gaussian integrals in Section 2.3.1.

In general, the method of steepest descent is to deform the contour C into a curve along which $\left|e^{-f(z)}\right|$ decays fastest. To see how such a contour looks like, let us write

$$f(z) = u(x,y) + iv(x,y), \qquad z = x + iy.$$

So $u = \operatorname{Re} f$ and $v = \operatorname{Im} f$. The steepest descent curve should follow the gradient of u since

$$|e^{-f}| = e^{-u}.$$

Since $f(z)$ is analytic, u and v satisfy the Cauchy-Riemann equations

$$\partial_x u = \partial_y v, \qquad \partial_y u = -\partial_x v.$$

It follows that

$$\nabla u \cdot \nabla v = \partial_x u \partial_x v + \partial_y u \partial_y v = 0.$$

In other words, ∇v is perpendicular to the gradient direction of u, thus the steepest descent curve will lie on a level set of v. This motivates the following strategy: we deform the contour C into a contour C' such that

① $\operatorname{Im} f$ is constant along C'

② C' passes through one or more points where

$$f'(z) = 0.$$

These are called *saddle points*. They are also the critical points of $\operatorname{Re} f$ along C'. Then

$$I(\lambda) = \int_{C'} g(z) e^{-\lambda f(z)}\, dz = e^{-i\lambda \operatorname{Im} f} \int_{C'} g(z) e^{-\lambda \operatorname{Re} f}\, dz$$

and we can apply Laplace's method.

Let us assume there is one non-degenerate saddle point z_0 on the contour C' which is a global minimum on C'. The condition of non-degenerate saddle point says

$$f'(z_0) = 0, \qquad f''(z_0) \neq 0.$$

Then a local computation via Gaussian integral gives

$$\int_{C'} g(z)e^{-\lambda f(z)}\,dz \simeq \sqrt{\frac{2\pi}{\lambda f''(z_0)}}g(z_0)e^{-\lambda f(z_0)} \qquad \text{as} \quad \lambda \to +\infty.$$

There are similar results for n-dimensional complex integrals. The branch for the square root from the Gaussian integral is determined by the analytic continuation as in the above example.

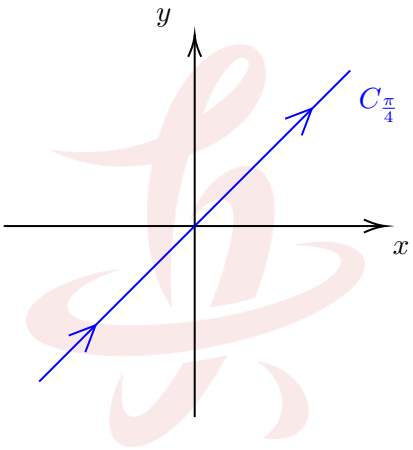
Example 2.5.3. *Consider the Gaussian integral*

$$\int_C e^{i\lambda z^2}\,dz, \qquad \lambda > 0.$$

Then $f(z) = -iz^2$ *and*

$$\operatorname{Re} f = 2xy, \qquad \operatorname{Im} f = y^2 - x^2.$$

The steepest descent contour is



2.5.3 Morse Flow

Concretely, curves of steepest descent can be constructed via Morse theory. We follow the presentation [49] to illustrate the basic idea in our case. Consider the following flow equation

$$\begin{cases} \dfrac{dz}{du} = -\overline{f'(z)} \\ \lim\limits_{u\to-\infty} z(u) = saddle \end{cases}$$

where $u \in \mathbb{R}$ *is the real parameter of the flow. Along the flow we have*

$$\frac{df(z)}{du} = -|f'(z)|^2.$$

So $\operatorname{Im} f$ *is constant and* $\operatorname{Re} f$ *is decreasing along the flow, leading to a steepest descent curve.*

Example 2.5.4. *Let us consider an example*

$$\int_C e^{\lambda f(z)}, \qquad f(z) = \frac{\alpha z^2}{2}, \qquad \alpha \in \mathbb{C}^*, \quad \lambda > 0.$$

The saddle point is at $z = 0$. The curve C of steepest descend satisfies

$$\operatorname{Im} f = 0, \quad \textit{and} \quad \operatorname{Re} f \to -\infty \quad \textit{along} \quad \partial C.$$

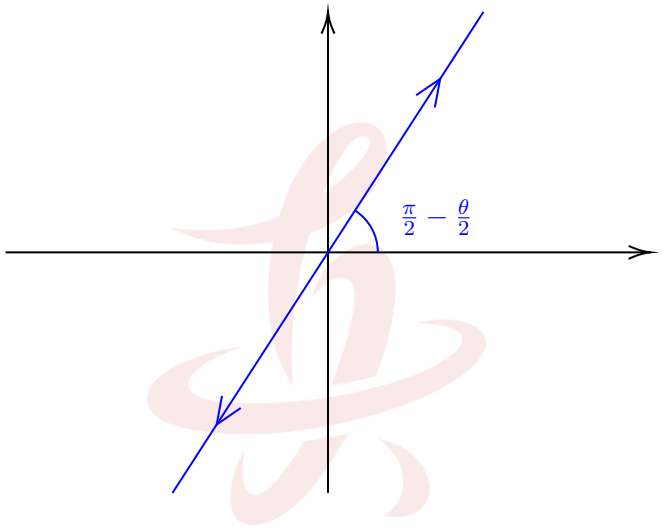
Such curve C can be constructed by solving the flow equation

$$\begin{cases} \dfrac{dz}{du} = -\overline{f'(z)} = -\overline{\alpha} z \\ \lim\limits_{u \to -\infty} z(u) = 0 \end{cases}$$

Let $\alpha = Ae^{i\theta}$, $A > 0$. There are two solutions pointing toward opposite directions

$$z(u) = \pm e^{Au} e^{\frac{i}{2}(\pi - \theta)}.$$

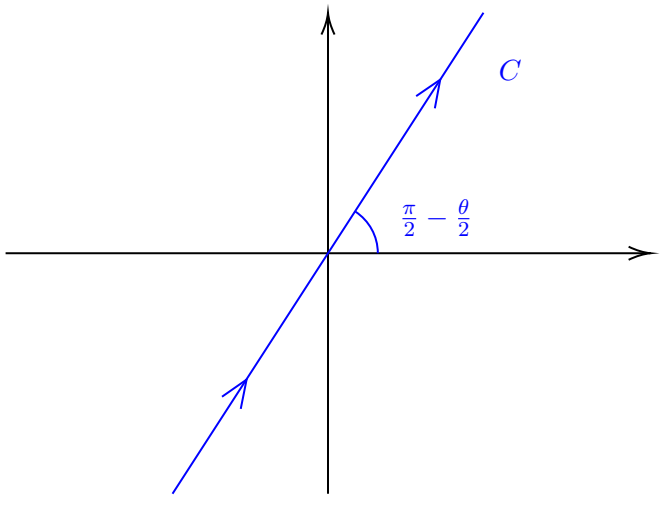
Here is the figure for the corresponding solutions (arrow indicates the flow direction)



The solutions flow along the direction with angle as in the figure

$$\frac{\pi}{2} - \frac{\theta}{2} = \frac{\pi}{2} - \frac{1}{2} \operatorname{Arg}(f''(0)).$$

With appropriate orientations chosen, these two flows combine to form the curve C.

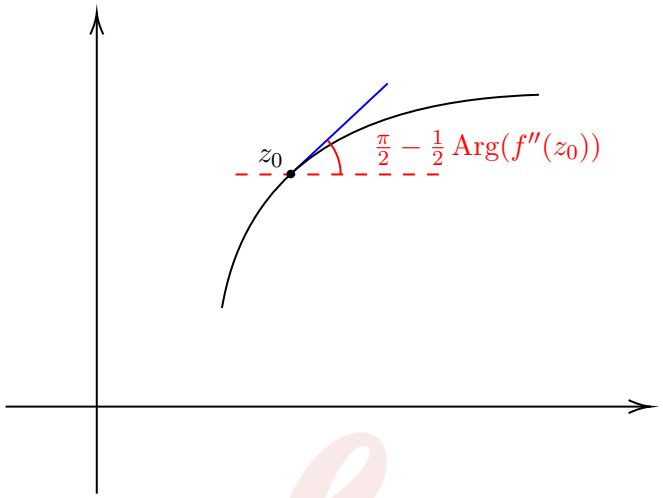


In general, suppose we are to describe the curve of steepest descend for the integral

$$\int_C e^{\lambda f(z)}$$

passing a saddle point z_0. Then the tangent line of C at z_0 is along the direction with angle

$$\frac{\pi}{2} - \frac{1}{2}\operatorname{Arg}(f''(z_0)).$$



2.5.4 Stokes Phenomenon

In applications of asymptotic method, we will often encounter cases when there are several saddle points and we need to sum them all. However, as we vary parameters of the model, the sum of the asymptotic expansions may exhibit discontinuous jump. This is known as the *Stokes phenomenon*. Such jump phenomenon actually displays important physical behaviors. We will explain the basic idea of Stokes phenomenon through a concrete example, the *Airy integral*.

Airy Function

We consider the following Airy integral along the real line

$$I(\lambda) := \int_{-\infty}^{+\infty} e^{i\lambda\left(\frac{z^3}{3}-z\right)}\, dz = 2\int_0^{+\infty} \cos\left(\lambda\left(\frac{z^3}{3} - z\right)\right)\, dz$$

for $\lambda \in \mathbb{R}_{>0}$. This integral is convergent and is related to the standard Airy function Ai

$$\operatorname{Ai}(x) = \frac{1}{\pi}\int_0^{+\infty} \cos\left(\frac{z^3}{3} + xz\right)\, dz$$

by

$$I(\lambda) = 2\pi\lambda^{-\frac{1}{3}} \operatorname{Ai}\left(-\lambda^{\frac{2}{3}}\right).$$

We are interested in the asymptotic behavior of $I(\lambda)$ as $\lambda \to +\infty$. As we discussed before, this can be analyzed by the method of steepest descent. To apply this method, the first step is to deform the contour $C = \mathbb{R}$ into contours of steepest descent. Let

$$f(z) = i\lambda\left(\frac{z^3}{3} - z\right).$$

It has two saddle points

$$f'(z) = 0 \qquad \Longrightarrow \qquad z = p_\pm = \pm 1.$$

A curve of steepest descent is a contour which passes a saddle point and satisfies

① $\operatorname{Im} f =$ constant

② $\operatorname{Re} f \to -\infty$ along the infinity endpoints of the curve.

Since

$$f(p_\pm) = \mp \frac{2}{3} i\lambda$$

we have two curves $C_\pm$ of steepest descent corresponding to the two saddle points $p_\pm$.

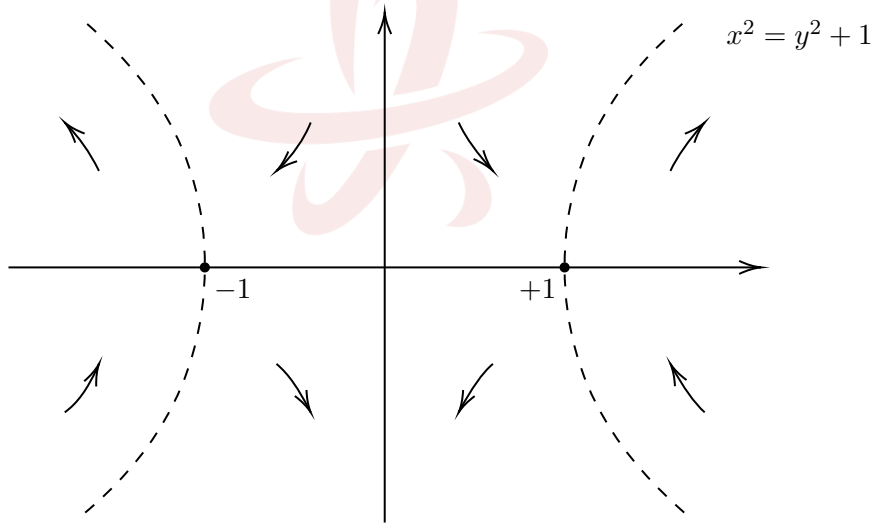
To describe these curves, let us consider the flow equation

$$\frac{dz}{du} = -\overline{f'(z)} = i\lambda(\overline{z}^2 - 1)$$

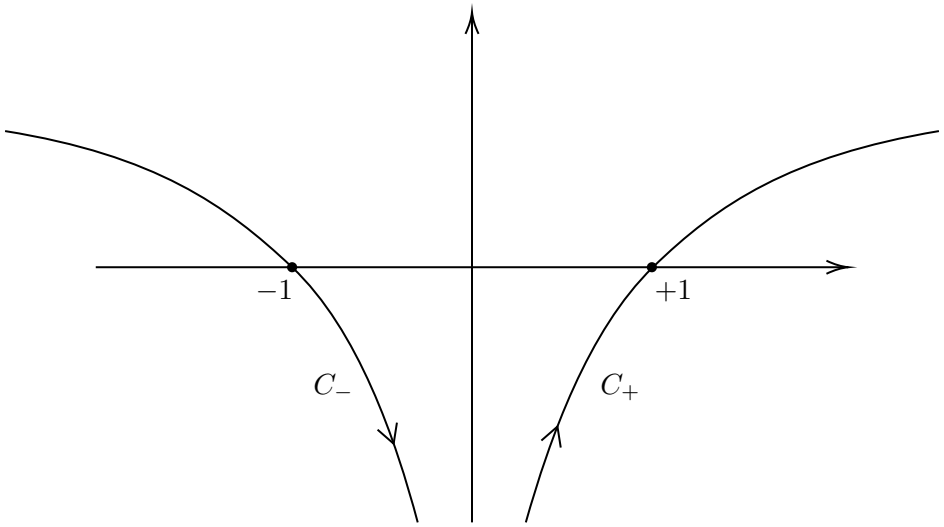
which can be written in real coordinates $z = x + iy$ as

$$\begin{cases} \dfrac{dx}{du} = 2\lambda xy \\ \dfrac{dy}{du} = \lambda(x^2 - y^2 - 1) \end{cases} \qquad (\lambda > 0)$$

We can draw the direction of the corresponding flow



This allows us to draw the curves $C_\pm$ as



It follows that for $\lambda > 0$

$$I(\lambda) = \int_{\mathbb{R}} e^{i\lambda\left(\frac{z^3}{3}-z\right)}dz = \int_{C_-} e^{i\lambda\left(\frac{z^3}{3}-z\right)}dz + \int_{C_+} e^{i\lambda\left(\frac{z^3}{3}-z\right)}dz$$

i.e., the contour $\mathbb{R}$ is deformed to $C_- + C_+$ for steepest descent. Thus $I(\lambda)$ has the asymptotic behavior via the method of steepest descent

$$I(\lambda) \simeq \sqrt{\frac{\pi}{i\lambda}} e^{\frac{2}{3}i\lambda}\left(1 + O\left(\frac{1}{\lambda}\right)\right) + \sqrt{\frac{\pi}{-i\lambda}} e^{-\frac{2}{3}i\lambda}\left(1 + O\left(\frac{1}{\lambda}\right)\right) \qquad \text{as} \quad \lambda \to +\infty.$$

Stokes Ray

Now we consider the analytic continuation of the Airy integral

$$\int_C e^{i\lambda\left(\frac{z^3}{3}-z\right)}dz$$

as λ varies. In particular, we would like to analyze the asymptotic behavior in the limit

$$\lambda \longrightarrow +\infty e^{i\theta}$$

as λ approaches ∞ in the direction of $e^{i\theta}$.

As λ varies, we need to deform the integration contour C accordingly so as to keep the integral convergent. Again, we can decompose C as a combination of curves $C_\pm^\lambda$ of steepest descent. The curves $C_\pm^\lambda$ are associated to the two saddle points and described by

① $C_\pm^\lambda$ passes the saddle point $p_\pm = \pm 1$

② $\operatorname{Im} f =$ constant along $C_\pm^\lambda$

③ $\operatorname{Re} f \to -\infty$ along the infinity endpoints of $C_\pm^\lambda$

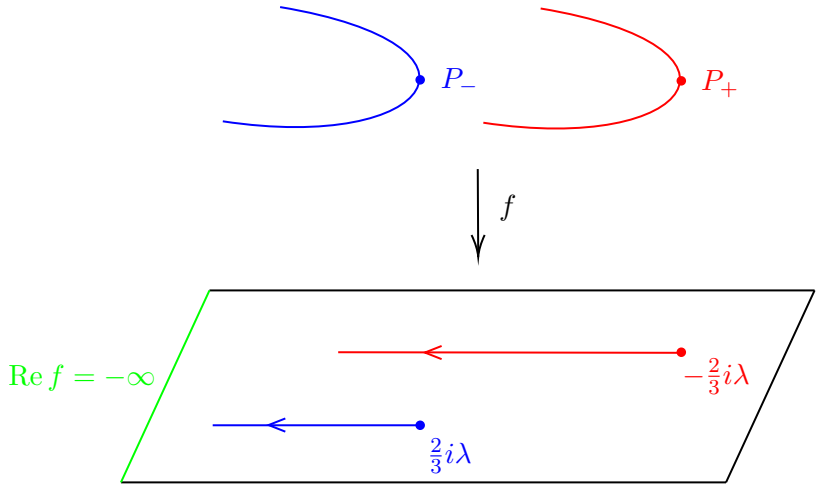
where

$$f = i\lambda\left(\frac{z^3}{3} - z\right).$$

Note that

$$\operatorname{Im}\left(f(p_\pm)\right) = \mp\frac{2}{3}\operatorname{Re}\lambda.$$

So as long as $\operatorname{Re}\lambda \neq 0$, curves $C_\pm^\lambda$ do not intersect and approaches ∞ in different regions.



If we deform the contour C into

$$C = n_- C_-^\lambda + n_+ C_+^\lambda,$$

then the Airy integral becomes

$$\int_C e^f dz = n_- \int_{C_-^\lambda} e^f dz + n_+ \int_{C_+^\lambda} e^f dz.$$

Now as we vary λ, the cycles $C_\pm^\lambda$ will rotate with λ. As long as λ does not hit the locus $\{\operatorname{Re}\lambda = 0\}$, the curves $C_\pm^\lambda$ will vary continuously. However, when

$$\operatorname{Re}\lambda = 0$$

so λ becomes pure imaginary,

$$\operatorname{Im}(f(p_-)) = \operatorname{Im}(f(p_+))$$

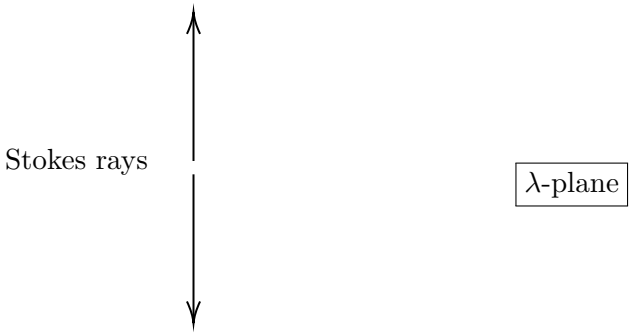
while

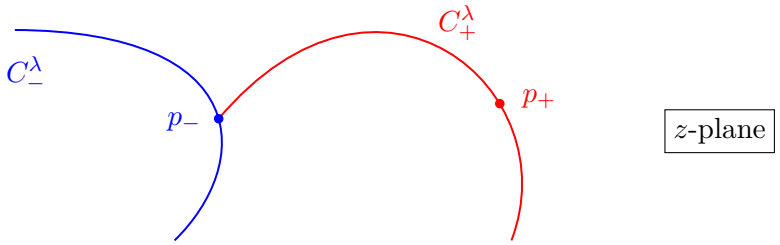
$$\operatorname{Re}(f(p_\pm)) = \pm\frac{2}{3}\operatorname{Im}\lambda.$$

Thus one of the curve of steepest descent connects the two saddle points. The two rays

$$\{\lambda \in i\mathbb{R}_{>0}\} \cup \{\lambda \in i\mathbb{R}_{<0}\}$$

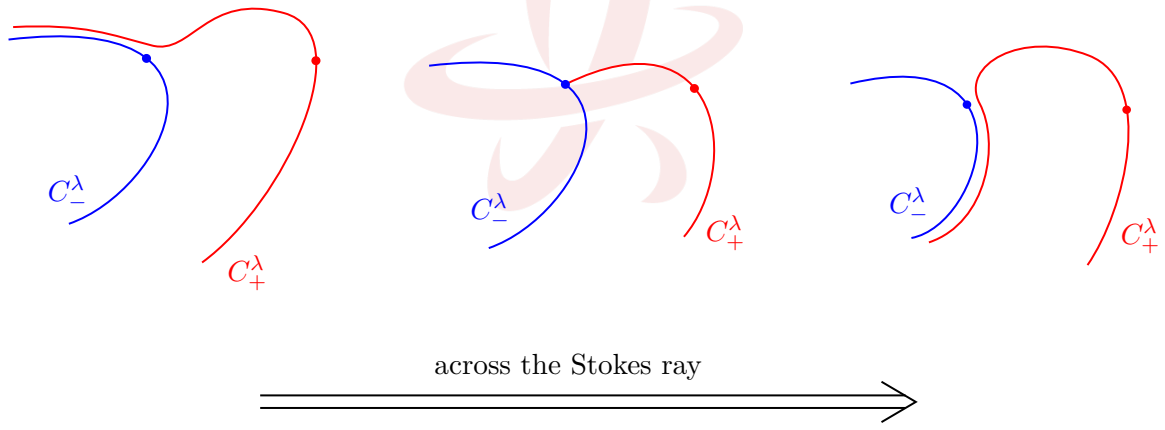
in the λ-plane are called *Stokes rays*.





on the Stokes ray $\lambda \in i\mathbb{R}_{>0}$: $\quad \mathrm{Re}(f(p_+)) > \mathrm{Re}(f(p_-))$

When we cross the Stokes ray, the curves $C_\pm^\lambda$ will display a discrete transformation. The following figure explains the crossing of one of the Stokes ray



The corresponding contours $C_\pm^\lambda$ display a transformation as explained by the figure

$$\begin{cases} C_-^\lambda \mapsto C_-^\lambda \\ C_+^\lambda \mapsto C_+^\lambda \pm C_-^\lambda \end{cases}$$

We apply the above result to the analytic continuation of

$$\int_C e^{i\lambda\left(\frac{z^3}{3}-z\right)}dz$$

as we vary λ and deform the contour C accordingly. We can decompose the contour C into a sum of curves of steepest descent $C_\pm^\lambda$

$$C = n_- C_-^\lambda + n_+ C_+^\lambda.$$

As a result, to keep the continuity of deformation of C along analytic continuation, the numbers (n_-, n_+) will be locally constant away from the Stokes ray but display a jump

$$\begin{cases} n_+ \mapsto n_+ \\ n_- \mapsto n_- \pm n_+ \end{cases}$$

when we cross a Stokes ray.

Asymptotic Sum

Now we consider the asymptotic behavior of the Airy integral

$$I(\lambda) = \int_C e^{i\lambda\left(\frac{z^3}{3} - z\right)} dz \qquad \text{as} \quad \lambda \to +\infty e^{i\theta}.$$

By the method of steepest descent, we first deform the contour C into a combination

$$C = n_- C_-^\lambda + n_+ C_+^\lambda.$$

Then the method of steepest descent gives the leading asymptotic behavior

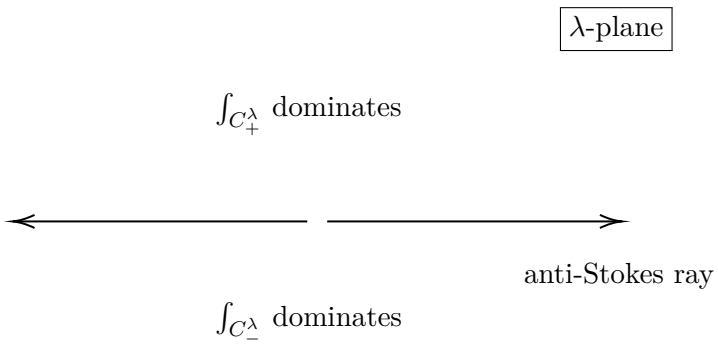
$$\begin{aligned} I(\lambda) &= n_- \int_{C_-^\lambda} e^{i\lambda\left(\frac{z^3}{3} - z\right)} dz + n_+ \int_{C_+^\lambda} e^{i\lambda\left(\frac{z^3}{3} - z\right)} dz \\ &\simeq n_- \sqrt{\frac{\pi}{i\lambda}} e^{\frac{2}{3}i\lambda} + n_+ \sqrt{\frac{\pi}{-i\lambda}} e^{-\frac{2}{3}i\lambda} \qquad \text{as} \quad \lambda \to +\infty e^{i\theta}. \end{aligned}$$

Note that

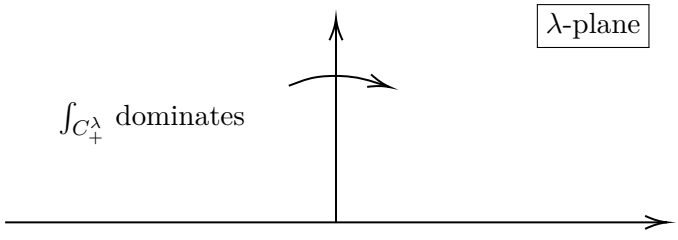
① if $\operatorname{Im}\lambda > 0$, then $\int_{C_+^\lambda}$ dominates;

② if $\operatorname{Im}\lambda < 0$, then $\int_{C_-^\lambda}$ dominates.

The rays $\{\operatorname{Im}\lambda = 0\}$ on the real line separating the dominant asymptotic behaviors are sometimes called *anti-Stokes rays*



This is compatible with our previous discussion on the Stokes jump. For example, consider the case when we cross the Stokes ray $\lambda \in \mathbb{R}_{>0}$.



The asymptotic expansion

$$I(\lambda) \simeq n_- \int_{C_-^\lambda} + n_+ \int_{C_+^\lambda}$$

will display a jump

$$\begin{cases} n_+ \mapsto n_+ \\ n_- \mapsto n_- \pm n_+ \end{cases}$$

This is possible since it does not alter the leading asymptotic behavior of $I(\lambda)$, which is given by the dominate term $n_+ \int_{C_+^\lambda}$.

2.6 Semi-classical Approximation

The goal of this section is to apply the method of steepest descent to compute the asymptotic leading contribution to the Feynman kernel

$$K(x'', t''; x', t') = \int_{x(t')=x'}^{x(t'')=x''} [Dx(t)]\ e^{\frac{i}{\hbar}S[x(t)]}$$

in the classical limit $\hbar \to 0$. For simplicity, we focus on the one-dimensional case.

2.6.1 Semi-classical Feynman Kernel

The saddle point of S is the classical trajectory $x_{cl}(t)$. We write a general path $x(t)$ by

$$x(t) = x_{cl}(t) + \gamma(t)$$

where $\gamma(t)$ satisfies the endpoint condition

$$\gamma(t') = \gamma(t'') = 0.$$

We can expand $S[x(t)]$ around the classical trajectory $x_{cl}(t)$ and find

$$S[x(t)] = \int_{t'}^{t''} \left(\frac{m}{2}\dot{x}^2 - V(x)\right) dt = S[x_{cl}(t)] + \int_{t'}^{t''} \left(\frac{m}{2}\dot{\gamma}^2 - \frac{1}{2}V''(x_{cl})\gamma^2\right) dt + O(\gamma^3).$$

Thus the method of steepest descent leads to the following leading asymptotic contribution

$$K(x'', t''; x', t') \simeq e^{\frac{i}{\hbar}S[x_{cl}(t)]} \int_{\gamma(t')=0}^{\gamma(t'')=0} [D\gamma(t)]\, e^{\frac{i}{\hbar}\int_{t'}^{t''}\left(\frac{m}{2}\dot{\gamma}^2 - \frac{1}{2}V''(x_{cl})\gamma^2\right)dt} \qquad \text{as} \quad \hbar \to 0.$$

This is called the *semi-classical approximation*.

Let us denote the semi-classical Feynman kernel by

$$K_{sc}(x'', t''; x', t') := e^{\frac{i}{\hbar}S[x_{cl}(t)]} \int_{\gamma(t')=0}^{\gamma(t'')=0} [D\gamma(t)]\, e^{\frac{i}{\hbar}\int_{t'}^{t''}\left(\frac{m}{2}\dot{\gamma}^2 - \frac{1}{2}V''(x_{cl})\gamma^2\right)dt}.$$

Applying our result on Gaussian path integral, the semi-classical Feynman kernel becomes

$$K_{sc}(x'', t''; x', t') = \left(\frac{m}{\pi i\hbar \det A}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S[x_{cl}(t)]}$$

where A is the elliptic operator

$$A = -\frac{d^2}{dt^2} - \frac{1}{m} V''\left(x_{cl}(t)\right).$$

The main goal of this subsection is to show the following semi-classical formula

$$K_{sc}(x'', t''; x', t') = \left(\frac{m}{2\pi i\hbar\varphi_0(t'')}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S[x_{cl}(t)]}$$

where $\varphi_0(t)$ is the solution to the initial value problem

$$\begin{cases} \left(-\dfrac{d^2}{dt^2} - \dfrac{1}{m}V''(x_{cl}(t))\right)\varphi_0(t) = 0 \\ \varphi_0(t') = 0, \qquad \varphi_0'(t') = 1. \end{cases}$$

Determinant Computation

Let us denote

$$\Theta(t) = \frac{1}{m} V''\left(x_{cl}(t)\right).$$

We present an intuitive computation of

$$\det A = \det\left(-\frac{d^2}{dt^2} - \Theta(t)\right)$$

due to Coleman [10].

The idea is to analyze the eigenvalue problem with initial condition at $t = t'$

$$\begin{cases} A\varphi_\lambda(t) = \lambda\varphi_\lambda(t) \\ \varphi_\lambda(t') = 0, \qquad \varphi_\lambda'(t') = 1. \end{cases}$$

For any λ, there exists a unique solution $\varphi_\lambda(t)$ for the above initial value problem. The key is to observe that

$$\varphi_\lambda(t'') = 0$$

if and only if λ is an eigenvalue of A for the corresponding Dirichlet boundary value problem

$$\begin{cases} A\varphi_\lambda(t) = \lambda\varphi_\lambda(t) \\ \varphi_\lambda(t') = \varphi_\lambda(t'') = 0. \end{cases}$$

Now let us consider another operator

$$\tilde{A} = -\frac{d^2}{dt^2} - \tilde{\Theta}(t)$$

and similarly solve $\tilde{\varphi}_\lambda(t)$ for

$$\begin{cases} \tilde{A}\tilde{\varphi}_\lambda(t) = \lambda\tilde{\varphi}_\lambda(t) \\ \tilde{\varphi}_\lambda(t') = 0, \qquad \tilde{\varphi}_\lambda'(t') = 1. \end{cases}$$

Then we claim that

$$\frac{\det(A-\lambda)}{\det(\tilde{A}-\lambda)} = \frac{\varphi_\lambda(t'')}{\tilde{\varphi}_\lambda(t'')} \tag{*}$$

Intuitively this follows by "observing" that both sides are meromorphic functions of λ with zeroes at eigenvalues of A and poles at eigenvalues of $\tilde{A}$ (a careful analysis shows that they are simple zeroes or poles). Let

$$f(\lambda) = \frac{\det(A-\lambda)}{\det(\tilde{A}-\lambda)}, \qquad g(\lambda) = \frac{\varphi_\lambda(t'')}{\tilde{\varphi}_\lambda(t'')}.$$

Then the above consideration says that $\frac{f(\lambda)}{g(\lambda)}$ is an entire function on $\mathbb{C}$.

We next analyze the behavior of $f(\lambda)$ and $g(\lambda)$ as $\lambda \to \infty$. Firstly, we have

$$\lim_{\substack{\lambda\to\infty \\ \lambda\notin\mathbb{R}_+}} f(\lambda) = 1.$$

Qualitatively this can be understood as follows. For Dirichlet boundary value problem, the operator $-\frac{d^2}{dt^2}$ has eigenvectors

$$u_n(t) = \sin\left(\frac{n\pi}{t''-t'}(t-t')\right)$$

with eigenvalues $\left(\frac{n\pi}{t''-t'}\right)^2$. Therefore the shifted operator $-\frac{d^2}{dt^2}-\lambda$ has eigenvalues

$$\mu_n = \left(\frac{n\pi}{t''-t'}\right)^2 - \lambda.$$

In the limit $\lambda \to \infty$ for $\lambda \notin \mathbb{R}_+$, all eigenvalues $|\mu_n| \to +\infty$. Thus $\Theta(t)$ is very small comparing to the operator $-\frac{d^2}{dt^2}-\lambda$ in the limit $\lambda\to\infty$, $\lambda\notin\mathbb{R}_+$. This small perturbation will cause negligible effect in this limit. Therefore it is natural to expect

$$\lim_{\substack{\lambda\to\infty \\ \lambda\notin\mathbb{R}_+}} f(\lambda) = 1.$$

Secondly, we consider the limit

$$\lim_{\substack{\lambda\to\infty \\ \lambda\notin\mathbb{R}_+}} g(\lambda).$$

To analyze this limit, we first consider the inhomogeneous problem

$$\begin{cases} \left(-\frac{d^2}{dt^2}-\lambda\right)u = f \\ u(t') = 0, \qquad u'(t') = 0. \end{cases}$$

This is uniquely solved by

$$u(t) = -\int_{t'}^{t} \frac{1}{\sqrt{\lambda}} \sin\left(\sqrt{\lambda}(t-s)\right) f(s)\, ds.$$

The corresponding Green's operator is

$$G(f)(t) := -\int_{t'}^{t} \frac{1}{\sqrt{\lambda}} \sin\left(\sqrt{\lambda}(t-s)\right) f(s)\, ds.$$

Consider the original boundary value problem

$$\begin{cases} \left(-\dfrac{d^2}{dt^2} - \lambda - \Theta(t)\right)\varphi_\lambda(t) = 0 \\ \varphi_\lambda(t') = 0, \qquad \varphi'_\lambda(t') = 1. \end{cases}$$

We will write $\varphi_\lambda(t)$ as

$$\varphi_\lambda(t) = \varphi_\lambda^{(0)}(t) + u(t)$$

where $\varphi_\lambda^{(0)}(t)$ solves

$$\begin{cases} \left(-\dfrac{d^2}{dt^2} - \lambda\right)\varphi_\lambda^{(0)} = 0 \\ \varphi_\lambda^{(0)}(t') = 0, \qquad \varphi_\lambda^{(0)\prime}(t') = 1. \end{cases}$$

Such $\varphi_\lambda^{(0)}$ is explicitly found by

$$\varphi_\lambda^{(0)}(t) = \frac{1}{\sqrt{\lambda}} \sin\left(\sqrt{\lambda}(t - t')\right).$$

Then the equation for $\varphi_\lambda(t)$ becomes

$$\begin{cases} \left(-\dfrac{d^2}{dt^2} - \lambda\right) u(t) = \Theta(t)\left(\varphi_\lambda^{(0)}(t) + u(t)\right) \\ u(t') = 0, \qquad u'(t') = 0. \end{cases}$$

Using the above Green's operator, this is equivalent to

$$u = G\left(\Theta\left(\varphi_\lambda^{(0)} + u\right)\right).$$

Let us rewrite this by

$$(1 - G \circ \hat{\Theta})u = G \circ \hat{\Theta}\left(\varphi_\lambda^{(0)}\right),$$

where $\hat{\Theta}$ is the operator

$$\hat{\Theta}(u)(t) = \Theta(t)u(t).$$

Then we find the perturbative solution

$$u = (1 - G \circ \hat{\Theta})^{-1} G \circ \hat{\Theta}\left(\varphi_\lambda^{(0)}\right) = \sum_{n=1}^{\infty} (G \circ \hat{\Theta})^n \left(\varphi_\lambda^{(0)}\right).$$

From this expression, we find that the correction u will have the asymptotic behavior

$$u = O\left(\frac{\Theta}{\sqrt{\lambda}}\right)\varphi_\lambda^{(0)}$$

which is small comparing to $\varphi_\lambda^{(0)}$ in the limit $\lambda \to \infty$, $\lambda \notin \mathbb{R}_+$. It follows that

$$\lim_{\substack{\lambda\to\infty \\ \lambda\notin\mathbb{R}_+}} g(\lambda) = \lim_{\substack{\lambda\to\infty \\ \lambda\notin\mathbb{R}_+}} \frac{\varphi_\lambda^{(0)}(t'')}{\tilde{\varphi}_\lambda^{(0)}(t'')} = 1.$$

Combining the above two results, we find

$$\lim_{\substack{\lambda\to\infty \\ \lambda\notin\mathbb{R}_+}} \frac{f(\lambda)}{g(\lambda)} = 1.$$

Since $f(\lambda)/g(\lambda)$ is an entire function, it follows that $f(\lambda)/g(\lambda) = 1$. This shows (*).

Let us rewrite (*) as

$$\frac{\det(A-\lambda)}{\varphi_\lambda(t'')} = \frac{\det(\tilde{A}-\lambda)}{\tilde{\varphi}_\lambda(t'')}.$$

This implies

$$\det A = c\varphi_0(t'')$$

where c is a constant that does not depend on the potential V. The constant c can determined by our result in the free case where $\tilde{A} = -\frac{d^2}{dt^2}$. In the free case, we know from Section 2.3.2

$$\det(\tilde{A}) = \det\left(-\frac{d^2}{dt^2}\right) = 2(t''-t').$$

On the other hand, the differential equation

$$\begin{cases} -\dfrac{d^2}{dt^2}\tilde{\varphi}_0(t) = 0 \\ \tilde{\varphi}_0(t') = 0, \qquad \tilde{\varphi}_0'(t') = 1 \end{cases}$$

is solved by

$$\tilde{\varphi}_0(t) = t - t'.$$

We find

$$c = \frac{\det\tilde{A}}{\tilde{\varphi}_0(t'')} = 2.$$

Thus

$$\det A = 2\varphi_0(t'').$$

We have arrived at the promised formula for the semi-classical Feynman kernel

$$K_{sc}(x'',t'';x',t') = \left(\frac{m}{2\pi i\hbar\varphi_0(t'')}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S[x_{cl}(t)]}$$

where $\varphi_0(t)$ is the solution to the initial value problem

$$\begin{cases} \left(-\dfrac{d^2}{dt^2} - \dfrac{1}{m}V''(x_{cl}(t))\right)\varphi_0(t) = 0 \\ \varphi_0(t') = 0, \qquad \varphi_0'(t') = 1. \end{cases}$$

2.6.2 Jacobi Field

The function $\varphi_0(t)$ appearing in the semi-classical Feynman kernel has a geometric interpretation in terms of Jacobi field. We illustrate this connection together with a few applications.

Consider all classical trajectories that start from x' at the initial time $t = t'$. They are parametrized by the initial velocity v' at $t = t'$. Let us denote $x_{cl}(t; v')$ for the classical trajectory that solves the initial value problem for the equation of motion

$$\begin{cases} m\ddot{x}_{cl} + V'(x_{cl}) = 0 \\ x_{cl}(t'; v') = 0, \qquad \dot{x}_{cl}(t'; v') = v'. \end{cases}$$

Here $\dot{(\,)}$ means $\frac{\partial(\,)}{\partial t}$. Thus $x_{cl}(t; v')$ gives a family of classical trajectories parametrized by v'.

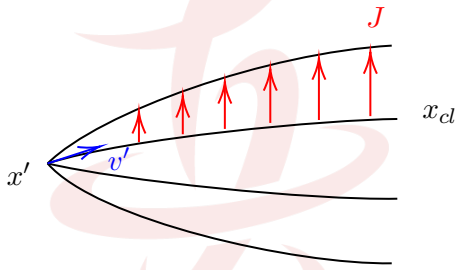
We consider the variation of this family with respect to the parameter v'

$$J(t; v') = \frac{\partial}{\partial v'} x_{cl}(t; v').$$

This is called the *Jacobi field*. Differentiating the equation of motion $m\ddot{x}_{cl} + V'(x_{cl}) = 0$ with respect to v', we find that the Jacobi field satisfies

$$m\frac{\partial^2}{\partial t^2} J + V''(x_{cl})J = 0$$

which is called the *Jacobi equation*.



The initial condition gives

$$\begin{cases} x_{cl}(t'; v') = 0 \\ \dot{x}_{cl}(t'; v') = v' \end{cases} \quad \Longrightarrow \quad \begin{cases} J(t'; v') = 0 \\ \dot{J}(t'; v') = 1 \end{cases}$$

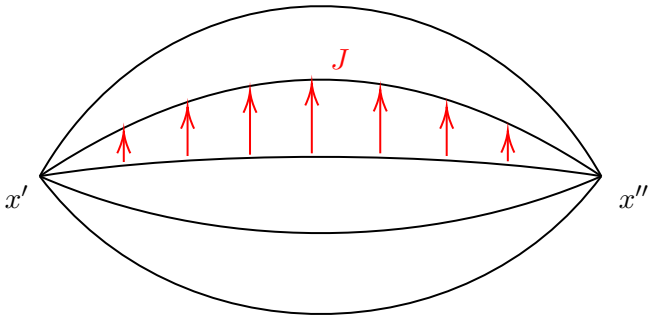
So $J(t; v')$ satisfies the following initial value problem

$$\begin{cases} \left(-\frac{\partial^2}{\partial t^2} - \frac{1}{m} V''(x_{cl}) \right) J = 0 \\ J|_{t=t'} = 0, \qquad \dot{J}|_{t=t'} = 1 \end{cases}$$

Thus the function $\varphi_0(t)$ from the determinant in Section 2.6.1 is precisely the Jacobi field

$$\varphi_0 = J.$$

Remark 2.6.1. The point t'' at which $J(t''; v') = 0$ is called a *conjugate point*. In presence of a conjugate point, there is a family of classical trajectories that start from the same point at $t = t'$ and end with the same point at $t = t''$.



Let us denote

$$S_{cl}(x'',t'';x',t') := \int_{t'}^{t''} \left(\frac{1}{2}m\dot{x_{cl}}^2 - V(x_{cl})\right) dt$$

for the action on the classical trajectory $x(t)$ that starts at $x(t') = x'$ and ends at $x(t'') = x''$. We learn from classical mechanics that $S_{cl}(x'',t'';x',t')$ satisfies the *Hamilton-Jacobi equation*

$$\begin{cases} \dfrac{\partial S_{cl}}{\partial x''} = p(t''), & \dfrac{\partial S_{cl}}{\partial x'} = -p(t') = -mv' \\ \dfrac{\partial S_{cl}}{\partial t''} = -E, & \dfrac{\partial S_{cl}}{\partial t'} = E. \end{cases}$$

Here $p(t) = m\dot{x}_{cl}(t)$ is the conjugate momentum at time t and $E = \frac{1}{2}m\dot{x_{cl}}^2 + V(x_{cl})$ is the energy along the trajectory x_{cl}. It follows that

$$\frac{\partial^2 S_{cl}}{\partial x' \partial x''} = -\frac{\partial p(t')}{\partial x''} = -m\frac{\partial v'}{\partial x''} = -\frac{m}{J(t'')} \quad \Longrightarrow \quad \frac{1}{J(t'')} = -\frac{1}{m}\frac{\partial^2 S_{cl}}{\partial x' \partial x''}.$$

Thus the semi-classical contribution of the classical path $x_{cl}(t)$ can be also written as

$$\left(\frac{m}{2\pi i\hbar\varphi_0(t'')}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S_{cl}} = \left(\frac{m}{2\pi i\hbar J(t'')}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S_{cl}} = \left(\frac{i}{2\pi\hbar}\frac{\partial^2 S_{cl}}{\partial x' \partial x''}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S_{cl}}.$$

In general, if we have several classical trajectories from x' at $t = t'$ to x'' at $t = t''$, then the semi-classical Feynman kernel is the sum of contributions from all classical trajectories

$$K_{sc}(x'',t'';x',t') = \sum_{\substack{x_{cl} \\ x_{cl}(t')=x' \\ x_{cl}(t'')=x''}} \left(\frac{i}{2\pi\hbar}\frac{\partial^2 S_{cl}}{\partial x' \partial x''}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S_{cl}}$$

where $S_{cl}(x'',t'';x',t') = S[x_{cl}(t)]$ is the value of the classical action on the corresponding classical trajectories. This is known as the *Van Vleck-Pauli-Morette formula*.

Example 2.6.2 (Free Particle)**.** *The classical trajectory is a straight line. Given initial point* (x',t') *and final point* (x'',t'')*, the unique classical trajectory is*

$$x_{cl}(t) = \frac{x'(t''-t)}{t''-t'} + \frac{x''(t-t')}{t''-t'}.$$

Then

$$S_{cl}(x'',t'';x',t') = \int_{t'}^{t''} \frac{1}{2}m\dot{x}_{cl}(t)^2\, dt = \frac{m}{2}\frac{(x''-x')^2}{t''-t'}$$

$$\Longrightarrow \qquad \frac{\partial^2 S_{cl}}{\partial x' \partial x''} = -\frac{m}{t''-t'}$$

$$\Longrightarrow \qquad K_{sc}(x'',t'';x',t') = \left(\frac{m}{2\pi i\hbar(t''-t')}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}\frac{m(x''-x')^2}{2(t''-t')}}.$$

In the free case, the semi-classical approximation is exact, i.e., $K_{sc} = K$.

Example 2.6.3 (Harmonic Oscillator)**.** *Consider the simple harmonic oscillator*

$$S[x(t)] = \int_{t'}^{t''} \left(\frac{m}{2}\dot{x}^2 - \frac{m}{2}\omega^2 x^2\right) dt.$$

The equation of motion for the classical trajectory is

$$\ddot{x} + \omega^2 x = 0.$$

When $\omega(t''-t') \notin \mathbb{Z}\pi$, there is a unique classical trajectory from x' at $t=t'$ to x'' at $t=t''$ by

$$x_{cl}(t) = \frac{\sin\omega(t''-t)}{\sin\omega(t''-t')}x' + \frac{\sin\omega(t-t')}{\sin\omega(t''-t')}x''.$$

Let

$$T := t''-t'$$

Then

$$\begin{aligned} S_{cl}(x'',t'';x',t') =& \int_{t'}^{t''} \left(\frac{m}{2}{\dot{x}_{cl}}^2 - \frac{m}{2}\omega^2 {x_{cl}}^2\right) dt \\ =& \frac{m\omega}{2\sin\omega T}\left[\left((x')^2+(x'')^2\right)\cos\omega T - 2x'x''\right] \end{aligned}$$

$$\Longrightarrow \qquad \frac{\partial^2 S_{cl}}{\partial x' \partial x''} = -\frac{m\omega}{\sin\omega T}$$

$$\Longrightarrow \qquad K_{sc}(x'',t'';x',t') = \left(\frac{i}{2\pi\hbar}\frac{\partial^2 S_{cl}}{\partial x'\partial x''}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S_{cl}} = \left(\frac{m\omega}{2\pi i\hbar\sin\omega T}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S_{cl}}.$$

For the harmonic oscillator, the semi-classical approximation is also exact: $K_{sc} = K$.

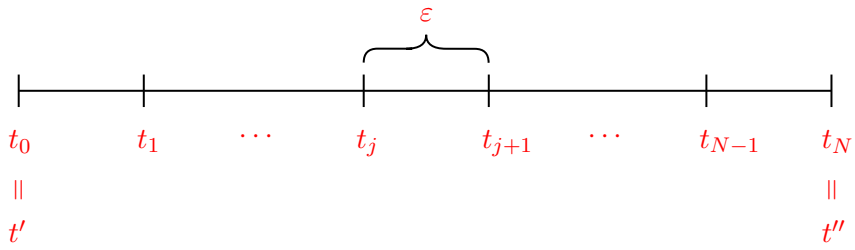
2.6.3 Time-slicing Method

The semi-classical contribution to the Feynman kernel from a classical path $x_{cl}(t)$

$$e^{\frac{i}{\hbar}S[x_{cl}(t)]} \int_{\gamma(t')=0}^{\gamma(t'')=0} [D\gamma(t)]\, e^{\frac{i}{\hbar}\int_{t'}^{t''}\left(\frac{m}{2}\dot{\gamma}^2 - \frac{1}{2}V''(x_{cl})\gamma^2\right)dt} = \left(\frac{m}{\pi i\hbar\det A}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S[x_{cl}(t)]}$$

$$\text{where} \quad A = -\frac{d^2}{dt^2} - \frac{1}{m}V''(x_{cl}(t))$$

can be also understood from a heuristic computation via limit process of time-slicing for paths.



Let us subdivite the time interval $[t', t'']$ into N small intervals of width $\epsilon = \frac{t''-t'}{N}$. Let

$$\omega_j^2 := \frac{V''(x_{cl}(t_j))}{m}$$

denote the value of $V''(x_{cl})$ at the discrete point $t = t_j$. By construction,

$$\begin{aligned}
&\int_{\gamma(t')=0}^{\gamma(t'')=0} [D\gamma(t)]\, e^{\frac{i}{\hbar}\int_{t'}^{t''}\left(\frac{m}{2}\dot\gamma^2 - \frac{1}{2}V''(x_{cl})\gamma^2\right)dt} \\
&= \lim_{\varepsilon\to 0}\left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{N}{2}} \int \prod_{j=1}^{N-1} dx_j\, e^{\frac{i}{\hbar}\sum_{j=0}^{N-1}\left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\varepsilon}\right)^2 - \frac{m\omega_j^2}{2}x_j^2\right]\varepsilon} \qquad \text{here} \quad x_0 := 0, x_N := 0 \\
&= \lim_{\varepsilon\to 0}\left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{N}{2}} \int \prod_{j=1}^{N-1} dx_j\, e^{\frac{im}{2\hbar\varepsilon}\mathbf{x}^t A_N \mathbf{x}} \qquad \text{here} \quad \mathbf{x} = (x_1, \cdots, x_{N-1}) \\
&= \lim_{\varepsilon\to 0}\left(\frac{m}{2\pi i\hbar\varepsilon \det A_N}\right)^{\frac{1}{2}}.
\end{aligned}$$

Here A_N is the $(N-1)\times(N-1)$ matrix

$$A_N = \begin{pmatrix}
2-\varepsilon^2\omega_1^2 & -1 & & & 0 \\
-1 & 2-\epsilon^2\omega_2^2 & \ddots & & \\
& \ddots & \ddots & \ddots & \\
& & \ddots & 2-\epsilon^2\omega_{N-2}^2 & -1 \\
0 & & & -1 & 2-\epsilon^2\omega_{N-1}^2
\end{pmatrix}.$$

Let us define $u_0 = \varepsilon$ and for $1 \le j \le N-1$

$$u_j = \varepsilon \det \begin{pmatrix}
2-\varepsilon^2\omega_1^2 & -1 & & & 0 \\
-1 & 2-\epsilon^2\omega_2^2 & \ddots & & \\
& \ddots & \ddots & \ddots & \\
& & \ddots & 2-\epsilon^2\omega_{j-1}^2 & -1 \\
0 & & & -1 & 2-\epsilon^2\omega_j^2
\end{pmatrix}.$$

Then we have the recursive relation

$$\frac{u_{j+1} - 2u_j + u_{j-1}}{\varepsilon^2} + \omega_{j+1}^2 u_j = 0, \qquad 1 \le j \le N-2.$$

In the continuum limit $\varepsilon \to 0$, this becomes a differential equation for $u(t)$ ($u_j = u(t_j)$)

$$\ddot u(t) + \omega^2(t)u(t) = 0.$$

Here $\omega^2(t) = V''(x_{cl}(t))/m$. The initial condition

$$u_0 = \varepsilon, \qquad \frac{u_1 - u_0}{\varepsilon} = 1 - \varepsilon^2\omega_1^2$$

becomes the initial condition

$$u(t') = 0, \qquad u'(t') = 1.$$

It follows that

$$\lim_{\varepsilon\to 0} \varepsilon \det A_N = u(t'')$$

where $u(t)$ solves

$$\begin{cases} \ddot{u}(t) + \dfrac{1}{m}V''(x_{cl}(t))u(t) = 0 \\ u(t') = 0, \qquad u'(t') = 1. \end{cases}$$

This is the same result as we find before.

2.7 Green's Function

2.7.1 Green's Function with Fixed Energy

In the study of Schrödinger equation, it is useful to go to energy eigenstates and study the stationary solutions with fixed energy. In the path integral formalism, we are thus led to define the Green's function G at fixed energy via the Fourier transform of the *retarded Feynman kernel* $\theta(t)K(x'', t; x', 0)$. Here

$$\theta(t) = \begin{cases} 1 & t \geq 0 \\ 0 & t < 0 \end{cases}$$

is the Heaviside step function. Precisely

$$\begin{aligned} G(x'', x'; E) &:= \frac{1}{i\hbar}\int_{-\infty}^{+\infty} dT\, e^{i(E+i\varepsilon)T/\hbar}\theta(T)K(x'', T; x', 0) \\ &= \frac{1}{i\hbar}\int_{0}^{+\infty} dT\, e^{i(E+i\varepsilon)T/\hbar}K(x'', T; x', 0) \\ &= \frac{1}{i\hbar}\int_{0}^{+\infty} dT\, e^{i(E+i\varepsilon)T/\hbar}\big\langle x''\big|e^{-i\,\widehat{\mathrm{H}}\,T/\hbar}\big|x'\big\rangle \\ &= \big\langle x''\big|\frac{1}{E - \widehat{\mathrm{H}} + i\varepsilon}\big|x'\big\rangle. \end{aligned}$$

Here, as often used in distributions, a small positive $\varepsilon > 0$ has been introduced to ensure convergence of the integral and we take $\varepsilon \to 0^+$ eventually.

The Green's function $G(x'', x'; E)$ is analytic in the region $\operatorname{Im} E > 0$, reflecting the retardation under Fourier transform. Knowing the Green's function, we can recover the Feynman kernel via the inverse Fourier transform

$$K(x'', T; x', 0) = \frac{i}{2\pi}\int_{\mathbb{R}} dE\, e^{-iET/\hbar}G(x'', x'; E).$$

Remark 2.7.1. As an illustration of the method $\varepsilon \to 0^+$, the following distributional identity is commonly used

$$\lim_{\varepsilon\to 0^+} \frac{1}{x \pm i\varepsilon} = \mp i\pi\delta(x) + \text{P.V.}\left(\frac{1}{x}\right).$$

Here $\delta(x)$ is the Dirac δ-function. P.V. $\left(\frac{1}{x}\right)$ is the Cauchy principal value defining the distribution

$$\begin{aligned}\text{P.V.}\left(\frac{1}{x}\right): \quad C_c^\infty(\mathbb{R}) &\longrightarrow \mathbb{R} \\ f &\longmapsto \lim_{\varepsilon\to 0^+} \int_{\mathbb{R}-[-\varepsilon,\varepsilon]} \frac{f(x)}{x}\, dx.\end{aligned}$$

We will simply drop the ε in formulae and keep in mind the meaning $\varepsilon \to 0^+$. Thus

$$G(x'', x'; E) = \big\langle x''\big|\frac{1}{E-\widehat{\mathrm{H}}}\big|x'\big\rangle.$$

In functional analysis, the operator $\frac{1}{A-z}$, for $z \in \mathbb{C}\backslash \operatorname{spec}(A)$, is called the *resolvent* of the operator A. Thus G is precisely the resolvent integral kernel of the Hamiltonian $\widehat{\mathrm{H}}$. It represents the inverse of $E - \widehat{\mathrm{H}}$ and satisfies

$$\left(E-\widehat{\mathrm{H}}\right) G(x'', x'; E) = \big\langle x''\big|x'\big\rangle = \delta(x''-x').$$

If the spectrum of $\widehat{\mathrm{H}}$ is the discrete set $\{E_k\}$ with orthonormal eigenstates $\{\psi_k\}$, then G can be written as a sum

$$G(x'', x'; E) = \sum_k \big\langle x''\big|\frac{1}{E-\widehat{\mathrm{H}}}|\psi_k\rangle\langle\psi_k|x'\big\rangle = \sum_k \frac{\psi_k(x'')\psi_k^*(x')}{E-E_k}.$$

Thus the energy eigenvalues $\{E_k\}$ are detected by the poles of G. In general when both bound and scattering states exist, we will have a spectral integral

$$G(x'', x'; E) = \int_{\mathbb{R}} \frac{dp}{2\pi\hbar}\, \frac{\psi_p(x'')\psi_p^*(x')}{E-E(p)}.$$

Example 2.7.2 (Free Particle)**.** *The Hamiltonian of the free particle is*

$$\widehat{\mathrm{H}}_0 = \frac{\hat{p}^2}{2m}$$

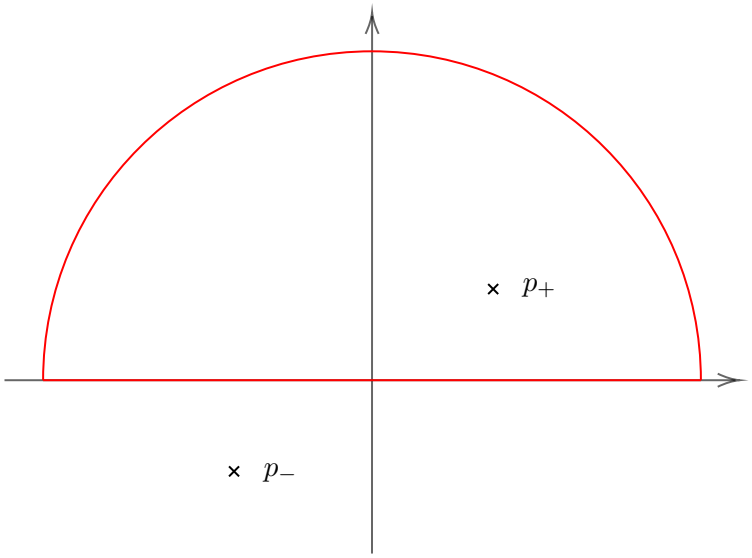
with the free Feynman kernel

$$K_0(x'', T; x', 0) = \Big(\frac{m}{2\pi\hbar i T}\Big)^{\frac{1}{2}} e^{\frac{im(x''-x')^2}{2\hbar T}}.$$

The energy spectrum is continuous. We can compute the free Green's function by

$$\begin{aligned} G_0(x'', x'; E) &= \big\langle x''\big|\frac{1}{E-\widehat{\mathrm{H}}}\big|x'\big\rangle \\ &= \frac{1}{2\pi\hbar}\int_{\mathbb{R}} dp\, \big\langle x''\big|\frac{1}{E-\widehat{\mathrm{H}}}|p\rangle\langle p|x'\big\rangle \\ &= \frac{1}{2\pi\hbar}\int_{\mathbb{R}} dp\, \frac{1}{E-p^2/2m+i\varepsilon} e^{ip(x''-x')/\hbar} \qquad (\varepsilon\to 0^+) \\ &= \frac{1}{2\pi\hbar}\int_{\mathbb{R}} dp\, \frac{1}{E-p^2/2m+i\varepsilon} e^{ip|x''-x'|/\hbar} \qquad (\varepsilon\to 0^+) \end{aligned}$$

We can compute the last integral by residue. The poles are located at $p_\pm = \pm\sqrt{2m}\sqrt{E+i\varepsilon}$*. The integral picks up a residue at* p_+



$$\Longrightarrow \quad G_0(x'',x';E) = \frac{i}{\hbar}\,\mathrm{Res}_{p=p_+}\left(\frac{e^{ip|x''-x'|/\hbar}}{E-p^2/2m+i\varepsilon}\right) \qquad (\varepsilon\to 0_+)$$
$$= \frac{1}{i\hbar}\sqrt{\frac{m}{2E}}e^{i\sqrt{2mE}|x''-x'|/\hbar}.$$

In the physical region $E>0$ with $E=\frac{\hbar^2k^2}{2m}$ $(k>0)$, we have

$$G_0(x'',x';E) = \frac{m}{i\hbar^2 k}e^{ik|x''-x'|}.$$

There is a standard way to construct Green's function that we briefly recall for the case at hand. Let $\psi_1(x)$ and $\psi_2(x)$ be two linearly independent solutions of

$$\left(E-\widehat{\mathrm{H}}\right)\psi_i(x)=0$$

i.e.,

$$\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-V(x)+E\right)\psi_i(x)=0.$$

Consider the following function

$$\xi(x,y;E) := \frac{2m}{\hbar^2 W}\left(\theta(x-y)\psi_1(x)\psi_2(y)+\theta(y-x)\psi_1(y)\psi_2(x)\right).$$

Here $W=\psi_1'(x)\psi_2(x)-\psi_2'(x)\psi_1(x)$ is called the *Wronskian* which is a constant by the equation. Using $\theta'(x-y)=\delta(x-y)$, it is direct to check that $\xi(x,y;E)$ satisfies the equation

$$\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-V(x)+E\right)\xi(x,y;E)=\delta(x-y).$$

In order for $\xi(x,y;E)=G(x,y;E)$ to hold, we need to choose ψ_1 and ψ_2 to satisfy appropriate boundary conditions. We illustrate this in the example of scattering problem.

Example 2.7.3. *Let us consider the case*

$$\lim_{|x|\to+\infty} V(x)=0$$

which is relevant for the scattering problem. Consider the inverse Fourier transform

$$K(x'', T; x', 0) = \frac{i}{2\pi} \int_{\mathbb{R}} dE\, e^{-iET/\hbar} G(x'', x'; E).$$

It can be viewed as a superposition of wavefunctions from different energies.

When $x'' \to +\infty$, the Feynman kernel should behave like an outgoing plane waves with positive momentum and energy. This tells

$$G(x'', x'; E) \propto e^{\frac{i}{\hbar}\sqrt{2mE}x''} \qquad as \quad x'' \to +\infty.$$

Similarly, behavior of an outgoing plane when $x'' \to -\infty$ tells

$$G(x'', x'; E) \propto e^{-\frac{i}{\hbar}\sqrt{2mE}x''} \qquad as \quad x'' \to -\infty.$$

This leads to the following asymptotic behavior for the solution ψ_1 and ψ_2

$$\begin{cases} \psi_1(x) \propto e^{\frac{i}{\hbar}\sqrt{2mE}x}, & x \to +\infty \\ \psi_2(x) \propto e^{-\frac{i}{\hbar}\sqrt{2mE}x}, & x \to -\infty \end{cases}$$

To illustrate this, consider the free particle when $V = 0$. The solutions

$$\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + E\right)\psi_i(x) = 0$$

for $E > 0$ with the expected boundary behavior is

$$\begin{cases} \psi_1(x) = e^{ikx} \\ \psi_2(x) = e^{-ikx} \end{cases}, \qquad k = \frac{\sqrt{2mE}}{\hbar}.$$

The Wronskian is $W = \psi_1'\psi_2 - \psi_1\psi_2' = 2ik$. Then the Green's function is

$$\begin{aligned} G(x'', x'; E) &= \frac{2m}{\hbar^2 2ik}\left(\theta(x'' - x')\psi_1(x'')\psi_2(x') + \theta(x' - x'')\psi_1(x')\psi_2(x'')\right) \\ &= \frac{m}{i\hbar^2 k}\left(\theta(x'' - x')e^{ik(x''-x')} + \theta(x' - x'')e^{ik(x'-x'')}\right) \\ &= \frac{m}{i\hbar^2 k}e^{ik|x''-x'|} \end{aligned}$$

which is precisely the formula we found above.

In general when a localized potential $V(x)$ is turned on, we are in the situation of scattering process. Consider the energy $E > 0$. Then the behavior

$$\psi_1(x) \propto e^{ikx}, \qquad x \to +\infty$$

can be more precisely described by

$$\psi_1(x) = \begin{cases} e^{ikx} + B(k)e^{-ikx} & x \to -\infty \\ A(k)e^{ikx} & x \to +\infty \end{cases}$$

This solution represents an incoming plane wave from $x = -\infty$ scattering through the potential region. The coefficient B represents the amplitude of the reflected wave, and A represents the amplitude of the transmitted wave.

Similarly, the behavior

$$\psi_2(x) \propto e^{-ikx}, \qquad x \to -\infty$$

can be precisely described by

$$\psi_2(x) = \begin{cases} A(k)e^{-ikx} & x \to -\infty \\ e^{-ikx} + C(k)e^{ikx} & x \to +\infty \end{cases}$$

This solution represents an incoming plane wave from $x = +\infty$ scattering through the potential region. The coefficient C represents the amplitude of the reflected wave, and A represents the amplitude of the transmitted wave. Note that the transmission amplitudes from the left and from the right are the same, due to time reversal symmetry.

We can compute the Wronskian from the behavior at $x = \pm\infty$ and find

$$W = \psi_1'(x)\psi_2(x) - \psi_1(x)\psi_2'(x) = 2ikA.$$

The Green's function is thus given by

$$G(x'', x'; E) = \frac{m}{ik\hbar^2 A}\left[\theta(x'' - x')\psi_1(x'')\psi_2(x') + \theta(x' - x'')\psi_1(x')\psi_2(x'')\right].$$

In the limit when $x' \to -\infty$, $x'' \to +\infty$, we find

$$G(x'', x'; E) = \frac{m}{ik\hbar^2} A e^{ik(x''-x')}, \qquad x' \to -\infty,\ x'' \to +\infty$$

which displays the information about the transmission amplitude. In Section 2.7.3, we will use this formula to compute A and derive the WKB formula for quantum tunneling.

2.7.2 Semi-classical Analysis

Now we perform a semi-classical analysis of the Green's function

$$G(x'', x'; E) = \frac{1}{i\hbar}\int_0^\infty dT\, e^{iET/\hbar} K(x'', T; x', 0)$$

in the asymptotic limit $\hbar \to 0$. Recall the Feynman kernel

$$K(x'', T; x', 0) = \int_{x(0)=x'}^{x(T)=x''} [Dx(t)]\, e^{\frac{i}{\hbar}S[x(t)]}.$$

Combining the above two formulae, we find

$$G(x'', x'; E) = \frac{1}{i\hbar}\int_0^\infty dT \int [Dx(t)]\, e^{\frac{i}{\hbar}(ET + S[x(t)])}.$$

We consider the semi-classical approximation in the limit $\hbar \to 0$ via the method of steepest descent. The saddle points are given by (x_{cl}, T_s) such that

$$\begin{cases} \dfrac{\delta}{\delta x}\left(ET + S[x(t)]\right)\Big|_{x(t)=x_{cl}, T=T_s} = 0 \\ \dfrac{\partial}{\partial T}\left(ET + S[x(t)]\right)\Big|_{x(t)=x_{cl}, T=T_s} = 0 \end{cases}$$

The first equation is the same as

$$\left.\frac{\delta S}{\delta x}\right|_{x=x_{cl},T=T_s} = 0$$

i.e., $x_{cl}(t)$ is a classical trajectory from $x_{cl}(0) = x'$ to $x_{cl}(T_s) = x''$. Plugging x_{cl} into the second equation and using the Hamilton-Jacobi equation, we find

$$E = -\frac{\partial S[x_{cl}]}{\partial T} = E_{cl}.$$

Here E_{cl} is the energy of the classical trajectory x_{cl}. Thus the saddle points are the set of pairs (x_{cl}, T_s) where x_{cl} is a classical trajectory from x' to x'' with energy E and travel time T_s.

Now let us compute the semi-classical contribution at a saddle point (x_{cl}, T_s). Let S_{cl} denote the action $S[x_{cl}]$ on the classical trajectory x_{cl}. Recall that we have the following semi-classical approximation for the Feynman kernel

$$K_{sc}(x'', T; x', 0) = \left(\frac{i}{2\pi\hbar}\frac{\partial^2 S_{cl}}{\partial x''\partial x'}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S_{cl}}.$$

This leads to the following semi-classical asymptotic behavior in the limit $\hbar \to 0$

$$\begin{aligned} G(x'', x'; E) &\simeq \sum_{(x_{cl},T_s)} \frac{1}{i\hbar}\left(\frac{i}{2\pi\hbar}\frac{\partial^2 S_{cl}}{\partial x''\partial x'}\right)^{\frac{1}{2}}\left(\frac{2\pi\hbar i}{\partial_T^2 S_{cl}}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}(ET_s+S_{cl})} \\ &= \frac{1}{\hbar}\sum_{(x_{cl},T_s)}\left(\frac{\frac{\partial^2 S_{cl}}{\partial x''\partial x'}}{-\frac{\partial E_{cl}}{\partial T}}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}(ET_s+S_{cl})}. \end{aligned}$$

This expression can be further simplified as follows. Recall from Section 2.6.2

$$\frac{\partial^2 S_{cl}}{\partial x''\partial x'} = -\frac{m}{J(T)}$$

where J is the Jacobi field solving

$$\begin{cases} \left(\frac{d^2}{dt^2} + \frac{1}{m}V''(x_{cl}(t))\right) J(t) = 0 \\ J(0) = 0, \qquad \dot{J}(0) = 1 \end{cases}$$

along the trajectory. Let $v_{cl}(t) = \dot{x}_{cl}(t)$ denote the velocity along the trajectory. Differentiating the trajectory equation

$$m\ddot{x}_{cl}(t) + V'(x_{cl}(t)) = 0$$

with respect to t, we find

$$\left(\frac{d^2}{dt^2} + \frac{1}{m}V''(x_{cl}(t))\right) v_{cl}(t) = 0$$

i.e., $v_{cl}(t)$ solves the same equation as J.

Since $v_{cl}(t)$ is tangent to the trajectory while $J(t)$ is along the normal direction, $\{v, J\}$ form two linearly independent solutions of the equation. The Wronskian

$$W = \dot{J}(t)v_{cl}(t) - J(t)\dot{v}_{cl}(t)$$

is a constant by the equation. Evaluating W at $t = 0$, we find $W = v_{cl}(0)$. Then

$$\frac{d}{dt}\left(\frac{J(t)}{v_{cl}(t)}\right) = \frac{W}{v_{cl}(t)^2} = \frac{v_{cl}(0)}{v_{cl}(t)^2} \qquad \Longrightarrow \qquad J(T) = v_{cl}(0)v_{cl}(T)\int_0^T \frac{dt}{v_{cl}(t)^2}.$$

On the other hand,

$$\begin{aligned} T = \int_0^T dt = \int_{x'}^{x''} \frac{dx}{v_{cl}(t)} &= \int_{x'}^{x''} \frac{dx}{\sqrt{2(E_{cl} - V(x))/m}} \\ \Longrightarrow \qquad \frac{dT}{dE_{cl}} = -\frac{1}{m}\int_{x'}^{x''} \frac{dx}{(2(E_{cl} - V(x))/m)^{3/2}} &= -\frac{1}{m}\int_{x'}^{x''} \frac{dx}{{v_{cl}}^3} = -\frac{1}{m}\int_0^T \frac{dt}{v_{cl}(t)^2} \\ \Longrightarrow \qquad \frac{\partial E_{cl}}{\partial T} &= -\frac{m}{\int_0^T \frac{dt}{v_{cl}(t)^2}}. \end{aligned}$$

It follows that

$$\frac{\frac{\partial^2 S_{cl}}{\partial x'' \partial x'}}{-\frac{\partial E_{cl}}{\partial T}} = \frac{-\frac{m}{J(T)}}{\frac{m}{\int_0^T \frac{dt}{v_{cl}(t)^2}}} = \frac{1}{-v_{cl}(0)v_{cl}(T)} = \frac{1}{-\dot{x}_{cl}(0)\dot{x}_{cl}(T)}.$$

Let us also define $W_{cl} = E_{cl}T_s + S_{cl}$. Then

$$\begin{aligned} W_{cl} &= E_{cl}T_s + \int_0^{T_s} \left(\frac{1}{2}m{\dot{x}_{cl}}^2 - V(x_{cl})\right) dt \\ &= E_{cl}T_s + \int_0^{T_s} m{\dot{x}_{cl}}^2\, dt - \int_0^{T_s} E_{cl}\, dt \\ &= \int_0^{T_s} m{\dot{x}_{cl}}^2\, dt = \int_{x'}^{x''} p dx. \end{aligned}$$

Here $p = m\dot{x} = \sqrt{2m(E - V(x))}$ is the classical momentum. Thus we have arrived at the following asymptotic semi-classical approximation

$$\begin{aligned} G(x', x''; E) \simeq &\frac{1}{\hbar} \sum_{(x_{cl}, T_s)} (-\dot{x}_{cl}(0)\dot{x}_{cl}(T_s))^{-\frac{1}{2}}\, e^{\frac{i}{\hbar}W_{cl}} \\ = &\frac{1}{\hbar} \sum_{(x_{cl}, T_s)} (-\dot{x}_{cl}(0)\dot{x}_{cl}(T_s))^{-\frac{1}{2}}\, e^{\frac{i}{\hbar}\int_{x'}^{x''} p dx}. \end{aligned}$$

Remark 2.7.4. It is worthwhile to emphasize one important point here. Since we have the integral contour

$$\int_0^\infty dT$$

for T, we are not summing over all possible classical trajectories (x_{cl}, T_s). In fact, to apply the method of steepest descent, we have to deform the integral contour

$$\int_0^\infty dT = \int_C dT$$

from $\mathbb{R}_{\geq 0}$ to contour C which is a combination of curves of steepest descent. As we vary the parameters x', x'', the sum of curves of steepest descent may display a discontinuous jump. This is precisely the Stokes phenomenon.

Example 2.7.5 (Free Particle). *Given energy $E > 0$, there exists a unique classical trajectory from x' to x'' by*

$$x_{cl}(t) = x' + \frac{x'' - x'}{T_s} t,$$

where

$$T_s = \sqrt{\frac{m}{2E}} |x'' - x'|.$$

The semi-classical Green's function is

$$\begin{aligned} G(x', x''; E) &\simeq \frac{1}{\hbar} \left(-\dot{x}_{cl}(0)\dot{x}_{cl}(T_s)\right)^{-\frac{1}{2}} e^{\frac{i}{\hbar}\int_{x'}^{x''} p_{cl}\, dx_{cl}} \\ &= \frac{1}{\hbar} \left(-\frac{2E}{m}\right)^{-\frac{1}{2}} e^{\frac{i}{\hbar}\sqrt{2mE}|x''-x'|} \\ &= \frac{m}{i\hbar^2 k} e^{ik|x''-x'|}, \qquad k = \frac{\sqrt{2mE}}{\hbar}. \end{aligned}$$

This is the same formula as we found before.

Example 2.7.6 (Linear Potential). *We consider the example of a linear potential*

$$V(x) = -\lambda x, \qquad \lambda > 0.$$

This example plays an important role in deriving the connection formula for WKB approximation. We shall understand a different perspective of the connection formula via semi-classical path integral in Section 2.7.3. We follow the presentation [9] to illustrate the basic idea first.

The equation of motion is

$$m\ddot{x} = \lambda.$$

Given T, there is a unique classical trajectory from $x(0) = x'$ to $x(T) = x''$ by

$$x_{cl}(t) = x' + \frac{x'' - x'}{T} t - \frac{\lambda T}{2m} t + \frac{\lambda}{2m} t^2.$$

The corresponding action value is

$$S_{cl} = \int_0^T \left(\frac{1}{2} m \dot{x}_{cl}{}^2 + \lambda x_{cl}\right) dt = \frac{m}{2T}(x'' - x')^2 + \frac{\lambda T}{2}(x'' + x') - \frac{\lambda^2 T^3}{24m}.$$

In the linear case, the semi-classical Feynman kernel is exact

$$K(x'', T; x', 0) = \left(\frac{i}{2\pi\hbar} \frac{\partial^2 S_{cl}}{\partial x'' \partial x'}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar} S_{cl}} = \left(\frac{m}{2\pi i\hbar T}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar} S_{cl}}.$$

Let us now consider the saddle points along the T-integral for the Green's function $G(x'', x'; E)$. Note that for a linear potential, a shift in energy is equivalent to a translation in x. Thus it is enough to consider the case $E = 0$, so we have

$$W_{cl} = S_{cl}.$$

We assume $E = 0$ in the following discussions.

The saddle point (x_{cl}, T_s) is located at the time T_s by

$$\begin{aligned} & E = -\left.\frac{\partial S_{cl}}{\partial T}\right|_{T=T_s} \\ \Longrightarrow \quad & \frac{m}{2T_s^2}(x''-x')^2 - \frac{\lambda}{2}(x''+x') + \frac{\lambda^2 T_s^2}{8m} = 0 \\ \Longrightarrow \quad & T_s = \left(\frac{2m}{\lambda}\right)^{\frac{1}{2}} (\pm\sqrt{x''} \pm \sqrt{x'}). \end{aligned}$$

There are four saddles in total, corresponding to all possible signs in the choice of square root of x' and x''. The value of the classical action is

$$S_{cl} = \frac{2}{3}(2m\lambda)^{\frac{1}{2}} \left(\pm\sqrt{x''}^3 \pm \sqrt{x'}^3\right)$$

with signs of $\sqrt{x''}$ and $\sqrt{x'}$ as that for T_s. The product of the initial and final velocities are

$$\begin{aligned} \dot{x}_{cl}(0)\dot{x}_{cl}(T_s) &= \left(\frac{x''-x'}{T_s} - \frac{\lambda T_s}{2m}\right)\left(\frac{x''-x'}{T_s} + \frac{\lambda T_s}{2m}\right) \\ &= \frac{(x''-x')^2}{T_s^2} - \frac{\lambda^2}{4m^2}T_s^2 \\ &= \frac{\lambda}{m}(x''+x') - \frac{\lambda^2}{2m^2}T_s^2 \\ &= -\frac{2\lambda}{m}(\pm\sqrt{x''})(\pm\sqrt{x'}). \end{aligned}$$

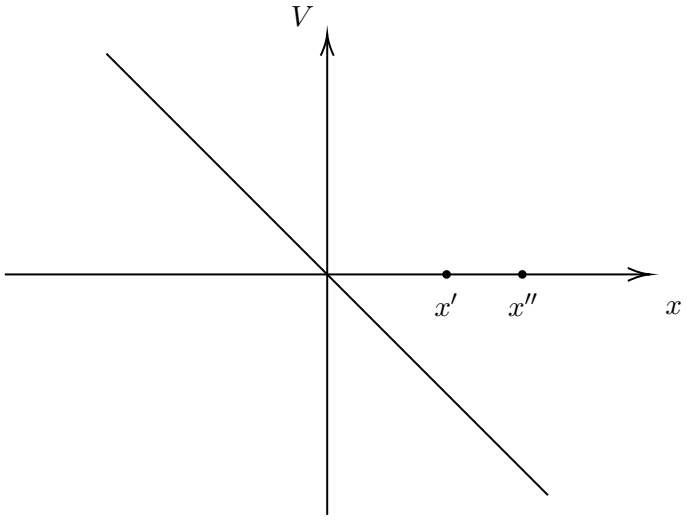
Thus the semi-classical contribution of the saddle (x_{cl}, T_s) to the Green's function is

$$\frac{1}{\hbar}\left(\frac{m}{2\lambda(\pm\sqrt{x''})(\pm\sqrt{x'})}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S_{cl}}.$$

Now let us identify which saddle points will contribute to the semi-classical Green's function. The situation will depend on the locus of x' and x''.

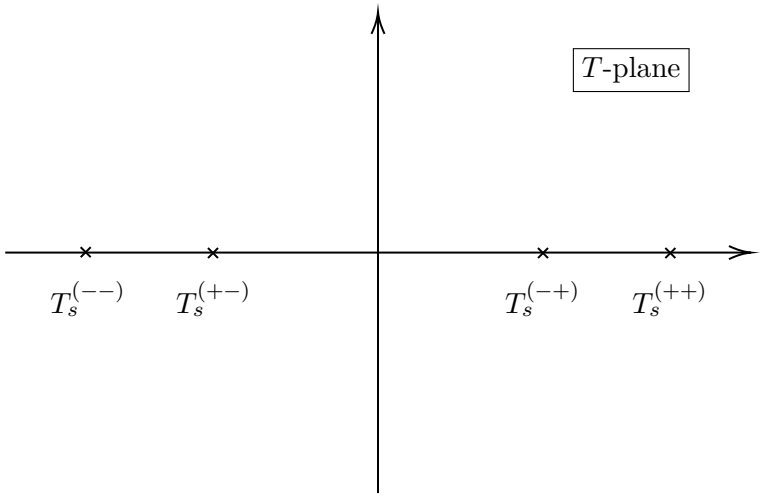
Case $0 < x' < x''$

Both x' and x'' lie in the classically allowed region ($x > 0$).



All the saddle points have real values and we denote them by

$$T_s^{(\pm\pm)} = \left(\frac{2m}{\lambda}\right)^{\frac{1}{2}} \left(\pm\sqrt{x'} \pm \sqrt{x''}\right).$$



Let us consider curves of steepest descent in the T-plane. The complex oscillatory integral is about the function ($E = 0$ here)

$$e^{\frac{i}{\hbar}(ET+S_{cl})} = e^{\frac{i}{\hbar}S_{cl}}.$$

The curves of steepest descent in the T-plane are described by

- $\mathrm{Im}(iS_{cl}) = \mathrm{Re}(S_{cl}) = \text{Constant}$
- $\mathrm{Re}(iS_{cl}) = -\mathrm{Im}(S_{cl}) \to -\infty$ along boundary
- Pass through some saddle point.

The classical action S_{cl} as a function of T is

$$S_{cl}(T) = \frac{m}{2T}(x'' - x')^2 + \frac{\lambda T}{2}(x'' + x') - \frac{\lambda^2 T^3}{24m}.$$

The corresponding values of S_{cl} on $T_s^{(\pm\pm)}$ are

$$S_{cl}\left(T_s^{(\pm\pm)}\right) = \frac{2}{3}(2m\lambda)^{\frac{1}{2}} \left(\pm\sqrt{x'}^3 \pm \sqrt{x''}^3\right).$$

So all $\mathrm{Re}\left(S_{cl}\left(T_s^{(\pm\pm)}\right)\right)$ are different and the corresponding four curves $C^{(\pm\pm)}$ of steepest descent do not intersect. They can be constructed by following the flow equation to $u \to +\infty$

$$\frac{dT}{du} = -\overline{iS_{cl}'(T)}$$

i.e.,

$$\frac{dT}{du} = i\left[-\frac{m}{2\overline{T}^2}(x'' - x')^2 + \frac{\lambda}{2}(x'' + x') - \frac{\lambda^2\overline{T}^2}{8m}\right]$$

with the initial condition $\lim_{u\to-\infty} T = \text{saddle point}$.

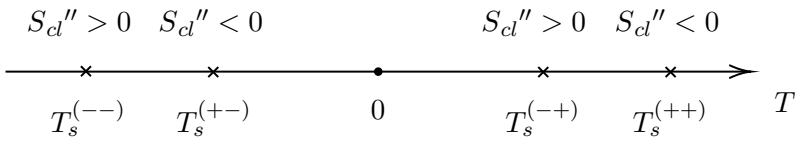
Now let us apply the method in Section 2.5.3 to

$$f(T) = iS_{cl}(T).$$

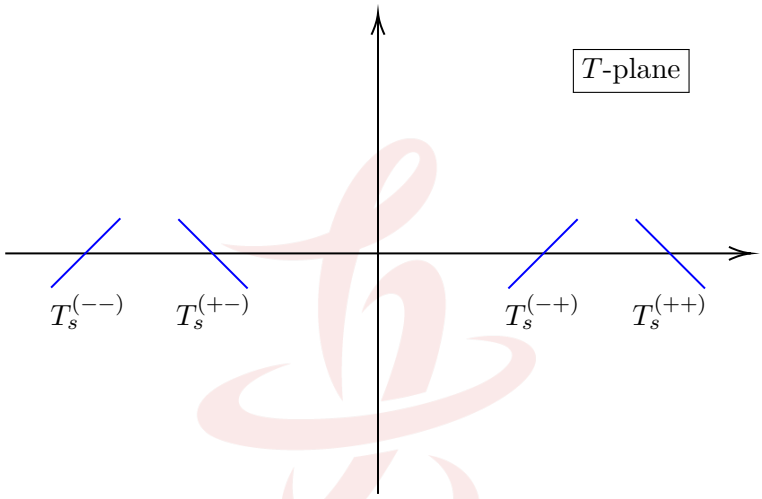
We have

$$S_{cl}{}'(T) = -\frac{\lambda^2}{8mT^2}\left(T - T_s^{(--)}\right)\left(T - T_s^{(+-)}\right)\left(T - T_s^{(-+)}\right)\left(T - T_s^{(++)}\right).$$

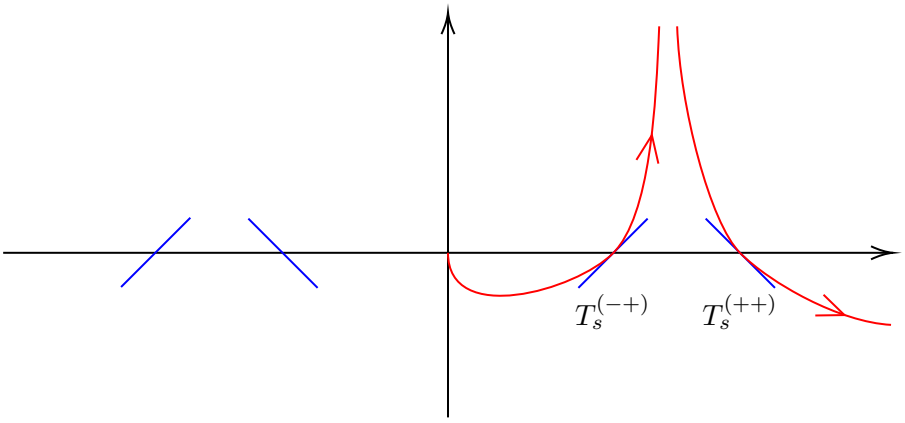
At the four saddle points,



So we can draw the tangent direction of steepest descent curve at each saddle point by



A bit further calculation shows that the integral contour $\{T \in \mathbb{R}_{\geq 0}\}$ is deformed into the sum of the following two curves of steepest descent



Case: $0 < x' < x''$.

Thus the semi-classical approximation of the Green's function $G(x'', x'; E)$ has contributions from two saddle points

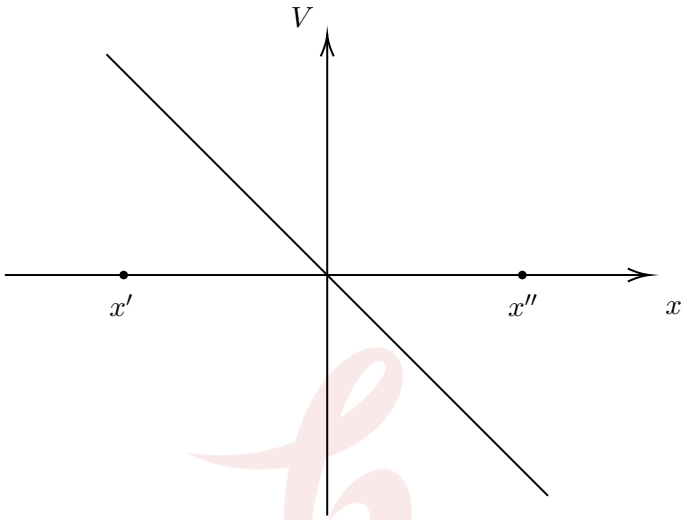
$$T_s^{(-+)} = \left(\frac{2m}{\lambda}\right)^{\frac{1}{2}}\left(-\sqrt{x'} + \sqrt{x''}\right)$$

$$T_s^{(++)} = \left(\frac{2m}{\lambda}\right)^{\frac{1}{2}} \left(\sqrt{x'} + \sqrt{x''}\right).$$

The saddle $T_s^{(-+)}$ corresponds to a direct path from x' to x''. The other saddle $T_s^{(++)}$ corresponds to a path that moves left from x', reflects at $x = 0$, then moves right to reach x''.

Case $x' < 0 < x''$

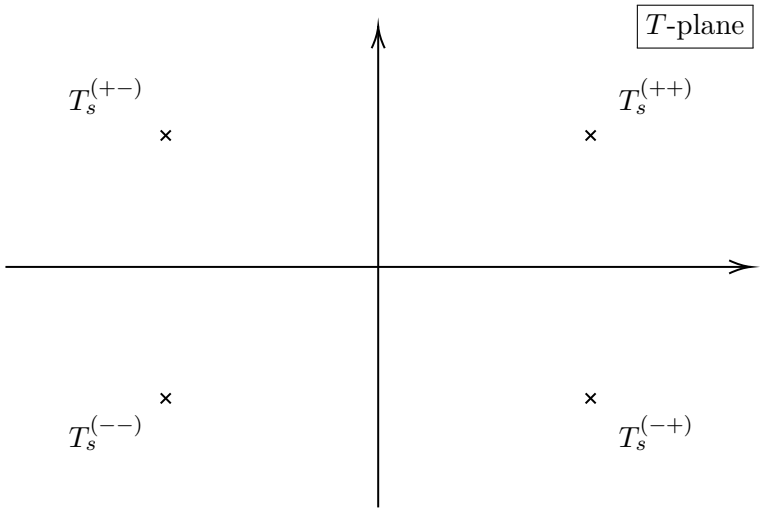
x' lies in the classically forbidden region and x'' lies in the classically allowed region.



The four saddle points

$$T_s^{(\pm\pm)} = \left(\frac{2m}{\lambda}\right)^{\frac{1}{2}} \left(\pm i\sqrt{|x'|} \pm \sqrt{x''}\right)$$

are all complex numbers.

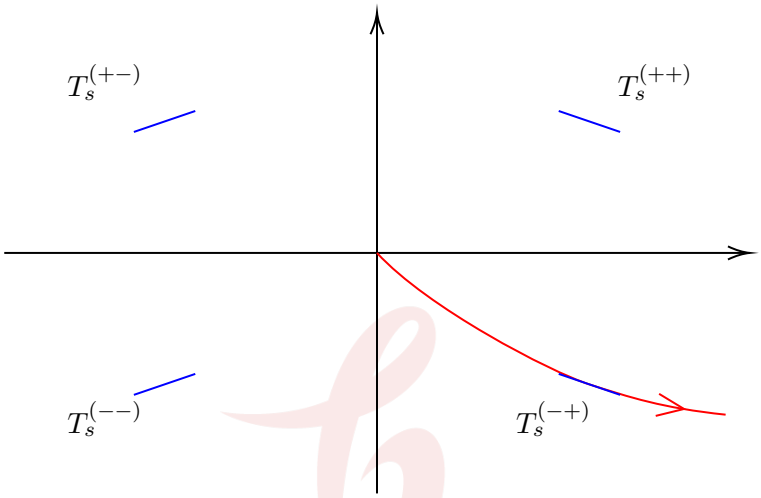


$$S_{cl}{}'(T) = -\frac{\lambda^2}{8mT^2} \left(T - T_s^{(--)}\right) \left(T - T_s^{(+-)}\right) \left(T - T_s^{(-+)}\right) \left(T - T_s^{(++)}\right).$$

At the saddle points, we have

$$\begin{aligned}
iS_{cl}''\left(T_s^{(++)}\right) &\in \left(T_s^{(++)}\right)^{-1}\mathbb{R}_{>0}\\
iS_{cl}''\left(T_s^{(+-)}\right) &\in -\left(T_s^{(+-)}\right)^{-1}\mathbb{R}_{>0}\\
iS_{cl}''\left(T_s^{(-+)}\right) &\in -\left(T_s^{(-+)}\right)^{-1}\mathbb{R}_{>0}\\
iS_{cl}''\left(T_s^{(--)}\right) &\in \left(T_s^{(--)}\right)^{-1}\mathbb{R}_{>0}
\end{aligned}$$

This allows us to draw the tangent directions of the steepest descent curves at saddles.



The integral contour $\{T \in \mathbb{R}_{\geq 0}\}$ is deformed to the curve of steepest descend passing

$$T_s^{(-+)} = \left(\frac{2m}{\lambda}\right)^{\frac{1}{2}}\left(-i\sqrt{|x'|}+\sqrt{x''}\right).$$

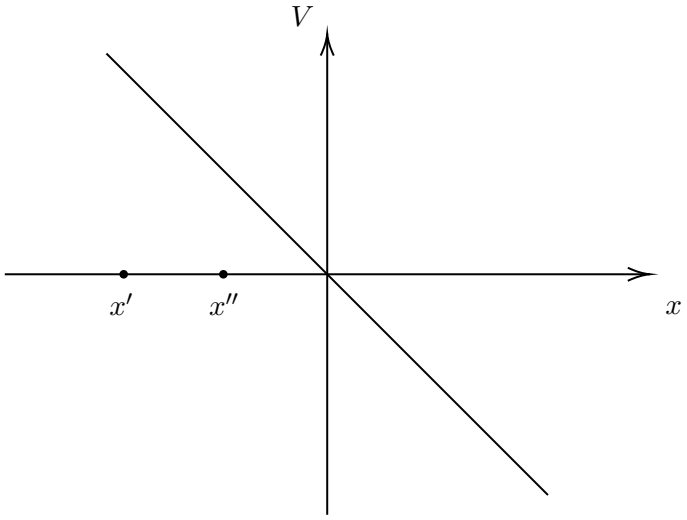
Note that the saddle $T_s^{(-+)}$ has imaginary part. It corresponds to a unique classical path from x' to x'', but has to go through non-real time! This non-real time is due to the fact that the path has to go through a portion of the classically forbidden region. Indeed

$$T = \int_0^T dt = \int_{x'}^{x''} \frac{dx}{\dot{x}} = \int_{x'}^{x''} \frac{dx}{\sqrt{2m(E-V(x))}}.$$

In the classical forbidden region, $E < V(x)$ hence the integration will give rise to imaginary contribution of the travel time.

Case $x' < x'' < 0$

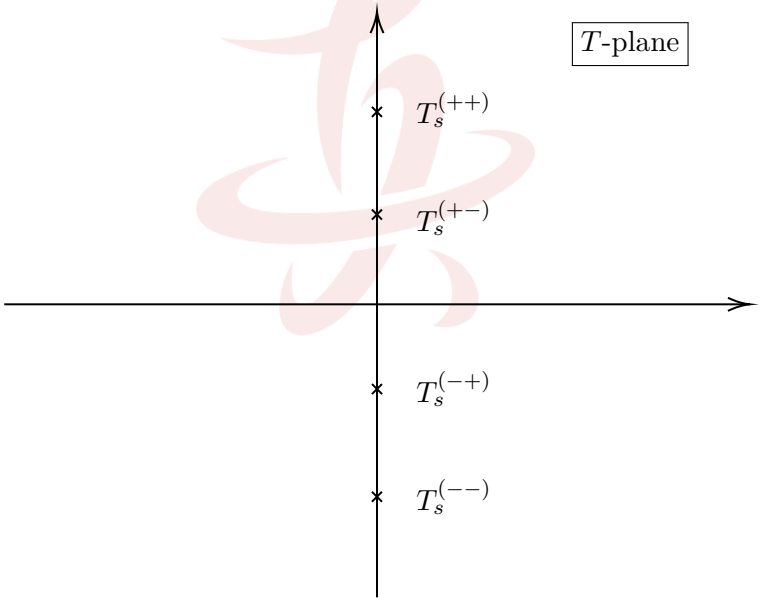
Both x' and x'' lie in the forbidden region.



The four saddle points

$$T_s^{(\pm\pm)} = \left(\frac{2m}{\lambda}\right)^{\frac{1}{2}} \left(\pm i\sqrt{|x'|} \pm i\sqrt{|x''|}\right)$$

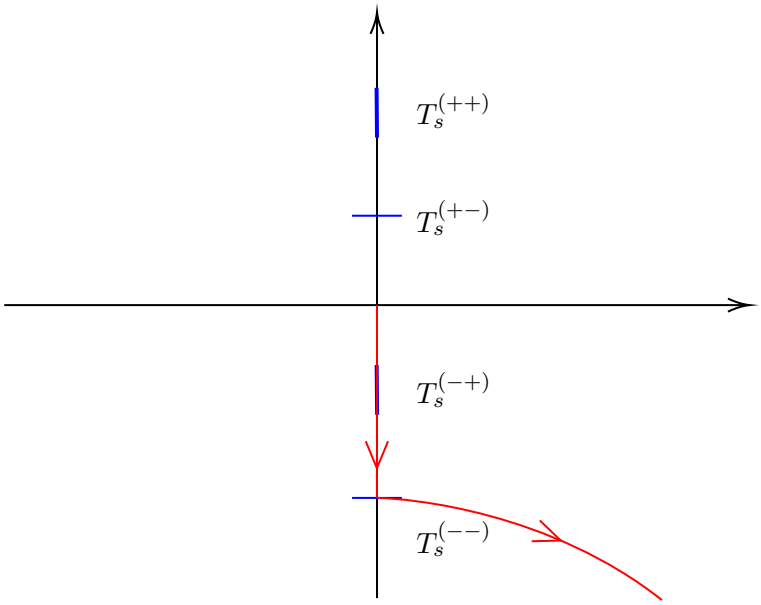
are all imaginary.



At the saddle points, we have

$$iS_{cl}{}''\left(T_s^{(++)}\right) \in \mathbb{R}_{>0}$$
$$iS_{cl}{}''\left(T_s^{(+-)}\right) \in \mathbb{R}_{<0}$$
$$iS_{cl}{}''\left(T_s^{(-+)}\right) \in \mathbb{R}_{>0}$$
$$iS_{cl}{}''\left(T_s^{(--)}\right) \in \mathbb{R}_{<0}$$

This allows us to draw the tangent directions of steepest descent curves at saddles.



The integral contour $\{T \in \mathbb{R}_{\geq 0}\}$ is deformed to two curves passing through $T_s^{(-+)}$ and $T_s^{(--)}$. The first curve goes from the origin, passes the saddle $T_s^{(-+)}$, and then ends up with the saddle $T_s^{(--)}$. The second curve starts from the saddle $T_s^{(--)}$ and goes to infinity. The contribution from the saddle $T_s^{(-+)}$ dominates.

2.7.3 WKB via Path Integral

Now we connect our discussion on the semi-classical approximation of path integrals to the WKB formalism on the semi-classical approximation of wave functions.

The Green's function

$$G(x'', x'; E) = \langle x'' | \frac{1}{E - \widehat{\mathrm{H}}} | x' \rangle$$

represents the inverse kernel of the operator $E - \widehat{\mathrm{H}}$ and satisfies

$$\left(E - \widehat{\mathrm{H}}_{x''}\right) G(x'', x'; E) = \delta(x'' - x').$$

Here $\widehat{\mathrm{H}}_{x''}$ is the Hamiltonian operator expressed in the x''-coordinate.

In the previous subsection, we have shown the asymptotic semi-classical formula

$$G(x'', x'; E) \simeq \frac{1}{\hbar} \sum_{(x_{cl}, T_s)} (-\dot{x}_{cl}(0)\dot{x}_{cl}(T_s))^{-\frac{1}{2}} \, e^{\frac{i}{\hbar} W_{cl}}$$

where the sum is over all classical trajectory x_{cl} from x' at time 0 to x'' at time T_s, with prescribed energy E. And

$$\begin{aligned} W_{cl} &= ET_s + S_{cl} = ET_s + S[x_{cl}] \\ &= \int_0^{T_s} \left(E + \frac{1}{2} m \dot{x}_{cl}{}^2 - V(x_{cl}) \right) dt \\ &= \int_0^{T_s} m \dot{x}_{cl}{}^2 \, dt = \int_{x'}^{x''} p \, dx \end{aligned}$$

where

$$p = m\dot{x} = \sqrt{2m(E - V(x))}$$

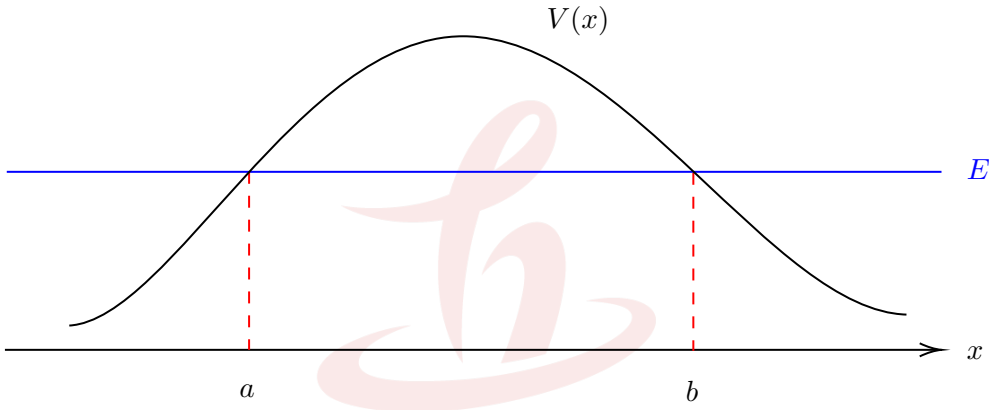
is the classical momentum. Thus semi-classically

$$G(x'', x'; E) \simeq \frac{1}{\hbar} \sum_{(x_{cl}, T_s)} \left(- \frac{1}{\sqrt{\frac{2(E-V(x'))}{m}} \sqrt{\frac{2(E-V(x''))}{m}}} \right)^{\frac{1}{2}} e^{\frac{i}{\hbar} \int_{x'}^{x''} p \, dx}.$$

We see that from the perspective of either x' or x'', the semi-classical Green's function produces the structure of WKB approximation.

Quantum Tunneling

Let us frist apply the semi-classical Green's function to the semi-classical computation of the transmission coefficient for the barrier tunneling of the localized potential $V(x)$.



As we have seen in Example 2.7.3, the Green's function has the behavior

$$G(x'', x'; E) = \frac{m}{ik\hbar^2} A e^{ik(x''-x')}, \qquad x' \to -\infty, \, x'' \to +\infty,$$

where A is the transmitted amplitude.

On the other hand, we have a semi-classical asymptotic result

$$G(x'', x'; E) \simeq \sum_{(x_{cl}, T_s)} \frac{1}{\hbar} \left(\frac{1}{-\dot{x}_{cl}(0)\dot{x}_{cl}(T_s)} \right)^{\frac{1}{2}} e^{\frac{i}{\hbar} W_{cl}}.$$

Note that in the limit region $x' \to -\infty$, $x'' \to +\infty$, the particle becomes free with velocity

$$\dot{x}(0) = \dot{x}(T_s) = \frac{\hbar k}{m}$$

where $k = \frac{\sqrt{2mE}}{\hbar}$.

To have a classical trajectory from x' to x'' along a time path from $t = 0$ to $t = T$, it is necessary to go through a region of complex time! This is because both x' and x'' lie in the classical allowed region, but the path has to go through the classically forbidden region in between. To penetrate the barrier, the time has to be complex. In fact,

$$\frac{dx}{dt} = \sqrt{\frac{2(E - V(x))}{m}}$$

thus in the region $E < V(x)$, t must go along the imaginary direction.

The total travel time for the trajectory is

$$\begin{aligned} T_s &= \int_0^{T_s} dt = \int_0^{T_s} \frac{dx}{\frac{dx}{dt}} = \int_{x'}^{x''} \sqrt{\frac{m}{2(E-V(x))}}\, dx \\ &= \int_{x'}^{a} \sqrt{\frac{m}{2(E-V(x))}}\, dx + \int_b^{x''} \sqrt{\frac{m}{2(E-V(x))}}\, dx \underbrace{-i \int_a^b \sqrt{\frac{m}{2(V(x)-E)}}\, dx}_{\text{imaginary contribution of the complex time}} . \end{aligned}$$

For this classical trajectory in the complex time, we have

$$W_{cl} = \int_{x'}^{x''} p\, dx = \int_{x'}^{a} \sqrt{2m(E-V(x))}\, dx + i \int_a^b \sqrt{2m(V(x)-E)}\, dx + \int_b^{x''} \sqrt{2m(E-V(x))}\, dx.$$

Thus the semi-classical Green's function in the limit region $x' \to -\infty$, $x'' \to +\infty$ is

$$G(x'', x'; E) \simeq \frac{m}{i\hbar^2 k} e^{\frac{i}{\hbar}\left(\int_{x'}^{a} + \int_b^{x''}\right)\sqrt{2m(E-V(x))}\, dx} e^{-\frac{1}{\hbar}\int_a^b \sqrt{2m(V(x)-E)}\, dx}.$$

Comparing with the result

$$G(x'', x'; E) = \frac{m}{ik\hbar^2} A e^{ik(x''-x')}, \qquad x' \to -\infty,\ x'' \to +\infty,$$

we deduce the semi-classical transmission coefficient

$$T \simeq |A|^2 = e^{-\frac{2}{\hbar}\int_a^b \sqrt{2m(V(x)-E)}\, dx}.$$

This is precisely the formula calculated from the WKB method in Section 1.10.5.

Connection Formula Revisited

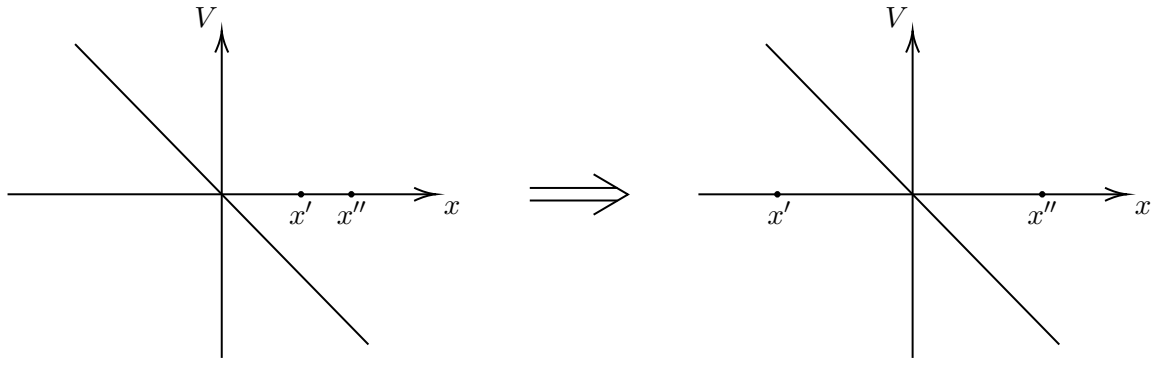
Next we investigate the connection formula of WKB approximation near the turning point where the potential is approximated by a linear potential, say

$$V(x) = -\lambda x, \qquad \lambda > 0.$$

We assume the energy $E = 0$, so the turning point is $x = 0$.

Consider the Green's function $G(x'', x'; E = 0)$. Let us fix $x'' > 0$ and vary x' from the region $x' > 0$ to the region $x' < 0$.

$$0 < x' < x'' \quad \Longrightarrow \quad x' < 0 < x''$$



We would like to keep track of the semi-classical approximation along the deformation of x'. However, if we simply change x' along the real axis, we will soon run into trouble when x' hits the turning point 0. In fact when $x' = 0$, the velocity at the turning point vanishes

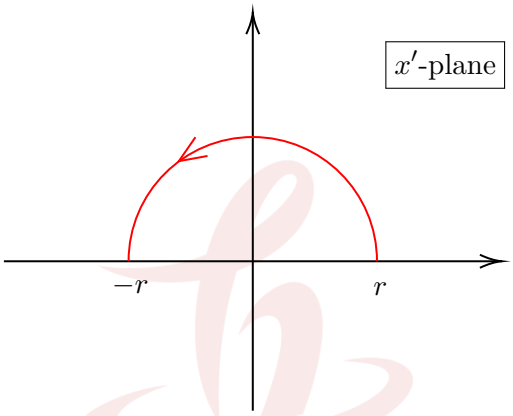
$$\sqrt{\frac{2(E-V)}{m}} = 0 \qquad \text{at} \quad x = 0.$$

So the semi-classical approximation fails and we lose track of the asymptotic information.

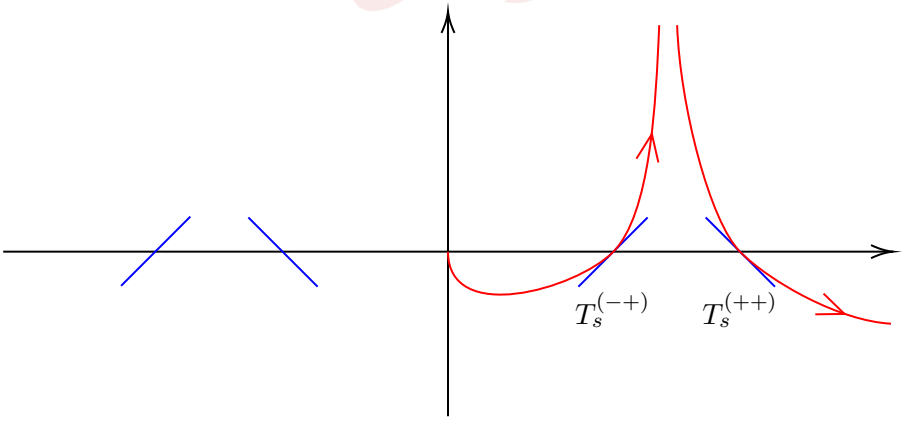
Instead, we can consider the analytic continuation in the complex plane to get around the turning point. For example, we will follow the change

$$x' = re^{i\theta}, \qquad r > 0$$

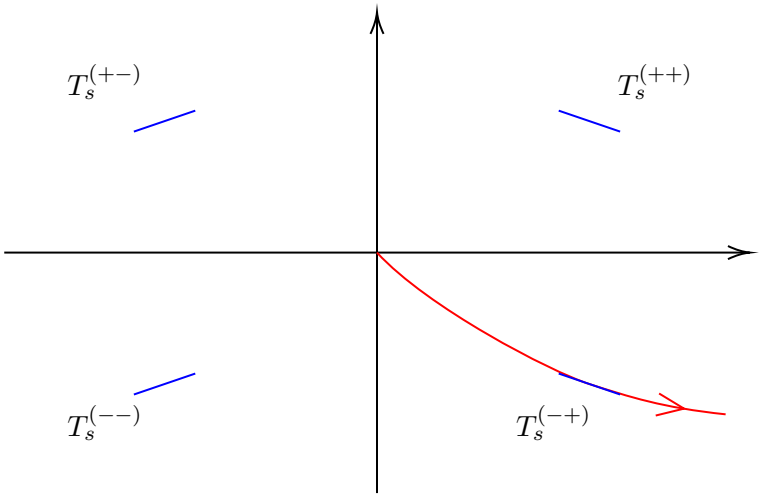
as θ varies from $\theta = 0$ to $\theta = \pi$.



As we have seen in Example 2.7.6, the semi-classical asymptotic behavior of $G(x'', x'; 0)$ is contributed by the curves of steepest descent as in the figure



when $0 < x' < x''$



when $x' < 0 < x''$

Let us analyze what happens in between as we vary θ. Recall the four saddle points

$$\begin{aligned} T_s^{(\pm\pm)} &= \left(\frac{2m}{\lambda}\right)^{\frac{1}{2}} \left(\pm\sqrt{x'} \pm \sqrt{x''}\right) \\ &= \left(\frac{2m}{\lambda}\right)^{\frac{1}{2}} \left(\pm e^{\frac{i}{2}\theta}\sqrt{r} \pm \sqrt{x''}\right) \qquad 0 < r < x''. \end{aligned}$$

The values of S_{cl} at these saddle points are

$$S_{cl}\left(T_s^{(\pm\pm)}\right) = \frac{2}{3}(2m\lambda)^{\frac{1}{2}} \left(\pm\sqrt{x'}^3 \pm \sqrt{x''}^3\right) = \frac{2}{3}(2m\lambda)^{\frac{1}{2}} \left(\pm e^{\frac{3}{2}i\theta}\sqrt{r}^3 \pm \sqrt{x''}^3\right).$$

Recall the curves of steepest descent satisfy

- $\mathrm{Im}(iS_{cl}) = \mathrm{Re}(S_{cl}) = \text{constant}$
- $\mathrm{Re}(iS_{cl}) = -\mathrm{Im}(S_{cl}) \to -\infty$ along boundary

At the initial stage

$$0 < x' < x''$$

there are two contributing saddles $T_s^{(-+)}$ and $T_s^{(++)}$. Consider

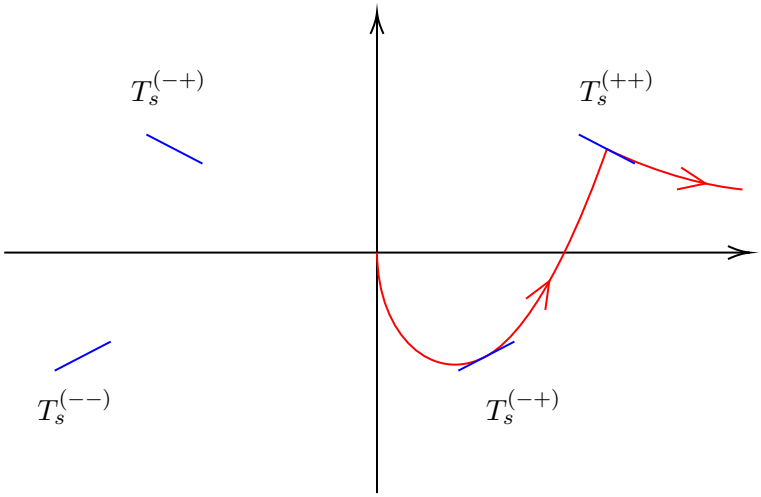
$$S_{cl}\left(T_s^{(-+)}\right) = \frac{2}{3}(2m\lambda)^{\frac{1}{2}} \left(-e^{\frac{3}{2}i\theta}\sqrt{r}^3 + \sqrt{x''}^3\right)$$

$$S_{cl}\left(T_s^{(++)}\right) = \frac{2}{3}(2m\lambda)^{\frac{1}{2}} \left(e^{\frac{3}{2}i\theta}\sqrt{r}^3 + \sqrt{x''}^3\right).$$

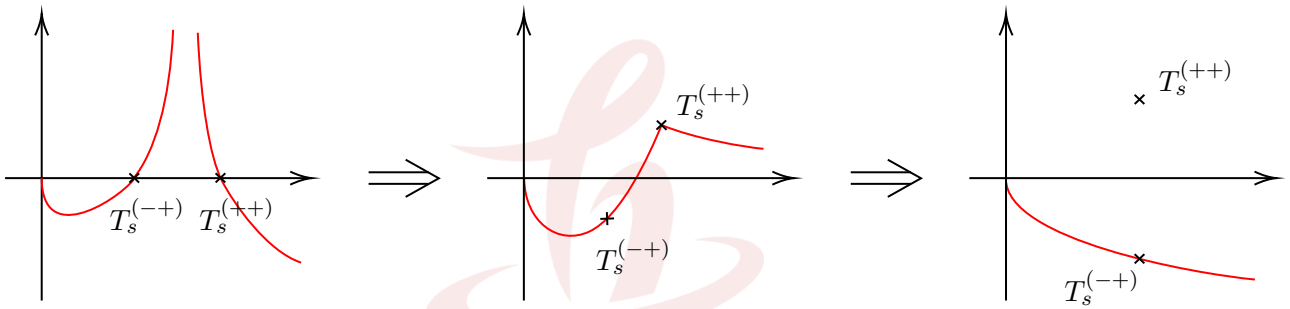
As we vary θ, the saddle contributions to the asymptotic behavior may jump by Stokes phenomenon, where one of the curve of steepest descent may hit another saddle point. The Stokes phenomenon happens when

$$\mathrm{Re}\left(S_{cl}\left(T_s^{(-+)}\right)\right) = \mathrm{Re}\left(S_{cl}\left(T_s^{(++)}\right)\right)$$

that is when $\theta = \frac{\pi}{3}$. We can draw the corresponding four saddles, the tangent directions of the steepest descent at saddles, and the contributing curves of steepest descent at $\theta = \frac{\pi}{3}$



After we pass $\theta = \frac{\pi}{3}$, only the saddle $T_s^{(-+)}$ contributes to the semi-classical Green's function. The process can be illustrated by the following picture



This process explains how the connection formula works. At $\theta = 0$, we have two saddle contributions from $T_s^{(-+)}$ and $T_s^{(++)}$ with phase factors

$$e^{\frac{i}{\hbar}S_{cl}(T_s^{(-+)})} = e^{\frac{i}{\hbar}\frac{2}{3}(2m\lambda)^{\frac{1}{2}}(-\sqrt{x'}^3+\sqrt{x''}^3)}$$

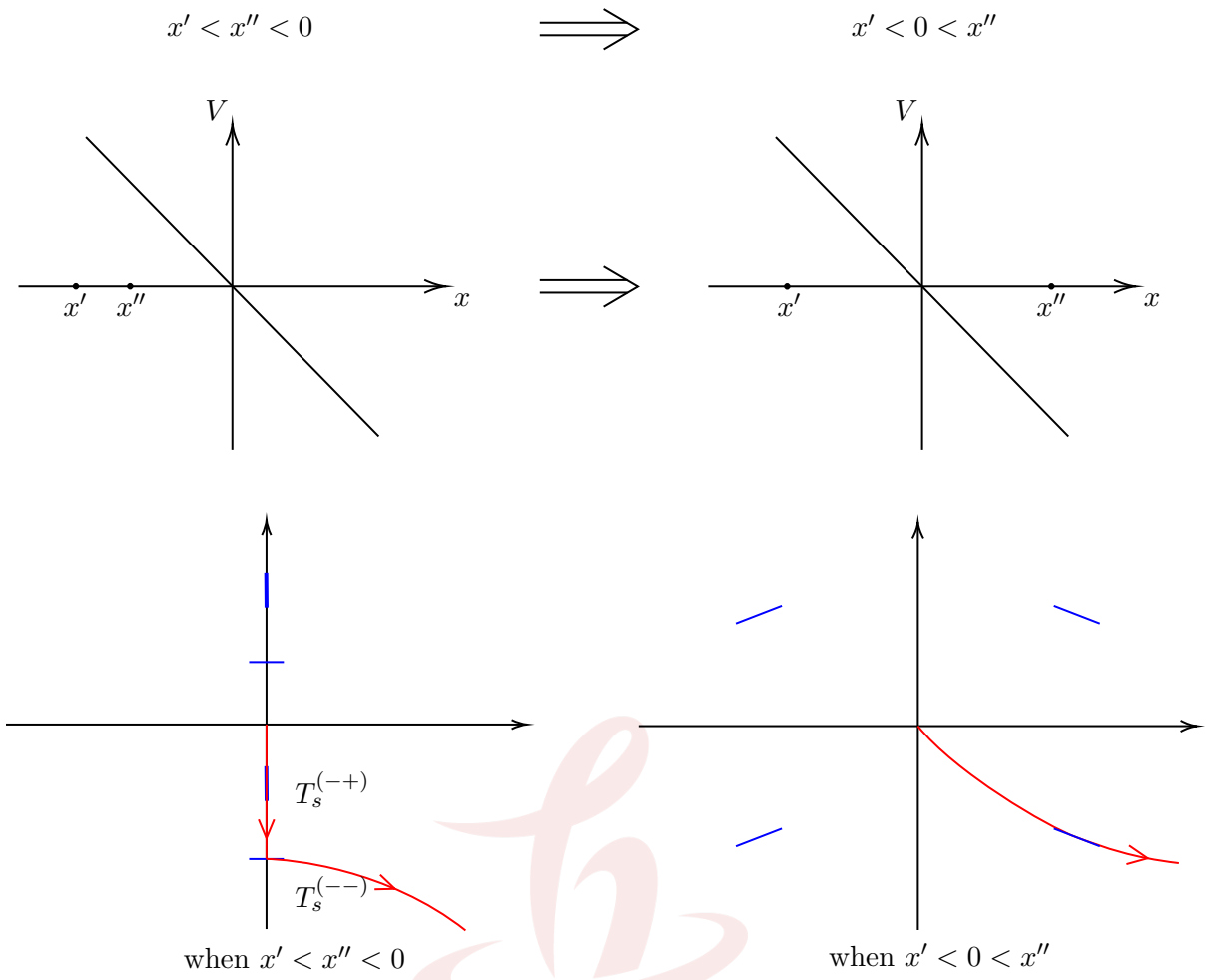
$$e^{\frac{i}{\hbar}S_{cl}(T_s^{(++)})} = e^{\frac{i}{\hbar}\frac{2}{3}(2m\lambda)^{\frac{1}{2}}(\sqrt{x'}^3+\sqrt{x''}^3)}.$$

They contribute equally dominant to the semi-classical asymptotic.

At $\theta = \pi$, after passing through $\theta = \frac{\pi}{3}$ by a Stokes jump, we have only $T_s^{(-+)}$ contributing to the semi-classical asymptotic with phase factor

$$e^{\frac{i}{\hbar}S_{cl}(T_s^{(-+)})} = e^{\frac{i}{\hbar}\frac{2}{3}(2m\lambda)^{\frac{1}{2}}\sqrt{x''}^3} e^{-\frac{1}{\hbar}\frac{2}{3}(2m\lambda)^{\frac{1}{2}}\sqrt{-x'}^3}.$$

Similarly, let us consider semi-classical behavior of the Green's function as we vary x''

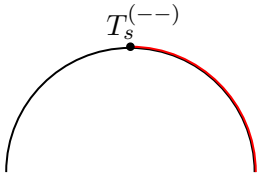


When $x' < x'' < 0$, we have two saddle contributions from $T_s^{(-+)}$ and $T_s^{(--)}$ with

$$e^{\frac{i}{\hbar}S_{cl}(T_s^{(-+)})} = e^{\frac{1}{\hbar}\frac{2}{3}(2m\lambda)^{\frac{1}{2}}(-\sqrt{-x'}^3+\sqrt{-x''}^3)}$$
$$e^{\frac{i}{\hbar}S_{cl}(T_s^{(--)})} = e^{\frac{1}{\hbar}\frac{2}{3}(2m\lambda)^{\frac{1}{2}}(-\sqrt{-x'}^3-\sqrt{-x''}^3)}.$$

The saddle contribution from $T_s^{(-+)}$ dominates that from $T_s^{(--)}$.

Another interesting phenomenon is that the steepest descent curve starting from $T_s^{(--)}$ has only half of the full curve of steepest descent from $T_s^{(--)}$



When we compute the semi-classical contribution, it gives $\frac{1}{2}$ of the usual formula from the Gaussian integral. Thus we write the saddle contribution in this case as

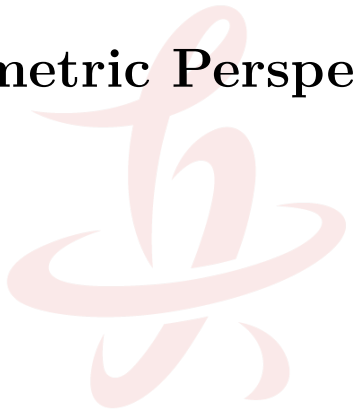
$$T_s^{(-+)} + \frac{1}{2}T_s^{(--)}.$$

As we vary x'' from the region $x'' < 0$ to the region $x'' > 0$, these two steepest descent curves will deform into one steepest descent curve as illustrated.

A careful calculation shows that the above relations between semi-classical asymptotics on two sides of the turning points precisely give rise to the WKB connection formula (see [9]).

Part II

Geometric Perspectives



Chapter 3 Phase Space Geometry

3.1 Symplectic Geometry of Phase Space

3.1.1 Symplectic Vector Space

Let V be a finite dimensional real vector space. Let

$$\begin{aligned}&\omega : V \times V \to \mathbb{R}\\ &\quad \omega(u,v) = -\omega(v,u), \qquad \forall u, v \in V\end{aligned}$$

be a skew-symmetric bilinear form. We denote the null space of ω by

$$N = \{u \in V \,|\, \omega(u,v) = 0,\ \forall v \in V\}.$$

We call ω non-degenerate or symplectic if its null space is trivial:

$$\omega \text{ is non-degenerate} \qquad \Longleftrightarrow \qquad N = \{0\}.$$

Definition 3.1.1. A symplectic vector space is a pair (V, ω) where ω is a non-degenerate skew-symmetric bilinear form on V. In this case we say ω is a symplectic pairing.

Let $c_1, \cdots, c_m$ be a basis of V. A skew-symmetric bilinear form ω is represented by a skew-symmetric matrix in this basis

$$\omega_{ij} = \omega(c_i, c_j), \qquad \omega_{ij} = -\omega_{ji}.$$

Then ω is non-degenerate if and only if the matrix (ω_{ij}) is invertible, i.e.,

$$\det(\omega_{ij}) \neq 0.$$

In the non-degenerate case, we can find a canonical representation of ω as follows:

Proposition 3.1.2. *Let ω be a symplectic pairing on V. Then there exists a basis $\{e_1, \cdots, e_n, f_1, \cdots, f_n\}$ of V such that*

$$\begin{cases}\omega(e_i, e_j) = \omega(f_i, f_j) = 0\\ \omega(e_i, f_j) = \delta_{ij} = -\omega(f_j, e_i)\end{cases} \quad \forall i, j.$$

In particular, $\dim V = 2n$ has to be even. In such a basis, ω is represented by the matrix

$$\omega_n := \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}.$$

Thus any symplectic vector space (V, ω) of $\dim = 2n$ is equivalent to the standard symplectic space $(\mathbb{R}^{2n}, \omega_n)$ under the choice of a basis as in Proposition 3.1.2.

Definition 3.1.3. Let (V, ω) be a symplectic vector space. The symplectic group $\mathrm{Sp}(V, \omega)$, or simply $\mathrm{Sp}(V)$, consists of invertible linear transformations $\varphi : V \to V$ such that

$$\omega(\varphi(u), \varphi(v)) = \omega(u, v), \qquad \forall u, v \in V.$$

When $(V, \omega) = (\mathbb{R}^{2n}, \omega_n)$ is the standard symplectic space, we denote the corresponding symplectic group by $\mathrm{Sp}(2n)$. Explicitly, let us represent $\varphi \in \mathrm{Sp}(2n)$ by

$$\varphi = \begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

where A, B, C, D are $n \times n$ matrices. Then the condition of preserving the symplectic pairing is

$$\varphi^T \omega_n \varphi = \omega_n,$$

i.e.,

$$\begin{pmatrix} A^T & C^T \\ B^T & D^T \end{pmatrix} \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}.$$

That is,

$$\begin{pmatrix} A^TC - C^TA & A^TD - C^TB \\ B^TC - D^TA & B^TD - D^TB \end{pmatrix} = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix} \quad \Longleftrightarrow \quad \begin{cases} A^TC - C^TA = 0 \\ B^TD - D^TB = 0 \\ A^TD - C^TB = I_n \end{cases}$$

Example 3.1.4. *In the case $n = 1$, we have $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{Sp}(2)$ if and only if $ad - bc = 1$. Thus*

$$\mathrm{Sp}(2) = \mathrm{SL}(2)$$

Definition 3.1.5. A complex structure on V is a real linear transformation $J : V \to V$ such that $J^2 = -1$. J is said to be compatible with the symplectic structure ω (or called ω-compatible) if

$$\omega(Ju, Jv) = \omega(u, v), \qquad \forall u, v \in V$$

and

$$\omega(u, Ju) > 0, \qquad \forall u \neq 0.$$

Let J be ω-compatible and define

$$g_J(-, -) := \omega(-, J(-)).$$

① g_J is symmetric:

$$g_J(u,v) = \omega(u, Jv) = \omega(Ju, J^2v) = -\omega(Ju, v) = \omega(v, Ju) = g_J(v,u).$$

② g_J is positive definite. This is by definition.

Thus g_J defines a positive definite inner product on V.

Example 3.1.6. *Let $\{e_1, \cdots, e_n, f_1, \cdots, f_n\}$ be a basis of V such that*

$$\begin{cases} \omega(e_i, e_j) = \omega(f_i, f_j) = 0 \\ \omega(e_i, f_j) = \delta_{ij} = -\omega(f_j, e_i) \end{cases}.$$

Consider $J : V \to V$ defined in the above basis by

$$J(e_i) = f_i, \qquad J(f_i) = -e_i.$$

Then J defines a ω-compatible complex structure

$$\begin{cases} g_J(e_i, f_j) = 0 \\ g_J(e_i, e_j) = g_J(f_i, f_j) = \delta_{ij} \end{cases}.$$

In particular, ω-compatible complex structure always exists.

Let J be a ω-compatible complex structure on V. Then V inherits a $\mathbb{C}$-linear structure by

$$(a + ib) \cdot u := au + bJ(u), \qquad \forall a + ib \in \mathbb{C}.$$

There is an induced Hermitian structure on V

$$\langle -, - \rangle : V \times V \longrightarrow \mathbb{C}$$

defined by

$$\langle -, - \rangle := g_J(-,-) + i\omega(-,-).$$

① Hermitian: for any $u, v \in V$,

$$\langle Ju, v \rangle = g_J(Ju, v) + i\omega(Ju, v) = \omega(Ju, Jv) - i\omega(u, Jv) = \omega(u, v) - ig_J(u, v) = -i \langle u, v \rangle$$

$$\langle u, Jv \rangle = g_J(u, Jv) + i\omega(u, Jv) = \omega(u, J^2v) + i\omega(u, Jv) = -\omega(u, v) + ig_J(u, v) = i \langle u, v \rangle$$

② Positivity: for any $u \in V$, $u \neq 0$,

$$\langle u, u \rangle = g_J(u, u) > 0.$$

Given (V, ω, J), let

$$\begin{aligned} \mathrm{Sp}(V) &= \{\varphi \in \mathrm{GL}(V) \,|\, \omega(\varphi(-), \varphi(-) = \omega(-,-)\} \\ \mathrm{GL}(V, J) &= \{\varphi \in \mathrm{GL}(V) \,|\, \varphi(J(-)) = J(\varphi(-))\} \\ \mathrm{O}(V) &= \{\varphi \in \mathrm{GL}(V) \,|\, g_J(\varphi(-), \varphi(-)) = g_J(-,-)\} \\ \mathrm{U}(V) &= \{\varphi \in \mathrm{GL}(V) \,|\, \langle \varphi(-), \varphi(-) \rangle = \langle -, - \rangle\} \end{aligned}$$

In terms of the standard symplectic space and the constructed J above, the above groups are

$$\mathrm{Sp}(2n), \quad \mathrm{GL}_n(\mathbb{C}), \quad \mathrm{O}(2n), \quad \mathrm{U}(n).$$

The relation

$$g_J(-,-) = \omega(-, J(-))$$

implies that if $\varphi \in \mathrm{GL}(V)$ preserves any two of $\{\omega, J, g_J\}$, then φ preserves the third and therefore preserves the Hermitian structure. Thus we have proved

Proposition 3.1.7.

$$\begin{aligned} \mathrm{Sp}(V) \cap \mathrm{GL}(V, J) &= \mathrm{U}(V) \\ \mathrm{Sp}(V) \cap \mathrm{O}(V) &= \mathrm{U}(V) \\ \mathrm{GL}(V, J) \cap \mathrm{O}(V) &= \mathrm{U}(V) \end{aligned}$$

Example 3.1.8. $\mathrm{Sp}(2n) \cap \mathrm{O}(2n) = \mathrm{U}(n)$ *can be explicitly realized as follows. Let*

$$A + iB \in \mathrm{U}(n), \qquad A, B \text{ are real } n \times n \text{ matrices.}$$

The unitary condition says

$$(A^T - iB^T)(A + iB) = I_n \quad \Longleftrightarrow \quad \begin{cases} A^T A + B^T B = I_n \\ A^T B - B^T A = 0 \end{cases}.$$

This implies

$$\begin{pmatrix} A & -B \\ B & A \end{pmatrix} \in \mathrm{Sp}(2n) \cap \mathrm{O}(2n).$$

Thus $\mathrm{Sp}(2n) \cap \mathrm{O}(2n) = \mathrm{U}(n)$ *is realized explicitly by the map*

$$A + iB \longmapsto \begin{pmatrix} A & -B \\ B & A \end{pmatrix}.$$

Let

$$\begin{aligned} \mathcal{J} &= \{\omega\text{-compatible complex structure}\} \\ \mathcal{P} &= \{\text{symmetric positive definite inner product}\} \end{aligned}$$

The map $J \mapsto g_J$ defines

$$j : \mathcal{J} \hookrightarrow \mathcal{P}.$$

On the other hand, given $g \in \mathcal{P}$, define $K : V \to V$ by the relation

$$\omega(u, v) = g(Ku, v).$$

K may not lie in $\mathcal{J}$. Nevertheless, K is invertible and skew-symmetric with respect to g

$$g(Ku, v) = \omega(u, v) = -\omega(v, u) = -g(Kv, u) = -g(u, Kv).$$

Let $K = RJ$ be the polar decomposition where R is symmetric positive definite and J is orthogonal with respect to g. Since K is skew-adjoint (hence normal), $RJ = JR$. Then

$$K^T = -K, \quad R^T = R \qquad \Longrightarrow \qquad J^T = -J \qquad \Longrightarrow \qquad J^2 = -J^T J = -1$$

i.e., J defines a complex structure on V. Moreover,

$$\omega(Ju, Jv) = g(KJu, Jv) = g(JKu, Jv) = g(Ku, v) = \omega(u, v)$$

$$\omega(u, Ju) = g(Ku, Ju) = g(R(Ju), Ju) > 0 \qquad \text{if } u \neq 0$$

i.e., J is ω-compatible. Thus the map

$$\begin{aligned} r : \mathcal{P} &\longrightarrow \mathcal{J} \\ g &\longmapsto J \end{aligned}$$

defines a retraction of $j : \mathcal{J} \to \mathcal{P}$.

Proposition 3.1.9. *The space $\mathcal{J}$ of ω-compatible complex structures on (V, ω) is contractible.*

Proof: We only need to show $\mathcal{P}$ is contractible. Given any $g_0 \in \mathcal{P}$, we define a homotopy

$$\begin{aligned} \varphi_t : \mathcal{P} &\longrightarrow \mathcal{P} \qquad\qquad 0 \leq t \leq 1 \\ g &\longmapsto tg + (1-t)g_0 \end{aligned}$$

Since $\varphi_1 = \text{identity}$ and $\varphi_0 = \text{const map to } g_0$, this shows the contractibility of $\mathcal{P}$. □

Example 3.1.10. *Consider $(\mathbb{R}^2, \omega_1)$. Let J be a ω_1-compatible complex structure. Preserving ω_1 says that $J \in \mathrm{SL}(2)$. $J^2 = -1$ implies further that J can be written as*

$$J = \begin{pmatrix} a & -b \\ \frac{1+a^2}{b} & -a \end{pmatrix} \qquad a \in \mathbb{R},\ b \in \mathbb{R} - \{0\}$$

Positivity of $\omega_1(-, J(-))$ says

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} a & -b \\ \frac{1+a^2}{b} & -a \end{pmatrix} = \begin{pmatrix} \frac{1+a^2}{b} & -a \\ -a & b \end{pmatrix}$$

is a symmetric positive definite matrix, that is $b > 0$. Therefore

$$\mathcal{J} = \left\{ \begin{pmatrix} a & -b \\ \frac{1+a^2}{b} & -a \end{pmatrix} \,\middle|\, a \in \mathbb{R},\ b \in \mathbb{R}^{>0} \right\}$$

3.1.2 Lagrangian Grassmannian

Definition 3.1.11. Let (V, ω) be a symplectic vector space. A linear subspace $L \subset V$ is called isotropic if $\omega|_{L \times L} = 0$, i.e.,

$$\omega(u, v) = 0, \qquad \forall u, v \in L.$$

Proposition 3.1.12. *Let L be an isotropic subspace of (V, ω). Then* $\dim L \leq \frac{1}{2} \dim V$.

Proof: The symplectic pairing ω induces a linear map

$$\begin{aligned} \tilde{\omega} : V &\longrightarrow V^* \\ v &\longmapsto \omega(v, -) \end{aligned}$$

which is an isomorphism by the non-degeneracy of ω. Let $L \subset V$ be an isotropic subspace, then $\tilde{\omega}$ induces

$$\begin{aligned} \tilde{\omega}_L : L &\longrightarrow (V/L)^* \\ u &\longmapsto \omega(u, -) \end{aligned}$$

Observe $\tilde{\omega}_L$ is injective: if $u \in L$ and $\tilde{\omega}_L(u) = 0$, then

$$\omega(u, v) = 0 \quad \forall v \in V \qquad \Longrightarrow \qquad u = 0.$$

Therefore $\dim L \leq \dim (V/L)$, i.e.,

$$\dim L \leq \frac{1}{2} \dim V.$$

□

Definition 3.1.13. A linear subspace L of a symplectic vector space (V, ω) is called a Lagrangian subspace if L is isotropic and $\dim L = \frac{1}{2} \dim V$.

Example 3.1.14. *Let* $\{e_1, \cdots, e_n, f_1, \cdots, f_n\}$ *be a basis of* V *such that*

$$\begin{cases} \omega(e_i, e_j) = \omega(f_i, f_j) = 0 \\ \omega(e_i, f_j) = \delta_{ij} \end{cases}$$

Then $\mathrm{Span}\{e_1, \cdots, e_n\}$ *and* $\mathrm{Span}\{f_1, \cdots, f_n\}$ *are Lagrangian subspaces of* (V, ω).

Definition 3.1.15. Let $N \subset V$ be a linear subspace. Define its ω-orthogonal complement by

$$N^{\perp} := \{u \in V \,|\, \omega(u, n) = 0, \ \forall n \in N\}.$$

It is clear that

$$N \subset V \text{ isotropic} \qquad \Longleftrightarrow \qquad N \subset N^{\perp}.$$

Since ω is non-degenerate, we have

$$\dim N^{\perp} = \dim V - \dim N.$$

It follows by dimension counting that

$$L \text{ is a Lagrangian subspace} \qquad \Longleftrightarrow \qquad L = L^{\perp}.$$

The collection of all Lagrangian subspaces of (V, ω) will be denoted by $\mathscr{L}(V)$, called the Lagrangian Grassmannian of V. The symplectic group $\mathrm{Sp}(V)$ acts naturally on $\mathscr{L}(V)$:

$$\begin{aligned} \mathrm{Sp}(V) \times \mathscr{L}(V) &\longrightarrow \mathscr{L}(V) \\ \varphi \times L &\mapsto \varphi(L) \end{aligned}$$

Let J be a ω-compatible complex structure. It induces a Hermitian structure on V and

$$\mathrm{U}(V) = \mathrm{Sp}(V) \cap \mathrm{O}(V).$$

Thus $\mathrm{U}(V)$ acts on $\mathscr{L}(V)$:

$$\mathrm{U}(V) \times \mathscr{L}(V) \longrightarrow \mathscr{L}(V).$$

Let $g(-,-) = \omega(-, J(-))$ be the corresponding symmetric positive-definite inner product. Let $L \in \mathscr{L}(V)$ be a Lagrangian subspace. Denote

$$L^* := \{u \in V \,|\, g(u,v) = 0,\ \forall v \in L\}$$

to be the g-orthogonal complement of L. Then

$$V = L \oplus L^*.$$

By definition, we also have $L^* = J(L)^\perp$. Since J is ω-compatible, $J(L)$ is also a Lagrangian subspace, thus $J(L)^\perp = J(L)$. Therefore we have the g-orthogonal decomposition

$$V = L \oplus J(L)$$

of V into a direct sum of two Lagrangian subspaces.

Proposition 3.1.16. $\mathrm{U}(V)$ *acts transitively on* $\mathscr{L}(V)$*. Its stabilizer at* $L \in \mathscr{L}(V)$ *is* $\mathrm{O}(L)$*, the orthogonal group of* L*. Thus we can identify* $\mathscr{L}(V)$ *as the homogeneous space*

$$\mathscr{L}(V) = \mathrm{U}(V)/\,\mathrm{O}(L).$$

Proof: For all $L_1, L_2 \in \mathscr{L}(V)$, let

$$\varphi : L_1 \longrightarrow L_2$$

be a g-orthogonal transformation. Then φ induces

$$\begin{array}{rccc} \tilde{\varphi}: & L_1 \oplus JL_1 & \xrightarrow{\varphi \oplus J \circ \varphi \circ J^{-1}} & L_2 \oplus JL_2 \\ & \| & & \| \\ & V & & V \end{array}$$

By construction, $\tilde{\varphi}$ is compatible with J and g, so

$$\tilde{\varphi} \in \mathrm{U}(V) \quad \text{and} \quad \tilde{\varphi}(L_1) = L_2.$$

This proves the transitivity of the $\mathrm{U}(V)$-action.

Let $\tilde{\varphi} \in \mathrm{U}(V)$ and $\tilde{\varphi}(L) = L$. Then $\varphi = \tilde{\varphi}|_L \in \mathrm{O}(L)$. Conversely, any $\varphi \in \mathrm{O}(L)$ leads to a stabilizer $\tilde{\varphi}$ of L as above. □

3.1.3 Maslov Index

Let (V,ω) be a $2n$-dimensional symplectic vector space, with a ω-compatible complex structure J and a Lagrangian subspace L. By Proposition 3.1.16, we can identify

$$\mathscr{L}(V) \simeq \mathrm{U}(V)/\,\mathrm{O}(L) \simeq \mathrm{U}(n)/\,\mathrm{O}(n).$$

Let "det" be the determinant mapping

$$\det : \mathrm{U}(V) \longrightarrow S^1 = \{z \in \mathbb{C} |\ |z| = 1\}.$$

Restricting to the subgroup $\mathrm{O}(n)$, we have

$$\det : \mathrm{O}(n) \longrightarrow \{\pm 1\}.$$

This leads to a well-defined map

$$\det{}^2 : \mathscr{L}(V) \longrightarrow S^1.$$

Let $F = \left(\det{}^2\right)^{-1}(1)$ be the fiber over $1 \in S^1$. If $[u] \in F$ is represented by $u \in \mathrm{U}(V)$ with

$$\det U = -1$$

then we can find $O \in \mathrm{O}(L)$ with $\det O = -1$ such that

$$[u] = [uO] \in \mathscr{L}(V) \quad \text{and} \quad \det(uO) = 1.$$

This implies that $\mathrm{SU}(V)$ acts transitively on F with stabilizer at L by $\mathrm{SO}(L)$. Thus

$$F = \mathrm{SU}(V)/\,\mathrm{SO}(L)$$

and we have a fibration

$$\begin{array}{ccc} \mathrm{SU}(n)/\,\mathrm{SO}(n) & \longrightarrow & \mathscr{L}(V) \\ & & \downarrow{\scriptstyle \det^2} \\ & & S^1 \end{array}$$

$\mathrm{SU}(n)$ is simply connected. To see this, consider $\mathrm{SU}(n)$ acting on $\mathbb{C}^n$ by standard matrix multiplication. It preserves the unit sphere S^{2n-1} where $\mathrm{SU}(n)$ acts transitively. The stabilizer is $\mathrm{SU}(n-1)$. This gives a fibration ($n \geq 3$)

$$\begin{array}{ccc} \mathrm{SU}(n-1) & \longrightarrow & \mathrm{SU}(n) \\ & & \downarrow \\ & & S^{2n-1} \end{array}$$

The homotopy exact sequence of this fibration gives

$$\pi_1(\mathrm{SU}(n)) \simeq \pi_1(\mathrm{SU}(n-1)) \simeq \cdots \simeq \pi_1(\mathrm{SU}(2)) = \pi_1(S^3) = 1.$$

Since $\mathrm{SO}(n)$ is connected, the homotopy exact sequence of the fibration

$$\begin{array}{ccc} \mathrm{SO}(n) & \longrightarrow & \mathrm{SU}(n) \\ & & \downarrow \\ & & \mathrm{SU}(n)/\mathrm{SO}(n) \end{array}$$

leads to

$$\pi_1(\mathrm{SU}(n)/\mathrm{SO}(n)) = 1.$$

Back to the fibration

$$\begin{array}{ccc} \mathrm{SU}(n)/\mathrm{SO}(n) & \longrightarrow & \mathscr{L}(V) \\ & & \downarrow{\scriptstyle \det^2} \\ & & S^1 \end{array}$$

we find that $\det^2$ induces an isomorphism

$$\pi_1(\mathscr{L}(V)) \xrightarrow{\det^2} \pi_1(S^1) = \mathbb{Z}.$$

This isomorphism does not depend on the choice of complex structure J (the collection of all ω-compatible J's is connected, actually contractible by Proposition 3.1.9) and does not depend on the choice of the reference Lagrangian L (since $\mathrm{U}(n)$ is connected). Thus for any loop

$$\gamma : S^1 \longrightarrow \mathscr{L}(V)$$

we can associate an integer $m(\gamma) \in \mathbb{Z}$ representing $[\gamma] \in \pi_1(\mathscr{L}(V)) \simeq \mathbb{Z}$. This integer is called the Maslov index. Explicitly, $m(\gamma)$ is the winding number of

$$\det^2 \circ \gamma : S^1 \longrightarrow S^1.$$

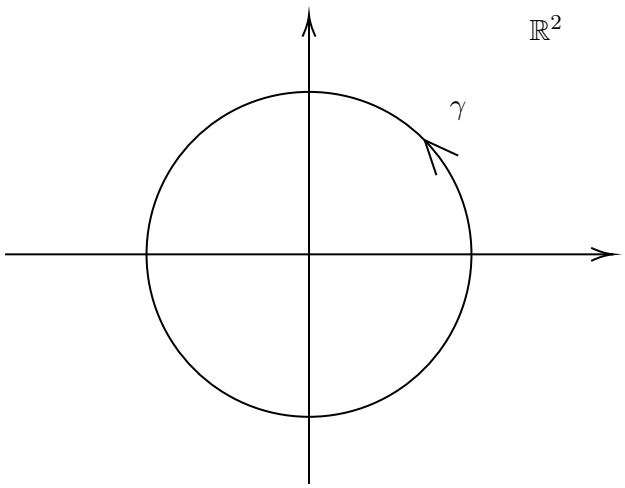
Example 3.1.17. *Consider $(V = \mathbb{R}^2, \omega)$. Any line L in $\mathbb{R}^2$ is a Lagrangian subspace. Thus*

$$\mathscr{L}(\mathbb{R}^2) = \mathbb{R}P^1 = \mathrm{U}(1)/\mathrm{O}(1) = S^1/Z_2.$$

Let

$$\begin{aligned} \gamma : S^1 &\longrightarrow \mathscr{L}(\mathbb{R}^2) \\ \theta &\longmapsto e^{i\theta} \end{aligned}$$

which winds around the unit circle.



The composition $\det^2 \circ \gamma$ *is*

$$\begin{aligned} \det^2 \circ \gamma : S^1 &\longrightarrow S^1 \\ e^{i\theta} &\longmapsto e^{2i\theta} \end{aligned}$$

Thus the Maslov index of γ *is*

$$m(\gamma) = 2.$$

3.1.4 Symplectic Manifold

Definition 3.1.18. A symplectic manifold is a pair (M, ω) where M is a smooth manifold and ω is a smooth 2-form on M such that

① ω is closed: $d\omega = 0$

② ω is non-degenerate: $\forall p \in M$,

$$\omega|_p : T_pM \times T_pM \longrightarrow \mathbb{R}$$

defines a symplectic pairing on T_pM.

In local coordinates $\{x^i\}$, ω can be written as

$$\omega = \frac{1}{2} \sum_{i,j} \omega_{ij}(x) dx^i \wedge dx^j$$

where $\omega_{ij}(x) = -\omega_{ji}(x)$. Condition $d\omega = 0$ becomes

$$\partial_i \omega_{jk} + \partial_j \omega_{ki} + \partial_k \omega_{ij} = 0, \qquad \forall i, j, k.$$

The non-degeneracy condition says

$$\det\left(\omega_{ij}(x)\right) \neq 0, \qquad \forall x.$$

Definition 3.1.19. Given a smooth function f on M, we define its associated Hamiltonian vector field $V_f \in \mathrm{Vect}(M)$ by the equation

$$\iota_{V_f} \omega = df.$$

Explicitly in local coordinates,

$$V_f = \sum_{i,j} \omega^{ij} \partial_i f \frac{\partial}{\partial x^j}$$

where $\{\omega^{ij}\}$ is the inverse matrix of $\{\omega_{ij}\}$,i.e., satisfies

$$\sum_k \omega^{ik} \omega_{kj} = \delta^i_j.$$

In fact,

$$\sum_{i,j} \omega^{ij} \partial_i f \iota_{\partial_j} \omega = \sum_{i,j,k} \omega^{ij} \partial_i f \omega_{jk} dx^k = \sum_i \partial_i f dx^i = df.$$

Definition 3.1.20. The Poisson bracket of two smooth functions f, g on M is defined to be

$$\{f, g\} := \iota_{V_f} \iota_{V_g} \omega.$$

Using $\iota_{V_g}\omega = dg$, this can be equivalently written as

$$\{f, g\} = \iota_{V_f}(dg) = V_f(g).$$

In local coordinates,

$$\{f, g\} = \sum_{i,j} \omega^{ij} \partial_i f \partial_j g.$$

Proposition 3.1.21. *Hamiltonian vector fields preserve the symplectic form ω, i.e., $\mathscr{L}_{V_f}\omega = 0$.*

Proof: Using Cartan's formula, we have

$$\mathscr{L}_{V_f}\omega = \left(d\iota_{V_f} + \iota_{V_f} d\right)\omega = d(df) + 0 = 0.$$

□

The symplectic form ω induces a volume form on M by

$$\frac{1}{n!}\omega^n, \qquad n = \dim M.$$

As a corollary, Hamiltonian vector fields preserve the volume density (Liouville's Theorem)

$$\mathscr{L}_{V_f}\left(\frac{1}{n!}\omega^n\right) = 0.$$

Proposition 3.1.22. $V_{\{f,g\}} = [V_f, V_g]$.

Proof: Using Cartan's formula

$$\iota_{V_{\{f,g\}}}\omega = d\{f, g\} = d\iota_{V_f}\iota_{V_g}\omega = \mathscr{L}_{V_f}\iota_{V_g}\omega - \iota_{V_f} d\iota_{V_g}\omega = \left(\mathscr{L}_{V_f}\iota_{V_g} - \iota_{V_g}\mathscr{L}_{V_f}\right)\omega - \iota_{V_f} ddg = \iota_{[V_f,V_g]}\omega.$$

By the non-degeneracy of ω,

$$V_{\{f,g\}} = [V_f, V_g].$$

□

Proposition 3.1.23. *$(C^\infty(M), \{-,-\})$ defines a Lie algebra. The map*

$$C^\infty(M) \longrightarrow \mathrm{Vect}(M)$$
$$f \longmapsto V_f$$

is a Lie algebra homomorphism.

Proof: $\{-,-\}$ is clearly skew-symmetric. We need to check Jacobi-identity:

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0.$$

In fact, using Proposition 3.1.22 and skew-symmetry of $\{-,-\}$

$$\begin{aligned}\{\{f, g\}, h\} &= V_{\{f,g\}}(h) = [V_f, V_g](h) = V_f(\{g, h\}) - V_g(\{f, h\}) \\ &= \{f, \{g, h\}\} - \{g, \{f, h\}\} = -\{\{g, h\}, f\} - \{\{h, f\}, g\}.\end{aligned}$$

The Lie algebra morphism follows from Proposition 3.1.22. □

Example 3.1.24 (Cotangent Bundle)**.** *For any smooth manifold X, the total space of its cotangent bundle $M = T^*X$ is canonically a symplectic manifold.*

Let $\{q^i\}$ be local coordinates on X. The frame $\left\{\frac{\partial}{\partial q^i}\right\}$ defines naturally linear coordinates $\{p_i\}$ along fibers of T^*X. Thus $\{q^i, p_i\}$ form local coordinates on T^*X. Consider the 1-form

$$\lambda = \sum_i p_i dq^i.$$

It is easy to check that this expression is independent of the choice of local coordinates and λ is a globally defined 1-form on T^*X. λ is called the Liouville 1-form. The 2-form

$$\omega = d\lambda = \sum_i dp_i \wedge dq^i$$

defines a symplectic form on T^*X.

Definition 3.1.25. Let (M, ω) be a symplectic manifold. A submanifold $L \subset M$ is called a Lagrangian submanifold if $\dim L = \frac{1}{2}\dim M$ and $\omega|_L = 0$.

This is equivalent to saying that for all $p \in L$, the tangent space T_pL is a linear Lagrangian subspace of $(T_pM, \omega|_p)$.

Let $M = T^*X$ and ω be the canonical symplectic form. A submanifold $L \subset M$ of $\dim L = \frac{1}{2}\dim M$ is a Lagrangian submanifold if

$$\omega|_L = d\lambda|_L = 0,$$

i.e., the restriction $\lambda|_L$ of the Liouville 1-form on L is a closed 1-form.

Let us consider a special case. Let $S : X \to T^*X$ be a section of the cotangent bundle. Such a section is the same as specifying a 1-form α on X, and we denote it by

$$S_\alpha : X \longrightarrow T^*X.$$

The image of S_α defines a submanifold

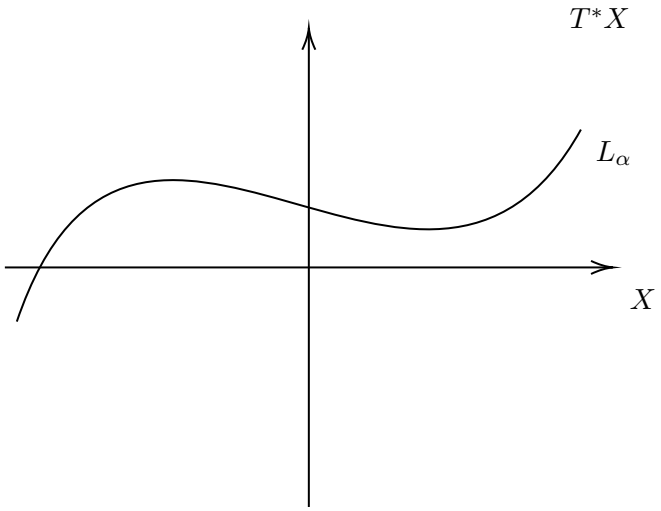
$$L_\alpha := S_\alpha(X) \subset T^*X.$$

One nice property of S_α is that we have tautologically

$$S_\alpha^*(\lambda) = \alpha.$$

This immediately leads to the following

Proposition 3.1.26. *$L_\alpha \subset T^*X$ is a Lagrangian submanifold if and only if α is a closed 1-form: $d\alpha = 0$.*



Definition 3.1.27. A Lagrangian submanifold of the form $L_\alpha \subset T^*X$ associated to a closed 1-form α is called a projectable Lagrangian submanifold of T^*X. L_α is called an exact Lagrangian if $\alpha = df$ is an exact 1-form.

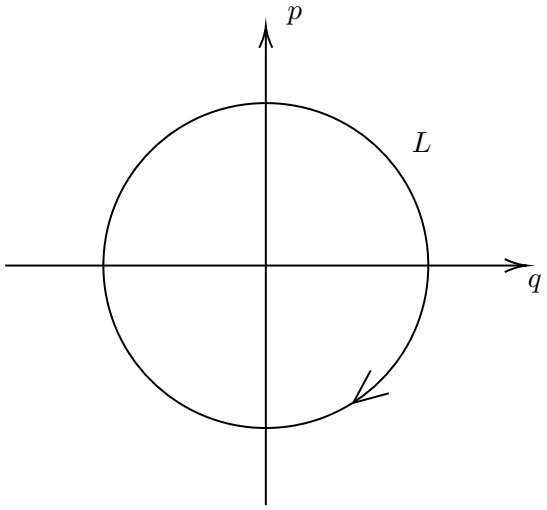
Example 3.1.28. *For an exact Lagrangian L_{df}, it is described by the equations*

$$p_i = \frac{\partial}{\partial q^i} f(q).$$

In this case, f is called a phase function of L. Note that the phase function is only determined up to a shift by a constant.

Example 3.1.29. $\mathbb{R}^2 = T^*\mathbb{R}$, $\omega = dp \wedge dq$. *Then any curve in $\mathbb{R}^2$ defines a Lagrangian submanifold. Consider*

$$L = \left\{p^2 + q^2 = R^2\right\} \subset T^*\mathbb{R}.$$



The restriction to L of the Liouville 1-form $\lambda = pdq$ is closed but not exact since

$$\int_L \lambda = \pm\pi R^2$$

where the sign $\pm$ depends on the orientation of L.

Definition 3.1.30. A diffeomorphism $\varphi : M \to M$ is called a symplectomorphism if φ preserves the symplectic structure, i.e.,

$$\varphi^* \omega = \omega.$$

Proposition 3.1.31. *Let $\varphi : M \to M$ be a symplectomorphism and $L \subset M$ be a Lagrangian submanifold. Then $\varphi(L)$ is also a Lagrangian submanifold.*

Example 3.1.32. *The flow $\phi_t : M \to M$ generated by a Hamiltonian vector field V_f is a symplectomorphism. In fact,*

$$\frac{d}{dt}\left(\phi_t^* \omega\right) = \phi_t^* \left(\mathscr{L}_{V_f} \omega\right) = 0 \qquad \Longrightarrow \qquad \phi_t^* \omega = \omega, \quad \forall t.$$

Let us now specialize this example to the case

$$M = T^* X \qquad \text{and} \qquad f : X \to \mathbb{R}.$$

Viewed as a function on M, the corresponding Hamiltonian vector field of f is

$$V_f = \sum_i \partial_{q^i} f \frac{\partial}{\partial p_i}.$$

The symplectomorphism $\phi_t : T^* X \to T^* X$ generated by V_f translates the fiber by tdf, thus

$$\phi_1(L_\alpha) = L_{\alpha + df}.$$

In particular, ϕ_1 transforms the zero section to

$$\phi_1(L_0) = L_{df}.$$

3.2 Semi-classical Quantization

3.2.1 Semi-classical Solution

We consider quantum particle moving in $\mathbb{R}^n$ in the potential $V(\mathbf{x})$. The quantum Hamiltonian operator is

$$\widehat{\mathrm{H}} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})$$

and the Schrödinger equation takes the form

$$i\hbar \frac{\partial}{\partial t}\Psi = \widehat{\mathrm{H}}\,\Psi.$$

We consider solutions of the form (called stationary states)

$$\Psi(\mathbf{x}, t) = e^{-iEt/\hbar}\psi(\mathbf{x})$$

Plugging into the Schrödinger equation, we find

$$\widehat{\mathrm{H}}\,\psi(\mathbf{x}) = E\psi(\mathbf{x}) \qquad (*)$$

Thus $\psi(\mathbf{x})$ is an eigenstate of $\widehat{\mathrm{H}}$ with eigenvalue E, which is interpreted as the energy. Equation $(*)$ is called the time-independent Schrödinger equation.

Let us consider a solution of $(*)$ by the form

$$\psi = e^{\frac{i}{\hbar}S(\mathbf{x})}a(\mathbf{x},\hbar).$$

$S(\mathbf{x})$ is called the phase function, and $a(\mathbf{x},\hbar)$ is called the amplitude. Observe

$$\begin{aligned}&\left(-\frac{\hbar^2}{2m}\nabla^2+(V-E)\right)\left(ae^{\frac{i}{\hbar}S}\right)\\&=\left[a\left(\frac{(\nabla S)^2}{2m}+(V-E)\right)-\frac{\hbar^2}{2m}\nabla^2 a-\frac{i\hbar}{2m}\left(a\nabla^2 S+2\nabla S\cdot\nabla a\right)\right]e^{\frac{i}{\hbar}S}.\end{aligned}$$

The idea of WKB method is to look for $\hbar$-asymptotic solutions of the form

$$\psi = e^{\frac{i}{\hbar}S(\mathbf{x})}\left(a_0(\mathbf{x})+a_1(\mathbf{x})\hbar+\cdots\right)$$

i.e., $a(\mathbf{x},\hbar)$ has the $\hbar$-asymptotic series

$$a(\mathbf{x},\hbar)\sim\sum_{k=0}^{\infty}a_k(\mathbf{x})\hbar^k,\qquad a_0(\mathbf{x})\neq 0.$$

Plugging this WKB ansatz into the above equation, we find

$$\begin{cases}\dfrac{(\nabla S)^2}{2m}+V=E\\ a_0\nabla^2 S+2\nabla S\cdot\nabla a_0=0\\ a_k\nabla^2 S+2\nabla S\cdot\nabla a_k=i\nabla^2 a_{k-1},\qquad k\geq 1\end{cases}$$

The approximate solution

$$e^{\frac{i}{\hbar}S(\mathbf{x})}a_0(\mathbf{x})$$

is called the **semi-classical approximation**.

The leading order equation for S can be written as

$$\mathscr{H}(\mathbf{x},\mathbf{p}=\nabla S)=E \qquad (**)$$

Here $\mathscr{H}(\mathbf{x},\mathbf{p})=\frac{\mathbf{p}^2}{2m}+V(\mathbf{x})$ is the classical Hamiltonian function. Equation $(**)$ is precisely the Hamilton-Jacobi equation.

Geometrically, S defines an exact projectable Lagrangian submanifold

$$L_{dS}\subset T^*\mathbb{R}^n$$

and the Hamilton-Jacobi equation says that $\mathscr{H}$ is constant $(=E)$ on L_{dS}, i.e.

$$d\mathscr{H}|_{L_{dS}}=0.$$

In terms of the Hamiltonian vector field $V_{\mathscr{H}}$, this is

$$\iota_{V_{\mathscr{H}}}\omega|_{L_{dS}}=0$$

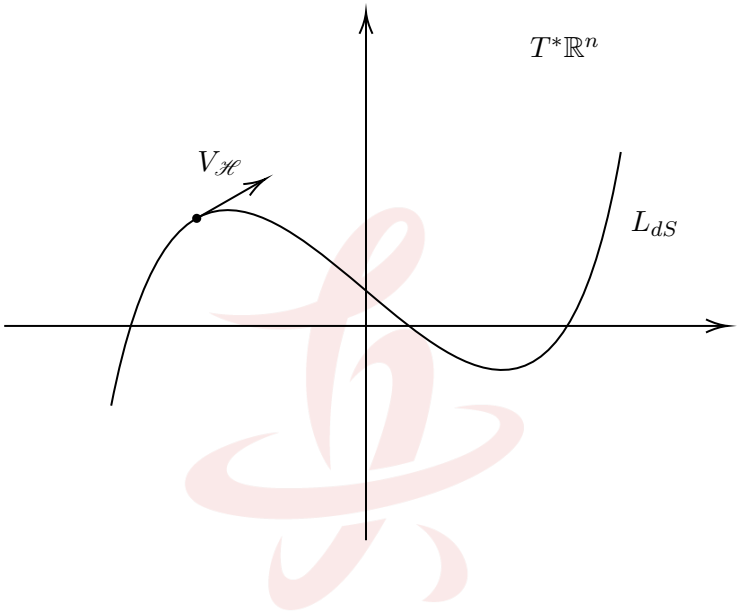
i.e.,

$$\omega\left(V_{\mathscr{H}}(p), T_p L_{dS}\right) = 0, \qquad \forall p \in L_{dS}.$$

Since L_{dS} is a Lagrangian submanifold, this is equivalent to

$$V_{\mathscr{H}}(p) \in T_p L_{dS}, \qquad \forall p \in L_{dS},$$

i.e., the Hamiltonian vector field $V_{\mathscr{H}}$ is tangent to L_{dS}.



Thus the Hamilton-Jacobi equation leads to an exact projectable Lagrangian submanifold L_{dS} with phase function S such that the Hamiltonian vector field $V_{\mathscr{H}}$ is tangent to L_{dS} at every point of L_{dS}.

Now we consider the subleading order equation

$$a_0 \nabla^2 S + 2\nabla S \cdot \nabla a_0 = 0$$

which is called the *homogeneous transport equation*. It can be written as

$$\nabla \cdot \left(a_0^2 \nabla S\right) = 0.$$

This allows us to interpret it as

$$\mathscr{L}_{\nabla S}\left(a_0^2 \left|d^n x\right|\right) = 0.$$

Here $|d^n x| = |dx^1 \wedge \cdots \wedge dx^n|$ is the canonical volume density on $\mathbb{R}^n$. $\mathscr{L}_{\nabla S}$ is the Lie derivative with respect to the vector field

$$\sum_i \partial_i S \frac{\partial}{\partial x^i}.$$

Geometrically, let π denote the diffeomorphism

$$\begin{aligned} \pi : \quad L_{dS} &\longrightarrow \mathbb{R}^n \\ (x^i, p_i = \partial_i S) &\longmapsto (x^i) \end{aligned}$$

The Hamiltonian vector field $V_{\mathscr{H}}$ is

$$V_{\mathscr{H}} = \sum_i \left(\frac{\partial \mathscr{H}}{\partial x^i} \frac{\partial}{\partial p_i} - \frac{\partial \mathscr{H}}{\partial p^i} \frac{\partial}{\partial x_i} \right) = \sum_i \left(\partial_i V \frac{\partial}{\partial p_i} - \frac{1}{m} p_i \frac{\partial}{\partial x_i} \right).$$

Observe

$$\pi_*(V_{\mathscr{H}}|_{L_{dS}}) = -\frac{1}{m} \sum_i \partial_i S \frac{\partial}{\partial x_i}.$$

Thus the homogeneous transport equation becomes

$$\mathscr{L}_{\pi_*(V_{\mathscr{H}}|_{L_{dS}})} \left(a_0^2 \, |d^n x| \right) = 0.$$

Since $\pi : L_{dS} \to \mathbb{R}^n$ is a diffeomorphism, we can equivalently describe this on L_{dS} as

$$\mathscr{L}_{V_{\mathscr{H}}|_{L_{dS}}} \left(\pi^* \left(a_0^2 \, |d^n x| \right) \right) = 0.$$

3.2.2 Half-Density

Recall that the density line bundle Dens_M on a manifold M is described by sections which in local coordinates $\left\{x^i\right\}$ are of the form

$$\rho_x(x) \, |d^n x|, \qquad \rho_x(x) \text{ smooth function.}$$

Under coordinate transformation $\left\{x^i\right\} \to \left\{y^i\right\}$, ρ_x and ρ_y in two coordinates are related by

$$\rho_x = \rho_y \left| \det \left(\frac{\partial y}{\partial x} \right) \right|.$$

Here $\left(\frac{\partial y}{\partial x}\right) = \left(\frac{\partial y^i}{\partial x^j}\right)$ is the Jacobian matrix. In other words, the transition function of the density line bundle is $\left|\det \left(\frac{\partial y}{\partial x}\right)\right|$. Invariantly, we can write it as

$$\rho_x \, |d^n x| = \rho_y \, |d^n y|.$$

This property allows us to integrate densities on manifold

$$\begin{aligned} \int_M : \Gamma(M, \mathrm{Dens}_M) &\longrightarrow \mathbb{R} \\ \rho &\longmapsto \int_M \rho \end{aligned}$$

Remark 3.2.1. If M is orientable, we can identify

$$\mathrm{Dens}_M \simeq \bigwedge^n T^*M, \qquad n = \dim M$$

via a choice of orientation. Thus a section of Dens_M becomes an n-form. When M is unorientable, these two bundles are different.

Similarly, for any $\alpha > 0$, we can define the α-density line bundle Dens_M^α whose transition function is given by

$$\left|\det\left(\frac{\partial y}{\partial x}\right)\right|^\alpha.$$

Invariantly, we can write an α-density locally by

$$\rho_x \left|d^n x\right|^\alpha.$$

The transition function says that under coordinate transformation $\left\{x^i\right\} \to \left\{y^i\right\}$, we have

$$\rho_x \left|d^n x\right|^\alpha = \rho_y \left|d^n y\right|^\alpha.$$

Back to the semi-classical solution, it is better to identify $a_0(\mathbf{x})$ as a half-density

$$a_0 \left|d^n x\right|^{1/2}.$$

Under the diffeomorphism $\pi : L_{dS} \to \mathbb{R}^n$, it gives a half-density $\pi^*\left(a_0 \left|d^n x\right|^{1/2}\right)$ on L_{dS}. Then the homogeneous transport equation can be written as

$$\mathscr{L}_{V_{\mathscr{H}}|_{L_{dS}}}\left(\pi^*\left(a_0 \left|d^n x\right|^{1/2}\right)\right) = 0.$$

In summary, we have arrived at the following description: a semi-classical solution of the time-independent Schrödinger equation is equivalent to the following geometric data:

① an exact projectable Lagrangian submanifold L which lies in a level set of the Hamiltonian function $\mathscr{H}$ (equivalently, $V_{\mathscr{H}}$ is tangent to L).

② a half-density Ω on L which is $V_{\mathscr{H}}$-invariant.

Given such data, we can write S for the phase function of L (defined up to a constant). Let

$$\begin{aligned} s : \mathbb{R}^n &\longrightarrow L \\ (x^i) &\longmapsto (x^i, p_i = \partial_i S) \end{aligned}$$

denote the diffeomorphism by the section map. Let

$$s^*\Omega = a_0(x) \left|d^n x\right|^{1/2}$$

be the corresponding half-density expressed on $\mathbb{R}^n$. Then

$$e^{\frac{i}{\hbar}S(x)} a_0(x)$$

gives a semi-classical solution.

There is an immediate advantage of such geometric description: L can be a general Lagrangian submanifold instead of an exact projectable one. For such L in a level set of $\mathscr{H}$, the notion of $V_{\mathscr{H}}$-invariant half-density is still well-defined. This leads to the geometric semi-classical state that we will discuss next.

3.2.3 Maslov Correction

Now we consider quantization on the Lagrangian submanifold $L \subset T^*\mathbb{R}^n$ which is not necessarily projectable. The points of L where

$$\pi : L \longrightarrow \mathbb{R}^n$$

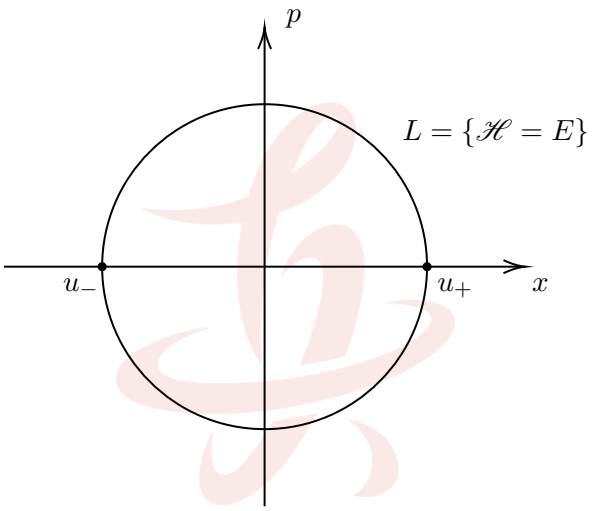
fail to become local diffeomorphisms are called *caustics*.

Example 3.2.2. *Consider the one dimensional Harmonic oscillator*

$$\mathscr{H} = \frac{p^2}{2m} + \frac{1}{2}kx^2.$$

The level set $\mathscr{H} = E > 0$ *is a Lagrangian submanifold*

$$L = \{(x,p) \,|\, \mathscr{H}(x,p) = E\}\,.$$



There are two caustics of L *by*

$$u_\pm = \left(\pm\sqrt{\frac{2E}{k}}, 0\right).$$

Caustics are not singularities of L. They actually reflect the way we choose the coordinate x from the configuration space. In fact, if we consider the projection to the p-coordinate

$$\pi_P : L \longrightarrow \mathbb{R}$$
$$(x,p) \longmapsto p$$

then π_p is a local diffeomorphism around $u_\pm$. It suggests that we could use appropriate coordinates locally around the Lagrangian to quantize and then glue. This is precisely Maslov's technique.

Motivated by the projectable case, we define a geometric semi-classical state as follows.

Definition 3.2.3. A geometric semi-classical stationary state is a pair (L, Ω) where
① $L \subset T^*X$ is a Lagrangian submanifold which lies in a level set of the Hamiltonian $\mathscr{H}$,
② Ω is a half-density on L which is invariant under the Hamiltonian vector field $V_{\mathscr{H}}$.

Let us next explore how to implement the analogue of the semi-classical solution

$$e^{\frac{i}{\hbar}S} a \, |d^n x|^{1/2}$$

on a geometric semi-classical state (L, Ω).

When $L = L_{dS}$ is exact projectable, the phase function S (viewed as a function of L) is

$$S = \int \lambda$$

up to a constant. Here $\lambda = \sum_i p_i dx^i$ is the Liouville 1-form. This is the same as saying that

$$\lambda|_L = dS.$$

For a general Lagrangian L, we have

$$\lambda|_L \text{ is closed}$$

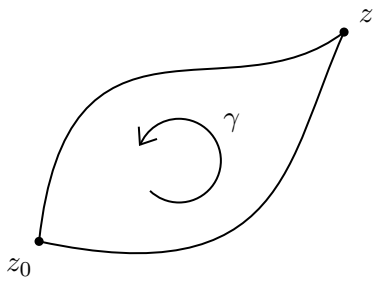
but may not be exact. Nevertheless, we still wish to define the phase factor by

$$e^{\frac{i}{\hbar}\int_{z_0}^{z} \lambda} \qquad \text{for } z \in L.$$

Here $z_0 \in L$ is some reference base point. The integral $\int_{z_0}^{z} \lambda$ is multi-valued and depends on the integration path from z_0 to z. Two paths from z_0 to z will differ by a closed cycle γ, and the corresponding integrations $\int_{z_0}^{z} \lambda$ differs by

$$\oint_\gamma \lambda.$$

Note that since λ is closed on L, the cycle integration $\oint_\gamma \lambda$ only depends on the topological class of γ in $H_1(L)$.



Thus if $\frac{1}{\hbar}\oint_\gamma \lambda \in 2\pi\mathbb{Z}$ for all $\gamma \in H_1(L)$, then $e^{\frac{i}{\hbar}\int_{z_0}^{z} \lambda}$ would be a well-defined function on L. This suggests the following integrality condition (*Bohr-Sommerfeld quantization condition*)

$$\frac{1}{2\pi\hbar}\oint_\gamma \lambda \in \mathbb{Z}$$

for all closed 1-cycle γ on L. This would be satisfied when L is projectable. However, when caustics appear, there is a further modification called the *Maslov correction*.

The issue comes from the half-density piece of the semi-classical solution. In the projectable case, L can be identified with $\mathbb{R}^n$ under the projection, and we can take the square root $|d^n x|^{1/2}$ uniformly on $\mathbb{R}^n$ and write

$$\pi_* \Omega = a(x) \, |d^n x|^{1/2}.$$

Then $e^{\frac{i}{\hbar} S} a$ leads to the semi-classical solution. In general, we need to understand how to take the square root of a volume density consistently on L.

Let us assume L is oriented and we identify the density bundle with

$$\mathrm{Dens}_L \simeq \bigwedge^n T^* L$$

which is the dual of $\bigwedge^n T_* L$. At each point $z \in L$, the tangent plane

$$T_z L \subset T_z(T^* \mathbb{R}^n) = \mathbb{R}^{2n}$$

defines a Lagrangian linear subspace, i.e.,

$$T_z L \in \mathscr{L}(\mathbb{R}^{2n})$$

defines an element of the Lagrangian Grassmannian.

Recall we can identify

$$\mathscr{L}(\mathbb{R}^{2n}) \simeq \mathrm{U}(n) / \mathrm{O}(n)$$

together with

$$\mathscr{L}(\mathbb{R}^{2n}) \xrightarrow{\det^2} S^1$$

which induces an isomorphism

$$\pi_1(\mathscr{L}(\mathbb{R}^{2n})) \simeq \pi_1(S^1).$$

Explicitly, let us choose the standard complex structure to identify

$$\mathbb{R}^{2n} \overset{J}{\simeq} \mathbb{C}^n = \mathbb{R}^n \oplus J\mathbb{R}^n,$$

where $\mathbb{R}^n = \mathrm{Span}\{e_1, \cdots, e_n\}$ and $J\mathbb{R}^n = \mathrm{Span}\{f_1, \cdots, f_n\}$. Then $\{e_1, \cdots, e_n\}$ defines a $\mathbb{C}$-basis of $\mathbb{C}^n = \mathbb{R}^{2n}$. For a Lagrangian subspace L_0, we choose an orthonormal basis $\{c_1, \cdots, c_n\}$ of L_0. Then

$$\det{}^2(L_0) = \left[\frac{c_1 \wedge_{\mathbb{C}} \cdots \wedge_{\mathbb{C}} c_n}{e_1 \wedge_{\mathbb{C}} \cdots \wedge_{\mathbb{C}} e_n} \right]^2 \in S^1.$$

Here $\wedge_{\mathbb{C}}$ is the $\mathbb{C}$-linear wedge product on $\mathbb{C}^n$. This allows us to define a map

$$\begin{aligned} \varphi : \left(\bigwedge^n L_0^\vee \right)^2 - \{0\} &\longrightarrow \mathbb{C}^* \\ (\alpha)^2 &\longmapsto r e^{-i\theta} \end{aligned}$$

where

$$r = (\alpha(c_1, \cdots, c_n))^2, \qquad e^{i\theta} = \det{}^2(L_0).$$

This map φ does not depend on the choice of the basis $\{c_1, \cdots, c_n\}$ of L_0.

Let us apply this construction to the Lagrangian submanifold $L \subset T^*\mathbb{R}^n$. We obtain a map

$$\varphi : \left(\bigwedge^n T^*L\right)^2 - \{\text{zero section}\} \longrightarrow \mathbb{C}^*.$$

The map φ can be viewed as describing the geometric change of 2-densities on L relative to a fixed reference 2-density on $\mathbb{R}^n$. Let us write the S^1-phase part of φ by

$$\Theta = \frac{\varphi}{|\varphi|} : \left(\bigwedge^n T^*L\right)^2 - \{\text{zero section}\} \longrightarrow S^1.$$

Θ represents the geometric phase change for 2-densities along L.

Let us now consider the half-density Ω on L. To describe a semi-classical solution, we need to compare Ω with the standard half-density on the configuration space $\mathbb{R}^n$. To go around caustics where a direct comparison with respect to the Jacobian blows up, we will use the geometric comparison φ as above. By construction, we can think about φ as a continuous parametrization of a 2-density relative to a reference one at a fixed point. For the half-density Ω on L, Ω^4 is a 2-density. Thus we can parametrize the half-density Ω by

$$\varphi(\Omega^4)^{1/4} = \Theta^{1/4}|\varphi(\Omega^4)|^{1/4}.$$

However, $\Theta^{1/4}$ is multi-valued on L. $\Theta^{1/4}$ changes by

$$e^{-\frac{i}{4}(2\pi m(\gamma))}$$

when it goes around a closed loop γ in L. Here $m(\gamma)$ is the Maslov index.

Let us now combine the half-density with the phase function and consider the geometric semi-classical wave

$$e^{\frac{i}{\hbar}\int^z \lambda}\Theta^{1/4}|\varphi(\Omega^4)|^{1/4}.$$

Its multi-valueness is now reflected by the change along a closed 1-cycle γ via the phase factor

$$e^{\frac{i}{\hbar}\oint_\gamma \lambda - \frac{i}{4}(2\pi m(\gamma))}.$$

Therefore the above geometric semi-classical wave is globally defined on L if and only if

$$\frac{1}{2\pi\hbar}\oint_\gamma \lambda - \frac{1}{4}m(\gamma) \in \mathbb{Z}$$

for each closed 1-cycle γ in L. This rule is the *Keller-Maslov* quantization condition. The factor $\frac{1}{4}m(\gamma)$ is the *Maslov correction*. In physics literature, this is known as *Einstein-Brillouin-Keller* (EBK) semi-classical quantization condition which improves the Bohr-Sommerfeld rule via the Maslov index.

Example 3.2.4. *Consider the one dimensional harmonic oscillator*

$$\mathscr{H} = \frac{p^2}{2m} + \frac{1}{2}kx^2.$$

The level set

$$C = \{\mathscr{H}(x,p) = E\}$$

is a Lagrangian submanifold. We have

$$\frac{1}{2\pi}\oint_C \lambda = \frac{1}{2\pi}\oint_C p dx = \frac{E}{\omega}, \qquad \omega = \sqrt{\frac{k}{m}}, \qquad m(C) = 2.$$

The Keller-Maslov quantization condition reads

$$\frac{E}{\hbar\omega} - \frac{1}{2} \in \mathbb{Z}.$$

This is compatible with the well-known spectrum

$$E = \hbar\omega\left(n + \frac{1}{2}\right), \qquad n = 0, 1, 2, \cdots.$$

3.3 Heisenberg Group

3.3.1 Heisenberg Lie Algebra

Let (V, ω) be a symplectic vector space of dimension $2n$. Consider the vector space of dimension $2n + 1$

$$h_V := V \oplus \mathbb{R}K$$

where we use K for the basis of the new dimension. We can define a bracket on h_V by

$$[u, v] = \omega(u, v)K \qquad \text{if } u, v \in V$$
$$[-, K] = 0 \qquad \text{i.e., } K \text{ is a center element}$$

It is easy to check that $(h_V, [-,-])$ forms a Lie algebra. This is called the **Heisenberg Lie algebra**. Explicitly, let $\{e_1, \cdots, e_n, f_1, \cdots, f_n\}$ be a symplectic basis of (V, ω). Then

$$[e_i, f_j] = \delta_{ij}K$$
$$[e_i, e_j] = [f_i, f_j] = 0$$
$$[e_i, K] = [f_i, K] = 0$$

give the explicit bracket relations in the Heisenberg Lie algebra.

When $V = \mathbb{R}^{2n}$ is the standard symplectic space, we denote

$$h_n := h_{\mathbb{R}^{2n}}.$$

Since any symplectic vector space (V, ω) of dimension $2n$ is symplectomorphic to the standard $\mathbb{R}^{2n}$, we have a Lie algebra isomorphism

$$h_V \simeq h_n.$$

Let $\varphi \in \mathrm{Sp}(V)$ be an element of the symplectic group. Since φ preserves the symplectic pairing, it induces a Lie algebra isomorphism

$$\begin{aligned} \varphi : \qquad h_V &\longrightarrow h_V \\ u + \lambda K &\longmapsto \varphi(u) + \lambda K \end{aligned}$$

This induces a group homomorphism

$$\mathrm{Sp}(V) \longrightarrow \mathrm{Aut}(h_V).$$

3.3.2 Heisenberg Group

The Heisenberg Group H_V is the simply connected Lie group associated to the Lie algebra h_V. As a set, H_V can be identified with h_V via the exponential map

$$H_V = \left\{ e^{u+\lambda K} \right\}_{u+\lambda K \in h_V}.$$

The multiplication law can be obtained via the Baker-Campbell-Hausdorff formula

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\text{higher brackets}}.$$

Since $[h_V, h_V] = \mathbb{R}K$ is the center, all higher brackets vanish here. Thus

$$e^{u_1+\lambda_1 K} \cdot e^{u_2+\lambda_2 K} = e^{u_1+u_2+\left(\lambda_1+\lambda_2+\frac{1}{2}\omega(u_1,u_2)\right)K}, \qquad u_1, u_2 \in V.$$

When $V = \mathbb{R}^{2n}$ is the standard symplectic space, we denote

$$H_n := H_{\mathbb{R}^{2n}}.$$

For general symplectic vector space V of dimension $2n$, a choice of symplectic basis gives a group isomorphism

$$H_V \simeq H_n.$$

There is also a group homomorphism

$$\mathrm{Sp}(V) \longrightarrow \mathrm{Aut}(H_V).$$

Given $\varphi \in \mathrm{Sp}(V)$, the induced group isomorphism is

$$\begin{aligned} H_V &\longrightarrow H_V \\ e^{u+\lambda K} &\longmapsto e^{\varphi(u)+\lambda K} \end{aligned}$$

This is compatible with the corresponding transformation on Heisenberg Lie algebra.

3.3.3 Schrödinger Representation

Let us consider $V = \mathbb{R}^{2n}$ with standard symplectic basis $\{e_1, \cdots, e_n, f_1, \cdots, f_n\}$. Let

$$S(\mathbb{R}^n) = \{ f(\mathbf{x}) \,|\, f \text{ is a } \mathbb{C}\text{-valued Schwartz function on } \mathbb{R}^n \}.$$

$S(\mathbb{R}^n)$ defines a representation of the Heisenberg Lie algebra h_n by

$$\begin{aligned} e_i &\longmapsto \frac{i}{\hbar}\hat{x}^i = \frac{i}{\hbar}x^i \\ f_i &\longmapsto -\frac{i}{\hbar}\hat{p}_i = -\frac{\partial}{\partial x^i} \\ K &\longmapsto \frac{i}{\hbar} \end{aligned}$$

This can be exponentiated to a unitary representation of the Heisenberg group H_n. In fact, let us identify vectors in h_n as

$$\mathbf{r}\cdot\mathbf{e} + \mathbf{s}\cdot\mathbf{f} + \lambda K.$$

Here $\mathbf{r} = (r_1, \cdots r_n) \in \mathbb{R}^n$, $\mathbf{s} = (s_1, \cdots s_n) \in \mathbb{R}^n$ and

$$\mathbf{e} = (e_1, \cdots e_n), \qquad \mathbf{f} = (f_1, \cdots f_n)$$

is the above symplectic basis.

Given a function $\psi(\mathbf{x}) \in S(\mathbb{R}^n)$, we would like to define the transformed function

$$e^{\mathbf{r}\cdot\mathbf{e}+\mathbf{s}\cdot\mathbf{f}+\lambda K}\psi.$$

To motivate how this is defined, we first use the group law to rewrite

$$e^{\mathbf{r}\cdot\mathbf{e}+\mathbf{s}\cdot\mathbf{f}+\lambda K} = e^{\mathbf{r}\cdot\mathbf{e}+\left(\lambda-\frac{1}{2}\mathbf{r}\cdot\mathbf{s}\right)K}e^{\mathbf{s}\cdot\mathbf{f}}.$$

By the corresponding Lie algebra action and the fact that ∂_{x^i} generates translation

$$\left(e^{\mathbf{s}\cdot\mathbf{f}}\psi\right)(\mathbf{x}) = \left(e^{-\mathbf{s}\cdot\nabla}\psi\right)(\mathbf{x}) = \psi(\mathbf{x}-\mathbf{s})$$
$$e^{\mathbf{r}\cdot\mathbf{e}+\left(\lambda-\frac{1}{2}\mathbf{r}\cdot\mathbf{s}\right)K}\psi(\mathbf{x}) = e^{\frac{i}{\hbar}\left(\mathbf{r}\cdot\mathbf{x}-\frac{1}{2}\mathbf{r}\cdot\mathbf{s}+\lambda\right)}\psi(\mathbf{x})$$

Therefore the expected transformation law is

$$\left(e^{\mathbf{r}\cdot\mathbf{e}+\mathbf{s}\cdot\mathbf{f}+\lambda K}\psi\right)(\mathbf{x}) = e^{\frac{i}{\hbar}\left(\mathbf{r}\cdot\mathbf{x}-\frac{1}{2}\mathbf{r}\cdot\mathbf{s}+\lambda\right)}\psi(\mathbf{x}-\mathbf{s}).$$

Definition 3.3.1. Given $(\mathbf{r}, \mathbf{s}, \lambda) \in \mathbb{R}^{2n+1}$, we define

$$T_\hbar(\mathbf{r}, \mathbf{s}, \lambda) : S(\mathbb{R}^n) \longrightarrow S(\mathbb{R}^n)$$

by

$$\left(T_\hbar(\mathbf{r}, \mathbf{s}, \lambda)\psi\right)(\mathbf{x}) := e^{\frac{i}{\hbar}\left(\mathbf{r}\cdot\mathbf{x}-\frac{1}{2}\mathbf{r}\cdot\mathbf{s}+\lambda\right)}\psi(\mathbf{x}-\mathbf{s}).$$

Proposition 3.3.2. *The following composition law holds*

$$T_\hbar(\mathbf{r}_1, \mathbf{s}_1, \lambda_1)T_\hbar(\mathbf{r}_2, \mathbf{s}_2, \lambda_2) = T_\hbar\left(\mathbf{r}_1+\mathbf{r}_2, \mathbf{s}_1+\mathbf{s}_2, \lambda_1+\lambda_2+\frac{1}{2}\left(\mathbf{r}_1\cdot\mathbf{s}_2-\mathbf{r}_2\cdot\mathbf{s}_1\right)\right).$$

This follows from the above formal computation, and can be verified directly. Thus $T_\hbar$ defines a representation of the Heisenberg group H_n

$$e^{\mathbf{r}\cdot\mathbf{e}+\mathbf{s}\cdot\mathbf{f}+\lambda K}\psi := T_\hbar(\mathbf{r}, \mathbf{s}, \lambda)\psi.$$

It is clear that $T_\hbar$ preserves the Hermitian inner product. Thus we can extend $T_\hbar$ to

$$T_\hbar(\mathbf{r}, \mathbf{s}, \lambda) : L^2(\mathbb{R}^n) \longrightarrow L^2(\mathbb{R}^n).$$

$T_\hbar$ defines a unitary representation of H_n on $L^2(\mathbb{R}^n)$. Thus we have a group homomorphism

$$T_\hbar : H_n \to \mathrm{U}(L^2(\mathbb{R}^n))$$

where $\mathrm{U}(L^2(\mathbb{R}^n))$ is the unitary group of $L^2(\mathbb{R}^n)$. This is called the **Schrödinger representation** of H_n with parameter $\hbar$. The parameter indicates the value of the central element

$$K \longmapsto \frac{i}{\hbar}.$$

The unitary representation $T_\hbar$ leads to a transformation of quantum operators via

$$\mathrm{Ad}_{T_\hbar} : \hat{\Theta} \longmapsto T_\hbar \hat{\Theta} T_\hbar^{-1}.$$

For example,

$$\mathrm{Ad}_{T_\hbar(\mathbf{r},\mathbf{s},\lambda)}(\hat{x}^i) = \hat{x}^i - s_i$$
$$\mathrm{Ad}_{T_\hbar(\mathbf{r},\mathbf{s},\lambda)}(\hat{p}_i) = \hat{p}_i - r_i$$

It turns out that the unitary representation $T_\hbar$ of the Heisenberg group H_n on $L^2(\mathbb{R}^n)$ is irreducible, i.e., the only closed subspaces of $L^2(\mathbb{R}^n)$ which are invariant under all H_n actions are $\{0\}$ and $L^2(\mathbb{R}^n)$ itself. Furthermore, the celebrated Stone-Von Neumann Theorem asserts that this is essentially the only irreducible unitary representation of H_n on Hilbert spaces.

Theorem 3.3.3 (Stone-Von Neumann)**.** *Let ρ be any irreducible unitary representation of H_n with center action by $\rho(e^K) = e^{\frac{i}{\hbar}}$ on a Hilbert space $\mathbb{H}$. Then there exists a unitary operator $U : \mathbb{H} \to L^2(\mathbb{R}^n)$ such that*

$$U\rho U^{-1} = T_\hbar.$$

Such U is uniquely determined up to a phase factor ξ with $|\xi| = 1$.

We refer to [21] for a proof of Theorem 3.3.3.

3.3.4 Bargmann-Fock Representation

There is another way to obtain the irreducible representation of the Heisenberg group in terms of holomorphic functions. This is closely related to the Fock space construction.

Let us first define a Hermitian inner product between two functions on $\mathbb{C}^n$ by

$$\langle f|g\rangle_\hbar := \frac{1}{(\pi\hbar)^n}\int_{\mathbb{C}^n} d^{2n}\mathbf{z}\,\overline{f(\mathbf{z})}g(\mathbf{z})e^{-|\mathbf{z}|^2/\hbar}.$$

Here f, g are not necessarily holomorphic, though we will restrict to holomorphic functions below for Segal-Bargmann space. The normalization constant is chosen such that

$$\langle 1|1\rangle_\hbar = 1.$$

The corresponding L^2-norm is denoted by

$$||f||_\hbar^2 = \langle f|f\rangle_\hbar = \frac{1}{(\pi\hbar)^n}\int_{\mathbb{C}^n} d^{2n}\mathbf{z}\,|f(\mathbf{z})|^2 e^{-|\mathbf{z}|^2/\hbar}.$$

Definition 3.3.4. The Segal-Bargmann space (or Bargmann-Fock space) is

$$\mathcal{F}_n := \left\{ f(\mathbf{z}) \text{ holomorphic in } \mathbb{C}^n \text{ and } ||f||_\hbar^2 < \infty \right\}.$$

Proposition 3.3.5. *$\mathcal{F}_n$ is a Hilbert space.*

Proof: We need to show $\mathcal{F}_n$ is complete with respect to the norm $||-||_\hbar$. Let $P_R(\mathbf{z}_0)$ denote the polydisk of radius R centered at $\mathbf{z}_0$:

$$P_R(\mathbf{z}_0) = \left\{\mathbf{z} \in \mathbb{C}^n \,|\, |z^i - z_0^i| < R \text{ for } i = 1, \cdots, n\right\}.$$

For any holomorphic function $f(\mathbf{z})$, we have the average property

$$f(\mathbf{z}_0) = \frac{1}{(\pi R^2)^n} \int_{P_R(\mathbf{z}_0)} d^{2n}\mathbf{z}\, f(\mathbf{z}).$$

Using the Cauchy-Schwartz inequality,

$$\begin{aligned}
|f(\mathbf{z}_0)| &\leq \frac{1}{(\pi R^2)^n} \int_{P_R(\mathbf{z}_0)} d^{2n}\mathbf{z}\, |f(\mathbf{z})| e^{-|\mathbf{z}|^2/2\hbar} e^{|\mathbf{z}|^2/2\hbar} \\
&\leq \frac{1}{(\pi R^2)^n} \left(\int_{P_R(\mathbf{z}_0)} d^{2n}\mathbf{z}\, e^{|\mathbf{z}|^2/\hbar} \right)^{\frac{1}{2}} \left(\int_{P_R(\mathbf{z}_0)} d^{2n}\mathbf{z}\, |f(\mathbf{z})|^2 e^{-|\mathbf{z}|^2/\hbar} \right)^{\frac{1}{2}} \\
&\leq \frac{(\pi\hbar)^n}{(\pi R^2)^n} \left(\int_{P_R(\mathbf{z}_0)} d^{2n}\mathbf{z}\, e^{|\mathbf{z}|^2/\hbar} \right)^{\frac{1}{2}} ||f||_\hbar.
\end{aligned}$$

This implies that for an open neighborhood V of $\mathbf{z}_0$, we can choose a constant C_V depending on V such that

$$|f(\mathbf{z})| \leq C_V ||f||_\hbar, \qquad \forall \mathbf{z} \in V$$

holds for any $f \in \mathcal{F}_n$.

Now let $\{f_n\}$ be a Cauchy sequence in $\mathcal{F}_n$. The above estimate shows that $\{f_n\}$ converges locally uniformly to some limit function f, which must be holomorphic as well. So $f \in \mathcal{F}_n$. Therefore $\mathcal{F}_n$ is complete, i.e., a Hilbert space. □

Proposition 3.3.6. *Let f, g be polynomial functions in $\mathbf{z} = (z^1, \cdots, z^n)$. We have*

$$\left\langle z^i f \middle| g \right\rangle_\hbar = \langle f | \hbar \partial_{z^i} g \rangle_\hbar.$$

Proof:

$$\begin{aligned}
\left\langle z^i f \middle| g \right\rangle_\hbar &= \frac{1}{(\pi\hbar)^n} \int_{\mathbb{C}^n} d^{2n}\mathbf{z}\, \overline{z^i f(\mathbf{z})} g(\mathbf{z}) e^{-|\mathbf{z}|^2/\hbar} \\
&= \frac{1}{(\pi\hbar)^n} \int_{\mathbb{C}^n} d^{2n}\mathbf{z}\, \overline{f(\mathbf{z})} g(\mathbf{z}) \left(-\hbar \frac{\partial}{\partial z^i} e^{-|\mathbf{z}|^2/\hbar} \right) \\
&= \frac{1}{(\pi\hbar)^n} \int_{\mathbb{C}^n} d^{2n}\mathbf{z}\, \overline{f(\mathbf{z})} \left(\hbar \partial_{z^i} g(\mathbf{z}) \right) e^{-|\mathbf{z}|^2/\hbar} \\
&= \langle f | \hbar \partial_{z^i} g \rangle_\hbar.
\end{aligned}$$

□

We define the raising and lowering operators $a_i^\dagger$ and a_i by

$$a_i^\dagger = z^i, \qquad a_i = \hbar \frac{\partial}{\partial z^i}.$$

They are adjoint of each other and satisfy

$$[a_i, a_j^\dagger] = \delta_{ij}\hbar.$$

Given a multi-index $I = \{i_1, i_2, \cdots, i_n\}$, we define the polynomial

$$\lambda_I(\mathbf{z}) := \frac{z^I}{\sqrt{\hbar^{|I|} I!}}$$

where

$$z^I := (z^1)^{i_1}(z^2)^{i_2}\cdots(z^n)^{i_n}, \qquad |I| := i_1 + i_2 + \cdots + i_n, \qquad I! := i_1! i_2! \cdots i_n!.$$

If we identify 1 as the vacuum state, then

$$\lambda_I = \frac{(a_1^\dagger)^{i_1}}{\sqrt{\hbar^{i_1} i_1!}} \cdots \frac{(a_n^\dagger)^{i_n}}{\sqrt{\hbar^{i_n} i_n!}} 1$$

are expressions of the excited states in the physics Fock space.

Proposition 3.3.7. *$\{\lambda_I\}$ form an orthonormal basis of $\mathcal{F}_n$.*

Proof: Orthogonality follows by the adjointness of $a_i^\dagger$ and a_i. We can compute the norm

$$\begin{aligned}\left\langle z^I \middle| z^I \right\rangle_\hbar &= \left\langle 1 \middle| (a_1^\dagger)^{i_1} \cdots (a_n^\dagger)^{i_n} a_1^{i_1} \cdots a_n^{i_n} 1 \right\rangle_\hbar \\ &= \hbar^{|I|} I! \langle 1|1\rangle_\hbar = \hbar^{|I|} I!.\end{aligned}$$

Thus $\{\lambda_I\}$ form an orthonormal set. We next show they form a basis.

For all $f \in \mathcal{F}_n$, we consider its Taylor series

$$f(\mathbf{z}) = \sum_I c_I z^I.$$

This series converges to f uniformly on compact subsets of $\mathbb{C}^n$. Let χ_R denote the characteristic function on the polydisk of radius R

$$\chi_R(\mathbf{z}) = \begin{cases} 1 & \text{if } \mathbf{z} \in P_R(0) \\ 0 & \text{otherwise} \end{cases}.$$

A direct computation using polar coordinate shows

$$\left\langle z^I \chi_R \middle| z^J \chi_R \right\rangle_\hbar = \delta_{IJ} d_{I,R}$$

where the constant $d_{I,R}$ increases with R and

$$\lim_{R\to\infty} d_{I,R} = \hbar^{|I|} I!.$$

On $P_R(0)$, the uniform convergence of the series and the above orthogonality imply

$$||f\chi_R||_\hbar^2 = \sum_I |c_I|^2 \, d_{I,R}.$$

Taking $R \to \infty$, we find

$$||f||_\hbar^2 = \sum_I |c_I|^2 ||z^I||_\hbar^2$$

This implies that $\{\lambda_I\}$ form a basis. □

Proposition 3.3.8. *Let $f \in \mathcal{F}_n$. Then*

$$||z^i f||_\hbar^2 = \hbar||f||_\hbar^2 + ||\hbar\partial_{z^i} f||_\hbar^2$$

In particular, $a_i, a_i^\dagger$ have the same domain on $\mathcal{F}_n$.

Proof: The identity holds for $f = \lambda_I$, and in general by Parseval equation.

□

Next we consider representation of the Heisenberg group H_n on the Segal-Bargmann space $\mathcal{F}_n$. Recall the construction of raising operators and lowering operators in harmonic oscillator

$$\begin{cases} a^\dagger = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{p}) \\ a = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{p}) \end{cases}$$

or

$$\begin{cases} \hat{x} = \frac{1}{\sqrt{2}}(a + a^\dagger) \\ \hat{p} = \frac{i}{\sqrt{2}}(a^\dagger - a) \end{cases}$$

Let $\mathbb{R}^{2n}$ be the standard symplectic space with symplectic basis $\{e_1, \cdots, e_n, f_1, \cdots, f_n\}$. Recall that in the Schrödinger representation, we have

$$\begin{aligned} e_i &\longmapsto \frac{i}{\hbar}\hat{x}^i \\ f_i &\longmapsto -\frac{i}{\hbar}\hat{p}_i \\ K &\longmapsto \frac{i}{\hbar} \end{aligned}$$

Comparing with the above formula of raising and lowering operators, this suggests to define the representation ρ on $\mathcal{F}_n$ by

$$\begin{aligned} e_i &\longmapsto \frac{i}{\sqrt{2}\hbar}\left(z^i + \hbar\frac{\partial}{\partial z^i}\right) \\ f_i &\longmapsto \frac{1}{\sqrt{2}\hbar}\left(z^i - \hbar\frac{\partial}{\partial z^i}\right) \\ K &\longmapsto \frac{i}{\hbar} \end{aligned}$$

Thus

$$\mathbf{r}\cdot\mathbf{e} + \mathbf{s}\cdot\mathbf{f} \longmapsto \frac{1}{\sqrt{2}\hbar}(i\mathbf{r} + \mathbf{s})\cdot\mathbf{z} + \frac{1}{\sqrt{2}}(i\mathbf{r} - \mathbf{s})\cdot\nabla_z.$$

Let us identify $(\mathbf{r}, \mathbf{s})$ with complex coordinates $\mathbf{w} \in \mathbb{C}^n$ by

$$\begin{cases} \mathbf{w} = \frac{1}{\sqrt{2}}(\mathbf{s} - i\mathbf{r}) \\ \overline{\mathbf{w}} = \frac{1}{\sqrt{2}}(\mathbf{s} + i\mathbf{r}) \end{cases} \quad \text{or} \quad \begin{cases} \mathbf{r} = \frac{i}{\sqrt{2}}(\mathbf{w} - \overline{\mathbf{w}}) \\ \mathbf{s} = \frac{1}{\sqrt{2}}(\mathbf{w} + \overline{\mathbf{w}}) \end{cases}$$

Then we can write

$$\mathbf{r}\cdot\mathbf{e} + \mathbf{s}\cdot\mathbf{f} \longmapsto \frac{1}{\hbar}\overline{\mathbf{w}}\cdot\mathbf{z} - \mathbf{w}\cdot\nabla_z.$$

This leads us to define the representation ρ of the Heisenberg group by

$$\rho_\hbar(\mathbf{w}) = e^{\frac{1}{\hbar}\overline{\mathbf{w}}\cdot\mathbf{z} - \mathbf{w}\cdot\nabla_z}.$$

Using the Baker–Campbell–Hausdorff formula, these operators satisfy the composition law

$$\begin{aligned}\rho_\hbar(\mathbf{w}_1)\rho_\hbar(\mathbf{w}_2) &= \rho_\hbar(\mathbf{w}_1+\mathbf{w}_2)e^{\frac{1}{2\hbar}(\overline{\mathbf{w}}_1\cdot\mathbf{w}_2-\mathbf{w}_1\cdot\overline{\mathbf{w}}_2)}\\ &= \rho_\hbar(\mathbf{w}_1+\mathbf{w}_2)e^{\frac{i}{\hbar}\operatorname{Im}(\overline{\mathbf{w}}_1\cdot\mathbf{w}_2)}.\end{aligned}$$

In particular, we have

$$\rho_\hbar(\mathbf{w}) = e^{\frac{1}{\hbar}\overline{\mathbf{w}}\cdot\mathbf{z}-\frac{1}{2\hbar}|\mathbf{w}|^2}e^{-\mathbf{w}\cdot\nabla_z}$$

Thus we find the following explicit formula of the representation on $\mathcal{F}_n$

$$\left(\rho_\hbar(\mathbf{w})f\right)(\mathbf{z}) := e^{\frac{1}{\hbar}\overline{\mathbf{w}}\cdot\mathbf{z}-\frac{1}{2\hbar}|\mathbf{w}|^2}f(\mathbf{z}-\mathbf{w}).$$

This is the **Bargmann-Fock representation** of the Heisenberg group.

By the Stone-Von Newmann Theorem, there exists a unitary map

$$\mathcal{B} : L^2(\mathbb{R}^n) \longrightarrow \mathcal{F}_n$$

intertwining the Schrödinger representation $T_\hbar$ and the Bargmann-Fock representation $\rho_\hbar$

$$\begin{array}{ccc} L^2(\mathbb{R}^n) & \xrightarrow{\mathcal{B}} & \mathcal{F}_n \\ \big\downarrow{\scriptstyle T_\hbar} & & \big\downarrow{\scriptstyle \rho_\hbar} \\ L^2(\mathbb{R}^n) & \xrightarrow{\mathcal{B}} & \mathcal{F}_n \end{array}$$

Explicitly, such $\mathcal{B}$ is found by

$$\left(\mathcal{B}\psi\right)(\mathbf{z}) = \frac{1}{(\pi\hbar)^{n/4}}\int_{\mathbb{R}^n} d^n\mathbf{x}\, e^{-\frac{1}{2\hbar}(\mathbf{z}\cdot\mathbf{z}-2\sqrt{2}\mathbf{z}\cdot\mathbf{x}+\mathbf{x}\cdot\mathbf{x})}\psi(\mathbf{x}).$$

To understand this formula, let us check at the Lie algebra level.

$$\begin{aligned}\mathbf{r}\cdot\mathbf{e}+\mathbf{s}\cdot\mathbf{f} &\xrightarrow{T_\hbar} \frac{i}{\hbar}\mathbf{r}\cdot\mathbf{x}-\mathbf{s}\cdot\nabla_x\\ &= -\frac{1}{\sqrt{2}\hbar}(\mathbf{w}-\overline{\mathbf{w}})\cdot\mathbf{x}-\frac{1}{\sqrt{2}}(\mathbf{w}+\overline{\mathbf{w}})\cdot\nabla_x\\ &= \frac{1}{\hbar}\overline{\mathbf{w}}\cdot\left(\frac{1}{\sqrt{2}}\mathbf{x}-\frac{\hbar}{\sqrt{2}}\nabla_x\right)-\mathbf{w}\cdot\left(\frac{1}{\sqrt{2}\hbar}\mathbf{x}+\frac{1}{\sqrt{2}}\nabla_x\right)\\ \mathbf{r}\cdot\mathbf{e}+\mathbf{s}\cdot\mathbf{f} &\xrightarrow{\rho_\hbar} \frac{1}{\hbar}\overline{\mathbf{w}}\cdot\mathbf{z}-\mathbf{w}\cdot\nabla_z\end{aligned}$$

Comparing the above two infinitesimal transformations, $\mathcal{B}$ should have the properties

$$\begin{aligned}z^i\left(\mathcal{B}\psi\right) &= \mathcal{B}\left[\left(\frac{1}{\sqrt{2}}x^i-\frac{\hbar}{\sqrt{2}}\partial_{x^i}\right)\psi\right]\\ \partial_{z^i}\left(\mathcal{B}\psi\right) &= \mathcal{B}\left[\left(\frac{1}{\sqrt{2}\hbar}x^i+\frac{1}{\sqrt{2}}\partial_{x^i}\right)\psi\right]\end{aligned}$$

It is not hard to check that the above defined $\mathcal{B}$ is designed to satisfy these two equations.

Let us also check the unitarity. Let $\psi \in S(\mathbb{R}^n)$ be a Schwartz function. Then

$$\begin{aligned}
||\mathcal{B}\psi||_\hbar^2 =& \frac{1}{(\pi\hbar)^{3n/2}} \int d^n\mathbf{x} d^n\mathbf{y}\, \psi(\mathbf{x})\overline{\psi(\mathbf{y})} \int d^{2n}\mathbf{z}\, e^{-\frac{1}{2\hbar}(\mathbf{z}\cdot\mathbf{z}-2\sqrt{2}\mathbf{z}\cdot\mathbf{x}+\mathbf{x}\cdot\mathbf{x}+\bar{\mathbf{z}}\cdot\bar{\mathbf{z}}-2\sqrt{2}\bar{\mathbf{z}}\cdot\mathbf{y}+\mathbf{y}\cdot\mathbf{y})} e^{-|\mathbf{z}|^2/\hbar} \\
\underline{\underline{\mathbf{z}=(\mathbf{r}+i\mathbf{s})/\sqrt{2}}} & \frac{1}{2^n(\pi\hbar)^{3n/2}} \int d^n\mathbf{x} d^n\mathbf{y}\, \psi(\mathbf{x})\overline{\psi(\mathbf{y})} \int d^n\mathbf{r} d^n\mathbf{s}\, e^{-\frac{1}{\hbar}(\mathbf{r}^2-\mathbf{r}\cdot(\mathbf{x}+\mathbf{y})+i\mathbf{s}\cdot(\mathbf{x}-\mathbf{y})+\frac{1}{2}(\mathbf{x}\cdot\mathbf{x}+\mathbf{y}\cdot\mathbf{y}))} \\
=& \frac{1}{(2\pi\hbar)^n} \int d^n\mathbf{x} d^n\mathbf{y}\, \psi(\mathbf{x})\overline{\psi(\mathbf{y})} e^{-\frac{1}{4\hbar}(\mathbf{x}\cdot\mathbf{x}-\mathbf{y}\cdot\mathbf{y})^2} \int d^n\mathbf{s}\, e^{-\frac{i}{\hbar}\mathbf{s}\cdot(\mathbf{x}-\mathbf{y})} \\
=& \int d^n\mathbf{x} d^n\mathbf{y}\, \psi(\mathbf{x})\overline{\psi(\mathbf{y})} e^{-\frac{1}{4\hbar}(\mathbf{x}\cdot\mathbf{x}-\mathbf{y}\cdot\mathbf{y})^2} \delta(\mathbf{x}-\mathbf{y}) \\
=& \int d^n\mathbf{x}\, \psi(\mathbf{x})\overline{\psi(\mathbf{x})} = ||\psi||^2_{L^2(\mathbb{R}^n)}
\end{aligned}$$

as expected. The unitary map $\mathcal{B} : L^2(\mathbb{R}^n) \to \mathcal{F}_n$ is called the **Segal-Bargmann transform**.

3.4 Weyl–Wigner Transform

3.4.1 Weyl Quantization

Let $f(\mathbf{y}, \boldsymbol{\xi}) \in C_c^\infty(\mathbb{R}^{2n})$ be a smooth function on the phase space $\mathbb{R}^{2n}$ with compact support. We define the following operator on the state space

$$T_\hbar(f) := \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} d^n\boldsymbol{\xi} d^n\mathbf{y}\, f(\mathbf{y}, \boldsymbol{\xi}) T_\hbar(\boldsymbol{\xi}, \mathbf{y})$$

where we denote the operator (see Definition 3.3.1)

$$T_\hbar(\boldsymbol{\xi}, \mathbf{y}) := T_\hbar(\boldsymbol{\xi}, \mathbf{y}, 0)$$

for simplicity. Explicitly, given a wave function $\psi(\mathbf{x}) \in S(\mathbb{R}^n)$, the operator $T_\hbar(f)$ acts as

$$\begin{aligned}
T_\hbar(f)(\psi)(\mathbf{x}) =& \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} d^n\boldsymbol{\xi} d^n\mathbf{y}\, f(\mathbf{y}, \boldsymbol{\xi})(T_\hbar(\boldsymbol{\xi}, \mathbf{y})\psi)(\mathbf{x}) \\
=& \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} d^n\boldsymbol{\xi} d^n\mathbf{y}\, f(\mathbf{y}, \boldsymbol{\xi}) e^{\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\mathbf{x}-\frac{1}{2}\boldsymbol{\xi}\cdot\mathbf{y})} \psi(\mathbf{x}-\mathbf{y}) \\
\underline{\underline{\mathbf{y}\to\mathbf{x}-\mathbf{y}}} & \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} d^n\boldsymbol{\xi} d^n\mathbf{y}\, f(\mathbf{x}-\mathbf{y}, \boldsymbol{\xi}) e^{\frac{i}{\hbar}\boldsymbol{\xi}\cdot(\frac{\mathbf{x}+\mathbf{y}}{2})} \psi(\mathbf{y}) \\
=& \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} d^n\mathbf{y}\, K_f(\mathbf{x}, \mathbf{y})\psi(\mathbf{y}).
\end{aligned}$$

Here

$$K_f(\mathbf{x}, \mathbf{y}) = \int_{\mathbb{R}^n} d^n\boldsymbol{\xi}\, f(\mathbf{x}-\mathbf{y}, \boldsymbol{\xi}) e^{\frac{i}{\hbar}\boldsymbol{\xi}\cdot(\frac{\mathbf{x}+\mathbf{y}}{2})}.$$

This can be rewritten as

$$K_f\left(\mathbf{x}+\frac{1}{2}\mathbf{y}, \mathbf{x}-\frac{1}{2}\mathbf{y}\right) = \int_{\mathbb{R}^n} d^n\boldsymbol{\xi}\, f(\mathbf{y}, \boldsymbol{\xi}) e^{\frac{i}{\hbar}\boldsymbol{\xi}\cdot\mathbf{x}}$$

which is a partial Fourier transform of f in the variable $\boldsymbol{\xi}$. Since the transformation

$$(\mathbf{x}, \mathbf{y}) \longrightarrow \left(\mathbf{x}+\frac{1}{2}\mathbf{y}, \mathbf{x}-\frac{1}{2}\mathbf{y}\right)$$

also preserves the measure, the transformation

$$f \longmapsto K_f$$

preserves the L^2-norm.

Theorem 3.4.1. *$T_\hbar$ defines a unitary map from $L^2(\mathbb{R}^{2n})$ to the space of Hilbert-Schmidt operators on $L^2(\mathbb{R}^n)$.*

Proof: K_f is the kernel function of the operator $T_\hbar(f)$. The theorem follows from the above computation that $f \mapsto K_f$ is unitary. □

Moreover, it is clear that for $f \in L^1(\mathbb{R}^{2n})$, $T_\hbar(f)$ defines a bounded operator on $L^2(\mathbb{R}^n)$. By the Schwartz Kernel Theorem, $T_\hbar$ further extends to a bijection

$$T_\hbar : S'(\mathbb{R}^{2n}) \xrightarrow{\simeq} \mathscr{L}(S(\mathbb{R}^n), S'(\mathbb{R}^n)).$$

Here $S'(\mathbb{R}^n)$ is the space of tempered distributions and $\mathscr{L}(-,-)$ refers to continuous linear maps.

Example 3.4.2. *Let $f(\mathbf{y}, \boldsymbol{\xi}) = \delta(\mathbf{y} - \mathbf{y}_0, \boldsymbol{\xi} - \boldsymbol{\xi}_0)$ be the Dirac δ-distribution at $(\boldsymbol{\xi}_0, \mathbf{y}_0)$. Then*

$$T_\hbar(f) = \frac{1}{(2\pi\hbar)^n} T_\hbar(\boldsymbol{\xi}_0, \mathbf{y}_0).$$

Example 3.4.3. *Let $f = 1$ be the constant function. Then*

$$K_f = \int_{\mathbb{R}^n} d^n\boldsymbol{\xi}\, e^{\frac{i}{\hbar}\boldsymbol{\xi}\cdot(\frac{\mathbf{x}+\mathbf{y}}{2})} = (2\pi\hbar)^n \delta\left(\frac{\mathbf{x}+\mathbf{y}}{2}\right)$$

Thus

$$T_\hbar(f)(\psi)(\mathbf{x}) = 2^n \psi(-\mathbf{x})$$

is a reflection up to a rescaling.

Definition 3.4.4. Let $f(\mathbf{x}, \mathbf{p}) \in S'(\mathbb{R}^{2n})$ be a tempered distribution on the phase space. We define its Weyl transform to be

$$\mathcal{W}_\hbar(f) := T_\hbar(\widehat{f_\omega}) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} d^n\mathbf{y} d^n\boldsymbol{\xi}\, \widehat{f_\omega}(\mathbf{y}, \boldsymbol{\xi}) e^{\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\hat{\mathbf{x}} - \mathbf{y}\cdot\hat{\mathbf{p}})}$$

where $\widehat{f_\omega}$ is the symplectic Fourier transform (composition of the Fourier transform with J)

$$\widehat{f_\omega}(\mathbf{y}, \boldsymbol{\xi}) := \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} d^n\mathbf{x} d^n\mathbf{p}\, e^{-\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\mathbf{x} - \mathbf{y}\cdot\mathbf{p})} f(\mathbf{x}, \mathbf{p}).$$

Since Fourier transform extends to tempered distributions, $\widehat{f_\omega} \in S'(\mathbb{R}^{2n})$. Hence $\mathcal{W}_\hbar(f)$ defines a continuous linear map

$$\mathcal{W}_\hbar(f) : S(\mathbb{R}^n) \longrightarrow S'(\mathbb{R}^n).$$

If $f \in L^2(\mathbb{R}^{2n})$, then $\mathcal{W}_\hbar(f)$ defines a Hilbert-Schmidt operator

$$\mathcal{W}_\hbar(f) : L^2(\mathbb{R}^n) \longrightarrow L^2(\mathbb{R}^n).$$

The operator $\mathcal{W}_\hbar(f)$ is also called the **Weyl quantization** of the phase space function f.

Example 3.4.5. *Consider the function*

$$f(\mathbf{x}, \mathbf{p}) = e^{\frac{i}{\hbar}(\mathbf{a}\cdot\mathbf{x}+\mathbf{b}\cdot\mathbf{p})}, \qquad \mathbf{a}, \mathbf{b} \in \mathbb{R}^n.$$

Its symplectic Fourier transform is

$$\widehat{f_\omega}(\mathbf{y}, \boldsymbol{\xi}) = \frac{1}{(2\pi\hbar)^n} \int d^n\mathbf{x} d^n\mathbf{p}\, e^{\frac{i}{\hbar}(\mathbf{x}\cdot(\mathbf{a}-\boldsymbol{\xi})+\mathbf{p}\cdot(\mathbf{b}+\mathbf{y}))} = (2\pi\hbar)^n \delta(\mathbf{y}+\mathbf{b})\delta(\boldsymbol{\xi}-\mathbf{a}).$$

Thus

$$\mathcal{W}_\hbar(f) = T_\hbar\left((2\pi\hbar)^n \delta(\mathbf{y}+\mathbf{b})\delta(\boldsymbol{\xi}-\mathbf{a})\right) = T_\hbar(\mathbf{a}, -\mathbf{b}) = e^{\frac{i}{\hbar}(\mathbf{a}\cdot\hat{\mathbf{x}}+\mathbf{b}\cdot\hat{\mathbf{p}})}$$

i.e.

$$\mathcal{W}_\hbar\left(e^{\frac{i}{\hbar}(\mathbf{a}\cdot\mathbf{x}+\mathbf{b}\cdot\mathbf{p})}\right) = e^{\frac{i}{\hbar}(\mathbf{a}\cdot\hat{\mathbf{x}}+\mathbf{b}\cdot\hat{\mathbf{p}})}.$$

Expanding the above formula in powers of $\mathbf{a}$ and $\mathbf{b}$, we find

$$\mathcal{W}_\hbar(x^I p^K) = \mathrm{Sym}(\hat{x}^I \hat{p}^K).$$

Here I, K are multi-indices and $\mathrm{Sym}(-)$ is the symmetrized order average.

For example, consider the $n = 1$ case. Then

$$\begin{aligned}
\mathcal{W}_\hbar(xp) &= \mathrm{Sym}(\hat{x}\hat{p}) = \frac{1}{2}(\hat{x}\hat{p} + \hat{p}\hat{x}) \\
\mathcal{W}_\hbar(x^2 p) &= \frac{1}{3}(\hat{x}^2\hat{p} + \hat{x}\hat{p}\hat{x} + \hat{p}\hat{x}^2) \\
\mathcal{W}_\hbar(x^2 p^2) &= \frac{1}{6}(\hat{x}^2\hat{p}^2 + \hat{p}^2\hat{x}^2 + \hat{x}\hat{p}\hat{x}\hat{p} + \hat{x}\hat{p}^2\hat{x} + \hat{p}\hat{x}\hat{p}\hat{x} + \hat{p}\hat{x}^2\hat{p})
\end{aligned}$$

This symmetrized ordering is also called the **Weyl ordering**.

3.4.2 Moyal Product

The Weyl transform identifies a function on the phase space with an operator on the state space. Since composition of operators defines an associative product, it is natural to ask how such a product is reflected on phase space functions under the Weyl transform.

Recall from the composition law of the Heisenberg group, we have

$$T_\hbar(\boldsymbol{\xi}_1, \mathbf{y}_1) T_\hbar(\boldsymbol{\xi}_2, \mathbf{y}_2) = T_\hbar(\boldsymbol{\xi}_1 + \boldsymbol{\xi}_2, \mathbf{y}_1 + \mathbf{y}_2) e^{\frac{i}{\hbar}\left(\frac{\boldsymbol{\xi}_1\cdot\mathbf{y}_2 - \boldsymbol{\xi}_2\cdot\mathbf{y}_1}{2}\right)}.$$

Thus

$$\begin{aligned}
T_\hbar(\widehat{f_1}) T_\hbar(\widehat{f_2}) &= \frac{1}{(2\pi\hbar)^{2n}} \int_{\mathbb{R}^{2n}} d^n\boldsymbol{\xi}_1 d^n\mathbf{y}_1\, \widehat{f_1}(\mathbf{y}_1, \boldsymbol{\xi}_1) T_\hbar(\boldsymbol{\xi}_1, \mathbf{y}_1) \int_{\mathbb{R}^{2n}} d^n\boldsymbol{\xi}_2 d^n\mathbf{y}_2\, \widehat{f_2}(\mathbf{y}_2, \boldsymbol{\xi}_2) T_\hbar(\boldsymbol{\xi}_2, \mathbf{y}_2) \\
&= \frac{1}{(2\pi\hbar)^{2n}} \int d^n\boldsymbol{\xi}_1 d^n\mathbf{y}_1 d^n\boldsymbol{\xi}_2 d^n\mathbf{y}_2\, \widehat{f_1}(\mathbf{y}_1, \boldsymbol{\xi}_1) \widehat{f_2}(\mathbf{y}_2, \boldsymbol{\xi}_2) e^{\frac{i}{2\hbar}(\boldsymbol{\xi}_1\cdot\mathbf{y}_2 - \boldsymbol{\xi}_2\cdot\mathbf{y}_1)} T_\hbar(\boldsymbol{\xi}_1 + \boldsymbol{\xi}_2, \mathbf{y}_1 + \mathbf{y}_2) \\
&= \frac{1}{(2\pi\hbar)^n} \int d^n\boldsymbol{\xi} d^n\mathbf{y}\, \left(\widehat{f_1} \# \widehat{f_2}\right)(\mathbf{y}, \boldsymbol{\xi}) T_\hbar(\boldsymbol{\xi}, \mathbf{y})
\end{aligned}$$

where

$$\left(\widehat{f}_1\#\widehat{f}_2\right)(\boldsymbol{\xi},\mathbf{y}) := \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^{2n}} d^n\boldsymbol{\eta}d^n\mathbf{z}\,\widehat{f}_1(\boldsymbol{\xi}-\boldsymbol{\eta},\mathbf{y}-\mathbf{z})\widehat{f}_2(\boldsymbol{\eta},\mathbf{z})e^{\frac{i}{2\hbar}((\boldsymbol{\xi}-\boldsymbol{\eta})\cdot\mathbf{z}-\boldsymbol{\eta}\cdot(\mathbf{y}-\mathbf{z}))}$$
$$= \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^{2n}} d^n\boldsymbol{\eta}d^n\mathbf{z}\,\widehat{f}_1(\boldsymbol{\xi}-\boldsymbol{\eta},\mathbf{y}-\mathbf{z})\widehat{f}_2(\boldsymbol{\eta},\mathbf{z})e^{\frac{i}{2\hbar}(\boldsymbol{\xi}\cdot\mathbf{z}-\boldsymbol{\eta}\cdot\mathbf{y})}.$$

Applying this to the Weyl transform, we find

$$\mathcal{W}_\hbar(f)\mathcal{W}_\hbar(g) = T_\hbar(\widehat{f}_\omega)T_\hbar(\widehat{g}_\omega) = T_\hbar(\widehat{f}_\omega\#\widehat{g}_\omega).$$

Thus we are led to define a product $*_\hbar$ on phase space functions by requiring

$$\widehat{(f *_\hbar g)}_\omega = \widehat{f}_\omega\#\widehat{g}_\omega$$

i.e.

$$(f *_\hbar g)(\mathbf{x},\mathbf{p}) = \frac{1}{(2\pi\hbar)^n}\int d^n\boldsymbol{\xi}d^n\mathbf{y}\left(\widehat{f}_\omega\#\widehat{g}_\omega\right)(\mathbf{y},\boldsymbol{\xi})e^{\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\mathbf{x}-\mathbf{y}\cdot\mathbf{p})}$$
$$= \frac{1}{(2\pi\hbar)^{2n}}\int d^n\boldsymbol{\xi}d^n\mathbf{y}\int d^n\boldsymbol{\eta}d^n\mathbf{z}\,\widehat{f}_\omega(\mathbf{y}-\mathbf{z},\boldsymbol{\xi}-\boldsymbol{\eta})\widehat{g}_\omega(\mathbf{z},\boldsymbol{\eta})e^{\frac{i}{2\hbar}(\boldsymbol{\xi}\cdot\mathbf{z}-\boldsymbol{\eta}\cdot\mathbf{y})}e^{\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\mathbf{x}-\mathbf{p}\cdot\mathbf{y})}$$
$$= \frac{1}{(2\pi\hbar)^{2n}}\int d^n\boldsymbol{\xi}d^n\mathbf{y}d^n\boldsymbol{\eta}d^n\mathbf{z}\,\widehat{f}_\omega(\mathbf{y},\boldsymbol{\xi})\widehat{g}_\omega(\mathbf{z},\boldsymbol{\eta})e^{\frac{i}{\hbar}\left[(\boldsymbol{\xi}+\boldsymbol{\eta})\cdot\left(\mathbf{x}+\frac{1}{2}\mathbf{z}\right)-\left(\mathbf{p}+\frac{1}{2}\boldsymbol{\eta}\right)\cdot(\mathbf{y}+\mathbf{z})\right]}$$
$$= \frac{1}{(2\pi\hbar)^{2n}}\int d^n\boldsymbol{\xi}d^n\mathbf{y}d^n\boldsymbol{\eta}d^n\mathbf{z}\,\widehat{f}_\omega(\mathbf{y},\boldsymbol{\xi})\widehat{g}_\omega(\mathbf{z},\boldsymbol{\eta})e^{\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\mathbf{x}-\mathbf{p}\cdot\mathbf{y})}e^{\frac{i}{\hbar}(\boldsymbol{\eta}\cdot\mathbf{x}-\mathbf{p}\cdot\mathbf{z})}e^{\frac{i}{2\hbar}(\boldsymbol{\xi}\cdot\mathbf{z}-\boldsymbol{\eta}\cdot\mathbf{y})}.$$

From the expression of the Fourier transform

$$\widehat{f}_\omega(\mathbf{y},\boldsymbol{\xi}) = \frac{1}{(2\pi\hbar)^n}\int d^n\mathbf{p}d^n\mathbf{x}e^{-\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\mathbf{x}-\mathbf{p}\cdot\mathbf{y})}f(\mathbf{x},\mathbf{p})$$

we have

$$\xi_i\widehat{f}_\omega(\mathbf{y},\boldsymbol{\xi}) = \widehat{(-i\hbar\partial_{x^i}f)}_\omega$$
$$y_i\widehat{f}_\omega(\mathbf{y},\boldsymbol{\xi}) = \widehat{(i\hbar\partial_{p_i}f)}_\omega$$

Thus we can formally write the above product as

$$(f *_\hbar g)(\mathbf{x},\mathbf{p}) \sim f(\mathbf{x},\mathbf{p})e^{\frac{i\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial x^i}\frac{\overrightarrow{\partial}}{\partial p_i}-\frac{\overleftarrow{\partial}}{\partial p_i}\frac{\overrightarrow{\partial}}{\partial x^i}\right)}g(\mathbf{x},\mathbf{p}).$$

Here $\frac{\overleftarrow{\partial}}{\partial(-)}$ means applying the derivative to the function on the left, and $\frac{\overrightarrow{\partial}}{\partial(-)}$ means applying the derivative to the function on the right. This formal expression becomes an exact formula when f, g are polynomials.

The above defined $*_\hbar$ is called the **Moyal product**, or the **Moyal-Weyl product**. Thus we have established

$$\mathcal{W}_\hbar(f *_\hbar g) = \mathcal{W}_\hbar(f)W_\hbar(g).$$

3.4.3 Wigner Transform

Wigner transform and Wigner function

The Wigner transform is the inverse of the Weyl transform, thus takes an operator back to a function on the phase space. Recall the Weyl transform

$$\mathcal{W}_\hbar(f) = T_\hbar(\widehat{f}_\omega)$$

where $\widehat{f_\omega}$ is the symplectic Fourier transform

$$\widehat{f_\omega}(\mathbf{y},\boldsymbol{\xi}) := \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^{2n}} d^n\mathbf{x}d^n\mathbf{p}\, e^{-\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\mathbf{x}-\mathbf{y}\cdot\mathbf{p})} f(\mathbf{x},\mathbf{p}).$$

The operator $T_\hbar(\widehat{f_\omega})$ on $L^2(\mathbb{R}^n)$ has a kernel $\frac{1}{(2\pi\hbar)^n}K_{\widehat{f_\omega}}(\mathbf{x},\mathbf{y})$ where

$$K_{\widehat{f_\omega}}(\mathbf{x},\mathbf{y}) = \int_{\mathbb{R}^n} d^n\boldsymbol{\xi}\, \widehat{f_\omega}(\mathbf{x}-\mathbf{y},\boldsymbol{\xi}) e^{\frac{i}{\hbar}\boldsymbol{\xi}\cdot\left(\frac{\mathbf{x}+\mathbf{y}}{2}\right)}$$

or equivalently

$$K_{\widehat{f_\omega}}\left(\mathbf{x}+\frac{1}{2}\mathbf{y},\mathbf{x}-\frac{1}{2}\mathbf{y}\right) = \int_{\mathbb{R}^n} d^n\boldsymbol{\xi}\, \widehat{f_\omega}(\mathbf{y},\boldsymbol{\xi}) e^{\frac{i}{\hbar}\boldsymbol{\xi}\cdot\mathbf{x}}.$$

Via the inverse Fourier transform, we find

$$\begin{aligned} f(\mathbf{x},\mathbf{p}) &= \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^{2n}} d^n\mathbf{y}d^n\boldsymbol{\xi}\, e^{\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\mathbf{x}-\mathbf{y}\cdot\mathbf{p})}\widehat{f_\omega}(\mathbf{y},\boldsymbol{\xi}) \\ &= \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} d^n\mathbf{y}\, e^{-\frac{i}{\hbar}\mathbf{y}\cdot\mathbf{p}} K_{\widehat{f_\omega}}\left(\mathbf{x}+\frac{1}{2}\mathbf{y},\mathbf{x}-\frac{1}{2}\mathbf{y}\right). \end{aligned}$$

This formula leads to the inverse map of the Weyl transform defined as follows.

Definition 3.4.6. Let Θ be an operator on $L^2(\mathbb{R}^n)$ with kernel function $\frac{1}{(2\pi\hbar)^n}K_\Theta(\mathbf{x},\mathbf{y})$. Define the **Wigner transform** $\mathrm{Wig}[\Theta]$ as a function on the phase space by

$$\mathrm{Wig}[\Theta](\mathbf{x},\mathbf{p}) := \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} d^n\mathbf{y}\, e^{-\frac{i}{\hbar}\mathbf{y}\cdot\mathbf{p}} K_\Theta\left(\mathbf{x}+\frac{1}{2}\mathbf{y},\mathbf{x}-\frac{1}{2}\mathbf{y}\right).$$

It is clear from the above computation that

$$\mathrm{Wig}[\mathcal{W}_\hbar(f)] = f,$$

i.e., the Wigner transform is the inverse of the Weyl transform.

Example 3.4.7. *Let Θ be the operator with kernel function*

$$K_\Theta(\mathbf{x},\mathbf{y}) = \psi_1(\mathbf{x})\overline{\psi_2(\mathbf{y})}.$$

Its Wigner transform is

$$\mathrm{Wig}\left[\Theta\right](\mathbf{x},\mathbf{p}) = \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} d^n\mathbf{y}\, e^{-\frac{i}{\hbar}\mathbf{y}\cdot\mathbf{p}}\psi_1\left(\mathbf{x}+\frac{1}{2}\mathbf{y}\right)\overline{\psi_2\left(\mathbf{x}-\frac{1}{2}\mathbf{y}\right)}.$$

A particular case of great interest is when

$$K_\Theta(\mathbf{x},\mathbf{y}) = \psi(\mathbf{x})\overline{\psi(\mathbf{y})}.$$

This operator Θ projects any state to a state proportional to $|\psi\rangle$. We denote its Wigner transform by

$$\mathrm{Wig}(\psi) := \mathrm{Wig}\left[\Theta\right]$$

or

$$\mathrm{Wig}(\psi)(\mathbf{x},\mathbf{p}) = \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} d^n\mathbf{y}\, e^{-\frac{i}{\hbar}\mathbf{y}\cdot\mathbf{p}}\psi\left(\mathbf{x}+\frac{1}{2}\mathbf{y}\right)\overline{\psi\left(\mathbf{x}-\frac{1}{2}\mathbf{y}\right)}.$$

$\mathrm{Wig}(\psi)$ is called the **Wigner function**, or the Wigner distribution, of the state ψ. Wigner proposed it as a substitute for the the nonexistent joint probability distribution of momentum and position in the quantum state ψ. Note that it does not make sense to speak of a joint probability distribution for momentum and position due to uncertainty principle. Moreover, $\mathrm{Wig}(\psi)$ is usually not a genuine probability density since it could take negative values (see the example of harmonic oscillator below).

Proposition 3.4.8.

$$\int_{\mathbb{R}^n} d^n\mathbf{p}\ \mathrm{Wig}(\psi)(\mathbf{x},\mathbf{p}) = |\psi(\mathbf{x})|^2$$
$$\int_{\mathbb{R}^n} d^n\mathbf{x}\ \mathrm{Wig}(\psi)(\mathbf{x},\mathbf{p}) = |\hat{\psi}(\mathbf{p})|^2$$

Here $\hat{\psi}(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{n/2}} \int_{\mathbb{R}^n} d^n\mathbf{x}\, e^{-\frac{i}{\hbar}\mathbf{x}\cdot\mathbf{p}}\psi(\mathbf{x})$ *is the Fourier transform of* ψ.

Proof:

$$\begin{aligned}\int_{\mathbb{R}^n} d^n\mathbf{p}\ \mathrm{Wig}(\psi)(\mathbf{x},\mathbf{p}) &= \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} d^n\mathbf{p}\int_{\mathbb{R}^n} d^n\mathbf{y}\, e^{-\frac{i}{\hbar}\mathbf{y}\cdot\mathbf{p}}\psi\left(\mathbf{x}+\frac{1}{2}\mathbf{y}\right)\overline{\psi\left(\mathbf{x}-\frac{1}{2}\mathbf{y}\right)}\\ &= \int_{\mathbb{R}^n} d^n\mathbf{y}\,\delta(\mathbf{y})\psi\left(\mathbf{x}+\frac{1}{2}\mathbf{y}\right)\overline{\psi\left(\mathbf{x}-\frac{1}{2}\mathbf{y}\right)}\\ &= \psi(\mathbf{x})\overline{\psi(\mathbf{x})}.\end{aligned}$$

Similarly,

$$\begin{aligned}\int_{\mathbb{R}^n} d^n\mathbf{x}\ \mathrm{Wig}(\psi)(\mathbf{x},\mathbf{p}) =& \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} d^n\mathbf{x}\int_{\mathbb{R}^n} d^n\mathbf{y}\, e^{-\frac{i}{\hbar}\mathbf{y}\cdot\mathbf{p}}\psi\left(\mathbf{x}+\frac{1}{2}\mathbf{y}\right)\overline{\psi\left(\mathbf{x}-\frac{1}{2}\mathbf{y}\right)}\\ \xrightarrow[\mathbf{y}\to\mathbf{x}-\mathbf{y}]{\mathbf{x}\to(\mathbf{x}+\mathbf{y})/2}& \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} d^n\mathbf{x}\int_{\mathbb{R}^n} d^n\mathbf{y}\, e^{-\frac{i}{\hbar}(\mathbf{x}-\mathbf{y})\cdot\mathbf{p}}\psi(\mathbf{x})\overline{\psi(\mathbf{y})}\\ =& \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} d^n\mathbf{x}\, e^{-\frac{i}{\hbar}\mathbf{x}\cdot\mathbf{p}}\psi(\mathbf{x})\int_{\mathbb{R}^n} d^n\mathbf{y}\, e^{\frac{i}{\hbar}\mathbf{y}\cdot\mathbf{p}}\overline{\psi(\mathbf{y})}\\ =& \psi(\mathbf{p})\overline{\psi(\mathbf{p})}.\end{aligned}$$

□

This proposition says the integration of the Wigner function over the momentum space / position space produces the probability distribution of the quantum state in the position space / momentum space. In particular, we have

$$\int_{\mathbb{R}^{2n}} d^n\mathbf{x}d^n\mathbf{p}\ \mathrm{Wig}(\psi)(\mathbf{x},\mathbf{p}) = ||\psi||_{L^2}^2.$$

Assume $||\psi||_{L^2} = 1$ is normalized, then $\mathrm{Wig}(\psi)$ is also called the Wigner quasi-probability distribution.

Proposition 3.4.9. *Assume* $||\psi||_{L^2} = 1$ *is normalized. Then*

$$-\frac{1}{(\pi\hbar)^n} \le \mathrm{Wig}(\psi) \le \frac{1}{(\pi\hbar)^n}.$$

Proof:

$$\begin{aligned}|\operatorname{Wig}(\psi)(\mathbf{x},\mathbf{p})| &\le \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} d^n\mathbf{y}\left|\psi\left(\mathbf{x}+\frac{1}{2}\mathbf{y}\right)\right|\left|\psi\left(\mathbf{x}-\frac{1}{2}\mathbf{y}\right)\right| \\ &\le \frac{1}{(2\pi\hbar)^n}\left(\int_{\mathbb{R}^n} d^n\mathbf{y}\left|\psi\left(\mathbf{x}+\frac{1}{2}\mathbf{y}\right)\right|^2\int_{\mathbb{R}^n} d^n\mathbf{y}\left|\psi\left(\mathbf{x}-\frac{1}{2}\mathbf{y}\right)\right|^2\right)^{\frac{1}{2}} \\ &= \frac{1}{(\pi\hbar)^n}||\psi||_{L^2}^2 = \frac{1}{(\pi\hbar)^n}.\end{aligned}$$

□

As a corollary, let $\Omega \subset \mathbb{R}^{2n}$ be any region in the phase space. Assume $||\psi||_{L^2} = 1$ is normalized. Then

$$\left|\int_\Omega d^n\mathbf{x}d^n\mathbf{p}\ \operatorname{Wig}(\psi)(\mathbf{x},\mathbf{p})\right| \le \frac{\operatorname{Vol}(\Omega)}{(\pi\hbar)^n}.$$

On the other hand, we have

$$\int_{\mathbb{R}^{2n}} d^n\mathbf{x}d^n\mathbf{p}\ \operatorname{Wig}(\psi)(\mathbf{x},\mathbf{p}) = ||\psi||_{L^2} = 1.$$

Comparing the above two expressions, we find that it is impossible for $\operatorname{Wig}(\psi)$ to concentrate in some region Ω with $\operatorname{Vol}(\Omega) < (\pi\hbar)^n$. This is a reflection of the uncertainty principle.

Example 3.4.10. *Consider the one-dimensional harmonic oscillator*

$$\mathscr{H} = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2.$$

The energy levels are $E_n = \hbar\omega\left(n+\frac{1}{2}\right)$, $n = 0, 1, 2, \cdots$, *with the normalized eigenfunctions by*

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! a\sqrt{\pi}}} H_n\left(\frac{x}{a}\right) e^{-\frac{x^2}{2a^2}}$$

where $a = \sqrt{\frac{\hbar}{m\omega}}$ *and* H_n *are Hermite polynomials.*

Let us consider the following linear superposition (coherent state)

$$\begin{aligned}\psi_z(x) &= \sum_{n=0}^{\infty} e^{-\frac{|z|^2}{2}}\frac{z^n}{\sqrt{n!}}\psi_n(x) \\ &= \frac{1}{\sqrt{a\sqrt{\pi}}}\exp\left(-\frac{|z|^2+z^2}{2}+\frac{\sqrt{2}zx}{a}-\frac{x^2}{2a^2}\right).\end{aligned}$$

Let us consider the analogue of the Wigner function construction

$$\begin{aligned}&\mathcal{W}_{z_1,z_2}(x,p) \\ =&\frac{1}{2\pi\hbar}\int dy\, e^{\frac{i}{\hbar}yp}\psi_{z_1}\left(x+\frac{y}{2}\right)\overline{\psi_{z_2}\left(x-\frac{y}{2}\right)} \\ =&\frac{1}{(2\pi\hbar)\,a\sqrt{\pi}}\int dy\, e^{\frac{i}{\hbar}yp}\exp\left(-\frac{|z_1|^2+|z_2|^2}{2}\right)\exp\left(-\frac{z_1^2+\overline{z}_2^2}{2}\right) \\ &\qquad\exp\left(\frac{\sqrt{2}z_1(x+y/2)}{a}+\frac{\sqrt{2}\,\overline{z}_2(x-y/2)}{a}\right)\exp\left(-\frac{(x+y/2)^2}{2a^2}-\frac{(x-y/2)^2}{2a^2}\right) \\ =&\frac{1}{\pi\hbar}\exp\left(-\frac{x^2}{a^2}-\frac{a^2p^2}{\hbar^2}\right)\exp\left(-\frac{|z_1|^2+|z_2|^2}{2}-\overline{z}_1z_2\right)\exp\left(2z_2\frac{x/a-ipa/\hbar}{\sqrt{2}}+2\overline{z}_1\frac{x/a+ipa/\hbar}{\sqrt{2}}\right).\end{aligned}$$

We can expand into power series in z_1, z_2 and collect terms proportional to $\frac{(z_1\overline{z}_2)^n}{n!}$ to find

$$\begin{aligned}\mathrm{Wig}(\psi_n)(x,p) &= \frac{(-1)^n}{\pi\hbar}\exp\left(-\frac{x^2}{a^2}-\frac{a^2p^2}{\hbar^2}\right)\sum_{j=0}^{n}\binom{n}{j}\frac{(-1)^j 2^j}{j!}\left(\frac{x^2}{a^2}+\frac{a^2p^2}{\hbar^2}\right)^j \\ &= \frac{(-1)^n}{\pi\hbar}e^{-u}L_n(2u), \qquad u=\frac{x^2}{a^2}+\frac{a^2p^2}{\hbar^2}\end{aligned}$$

where L_n are the Laguerre polynomials

$$L_n(t) = \frac{e^t}{n!}\frac{d^n}{dt^n}(e^{-t}t^n).$$

We list a first few terms of Laguerre polynomials

$$\begin{aligned}L_0 &= 1 \\ L_1(t) &= -t+1 \\ L_2(t) &= \frac{1}{2}(t^2-4t+2) \\ L_3(t) &= \frac{1}{6}(-t^3+9t^2-18t+6) \\ L_4(t) &= \frac{1}{24}(t^4-16t^3+72t^2-96t+24) \\ &\vdots\end{aligned}$$

3.5 Geometric Quantization

3.5.1 Dirac Quantization Principle

Classical mechanics is rooted in the symplectic geometry of the phase space manifold M. The space $\mathrm{Obs}^{cl} := C^\infty(M)$ of classical observables carries a structure of Poisson bracket $\{-,-\}$. We say $\{f_1,\cdots,f_m\}$ is a complete set of classical observables if for $g\in\mathrm{Obs}^{cl}$,

$$\{g,f_1\}=\cdots=\{g,f_m\}=0 \qquad \Longrightarrow \qquad g=\text{constant}.$$

For example, on $M=\mathbb{R}^{2n}$, the set of position and momentum functions $\{x^1,\cdots,x^n,p_1,\cdots,p_n\}$ is complete.

In quantum mechanics, we have a Hilbert space $\mathbb{H}$ representing the space of quantum states. The space Obs^q of quantum observables is an appropriate collection of linear operators on $\mathbb{H}$ that carries the natural structure of operator commutator

$$[\mathcal{O}_1,\mathcal{O}_2]=\mathcal{O}_1\mathcal{O}_2-\mathcal{O}_2\mathcal{O}_1.$$

Similarly, we say quantum observables $\{\mathcal{O}_1,\cdots,\mathcal{O}_m\}$ is a complete set of quantum observables if for $\mathcal{O}\in\mathrm{Obs}^q$,

$$[\mathcal{O},\mathcal{O}_1]=\cdots=[\mathcal{O},\mathcal{O}_m]=0 \qquad \Longrightarrow \qquad \mathcal{O}=c\mathbf{1} \text{ is a multiple of the identity.}$$

In Dirac's Principle, quantization amounts to an assignment

$$Q : \mathrm{Obs}^{cl} \longrightarrow \mathrm{Obs}^{q}$$
$$f \longmapsto \hat{f}$$

of operators $\hat{f}$ on some Hilbert space to classical observables f. This assignment has to satisfy

Q1: Q is $\mathbb{R}$-linear

Q2: $\hat{1} = Q(1)$ is the identity operator

Q3: if f is real, then $\hat{f}$ is self-adjoint

Q4: $\left[\hat{f}, \hat{g}\right] = i\hbar\widehat{\{f, g\}}$

Q5: if $\{f_1, \cdots, f_m\}$ is a complete set of classical observables, then $\left\{\hat{f}_1, \cdots, \hat{f}_m\right\}$ is a complete set of quantum observables.

Q1,Q2,Q3 are natural requirements. Q4 is Dirac's observation that the operator commutator should be the quantum counterpart of the classical Poisson bracket. Q5 can be viewed as an irreducibility condition. The Hilbert space $\mathbb{H}$ is in general infinite dimensional. But it could be finite dimensional as well (such as describing internal symmetries).

Unfortunately, it is in general not possible to satisfy both Q4 and Q5. This is illustrated by a "no-go" type result for quantization that we will discuss in Section 3.5.2.

Before that, let us first take a look at Weyl quantization on Schrödinger representation. Let $f(\mathbf{x}, \mathbf{p})$ be a polynomial. Its Weyl quantization is the operator

$$\mathcal{W}_\hbar(f) = \mathrm{Sym}(f(\hat{x}^i, \hat{p}_i))$$

where

$$\hat{x}^i = x^i \qquad \hat{p}_i = -i\hbar\frac{\partial}{\partial x^i}$$

and $\mathrm{Sym}(-)$ is the symmetrized order average. We have

$$\mathcal{W}_\hbar(f)W_\hbar(g) = \mathcal{W}_\hbar(f *_\hbar g)$$

where $f *_\hbar g$ is the Moyal product

$$(f *_\hbar g)(\mathbf{x}, \mathbf{p}) = f(\mathbf{x}, \mathbf{p})e^{\frac{i\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial x^i}\frac{\overrightarrow{\partial}}{\partial p_i} - \frac{\overleftarrow{\partial}}{\partial p_i}\frac{\overrightarrow{\partial}}{\partial x^i}\right)}g(\mathbf{x}, \mathbf{p}).$$

In particular,

$$[\mathcal{W}_\hbar(f), W_\hbar(g)] = \mathcal{W}_\hbar([f, g]_*)$$

where

$$[f, g]_* := f *_\hbar g - g *_\hbar f$$

is the commutator of Moyal product. We compute

$$[f, g]_* = i\hbar\{f, g\} + \frac{(i\hbar)^3}{24}f\left(\frac{\overleftarrow{\partial}}{\partial x^i}\frac{\overrightarrow{\partial}}{\partial p_i} - \frac{\overleftarrow{\partial}}{\partial p_i}\frac{\overrightarrow{\partial}}{\partial x^i}\right)^3 g + \cdots.$$

Thus in the Schrödinger representation, the Weyl quantization violates Q4.

On the other hand, the above computation implies

$$[f,g]_* = i\hbar\{f,g\}$$

if f, g are polynomials of deg ≤ 2. We will see next that deg $= 4$ leads to the obstruction.

3.5.2 The Groenewold-Van Hove Theorem

The Groenewold-Van Hove Theorem established several "No-Go" type results for quantization. We describe the simplest version in the following.

Consider quantization on $\mathbb{R}^{2n}$. Let

$$P^{\leq k} := \left\{ f \in \mathbb{R}[x^i, p_i] | \deg f \leq k \right\}.$$

The Schrödinger representation assigns elements of $P^{\leq 1}$ to operators

$$\begin{aligned} 1 &\longmapsto \hat{1} = 1 \\ x^i &\longmapsto \hat{x}^i = x^i \\ p_i &\longmapsto \hat{p}_i = -i\hbar\frac{\partial}{\partial x^i} \end{aligned}$$

and

$$[\hat{x}^i, \hat{p}_j] = i\hbar\delta_{ij} = i\hbar\widehat{\{x^i, p_j\}}.$$

Theorem 3.5.1 (Groenewold)**.** *There is no $\mathbb{R}$-linear map*

$$Q : P^{\leq 4} \longrightarrow \textit{self-adjoint operators on } L^2(\mathbb{R}^n)$$

satisfying

(1) $Q(1) = 1$, $Q(x^i) = \hat{x}^i$, $Q(p_i) = \hat{p}_i$

(2) $[Q(f), Q(g)] = i\hbar Q(\{f,g\})$, $\forall f, g \in P^{\leq 4}$.

Proof: We prove the case for $n = 1$. The proof for the case $n > 1$ is similar. Assume such Q exists. Recall the Weyl quantization $\mathcal{W}_\hbar$. By assumption (1)

$$Q(f) = \mathcal{W}_\hbar(f) \qquad \text{for} \quad f \in P^{\leq 1}.$$

Observe the Poisson bracket satisfies

$$\left\{ P^{\leq 2}, P^{\leq 1} \right\} \subset P^{\leq 1}$$

and

$$[\mathcal{W}_\hbar(f), \mathcal{W}_\hbar(g)] = i\hbar\mathcal{W}_\hbar(\{f,g\}) \qquad \text{for} \quad f \in P^{\leq 2}, g \in P^{\leq 1}.$$

Therefore

$$[\mathcal{W}_\hbar(f), \hat{g}] = i\hbar\widehat{\{f,g\}} = [Q(f), \hat{g}] \qquad \text{for} \quad f \in P^{\leq 2}, g \in P^{\leq 1}.$$

Thus

$$[Q(f) - \mathcal{W}_\hbar(f), \hat{x}] = [Q(f) - \mathcal{W}_\hbar(f), \hat{p}] = 0.$$

It follows that the exponentiated one-parameter family of unitary operators $e^{i\alpha(Q(f)-\mathcal{W}_\hbar(f))}$ on $L^2(\mathbb{R}^n)$ commute with the Heisenberg group action and give rise to automorphisms of the Schrödinger representation. By Stone-von Neumann Theorem (Theorem 3.3.3), such automorphisms must be scalar multiplication so

$$Q(f) - \mathcal{W}_\hbar(f) = \text{const } 1 \qquad \text{for} \quad f \in P^{\leq 2}.$$

The above constants on the right are actually zero. In fact, using $x^2 = \frac{1}{2}\{x^2, xp\}$,

$$\begin{aligned} Q(x^2) &= \frac{1}{2i\hbar}[Q(x^2), Q(xp)] \\ &= \frac{1}{2i\hbar}[\mathcal{W}_\hbar(x^2) + c_1, \mathcal{W}_\hbar(xp) + c_2] \qquad c_1, c_2 \text{ are some constants} \\ &= \frac{1}{2i\hbar}[\mathcal{W}_\hbar(x^2), \mathcal{W}_\hbar(xp)] \\ &= \mathcal{W}_\hbar(x^2). \end{aligned}$$

Similarly we can show $Q(p^2) = \mathcal{W}_\hbar(p^2)$ and $Q(xp) = \mathcal{W}_\hbar(xp)$. Thus

$$Q(f) = \mathcal{W}_\hbar(f) \qquad \text{for} \quad f \in P^{\leq 2}.$$

Next we observe that for $f \in P^{\leq 3}$, $g \in P^{\leq 1}$,

$$[\mathcal{W}_\hbar(f), \mathcal{W}_\hbar(g)] = i\hbar\mathcal{W}_\hbar(\{f, g\})$$

still holds. Thus for $f \in P^{\leq 3}$, $g \in P^{\leq 1}$,

$$[Q(f) - \mathcal{W}_\hbar(f), \hat{g}] = i\hbar Q(\{f, g\}) - i\hbar\mathcal{W}_\hbar(\{f, g\}) = 0$$

since $\{f, g\} \in P^{\leq 2}$. By the same argument as above, we have

$$Q(f) - \mathcal{W}_\hbar(f) = \text{const } 1 \qquad \text{for} \quad f \in P^{\leq 3}.$$

Similarly, using

$$\begin{aligned} x^3 &= \frac{1}{3}\{x^3, xp\} & p^3 &= \frac{1}{3}\{xp, p^3\} \\ x^2p &= \frac{1}{6}\{x^3, p^2\} & xp^2 &= \frac{1}{6}\{x^2, p^3\} \end{aligned}$$

we can deduce that the above constants on the right are zero. Hence

$$Q(f) = \mathcal{W}_\hbar(f) \qquad \text{for} \quad f \in P^{\leq 3}.$$

Now we come to degree 4 polynomials. Consider

$$x^2p^2 = \frac{1}{9}\{x^3, p^3\} = \frac{1}{3}\{x^2p, xp^2\}.$$

By assumption (2), we would have

$$Q(x^2p^2) = \frac{1}{9i\hbar}[Q(x^3), Q(p^3)] = \frac{1}{3i\hbar}[Q(x^2p), Q(xp^2)].$$

On the other hand, using

$$[x^3, p^3]_* = 9(i\hbar)x^2p^2 + \frac{3}{2}(i\hbar)^3$$
$$[x^2p, xp^2]_* = 3(i\hbar)x^2p^2 - \frac{1}{2}(i\hbar)^3$$

we have

$$\frac{1}{9i\hbar}[Q(x^3), Q(p^3)] = \frac{1}{9i\hbar}[\mathcal{W}_\hbar(x^3), \mathcal{W}_\hbar(p^3)] = \frac{1}{9i\hbar}\mathcal{W}_\hbar([x^3, p^3]_*) = \mathcal{W}_\hbar(x^2p^2) - \frac{1}{6}\hbar^2$$

and

$$\begin{aligned}\frac{1}{3i\hbar}[Q(x^2p), Q(xp^2)] =& \frac{1}{3i\hbar}[\mathcal{W}_\hbar(x^2p), \mathcal{W}_\hbar(xp^2)] = \frac{1}{3i\hbar}\mathcal{W}_\hbar([x^2p, xp^2]_*) = \mathcal{W}_\hbar(x^2p^2) + \frac{1}{6}\hbar^2 \\ \neq& \frac{1}{9i\hbar}[Q(x^3), Q(p^3)].\end{aligned}$$

Contradiction. □

3.5.3 Prequantization

Since it is unrealistic to construct quantization satisfying all the conditions Q1-Q5, we have to relax either condition Q4 or Q5. There is a natural way to construct a quantization of a symplectic manifold which satisfies conditions Q1-Q4. This is known as the prequantization.

Let (M, ω) be a symplectic manifold. Recall the construction of Hamiltonian vector fields

$$\begin{aligned}C^\infty(M) &\longrightarrow \mathrm{Vect}(M) \\ f &\longmapsto V_f, \qquad \iota_{V_f}\omega = df\end{aligned}$$

which is a Lie algebra homomorphism

$$[V_f, V_g] = V_{\{f,g\}}.$$

If we think of V_f as a first order differential operator acting on $C^\infty(M)$, then the assignment

$$f \longmapsto i\hbar V_f$$

satisfies Q1, Q3, Q4 but not Q2 since it sends $1 \longmapsto 0$.

To remedy this, let $L \to M$ be a complex line bundle on M with a connection ∇. Let F_∇ be the curvature 2-form. For any vector fields X, Y, we have

$$[\nabla_X, \nabla_Y] - \nabla_{[X,Y]} = F_\nabla(X, Y).$$

Given a function f, we use ∇_f to denote the covariant derivative with respect to the Hamiltonian vector field V_f

$$\nabla_f := \nabla_{V_f}.$$

Then the above curvature formula reads

$$[\nabla_f, \nabla_g] - \nabla_{\{f,g\}} = F_\nabla(V_f, V_g) = \iota_{V_g}\iota_{V_f}F_\nabla.$$

Here ι_{V_f} is the interior product (contraction) with the vector field V_f.

Consider the following assignment of operators on $\Gamma(M, L)$

$$Q(f) := i\hbar\nabla_f + f.$$

We have

$$\begin{aligned}
[Q(f), Q(g)] =& [i\hbar\nabla_f + f, i\hbar\nabla_g + g] \\
=& (i\hbar)^2 \left(\nabla_{\{f,g\}} + F_\nabla(V_f, V_g)\right) + 2i\hbar \{f, g\} \\
=& (i\hbar) \left(i\hbar\nabla_{\{f,g\}} + \{f, g\}\right) + (i\hbar)^2 F_\nabla(V_f, V_g) + i\hbar \{f, g\} \\
=& i\hbar Q(\{f, g\}) + (i\hbar)^2 F_\nabla(V_f, V_g) + i\hbar \{f, g\} \\
=& i\hbar Q(\{f, g\}) + (i\hbar)^2 F_\nabla(V_f, V_g) + i\hbar \iota_{V_f}\iota_{V_g}\omega
\end{aligned}$$

Thus if the curvature 2-form is

$$F_\nabla = -\frac{i}{\hbar}\omega$$

then the following relation holds

$$[Q(f), Q(g)] = i\hbar Q(\{f, g\}).$$

This calculation motivates the following definition.

Definition 3.5.2. A prequantum line bundle on (M, ω) is a Hermitian line bundle $(\mathscr{L}, \langle -, - \rangle)$ with a compatible connection ∇ such that its curvature 2-form F_∇ satisfies

$$F_\nabla = -\frac{i}{\hbar}\omega.$$

Here we recall a Hermitian line bundle is a complex line bundle $\mathscr{L}$ with a smoothly varying family of Hermitian inner products $\langle -, - \rangle$ on fibers of $\mathscr{L}$. Our convention for Hermitian inner product is that $\langle -, - \rangle$ is complex-conjugate linear in the first argument and complex linear in the second. Thus for any local sections $s, s_1, s_2 \in \Gamma(U, \mathscr{L})$ and a local function $f \in C^\infty(U)$,

- $\overline{\langle s_1, s_2 \rangle} = \langle s_2, s_1 \rangle$
- $\langle f s_1, s_2 \rangle = \overline{f} \langle s_1, s_2 \rangle$
- $\langle s_1, f s_2 \rangle = f \langle s_1, s_2 \rangle$
- $\langle s, s \rangle \geq 0$ and $\langle s, s \rangle = 0 \iff s = 0$.

The connection ∇ is said to be compatible with the Hermitian inner product if for any real vector field X on M and local sections s_1, s_2 of $\mathscr{L}$,

$$X \langle s_1, s_2 \rangle = \langle \nabla_X s_1, s_2 \rangle + \langle s_1, \nabla_X s_2 \rangle .$$

The Hermitian structure $\langle -, - \rangle$ induces a Hermitian inner product $\langle - | - \rangle$ between global sections of $\mathscr{L}$ by

$$\langle s_1 | s_2 \rangle := \int_M \langle s_1, s_2 \rangle \frac{\omega^n}{n!}.$$

We obtain a Hilbert space $L^2(M,\mathscr{L})$ by square integrable measurable sections of $\mathscr{L}$. Thus

$$||s|| := \left(\int_M \langle s,s\rangle \frac{\omega^n}{n!}\right)^{\frac{1}{2}} < \infty \quad \text{for} \quad s \in L^2(M,\mathscr{L}).$$

Let $(\mathscr{L},\omega,\langle -,-\rangle)$ be a prequantum line bundle on (M,ω). For a smooth function f, we assign the following operator

$$Q(f) = i\hbar\nabla_f + f: \quad \Gamma(M,\mathscr{L}) \longrightarrow \Gamma(M,\mathscr{L}).$$

The curvature condition $F_\nabla = -\frac{i}{\hbar}\omega$ implies

$$[Q(f),Q(g)] = i\hbar Q(\{f,g\})$$

so condition Q4 is satisfied. Also we have

$$Q(1) = 1$$

so condition Q2 is satisfied. Condition Q1 on $\mathbb{R}$-linearity is obvious.

Let us examine condition Q3. Let $s_1, s_2 \in \Gamma_c(M,\mathscr{L})$ be two sections of $\mathscr{L}$ with compact support. Let f be a real smooth function on M. Compatibility of ∇ with $\langle -,-\rangle$ implies

$$\nabla_f \langle s_1,s_2\rangle = \langle \nabla_f s_1, s_2\rangle + \langle s_1, \nabla_f s_2\rangle .$$

Integrating over M with respect to the volume form $\frac{\omega^n}{n!}$, we find

$$\begin{aligned}
&\langle \nabla_f s_1|s_2\rangle + \langle s_1|\nabla_f s_2\rangle \\
=&\int_M \left(\langle \nabla_f s_1,s_2\rangle + \langle s_1,\nabla_f s_2\rangle\right)\frac{\omega^n}{n!} \\
=&\int_M \nabla_f \langle s_1,s_2\rangle \frac{\omega^n}{n!} \\
=&\int_M \left(\mathscr{L}_{V_f}\langle s_1,s_2\rangle\right)\frac{\omega^n}{n!} \\
=&-\int_M \langle s_1,s_2\rangle \mathscr{L}_{V_f}\left(\frac{\omega^n}{n!}\right) = 0.
\end{aligned}$$

Here in the last step, we have used the Liouville Theorem on the invariance of the Liouville volume form under Hamiltonian flows. This implies the self-adjoint relation

$$\langle Q(f)s_1|s_2\rangle = \langle s_1|Q(f)s_2\rangle.$$

Thus a prequantum line bundle leads to a quantization that satisfies conditions Q1-Q4.

The above discussion is based on a given prequantum line bundle. However, it is not clear whether prequantum line bundles exist or not. There is indeed a topological obstruction for it.

The 2-form

$$\frac{i}{2\pi}F_\nabla$$

is closed, and its de Rham cohomology class

$$\left[\frac{i}{2\pi}F_\nabla\right] = c_1(\mathscr{L})$$

represents the first Chern class of L. One remarkable feature of Chern class is the integrality:

$$\frac{i}{2\pi}\int_\Sigma F_\nabla \in \mathbb{Z}$$

for any closed surface Σ. Therefore $\frac{1}{2\pi\hbar}[\omega]$ represents an integral cohomology class. The converse is also true: if $\frac{1}{2\pi\hbar}[\omega]$ is integral, then there exists a prequantum line bundle.

Definition 3.5.3. We say the symplectic manifold (M,ω) is quantizable (for a particular value of $\hbar$) if

$$\frac{1}{2\pi\hbar}\int_\Sigma \omega \in \mathbb{Z}$$

for every closed surface Σ in M.

Thus on a quantizable phase space, we can construct a quantization satisfying Q1-Q4. Note that such a quantization is far from expectation in quantum mechanics. For example

$$Q(f) = i\hbar\nabla_f + f$$

is always a first order differential operator for any function f. But we should expect higher order differential operators, such as Schrödinger operator, in quantum mechanics. The problem is condition Q5, i.e., the above constructed Hilbert space $L^2(M,\mathscr{L})$ is too big. We will consider how to cut down the degrees of freedom in Section 3.5.4.

Example 3.5.4. *Consider the total space of the cotangent bundle*

$$M = T^*X, \quad \omega = d\theta$$

where θ is the Liouville 1-form. Since ω is exact,

$$\int_\Sigma \omega = \int_\Sigma d\theta = 0$$

for any closed surface $\Sigma \subset M$. Thus cotangent bundles are always quantizable. In fact, we can choose $\mathscr{L}$ to be the trivial line bundle and the connection by

$$\nabla = d - \frac{i}{\hbar}\theta.$$

Example 3.5.5. $M = S^2 = \left\{x^2+y^2+z^2=1\right\} \subset \mathbb{R}^3$.

$$\omega = A(xdydz + ydzdx + zdxdy), \qquad A > 0.$$

We have

$$\int_{S^2}\omega = \int_{x^2+y^2+z^2\le 1} d\omega = 4\pi A.$$

Thus (M,ω) is quantizable $\iff$ $A \in \frac{\hbar}{2}\mathbb{Z}$.

3.5.4 Polarization and Quantum States

The problem with the Hilbert space $L^2(M, \mathscr{L})$ arising from a prequantum line bundle $\mathscr{L}$ on a quantizable symplectic manifold M is that it is too big. For example on $M = \mathbb{R}^{2n}$, a section ψ of $\mathscr{L}$ depends on both the position $\mathbf{x}$ and the momentum $\mathbf{p}$, thus can not be the candidate of a wave function in quantum mechanics. We need a way to eliminate "half" of the variables. The notion of polarization serves for this purpose.

Let $T^{\mathbb{C}}M = TM \otimes_{\mathbb{R}} \mathbb{C}$ denote the complexification of the tangent bundle TM. Let

$$\begin{aligned} \overline{} : T^{\mathbb{C}}M &\longrightarrow T^{\mathbb{C}}M \\ X &\longmapsto \overline{X} \end{aligned}$$

denote the complex conjugate. The symplectic form ω extends $\mathbb{C}$-linearly to a non-degenerate pairing on $T^{\mathbb{C}}M$ and we still denote it by ω.

Assume $\dim_{\mathbb{R}}(M) = 2n$. For any $z \in M$, a $\mathbb{C}$-linear subspace $P \subset T_z^{\mathbb{C}}M$ is called a Lagrangian subspace if $\dim_{\mathbb{C}} P = n$ and

$$\omega(X, Y) = 0, \qquad \forall X, Y \in P.$$

Definition 3.5.6. A polarization of (M, ω) is a complex subbundle $P \subset T^{\mathbb{C}}M$ such that

① for any $z \in M$, P_z is a Lagrangian subspace of $T_z^{\mathbb{C}}M$

② integrability: for any open subset U,

$$X, Y \in \Gamma(U, P) \qquad \Longrightarrow \qquad [X, Y] \in \Gamma(U, P)$$

Here $[X, Y]$ is the Lie bracket of two vector fields.

③ $\dim(P_z \cap \overline{P}_z)$ is constant for $z \in M$.

Condition ③ is a technical assumption for the purpose of certain constructions.

We will be mainly interested in the following two types of polarizations:

a) Real Polarization: $P_z = \overline{P}_z$, $\forall z \in M$

b) Kähler Polarization: $P_z \cap \overline{P}_z = \{0\}$, $\forall z \in M$

Definition 3.5.7. Let $(\mathscr{L}, \nabla)$ be a prequantum line bundle on (M, ω) and P be a polarization. A section $s \in \Gamma(M, \mathscr{L})$ is called P-polarized if

$$\nabla_X s = 0$$

for any vector field X in P.

Let us check the consistency of the above condition. Let X, Y be two vector fields in P. Assume $\nabla_X s = \nabla_Y s = 0$ holds, then

$$[\nabla_X, \nabla_Y]s = 0.$$

On the other hand,

$$\begin{aligned}[\nabla_X, \nabla_Y] =& \nabla_{[X,Y]} + F_\nabla(X, Y) \\ =& \nabla_{[X,Y]} - \frac{i}{\hbar}\omega(X, Y).\end{aligned}$$

Since P is a polarization, $[X, Y]$ is still a vector in P and $\omega(X, Y) = 0$. This shows the consistency of the defining equation for polarized sections.

Thus we can define the quantum Hilbert space associated to a prequantum line bundle $\mathscr{L}$ and a polarization P by

$$L^2(M, \mathscr{L})_P := \left\{ s \in L^2(M, \mathscr{L}) \,|\, s \text{ is } P\text{-polarized} \right\}.$$

Example 3.5.8. *Consider the phase space $\mathbb{R}^{2n}$ with the following prequantum line bundle*

- *$\mathscr{L}$ is the trivial line bundle on $\mathbb{R}^{2n}$ with Hermitian inner product*

$$\langle f, g \rangle = \overline{f} g$$

- *The connection ∇ is*

$$\nabla = d - \frac{i}{\hbar}\theta$$

where $\theta = \sum_i p_i dx^i$ is the Liouville 1-form. The curvature of ∇

$$F_\nabla = -\frac{i}{\hbar} d\theta = -\frac{i}{\hbar}\omega$$

satisfies the prequantization condition.

We consider the polarization P spanned by vector fields along momentum directions

$$P = \text{Span}\left\{ \frac{\partial}{\partial p_i} \right\}.$$

For any function $f(\mathbf{x}, \mathbf{p})$,

$$\nabla_{\frac{\partial}{\partial p_i}} f = \frac{\partial f}{\partial p_i} - \frac{i}{\hbar}\theta\left(\frac{\partial}{\partial p_i}\right) f = \frac{\partial f}{\partial p_i}.$$

Thus f is P-polarized if and only if

$$f = f(\mathbf{x})$$

does not depend on $\mathbf{p}$. This gives the expected result for wave functions.

If we consider another polarization P' spanned by vector fields along position directions

$$P' = \text{Span}\left\{ \frac{\partial}{\partial x^i} \right\}.$$

Since

$$\nabla_{\frac{\partial}{\partial x^i}} f = \frac{\partial f}{\partial x^i} - \frac{i}{\hbar}\theta\left(\frac{\partial}{\partial x^i}\right) f = \frac{\partial f}{\partial x^i} - \frac{i}{\hbar} p_i f,$$

f is P'-polarized if and only if f is of the form

$$f = e^{\frac{i}{\hbar}\mathbf{x}\cdot\mathbf{p}} g(\mathbf{p}).$$

Example 3.5.9. *Consider the phase space $\mathbb{C}^n$ with Kähler symplectic form*

$$\omega = i\partial\bar{\partial}K.$$

Here K is a real function called the Kähler potential. We choose the prequantum line bundle $\mathscr{L}$ to be the trivial line bundle with Hermitian inner product

$$\langle f_1, f_2\rangle = \overline{f}_1 f_2 e^{-\frac{K}{\hbar}}$$

and compatible connection

$$\nabla = d - \frac{1}{\hbar}\partial K.$$

Its curvature

$$F_\nabla = -\frac{1}{\hbar} d(\partial K) = -\frac{1}{\hbar}\bar{\partial}\partial K = \frac{1}{\hbar}\partial\bar{\partial}K = -\frac{i}{\hbar}\omega$$

satisfies the prequantization condition.

We choose the Kähler polarization spanned by vector fields of $(0,1)$-type

$$P = \mathrm{Span}\left\{\frac{\partial}{\partial\overline{z}^1}, \cdots, \frac{\partial}{\partial\overline{z}^n}\right\}.$$

Since

$$\nabla_{\frac{\partial}{\partial\overline{z}^j}} f = \frac{\partial f}{\partial\overline{z}^j}$$

f is P-polarized if and only if $f = f(\mathbf{z})$ is holomorphic. The resulting quantum Hilbert space consists of holomorphic functions $f(\mathbf{z})$ such that

$$\int_{\mathbb{C}^n} |f(\mathbf{z})|^2 e^{-\frac{K}{\hbar}} \frac{\omega^n}{n!} < \infty.$$

For $K = |\mathbf{z}|^2$, we find precisely the Segal-Bargmann space.

Example 3.5.10. *We generalize the above construction to a complex manifold M with a hermitian holomorphic line bundle $\mathscr{L}$. Let ∇ be the compatible connection on $\mathscr{L}$ such that*

$$\nabla = \nabla^{1,0} + \nabla^{0,1} \qquad \text{where} \quad \nabla^{0,1} = \bar{\partial}.$$

Assume the first Chern class $\frac{i}{2\pi}F_\nabla$ defines a symplectic form on M.

We consider the phase space (M,ω) where

$$\omega = i\hbar F_\nabla.$$

By construction, $(\mathscr{L},\nabla)$ defines a prequantum line bundle. We choose the polarization

$$P = T^{0,1}M$$

spanned by vector fields of type $(0,1)$. *In local holomorphic coordinates* $\{z^i\}$, P *is spanned by* $\left\{\frac{\partial}{\partial \overline{z}^i}\right\}$. *Thus* P*-potential sections are holomorphic sections of* $\mathscr{L}$.

Assume M *is compact. Then the space* $H^0(M,\mathscr{L})$ *of holomorphic sections is finite dimensional. Thus we obtain a finite dimensional quantum Hilbert space*

$$\mathbb{H} = H^0(M,\mathscr{L}).$$

Such Hilbert space can be used to describe internal degrees of freedom in a quantum system.

As an example, we consider

$$M = \mathbb{C}P^1 = \{\textit{lines in } \mathbb{C}^2\}.$$

It is covered by two holomorphic charts

$$z \in U = \mathbb{C}, \qquad w \in V = \mathbb{C}$$

which are glued along $\mathbb{C}^*$ *by identifying*

$$z = \frac{1}{w}.$$

We consider the holomorphic line bundle

$$\mathscr{L} = \mathcal{O}_{\mathbb{C}P^1}(k), \qquad k \in \mathbb{Z}^{>0}$$

whose transition function from U *to* V *is* w^k *on the intersection* $U \cap V$. *A holomorphic section is given by a pair* $(f(z), g(w))$ *where*

- $f(z)$ *is holomorphic on* U
- $g(w)$ *is holomorphic on* V
- $f(z)w^k = g(w)$ *on* $U \cap V$

We find $f(z)$ *can only be a polynomial of* $\deg \leq k$, *and* $g(w) = f(w^{-1})w^k$. *Thus*

$$H^0(\mathbb{C}P^1,\mathscr{L}) = \mathrm{Span}_{\mathbb{C}}\left\{1, z, \cdots, z^k\right\}$$

which has $\dim = k+1$. *It is precisely the spin* $k/2$ *representation of* $\mathrm{su}(2)$.

We can also write down the symplectic form explicitly. In the holomorphic chart U,

$$\omega = ik\hbar \frac{dz \wedge d\overline{z}}{(1+|z|^2)^2}.$$

Example 3.5.11. *We continue with our previous example but change a point of view. Let* $(\mathscr{L}_0, \nabla_0)$ *be a fixed Hermitian holomorphic line bundle on the complex manifold* M *whose first Chern class gives a symplectic form*

$$\omega = \frac{i}{2\pi} F_{\nabla_0}.$$

Let us consider the k*-th tensor* $\mathscr{L} = \mathscr{L}_0^{\otimes k}$ *with induced connection* ∇ *from* ∇_0. *Then*

$$F_\nabla = kF_{\nabla_0} = -i(2\pi k)\omega.$$

Thus $(\mathscr{L}, \nabla)$ defines a prequantum line bundle if we identify

$$\hbar = \frac{1}{2\pi k}$$

In particular, the semi-classical limit $\hbar \to 0$ corresponds to $k \to \infty$.

Assume M is compact, so the quantum Hilbert space $H^0(M, \mathscr{L})$ is finite dimensional. Let

$$\chi(M, \mathscr{L}) := \sum_i (-1)^i \dim H^i(M, \mathscr{L})$$

be the Euler characteristic of $\mathscr{L}$. By Hirzebruch–Riemann–Roch Theorem,

$$\chi(M, \mathscr{L}) = \int_M \mathrm{ch}(\mathscr{L}) \,\mathrm{td}(M)$$

where $\mathrm{td}(M)$ is the Todd class of the tangent bundle of M. In the case above where $\mathscr{L}_0$ is a positive line bundle, we have

$$H^i(M, \mathscr{L}_0^{\otimes k}) = 0 \qquad \text{for } i > 0 \text{ and } k \text{ sufficiently large}$$

Thus in the $k \to \infty$ limit, we have the leading behavior for $\mathscr{L} = \mathscr{L}_0^{\otimes k}$

$$\begin{aligned} \dim H^0(M, \mathscr{L}) = \int_M e^{\frac{i}{2\pi} F_\nabla} \,\mathrm{td}(M) = \int_M e^{k\omega} \,\mathrm{td}(M) \\ \sim k^n \int_M \frac{\omega^n}{n!} = k^n \,\mathrm{Vol}_\omega(M) \end{aligned}$$

where $2n = \dim_{\mathbb{R}} M$ and $\mathrm{Vol}_\omega(M)$ is the Liouville volume of M. Under the identification $\hbar = \frac{1}{2\pi k}$, we find the semi-classical behavior

$$\dim H^0(M, \mathscr{L}) \sim \frac{1}{(2\pi\hbar)^n} \,\mathrm{Vol}_\omega(M).$$

This leads to the semi-classical intuition that the number of quantum states is approximately the number of cells in phase space measured in units of $\hbar$.

3.5.5 Quantum Operators

Let (M, ω) be a quantizable symplectic manifold, with a chosen prequantum line bundle $(\mathscr{L}, \nabla)$ and a polarization $P \subset T^{\mathbb{C}}M$. Next we consider how to quantize functions $f \in C^\infty(M)$ to operators on the quantum Hilbert space $L^2(M, \mathscr{L})_P$.

There is a special class of functions that are naturally quantized. These are functions that preserve the polarization P.

Definition 3.5.12. A function f is called P-preserving if its Hamiltonian vector field V_f satisfies

$$[V_f, P] \subset P$$

i.e., for any vector field X in P, the Lie bracket $[V_f, X]$ is still a vector field in P. The collection of P-preserving functions will be denoted by $C^\infty(M)_P$.

Proposition 3.5.13. *Let $\psi \in \Gamma(M, \mathscr{L})$ be a P-polarized section of $\mathscr{L}$, and $f \in C^\infty(M)_P$ be a P-preserving function. Then $Q(f)\psi$ is also a P-polarized section of $\mathscr{L}$.*

Proof: Recall the prequantization map

$$Q(f) = i\hbar\nabla_f + f.$$

Let X be any vector field in P. Then

$$\begin{aligned}
[\nabla_X, Q(f)] =& [\nabla_X, i\hbar\nabla_f + f] \\
=& i\hbar\nabla_{[X,V_f]} + i\hbar F_\nabla(X, V_f) + X(f) \\
=& i\hbar\nabla_{[X,V_f]} + \omega(X, V_f) + X(f) \\
=& i\hbar\nabla_{[X,V_f]} - \iota_X\iota_{V_f}\omega + X(f) \\
=& i\hbar\nabla_{[X,V_f]} - \iota_X df + X(f) \\
=& i\hbar\nabla_{[X,V_f]}.
\end{aligned}$$

By assumption, $[X, V_f]$ is still a vector field in P. Thus for a P-polarized section ψ,

$$\begin{aligned}
\nabla_X Q(f)\psi =& [\nabla_X, Q(f)]\psi && \text{since } \nabla_X\psi = 0 \\
=& i\hbar\nabla_{[X,V_f]}\psi \\
=& 0 && \text{since } [X, V_f] \text{ lies in } P.
\end{aligned}$$

Therefore $Q(f)\psi$ is also a P-polarized section. □

Thus for a P-preserving function f, we can simply quantize it to the operator $Q(f)$ on the quantum Hilbert space.

For functions that are not P-preserving, their quantization is more tricky. The basic idea is that their Hamiltonian flows will change the polarization, hence will change a P-polarized state to a state that is polarized with a different polarization. Then one can construct a map relating quantum Hilbert spaces associated to different polarizations. This is the idea of Blattner-Kostant-Sternberg (BKS) kernel construction. We will not go into further details here.

Example 3.5.14. *Consider the phase space*

$$\mathbb{R}^{2n}, \qquad \omega = \sum_i dp_i \wedge dx^i$$

with prequantum line bundle

$$\nabla = d - \frac{i}{\hbar}\theta, \qquad \theta = \sum_i p_i dx^i$$

and polarization

$$P = \text{Span}\left\{\frac{\partial}{\partial p_i}\right\}.$$

Consider a function $f(\mathbf{x}, \mathbf{p})$ whose Hamiltonian vector field is

$$V_f = \sum_i \left(\partial_{x^i} f \frac{\partial}{\partial p_i} - \partial_{p_i} f \frac{\partial}{\partial x^i}\right).$$

From

$$\left[\frac{\partial}{\partial p_k}, V_f\right] = \sum_i \left(\partial_{p_k}\partial_{x^i} f\right)\frac{\partial}{\partial p_i} - \sum_i \left(\partial_{p_k}\partial_{p_i} f\right)\frac{\partial}{\partial x^i}$$

we see that V_f *preserves* P *if and only if*

$$\partial_{p_k}\partial_{p_i} f = 0, \qquad \forall i, k.$$

Thus $C^\infty(\mathbb{R}^{2n})_P = \left\{a(\mathbf{x}) + \sum_i b_i(\mathbf{x})p_i\right\}$ *consists of functions at most linear in* p_i*. Such a function* $f = a(\mathbf{x}) + \sum_i b_i(\mathbf{x})p_i$ *is quantized to*

$$Q(f) = i\hbar\left(V_f - \frac{i}{\hbar}\theta(V_f)\right) + f = -i\hbar\sum_i b_i(\mathbf{x})\frac{\partial}{\partial x^i} + a(\mathbf{x})$$

as an operator acting on wave functions $\psi = \psi(\mathbf{x})$*.*

Example 3.5.15. *Consider the phase space*

$$\mathbb{C}^n, \qquad \omega = i\partial\bar{\partial}K$$

where K *is the Kähler potential. We choose the prequantum line bundle* $\mathscr{L}$ *to be the trivial line bundle with Hermitian inner product by*

$$\langle f_1, f_2\rangle = \overline{f}_1 f_2 e^{-\frac{K}{\hbar}}$$

and compatible connection by

$$\nabla = d - \frac{1}{\hbar}\partial K.$$

Its curvature

$$F_\nabla = -\frac{1}{\hbar}d(\partial K) = -\frac{1}{\hbar}\bar{\partial}\partial K = \frac{1}{\hbar}\partial\bar{\partial}K = -\frac{i}{\hbar}\omega$$

satisfies the prequantization condition. We choose the Kähler polarization

$$P = \mathrm{Span}\left\{\frac{\partial}{\partial\overline{z}^i}\right\}$$

so polarized sections of $\mathscr{L}$ *are holomorphic functions.*

Let us write the Kähler form as

$$\omega = \sum_{j,m} g_{j\overline{m}} dz^j \wedge d\overline{z}^m$$

where $g_{j\overline{m}} = i\partial_j\partial_{\overline{m}}K$*. Let* $g^{\overline{m}j}$ *denote the inverse matrix of* $g_{j\overline{m}}$*, i.e.,*

$$\sum_{\overline{m}} g_{i\overline{m}}g^{\overline{m}j} = \delta_i{}^j.$$

Let f *be a function on* $\mathbb{C}^n$*. Its Hamiltonian vector field is given by*

$$V_f = \sum_{j,\overline{m}}\left(g^{\overline{m}j}\partial_{\overline{m}} f\frac{\partial}{\partial z^j} - g^{\overline{m}j}\partial_j f\frac{\partial}{\partial\overline{z}^m}\right)$$

where $\partial_{\overline{m}} = \frac{\partial}{\partial \overline{z}^m}$ *and* $\partial_j = \frac{\partial}{\partial z^j}$. *Since*

$$\left[\frac{\partial}{\partial \overline{z}^i}, V_f\right] = \sum_{j,\overline{m}} \frac{\partial}{\partial \overline{z}^i}\left(g^{\overline{m}j}\partial_{\overline{m}} f\right)\frac{\partial}{\partial z^j} \qquad \textit{modulo } P$$

we see that f *is* P*-preserving if and only if*

$$\sum_{\overline{m}} \frac{\partial}{\partial \overline{z}^i}\left(g^{\overline{m}j}\frac{\partial}{\partial \overline{z}^m} f\right) = 0, \qquad \forall i, j.$$

Now we specialize to the case when

$$K = |\mathbf{z}|^2, \qquad g_{j\overline{m}} = i\delta_{jm}.$$

Then the condition for P*-preserving becomes*

$$\frac{\partial}{\partial \overline{z}^i}\frac{\partial}{\partial \overline{z}^j} f = 0, \qquad \forall i, j$$

i.e., f *is at most linear in* $\overline{z}^i$*'s. If we further require real condition, then the only real* P*-preserving functions are of the form*

$$f = a + b_k z^k + \overline{b}_k \overline{z}^k + c_{k\overline{j}} z^k \overline{z}^j,$$

where $a \in \mathbb{R}$, $b_k, c_{k\overline{j}} \in \mathbb{C}$ *and* $\overline{c_{k\overline{j}}} = c_{j\overline{k}}$. *The Hamiltonian vector of* f *is*

$$V_f = -i\sum_k \left(\partial_{\overline{k}} f \frac{\partial}{\partial z^k} - \partial_k f \frac{\partial}{\partial \overline{z}^k}\right).$$

Thus f *is quantized to*

$$\begin{aligned} Q(f) =& i\hbar\left(V_f - \frac{1}{\hbar}\partial K(V_f)\right) + f \\ =& \hbar\sum_k \partial_{\overline{k}} f \frac{\partial}{\partial z^k} - \sum_k \overline{z}^k \frac{\partial}{\partial \overline{z}^k} f + f \\ =& a + \sum_k b_k z^k + \hbar\sum_k \left(\overline{b}_k + c_{j\overline{k}} z^j\right)\frac{\partial}{\partial z^k} \end{aligned}$$

as an operator acting on holomorphic functions.

This makes holomorphic representation particularly useful for quantization of quadratic Hamiltonians. For example, consider one-dimensional Harmonic oscillator with Hamiltonian

$$\mathscr{H} = |z|^2 \qquad \text{on} \quad \mathbb{C}.$$

The above Kähler polarization quantizes $\mathscr{H}$ to the operator

$$Q(\mathscr{H}) = \hbar z \frac{\partial}{\partial z}$$

on the Segal-Bargmann space. Note that

$$Q(\mathscr{H}) z^n = n\hbar z^n,$$

thus eigenvalues of $Q(\mathscr{H})$ are non-negative integers in unit of $\hbar$. However, this is not the correct spectrum: the Maslov correction is missing.

This is the same problem that we have encountered in our discussion on semi-classical quantization. The way out is to modify our quantum Hilbert space by including half-densities. In the Kähler quantization, this modification amounts to define a quantum state ψ to be a section of $\mathscr{L} \otimes \sqrt{K_M}$ where K_M is the canonical line bundle and $\sqrt{K_M}$ is a square root of it.

In the Harmonic oscillator example above, this modification amounts to change the state

$$z^n \longrightarrow z^n \sqrt{dz}$$

which will then have the correct eigenvalue $\left(n + \frac{1}{2}\right)\hbar$ under $Q(\mathscr{H}) = \hbar z \frac{\partial}{\partial z}$.

3.6 Path Integral in Phase Space

Classical Hamiltonian mechanics is captured by the following action in the phase space

$$S = \int (pdq - \mathscr{H} dt) = \int \left(p_i(t)\dot{q}^i(t) - \mathscr{H}(p(t), q(t))\right) dt.$$

Here $\{p_i(t), q^i(t)\}$ represents a path of classical particle in the phase space and t is the time variable. Classical trajectories are extremals of this action and can be obtained via functional variation (with fixed boundary values of q^i)

$$\begin{aligned}
\delta S &= \int \left[\delta p_i \dot{q}^i + p_i \frac{d}{dt}(\delta q^i) - \left(\frac{\partial \mathscr{H}}{\partial p_i}\delta p_i + \frac{\partial \mathscr{H}}{\partial q^i}\delta q^i\right)\right] dt \\
&= \int \left(\delta p_i \dot{q}^i - \dot{p}_i \delta q^i - \frac{\partial \mathscr{H}}{\partial p_i}\delta p_i - \frac{\partial \mathscr{H}}{\partial q^i}\delta q^i\right) dt \\
&= \int \left[\left(\dot{q}^i - \frac{\partial \mathscr{H}}{\partial p_i}\right)\delta p_i - \left(\dot{p}_i + \frac{\partial \mathscr{H}}{\partial q^i}\right)\delta q^i\right] dt.
\end{aligned}$$

Requiring the extremal condition $\delta S = 0$, we obtain the Hamilton's equations

$$\begin{cases}
\dot{q}^i = \dfrac{\partial \mathscr{H}}{\partial p_i} \\
\dot{p}_i = -\dfrac{\partial \mathscr{H}}{\partial q^i}
\end{cases}$$

Quantum mechanically, transition amplitudes and correlation functions are captured by the form of path integral

$$\int [DqDp]\, e^{\frac{i}{\hbar}S} \mathcal{O}.$$

In this section, we will discuss perturbative approach to such path integral in the asymptotic $\hbar \to 0$ limit in terms of Feynman's combinatorial formula of graph expansion.

3.6.1 Wick's Theorem

Gaussian Integral

We start with the finite dimensional situation. Let

$$Q(x) = \sum_{i,j=1}^{n} Q_{ij} x^i x^j$$

be a positive definite quadratic form, i.e., the matrix (Q_{ij}) is positive definite. Consider the following volume form on $\mathbb{R}^n$

$$\Omega = \sqrt{\det Q} \prod_{i=1}^{n} \frac{dx^i}{\sqrt{2\pi\hbar}} e^{-\frac{1}{2\hbar}Q(x)}, \qquad \hbar > 0.$$

By the Gaussian integral $\int_{\mathbb{R}} dx\, e^{-\frac{1}{2}x^2} = \sqrt{2\pi}$, it is easy to find

$$\int_{\mathbb{R}^n} \Omega = 1.$$

Thus Ω defines a probability density on $\mathbb{R}^n$.

Consider for simplicity a polynomial function $f(x) \in \mathbb{R}[x^i]$. Define the following expectation value with respect to the probability density Ω:

$$\langle f(x) \rangle_x := \frac{\int_{\mathbb{R}^n} \Omega f(x)}{\int_{\mathbb{R}^n} \Omega} = \int_{\mathbb{R}^n} \Omega f(x).$$

The subscript x indicates the integration variable. This expectation value defines a map

$$\langle - \rangle_x : \mathbb{R}[x^i] \longrightarrow \mathbb{R}.$$

To compute this expectation map, let us consider the auxiliary integral

$$\begin{aligned} Z[J] :=& \left\langle e^{\sum_i x^i J_i} \right\rangle_x \qquad J = (J_1, \cdots, J_n) \\ =& \sqrt{\det Q} \int_{\mathbb{R}^n} \prod_{i=1}^{n} \frac{dx^i}{\sqrt{2\pi\hbar}} e^{-\frac{1}{2\hbar}Q(x) + \sum_i x^i J_i} \end{aligned}$$

Completing the square, we find

$$\frac{1}{2\hbar}Q(x) - \sum_i x^i J_i = \frac{1}{2\hbar}Q(x^i - \hbar \sum_j (Q^{-1})^{ij} J_j) - \frac{\hbar}{2} Q^{-1}(J).$$

Here $(Q^{-1})^{ij}$ is the inverse matrix of Q_{ij}

$$\sum_k Q_{ik} (Q^{-1})^{kj} = \delta_i{}^j$$

and $Q^{-1}(J)$ is the quadratic expression

$$Q^{-1}(J) = \sum_{i,j} (Q^{-1})^{ij} J_i J_j.$$

Thus

$$Z[J] = e^{\frac{\hbar}{2} Q^{-1}(J)} \int_{\mathbb{R}^n} \Omega = e^{\frac{\hbar}{2} Q^{-1}(J)}.$$

Now for a polynomial $f(x)$, Taylor series expansion at $x = 0$ gives

$$f(x) = e^{\sum_i x^i \frac{\partial}{\partial a^i}} f(a) \Big|_{a=0}.$$

Using this formula, we find

$$\begin{aligned} \langle f(x) \rangle_x =& \left\langle e^{\sum_i x^i \frac{\partial}{\partial a^i}} f(a) \Big|_{a=0} \right\rangle_x \\ \xlongequal{J = \frac{\partial}{\partial a}} & Z\left[\frac{\partial}{\partial a}\right] f(a) \Big|_{a=0} = e^{\frac{\hbar}{2} Q^{-1}\left(\frac{\partial}{\partial a}\right)} f(a) \Big|_{a=0} \end{aligned}$$

where $Q^{-1}\left(\frac{\partial}{\partial a}\right) = \sum_{i,j} (Q^{-1})^{ij} \frac{\partial}{\partial a^i} \frac{\partial}{\partial a^j}$ is a second-order differential operator.

Wick's Theorem

The obtained formula

$$\langle f(x)\rangle_x = e^{\frac{\hbar}{2}Q^{-1}(\frac{\partial}{\partial a})} f(a)\Big|_{a=0}$$

has a combinatorial interpretation as follows. Let

$$i_1, i_2, \cdots, i_{2m} \in \{1, 2, \cdots, n\}$$

be $2m$ indices. We consider the monomial $x^{i_1}x^{i_2}\cdots x^{i_{2m}}$ of degree $2m$ obtained from the index set. Let us compute its expectation from the above formula:

$$\left\langle x^{i_1}x^{i_2}\cdots x^{i_{2m}}\right\rangle_x = e^{\frac{\hbar}{2}Q^{-1}(\frac{\partial}{\partial a})} a^{i_1}a^{i_2}\cdots a^{i_{2m}}\Big|_{a=0} = \frac{\hbar^m}{m!}\left[\frac{1}{2}\sum_{i,j}(Q^{-1})^{ij}\frac{\partial}{\partial a^i}\frac{\partial}{\partial a^j}\right]^m a^{i_1}a^{i_2}\cdots a^{i_{2m}} \tag{*}$$

To compute this value, let

$$P(2m) = \text{ set of partitions of } \{1, 2, \cdots, 2m\} \text{ into unordered } m \text{ pairs.}$$

An element $\sigma \in P(2m)$ can be described by a permutation $\sigma \in S_{2m}$ such that

$$\sigma(1) < \sigma(2), \quad \sigma(3) < \sigma(4), \quad \cdots, \quad \sigma(2m-1) < \sigma(2m)$$

and

$$\sigma(1) < \sigma(3) < \cdots < \sigma(2m-3) < \sigma(2m-1).$$

Then we identify this permutation

$$\begin{bmatrix} 1 & 2 & 3 & \cdots & 2m-1 & 2m \\ \sigma(1) & \sigma(2) & \sigma(3) & \cdots & \sigma(2m-1) & \sigma(2m) \end{bmatrix}$$

with an element of $P(2m)$ by pairing

$$\underbrace{\sigma(1)\sigma(2)}_{\text{pair}} \quad \underbrace{\sigma(3)\sigma(4)}_{\text{pair}} \quad \cdots \quad \underbrace{\sigma(2m-1)\sigma(2m)}_{\text{pair}}$$

In the above formula (*), it is computed to become the following sum

$$\boxed{\left\langle x^{i_1}x^{i_2}\cdots x^{i_{2m}}\right\rangle_x = \hbar^m \sum_{\sigma\in P(2m)} (Q^{-1})^{\sigma(1)\sigma(2)}(Q^{-1})^{\sigma(3)\sigma(4)}\cdots(Q^{-1})^{\sigma(2m-1)\sigma(2m)}}.$$

This is called the **Wick's Theorem**.

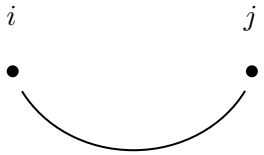
We can also draw each sum as

For each edge connecting i and j, we assign the factor $\hbar(Q^{-1})^{ij}$ to it.

Example 3.6.1 (Two-point function)**.** *The two-point function*

$$\left\langle x^i x^j \right\rangle_x = \hbar(Q^{-1})^{ij}$$

*is given by the inverse matrix of Q. $(Q^{-1})^{ij}$ is also called the "**propagator**".*



Example 3.6.2. *The following four-point function is computed by*

$$\begin{aligned}\left\langle x^i x^j x^k x^l \right\rangle_x =& \sqcap\!\!\sqcap ijkl + \sqcap\!\sqcap\!\sqcap ijkl + \sqcap\!\sqcap\!\sqcap ijkl \\ =& \hbar^2 \left[(Q^{-1})^{ij}(Q^{-1})^{kl} + (Q^{-1})^{ik}(Q^{-1})^{jl} + (Q^{-1})^{il}(Q^{-1})^{jk} \right].\end{aligned}$$

We can also add "background" by considering the shift $x \to x + a$

$$\langle f(x+a) \rangle_x = \int_{\mathbb{R}^n} \Omega\, f(x+a)$$

which is now a function of a. A similar argument shows

$$\langle f(x+a) \rangle_x = e^{\frac{\hbar}{2} Q^{-1}\left(\frac{\partial}{\partial a}\right)} f(a).$$

If $f(x) = x^{i_1} x^{i_2} \cdots x^{i_k}$, then Wick's Theorem in this case is a sum over partial pairings

We assign the propagator to the paired indices and assign a^i to unpaired index i.

Example 3.6.3. *Let $f(x) = x^i x^j x^k x^l$. Then*

$$\begin{aligned}\langle f(x+a) \rangle_x =& ijkl + \sqcap ijkl + \sqcap\!\!\sqcap ijkl + \sqcap\!\!\sqcap\!\!\sqcap ijkl + \sqcap ijkl + \sqcap\!\!\sqcap ijkl + \sqcap ijkl + \sqcap\!\!\sqcap ijkl + \sqcap\!\sqcap\!\sqcap ijkl + \sqcap\!\sqcap\!\sqcap ijkl \\ =& a^i a^j a^k a^l + \hbar \left[(Q^{-1})^{ij} a^k a^l + (Q^{-1})^{ik} a^j a^l + (Q^{-1})^{il} a^j a^k \right. \\ & \left. + (Q^{-1})^{jk} a^i a^l + (Q^{-1})^{jl} a^i a^k + (Q^{-1})^{kl} a^i a^j \right] \\ & + \hbar^2 \left[(Q^{-1})^{ij}(Q^{-1})^{kl} + (Q^{-1})^{ik}(Q^{-1})^{jl} + (Q^{-1})^{il}(Q^{-1})^{jk} \right].\end{aligned}$$

3.6.2 Feynman Graph Expansion

Now we consider integrals of the form

$$\sqrt{\det Q}\int_{\mathbb{R}^n}\prod_{i=1}^{n}\frac{dx^i}{\sqrt{2\pi\hbar}}\,e^{-\frac{1}{\hbar}S(x)}$$

where

$$S(x)=\frac{1}{2}Q(x)-\frac{\lambda}{3!}I(x).$$

Here $Q(x)=\sum_{i,j}Q_{ij}x^ix^j$ is a positive quadratic as before, and

$$I(x)=\sum_{i,j,k}I_{ijk}x^ix^jx^k$$

is a cubic polynomial, called the "**interaction**". The constants I_{ijk} parametrize the cubics. The constant λ is called the "**coupling constant**".

Since the cubic approaches both $\pm\infty$ and grows faster than quadratic, the above integral is simply "divergent". There are essentially two ways out to make sense of it:

① Complexify x^i to complex variables z^i and change the integration contour

$$\mathbb{R}^n\subset\mathbb{C}^n\qquad\Longrightarrow\qquad\Gamma\subset\mathbb{C}^n$$

to some other contour Γ such that the integration becomes convergent. "Airy integral" is such an example. This method is usually referred to as the non-perturbative method.

② Treat λ as a perturbative parameter and compute the asymptotic series. This method is usually referred to as the perturbative method.

We will focus on the perturbative method ② here. Let us rewrite

$$\text{“}\sqrt{\det Q}\int_{\mathbb{R}^n}\prod_{i=1}^{n}\frac{dx^i}{\sqrt{2\pi\hbar}}\,e^{-\frac{1}{\hbar}S(x)}\text{”}=\text{“}\int_{\mathbb{R}^n}\Omega\,e^{\frac{\lambda}{3!\hbar}I(x)}\text{”}=\text{“}\left\langle e^{\frac{\lambda}{3!\hbar}I(x)}\right\rangle_x\text{”}.$$

Here $\Omega=\sqrt{\det Q}\prod_{i=1}^{n}\frac{dx^i}{\sqrt{2\pi\hbar}}e^{-\frac{1}{2\hbar}Q(x)}$ is the probability density as before. Now we can redefine the above divergent integral as a power series by

$$\sum_{m=0}^{\infty}\frac{\lambda^m}{m!\hbar^m}\left\langle\left(\frac{1}{3!}I(x)\right)^m\right\rangle_x.$$

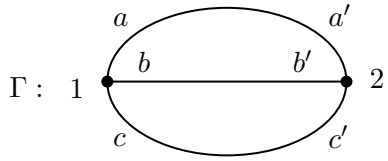
Here each term $\left\langle\left(\frac{1}{3!}I(x)\right)^m\right\rangle_x$ has a well-defined value which can be computed by Wick's Theorem. This will lead to a combinatorial graph formula for this power series.

Definition 3.6.4. By a graph γ, we refer to the following data

- $V(\gamma)=$ set of vertices
- $HE(\Gamma)=$ set of half-edges

- $i_\Gamma : HE(\Gamma) \to V(\gamma)$ incidence map
- $E(\Gamma)$: a perfect matching on $HE(\Gamma)$ into pairs of two elements. Each pair is called an "edge".
- For each $v \in V(\Gamma)$, $\#\left\{i_\Gamma^{-1}(v)\right\}$ is called the valency of v.

Example 3.6.5. *Consider the following* Θ *graph*



Here $V = \{1, 2\}$, $HE = \{a, b, c, a', b', c'\}$, $E = \{(a, a'), (b, b'), (c, c')\}$. *The incidence map is*

$$\begin{aligned} i_\Gamma : HE &\longrightarrow V \\ \{a, b, c\} &\longmapsto 1 \\ \{a', b', c'\} &\longmapsto 2 \end{aligned}$$

Both vertex 1 *and* 2 *have valency* 3.

Definition 3.6.6. A graph isomorphism between two graphs Γ and Γ' is a pair of bijections

$$\begin{aligned} \sigma_V &: V(\Gamma) \longrightarrow V(\Gamma') \\ \sigma_{HE} &: HE(\Gamma) \longrightarrow HE(\Gamma') \end{aligned}$$

which are compatible with incident maps (the following diagram commutes)

$$\begin{array}{ccc} HE(\Gamma) & \xrightarrow{\sigma_{HE}} & HE(\Gamma') \\ \downarrow{\scriptstyle i_\Gamma} & & \downarrow{\scriptstyle i'_\Gamma} \\ V(\Gamma) & \xrightarrow{\sigma_V} & V(\Gamma') \end{array}$$

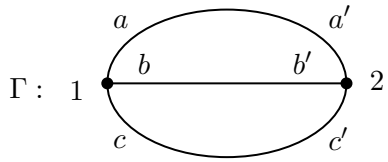
and compatible with edges: for any $a, b \in HE(\Gamma)$,

$$(a, b) \in E(\Gamma) \qquad \Longleftrightarrow \qquad (\sigma_{HE}(a), \sigma_{HE}(b)) \in E(\Gamma').$$

An automorphism of Γ is an isomorphism $\sigma : \Gamma \to \Gamma$. Denote

$$\mathrm{Aut}(\Gamma) = \text{Group of automorphisms of } \Gamma.$$

Example 3.6.7. *Consider*



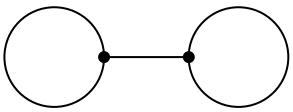
Here $HE = \{a, b, c, a', b', c'\}$, $V = \{1, 2\}$, $E = \{(a, a'), (b, b'), (c, c')\}$. *The incidence map is as above. Here are two examples of automorphisms of* Γ

① $\sigma_V : (1,2) \longrightarrow (2,1)$
$\sigma_{HE} : (a,b,c,a',b',c') \longrightarrow (a',b',c',a,b,c)$

② $\sigma_V : (1,2) \longrightarrow (1,2)$
$\sigma_{HE} : (a,b,c,a',b',c') \longrightarrow (b,c,a,b',c',a')$

Similarly, we find $\mathrm{Aut}(\Gamma) = \mathbb{Z}_2 \times S_3$. *Here,* $\mathbb{Z}_2$ *corresponds to permutation of the two vertices, and* S_3 *correponds to permutation of the three edges.*

Example 3.6.8. *Consider*

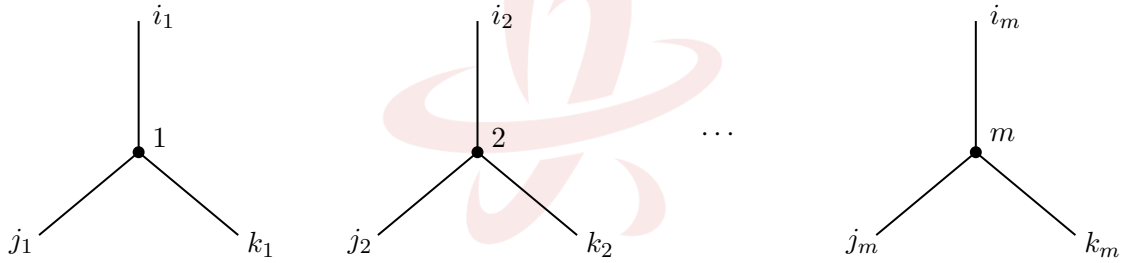
$\Gamma :$ 

We find $\mathrm{Aut}(\Gamma) = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$.

Now let us consider the computation of

$$\langle I(x)^m \rangle_x = \langle \underbrace{I(x)I(x)\cdots I(x)}_{m} \rangle_x$$

Each $I(x)$ gives a vertex with 3 half-edges



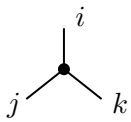
Vertex set	$V = \{1, 2, \cdots, m\}$
Half-edge set	$HE = \{i_1, j_1, k_1, i_2, j_2, k_2, , \cdots, i_m, j_m, k_m, \}$
Incidence map	$i : \{i_s, j_s, k_s\} \longrightarrow \{s\}$

By Wick's Theorem, $\langle I(x)^m \rangle_x$ is a sum over perfect matching E

$$\langle I(x)^m \rangle_x = \sum_{E \in Y} \hbar^{|E(\Gamma_E)|} \omega_{\Gamma_E}.$$

Here $Y = \{\text{perfect matchings of } HE\}$ and Γ_E is the graph by assigning the pairing E to the vertex set V and the half-edge set HE.

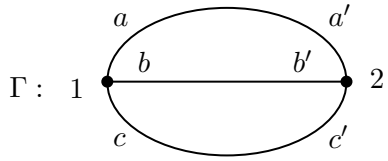
For each graph Γ, ω_Γ is the number by assigning

① each vertex  $\Longrightarrow$ I_{ijk}

② each edge i —— j $\Longrightarrow$ $(Q^{-1})^{ij}$

③ sum over indices

Example 3.6.9. *Consider*



$$\omega_\Gamma = \sum_{\substack{i_1,j_1,k_1\\ i_2,j_2,k_2}} I_{i_1j_1k_1} I_{i_2j_2k_2} (Q^{-1})^{i_1i_2} (Q^{-1})^{j_1j_2} (Q^{-1})^{k_1k_2}$$

It is clear that

$$\omega_\Gamma = \omega_{\Gamma'} \quad \text{if } \Gamma \text{ is isomorphic to } \Gamma'.$$

All graphs here are trivalent (valency 3 for each vertex). The set of bijections

$$\sigma_V : V \longrightarrow V$$
$$\sigma_{HE} : HE \longrightarrow HE$$

that preserve the incidence map is

$$G = \underbrace{S_m}_{\text{permuting vertices}} \times \underbrace{(S_3)^m}_{\text{permuting half-edges}} .$$

We have a natural G-action on Y with orbits

$$Y/G = \{\text{isomorphic class of trivalent graphs consisting of } m\text{-vertices}\}.$$

Thus

$$\begin{aligned}\frac{1}{m!(3!)^m} \langle I(x)^m \rangle_x =& \frac{1}{|G|} \sum_{\Gamma \in Y/G} \frac{|G|}{|\operatorname{Aut}(\Gamma)|} \omega_\Gamma \hbar^{|E(\Gamma)|} \\ =& \sum_{\substack{\Gamma\text{: trivalent graph}\\ \text{with } m \text{ vertices}}} \frac{\omega_\Gamma}{|\operatorname{Aut}(\Gamma)|} \hbar^{|E(\Gamma)|}\end{aligned}$$

We can also refine this formula by grouping disconnected graphs into connected isomorphic ones. This leads to the following Feynman graph expansion formula (details left to the reader).

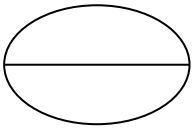
Proposition 3.6.10 (Feynman Graph Expansion Formula)**.** *We have the following combinatorial graph expansion formula for the asymptotic power series*

$$\begin{aligned}\left\langle e^{\frac{\lambda}{3!\hbar} I(x)} \right\rangle_x :=& \sum_{m=0}^{\infty} \frac{\lambda^m}{m!\hbar^m} \left\langle \left(\frac{1}{3!} I(x) \right)^m \right\rangle_x \\ =& \sum_{\Gamma\text{: } trivalent} \hbar^{|E(\Gamma)|-|V(\Gamma)|} \lambda^{|V(\Gamma)|} \frac{\omega_\Gamma}{|\operatorname{Aut}(\Gamma)|} \\ =& \exp\left(\sum_{\substack{\Gamma\text{: } connected\\ trivalent}} \lambda^{|V(\Gamma)|} \hbar^{l(\Gamma)-1} \frac{\omega_\Gamma}{|\operatorname{Aut}(\Gamma)|} \right).\end{aligned}$$

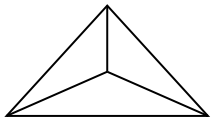
Here for a connected graph Γ*,*

$$l(\Gamma) = |E(\Gamma)| - |V(\Gamma)| + 1 = 1 - \chi(\Gamma)$$

is called the loop number of Γ*.*



$l(\Gamma) = 3 - 2 + 1 = 2$



$l(\Gamma) = 6 - 4 + 1 = 3$

In general, if the interaction contains terms of all possible degrees

$$\frac{\lambda_3}{3!} I_3(x) + \frac{\lambda_4}{4!} I_4(x) + \cdots + \frac{\lambda_m}{m!} I_m(x) + \cdots$$

then the series expension will have all possible graphs, where each vertex of valency m is associated the value I_m similarly. The general Feynman graph expansion formula reads

$$\left\langle e^{\frac{1}{\hbar}\left(\sum_{m\geq 3} \frac{\lambda_m}{m!} I_m(x)\right)} \right\rangle_x \overset{\text{asymptotic}}{=\!=\!=} \exp\left(\sum_{\substack{\Gamma\text{: connected} \\ \text{graph}}} \left(\prod_{m\geq 3} \lambda_m^{|V_m(\Gamma)|} \right) \hbar^{l(\Gamma)-1} \frac{\omega_\Gamma}{|\operatorname{Aut}(\Gamma)|} \right)$$

where $V_m(\Gamma)$ is the set of vertices with valency m.

3.6.3 Weyl Quantization Revisited

Let us apply the combinatorial formula of Feynman graph to the quantum mechanical situation. The relevant space consists of paths on the phase space parametrized by the time. For simplicity, we consider the phase space $\mathbb{R}^2$. The discussion generalizes easily to $\mathbb{R}^{2n}$.

We use $\gamma(t) = (\mathbb{X}(t), \mathbb{P}(t))$ to represent a particle trajectory on the phase space $\mathbb{R}^2$. Thus γ can be viewed as a map

$$\begin{aligned} \gamma : \mathbb{R} &\longrightarrow \mathbb{R}^2 \\ t &\longmapsto (\mathbb{X}(t), \mathbb{P}(t)) \end{aligned}$$

Let us denote

$$\mathcal{E} = \operatorname{Map}(\mathbb{R}, \mathbb{R}^2)$$

The action S can be viewed as a function on $\mathcal{E}$ (with a suitable domain which is not relevant in our current discussion)

$$\begin{aligned} S : \mathcal{E} &\longrightarrow \mathbb{R} \\ S[\gamma] &= \int \left(\mathbb{P}\dot{\mathbb{X}} - \mathscr{H} \right) dt \end{aligned}$$

We are interested in the following expectation

$$\langle \mathcal{O} \rangle_\gamma = \frac{\int_{\mathcal{E}} [D\gamma]\, e^{\frac{i}{\hbar} S[\gamma]} \mathcal{O}[\gamma]}{\int_{\mathcal{E}} [D\gamma]\, e^{\frac{i}{\hbar} S[\gamma]}}$$

where $\mathcal{O}$ is some appropriate function on $\mathcal{E}$ and is called an observable. Let us first consider the free case without Hamiltonian $\mathscr{H}$, i.e.,

$$S[\gamma] = S_0[\gamma] = \int \mathbb{P}\dot{\mathbb{X}}\, dt.$$

As we will see, the zero Hamiltonian case has a topological nature.

The above integration is on the infinite-dimensional path space $\mathcal{E}$, thus not well-defined in the first space. In Chapter 2, we have treated path integral as a limit of finite dimensional appproximation. When time is imaginary, this is related to Wienner measure integration.

In this section, we use an alternate perturbative approach. It turns out that we can borrow the finite dimensional result and design the parallel combinatorial formula into the infinite-dimensional setting. Let us see how this works in practice.

Let us first compare the finite-dimensional with the infinite-dimensional setting.

	Finite Dim	Infinite Dim
space	$\mathbb{R}^n$	$\mathcal{E} = \mathrm{Map}(\mathbb{R}, \mathbb{R}^2)$
variable	x^i	$\gamma(t)$
index	$i \in \{1, 2, \cdots, n\}$	$t \in \mathbb{R}$
sum	$\sum_i$	$\int_{\mathbb{R}} dt$
action	$Q(x) = \sum_{i,j} Q_{ij} x^i x^j$	$S_0[\gamma] = \int \mathbb{P}\dot{\mathbb{X}}\, dt$
density	$e^{-\frac{1}{2\hbar}Q(x)}$	$e^{\frac{i}{\hbar}S_0[\gamma]}$

In the finite-dimensional case, the two point function

$$\left\langle x^i x^j \right\rangle_x = \hbar (Q^{-1})^{ij}$$

plays the fundamental role as building block in computing general expectation values. It is called the "propagator" and is given by the inverse matrix of the quadratic pairing Q.

The infinite-dimensional situation looks exactly the same. The free action

$$S_0[\gamma] = \int \mathbb{P}\dot{\mathbb{X}}\, dt$$

is quadratic in $\gamma = (\mathbb{X}, \mathbb{P})$. Let us write (ignore the boundary behavior so far)

$$\begin{aligned} S_0[\gamma] =& \frac{1}{2} \int \left(\mathbb{P}\dot{\mathbb{X}} - \mathbb{X}\dot{\mathbb{P}} \right) dt \\ =& \frac{1}{2} \int \begin{bmatrix} \mathbb{X} & \mathbb{P} \end{bmatrix} \begin{bmatrix} & -\frac{d}{dt} \\ \frac{d}{dt} & \end{bmatrix} \begin{bmatrix} \mathbb{X} \\ \mathbb{P} \end{bmatrix} dt \end{aligned}$$

Thus

$$e^{\frac{i}{\hbar}S_0[\gamma]} = \exp\left(-\frac{1}{2\hbar} \left(\frac{1}{i} \int \begin{bmatrix} \mathbb{X}(t) & \mathbb{P}(t) \end{bmatrix} \begin{bmatrix} 0 & -\frac{d}{dt} \\ \frac{d}{dt} & 0 \end{bmatrix} \begin{bmatrix} \mathbb{X}(t) \\ \mathbb{P}(t) \end{bmatrix} dt \right) \right).$$

Comparing with the finite-dimensional situation

$$e^{-\frac{1}{2\hbar}\sum_{i,j} Q_{ij} x^i x^j}$$

the analogue of the inverse matrix Q^{-1} is

$$i\begin{bmatrix} 0 & -\frac{d}{dt} \\ \frac{d}{dt} & 0 \end{bmatrix}^{-1}$$

In analysis, the inverse of a differential operator is usually represented by an integral kernel called the Green's function. The Green's function of $\frac{d}{dt}$ is a function $G(t_1, t_2)$ satisfying

$$\frac{\partial}{\partial t_1} G(t_1, t_2) = \delta(t_1 - t_2).$$

Here $\delta(t_1 - t_2)$ can be viewed as the infinite-dimensional analogue of δ_{ij}.

In terms of $G(t_1, t_2)$, we have

$$\begin{bmatrix} 0 & -\frac{\partial}{\partial t_1} \\ \frac{\partial}{\partial t_1} & 0 \end{bmatrix} \begin{bmatrix} 0 & G(t_1, t_2) \\ -G(t_1, t_2) & 0 \end{bmatrix} = \begin{bmatrix} \delta(t_1 - t_2) & 0 \\ 0 & \delta(t_1 - t_2) \end{bmatrix}$$

The right hand side can be viewed as the (t_1, t_2)-entry of the infinite-dimensional identity matrix. Thus the (t_1, t_2)-entry of the above inverse can be written as

$$i\begin{bmatrix} 0 & -\frac{d}{dt} \\ \frac{d}{dt} & 0 \end{bmatrix}^{-1}_{t_1, t_2} = \begin{bmatrix} 0 & iG(t_1, t_2) \\ -iG(t_1, t_2) & 0 \end{bmatrix}.$$

Then we could "define" the two-point functions in terms of this inverse by

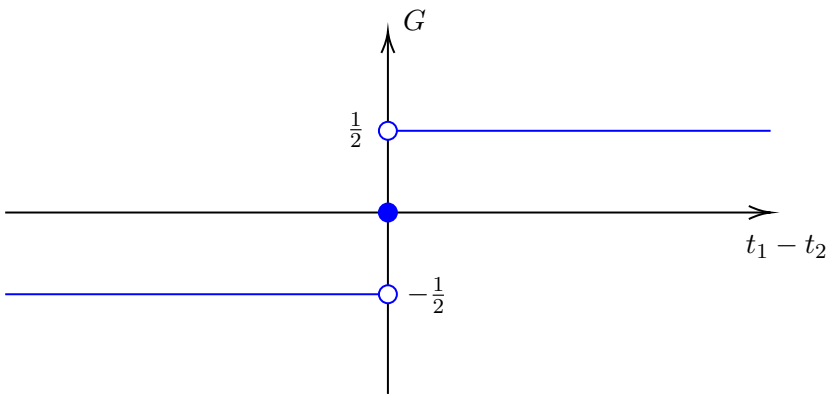
$$\begin{cases} \langle \mathbb{X}(t_1)\mathbb{P}(t_2) \rangle_\gamma := i\hbar G(t_1, t_2) \\ \langle \mathbb{P}(t_1)\mathbb{X}(t_2) \rangle_\gamma := -i\hbar G(t_1, t_2) \\ \langle \mathbb{X}(t_1)\mathbb{X}(t_2) \rangle_\gamma = \langle \mathbb{P}(t_1)\mathbb{P}(t_2) \rangle_\gamma = 0 \end{cases}$$

We are left to solve $G(t_1, t_2)$. The above expression asks for $G(t_1, t_2)$ such that

$$G(t_1, t_2) = -G(t_2, t_1).$$

Such Green's function of $\frac{d}{dt}$ is explicitly given by

$$G(t_1, t_2) = \frac{1}{2}\operatorname{sgn}(t_1 - t_2) = \begin{cases} \frac{1}{2} & t_1 > t_2 \\ 0 & t_1 = t_2 \\ -\frac{1}{2} & t_1 < t_2 \end{cases}$$



In fact, for any compactly supported test function $f(t)$

$$-\int_{\mathbb{R}} dt_1\, G(t_1,t_2)f'(t_1) = \frac{1}{2}\int_{-\infty}^{t_2} dt_1\, f'(t_1) - \frac{1}{2}\int_{t_2}^{\infty} dt_1\, f'(t_1) = \frac{1}{2}f(t_2) - \frac{1}{2}\left(-f(t_2)\right) = f(t_2).$$

So

$$\frac{\partial}{\partial t_1}G(t_1,t_2) = \delta(t_1-t_2)$$

holds as a distributional equation.

In summary, we are interested in the following two-point function

$$\langle \mathbb{X}(t_1)\mathbb{P}(t_2)\rangle_\gamma \text{“}= \text{”} \frac{\int [D\gamma]\, e^{\frac{i}{\hbar}S_0[\gamma]}\, \mathbb{X}(t_1)\mathbb{P}(t_2)}{\int [D\gamma]\, e^{\frac{i}{\hbar}S_0[\gamma]}}$$

Although we do not know a prior the precise information about the path integral measure, we can still derive a reasonable result in comparison with the finite dimensional Gaussian integral

$$\langle \mathbb{X}(t_1)\mathbb{P}(t_2)\rangle_\gamma := i\hbar G(t_1,t_2) = \frac{i\hbar}{2}\,\mathrm{sgn}(t_1-t_2).$$

In the following, we use this formula to define our two-point function.

Note that this two-point function, or the propagator, does not depend on the precise value of t_1, t_2, but only on the relative position

$$\langle \mathbb{X}(t_1)\mathbb{P}(t_2)\rangle_\gamma = \begin{cases} \frac{i\hbar}{2} & t_1 > t_2 \\ 0 & t_1 = t_2 \\ -\frac{i\hbar}{2} & t_1 < t_2 \end{cases}$$

This indicates a topological nature of this model, which is indeed the case.

Now let $f(x,p)$ and $g(x,p)$ be two polynomials . We plot them on the time line as

We define a new function on the phase space by the following correlation

$$\langle f(x+\mathbb{X}(t_2), p+\mathbb{P}(t_2))g(x+\mathbb{X}(t_1), p+\mathbb{P}(t_1))\rangle_\gamma .$$

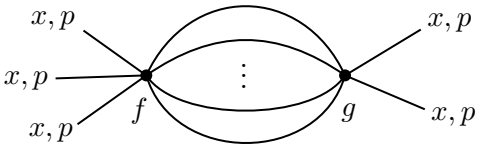
Here we perturb the variables x, p by quantum fluctuations $\mathbb{X}(t), \mathbb{P}(t)$ at time t_1 for g and at time t_2 for f. Equivalently, we can treat x and p as "background" shift. This correlation function depends on the background variable $\{x,p\}$ and defines a function on the phase space.

Let us apply Wick's Theorem to compute this correlation. We represent each f and g as a vertex whose valency is the polynomial degree

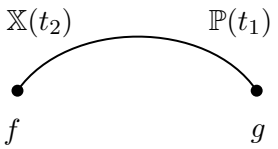
Then Wick's Theorem says

$$\langle f(x+\mathbb{X}(t_2),p+\mathbb{P}(t_2))g(x+\mathbb{X}(t_1),p+\mathbb{P}(t_1))\rangle_\gamma$$

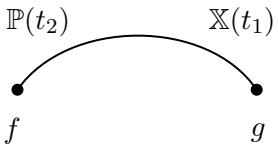
$$= \sum$$



Here for each unpaired half-edge, we assign x or p as in the original vertex. For paired half-edges



$$\Longrightarrow \qquad \langle \mathbb{X}(t_2)\mathbb{P}(t_1)\rangle_\gamma = \frac{i}{2}\hbar$$



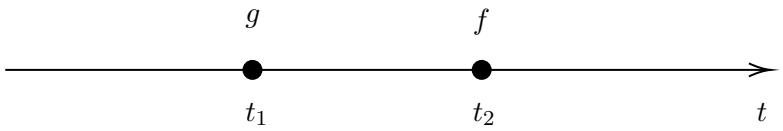
$$\Longrightarrow \qquad \langle \mathbb{P}(t_2)\mathbb{X}(t_1)\rangle_\gamma = -\frac{i}{2}\hbar$$

For a graph with m propagators, there will be an automorphism group S_m by permuting the edges, contributing $\frac{1}{m!}$ in the Feynman graph expansion. Thus we find

$$\begin{aligned}&\langle f(x+\mathbb{X}(t_2),p+\mathbb{P}(t_2))g(x+\mathbb{X}(t_1),p+\mathbb{P}(t_1))\rangle_\gamma \\ =&f(x,p)e^{\frac{i}{2}\hbar\left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p}-\frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)}g(x,p) = (f *_\hbar g)(x,p)\end{aligned}$$

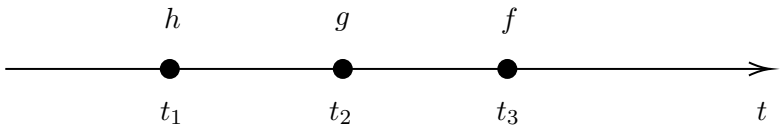
which is precisely the Moyal product.

We can think about



as inserting an operator g at time t_1, and then inserting another operator f at a later time t_2. The total effect is the composition of two operators, which is represented quantum mechanically by the Moyal product $f *_\hbar g$.

This picture also gives a simple explanation of the associativity of the Moyal product $*_\hbar$. Given three functions f, g, h, we insert them in time order



Consider the correlation

$$\langle f(x+\mathbb{X}(t_3),p+\mathbb{P}(t_3))g(x+\mathbb{X}(t_2),p+\mathbb{P}(t_2))h(x+\mathbb{X}(t_1),p+\mathbb{P}(t_1))\rangle_\gamma .$$

This value is invariant under local deformations of the time positions and only the order is relevant. By our previous computation

$$(f *_\hbar g)*_\hbar h = \lim_{t_1\to t_2^-}\lim_{t_3\to t_2^+} \langle f(x+\mathbb{X}(t_3),p+\mathbb{P}(t_3))g(x+\mathbb{X}(t_2),p+\mathbb{P}(t_2))h(x+\mathbb{X}(t_1),p+\mathbb{P}(t_1))\rangle_\gamma$$

$$f*_\hbar(g *_\hbar h) = \lim_{t_3\to t_2^+}\lim_{t_1\to t_2^-} \langle f(x+\mathbb{X}(t_3),p+\mathbb{P}(t_3))g(x+\mathbb{X}(t_2),p+\mathbb{P}(t_2))h(x+\mathbb{X}(t_1),p+\mathbb{P}(t_1))\rangle_\gamma$$

The topological nature of the above correlation implies

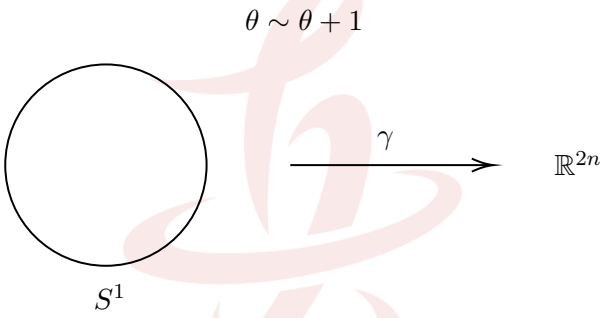
$$(f *_\hbar g) *_\hbar h = f *_\hbar (g *_\hbar h)\,.$$

3.6.4 S^1-Correlation

Let us now introduce topology and put our quantum mechanical model on S^1

$$\gamma(\theta) = \big(\mathbb{X}^i(\theta),\mathbb{P}_i(\theta)\big) : S^1 \longrightarrow \mathbb{R}^{2n}.$$

Here $\theta \in S^1$ is the angle variable and we identify



S^1-Propagator

We consider the free action as before

$$S_0[\gamma] = \int_{S^1} \mathbb{P}_i(\theta)\dot{\mathbb{X}}^i(\theta)\,d\theta, \qquad \dot{\mathbb{X}}^i(\theta) = \frac{d\mathbb{X}^i}{d\theta}.$$

We use Feynman graph expansion to define correlation function in this model. The propagator is given by the two-point function

$$\Big\langle \mathbb{X}^k(\theta_1)\mathbb{P}_j(\theta_2)\Big\rangle_\gamma^{S^1} = i\hbar G(\theta_1,\theta_2)\delta^k_j$$

where $G(\theta_1,\theta_2)$ is the Green's function representing the integral kernel of the operator "$\big(\frac{d}{d\theta}\big)^{-1}$".

On S^1, we have a Fourier basis of functions

$$\Big\{e^{2\pi i n\theta}\Big\}_{n\in\mathbb{Z}}.$$

The δ-function can be represented by

$$\delta(\theta_1,\theta_2) = \sum_{n\in\mathbb{Z}} e^{2\pi i n(\theta_2-\theta_1)}.$$

Note that for $n = 0$, the constant function "1" can not be inverted by "$\frac{d}{d\theta}$". This is called the zero mode, which is related to the nontrivial harmonics on S^1. Let

$$\widehat{\delta}(\theta_1, \theta_2) = \sum_{n \in \mathbb{Z}\setminus\{0\}} e^{2\pi i n(\theta_2 - \theta_1)}$$

where we have deleted the zero mode. The Green's function $G(\theta_1, \theta_2)$ solves

$$\frac{\partial}{\partial \theta_1} G(\theta_1, \theta_2) = \widehat{\delta}(\theta_1, \theta_2)$$

$$\Longrightarrow \qquad G(\theta_1, \theta_2) = \sum_{n \in \mathbb{Z}\setminus\{0\}} \frac{i}{2\pi n} e^{2\pi i n(\theta_2 - \theta_1)} = g(\theta_2 - \theta_1)$$

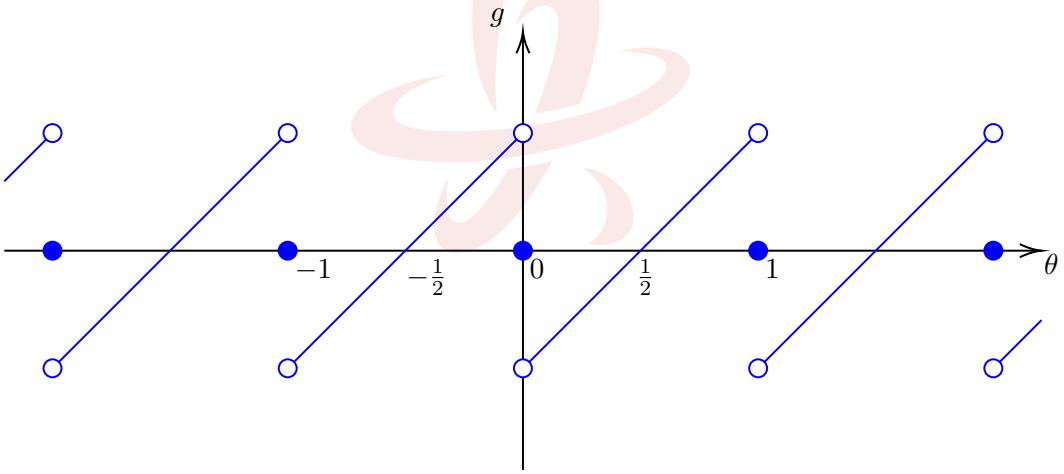
where $g(\theta)$ is the following function on S^1

$$g(\theta) = \sum_{n \in \mathbb{Z}\setminus\{0\}} \frac{i}{2\pi n} e^{2\pi i n \theta}.$$

Proposition 3.6.11. *Viewed as a periodic function on $\mathbb{R}$ with $g(\theta + 1) = g(\theta)$, the value of $g(\theta)$ on $[0, 1)$ is*

$$g(\theta) = \begin{cases} 0 & \theta = 0 \\ \theta - \frac{1}{2} & 0 < \theta < 1 \end{cases}$$

Here we impose $g(0) = 0$ to ensure $g(-\theta) = -g(\theta)$.



Proof: Let $g(\theta)$ be the periodic function as above. We can compute its Fourier expansion

$$\begin{aligned} &\int_0^1 e^{-2\pi i n\theta} \left(\theta - \frac{1}{2}\right) d\theta \qquad (\text{ for } n \neq 0\ ) \\ =&\frac{i}{2\pi n} e^{-2\pi i n\theta} \left(\theta - \frac{1}{2}\right)\Big|_0^1 - \int_0^1 e^{-2\pi i n\theta}\, d\theta \\ =&\frac{i}{2\pi n}. \end{aligned}$$

For $n = 0$, we have $\int_0^1 \left(\theta - \frac{1}{2}\right) d\theta = 0$. Thus

$$\theta - \frac{1}{2} = \sum_{n \in \mathbb{Z}\setminus\{0\}} \frac{i}{2\pi n} e^{2\pi i n\theta}, \qquad 0 < \theta < 1$$

as expected. □

We can also check the distributional equation

$$\frac{\partial}{\partial\theta_1}G(\theta_1,\theta_2)=\widehat{\delta}(\theta_1,\theta_2)=\delta(\theta_1,\theta_2)-1$$

directly. For any smooth test function $f(\theta)$ on S^1,

$$\begin{aligned}
-\int_{S^1}G(\theta_1,\theta_2)f'(\theta_1)\,d\theta_1=&-\int_{\theta_2-1}^{\theta_2}g(\theta_2-\theta_1)f'(\theta_1)\,d\theta_1\\
=&-\int_{\theta_2-1}^{\theta_2}\left(\theta_2-\theta_1-\frac{1}{2}\right)f'(\theta_1)\,d\theta_1\\
=&-\left(\theta_2-\theta_1-\frac{1}{2}\right)f(\theta_1)\Big|_{\theta_2-1}^{\theta_2}-\int_{\theta_2-1}^{\theta_2}f(\theta_1)\,d\theta_1\\
=&f(\theta_2)-\int_{S^1}f(\theta)d\theta\\
=&\int_0^1\left(\delta(\theta_1,\theta_2)-1\right)f(\theta_1)\,d\theta_1
\end{aligned}$$

as expected.

Thus we have found the two-point function

$$\left\langle\mathbb{X}^k(\theta_1)\mathbb{P}_j(\theta_2)\right\rangle_\gamma^{S^1}=i\hbar G(\theta_1,\theta_2)\delta_j^k=i\hbar g(\theta_2-\theta_1)\delta_j^k.$$

Note that in the limit $\theta_1\to\theta_2$

$$\begin{aligned}
\lim_{\theta_1\to\theta_2^-}\left\langle\mathbb{X}^k(\theta_1)\mathbb{P}_j(\theta_2)\right\rangle_\gamma^{S^1}&=-\frac{i\hbar}{2}\delta_j^k\\
\lim_{\theta_1\to\theta_2^+}\left\langle\mathbb{X}^k(\theta_1)\mathbb{P}_j(\theta_2)\right\rangle_\gamma^{S^1}&=\frac{i\hbar}{2}\delta_j^k
\end{aligned}$$

Thus when θ_1 and θ_2 are close to each other, this two-point function becomes the two point function on $\mathbb{R}$. This is expected as the local geometry on S^1 is precisely $\mathbb{R}$.

S^1-Correlation

Let $\mathcal{A}=\mathbb{R}[x^i,p_i]$ denote the ring of polynomial functions on the phase space. Recall we have a natural multiplication map

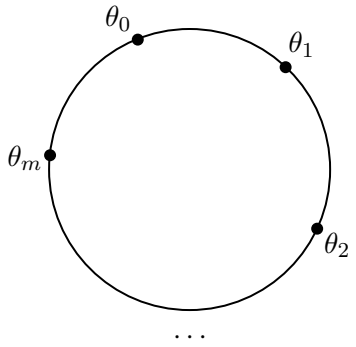
$$\begin{aligned}
\mathcal{A}\otimes\mathcal{A}\otimes\cdots\otimes\mathcal{A}&\longrightarrow\mathcal{A}\\
f_0\otimes f_1\otimes\cdots\otimes f_m&\longmapsto f_0f_1\cdots f_m
\end{aligned}$$

As an application of the S^1-quantum mechanical model, we construct a version of quantization $\langle f_0\otimes f_1\otimes\cdots\otimes f_m\rangle_{S^1}$ of the above multiplication map such that

$$\langle f_0\otimes f_1\otimes\cdots\otimes f_m\rangle_{S^1}=f_0f_1\cdots f_m+O(\hbar).$$

Let

$$\mathrm{Cyc}_{m+1}(S^1)=\left\{(\theta_0,\theta_1,\cdots,\theta_m)\in(S^1)^{m+1}\,|\,\theta_0,\theta_1,\cdots,\theta_m\text{ are distinct in clockwise cyclic order}\right\}.$$



Using rotation invariance, we have

$$\int_{\mathrm{Cyc}_{m+1}(S^1)} d\theta_0 d\theta_1 \cdots d\theta_m = \int_{1\geq\theta_1\geq\cdots\geq\theta_m\geq 0} d\theta_1 \cdots d\theta_m = \frac{1}{m!}.$$

Definition 3.6.12. Let $f_i \in \mathcal{A}$. We define their S^1-correlation

$$\langle f_0 \otimes f_1 \otimes \cdots \otimes f_m \rangle_{S^1} \in \mathcal{A}[\hbar]$$

by

$$\begin{aligned}&\langle f_0 \otimes f_1 \otimes \cdots \otimes f_m \rangle_{S^1} (\mathbf{x}, \mathbf{p}) \\ =&m! \int_{\mathrm{Cyc}_{m+1}(S^1)} d\theta_0 d\theta_1 \cdots d\theta_m \, \langle f_0(\mathbf{x} + \mathbb{X}(\theta_0), \mathbf{p} + \mathbb{P}(\theta_0)) \cdots f_m(\mathbf{x} + \mathbb{X}(\theta_m), \mathbf{p} + \mathbb{P}(\theta_m)) \rangle_\gamma^{S^1}.\end{aligned}$$

Here the correlation $\langle - \rangle_\gamma^{S^1}$ is defined via Wick's Theorem and Feynman graphs. Explicitly,

$$\begin{aligned}&\langle f_0(\mathbf{x} + \mathbb{X}(\theta_0), \mathbf{p} + \mathbb{P}(\theta_0)) \cdots f_m(\mathbf{x} + \mathbb{X}(\theta_m), \mathbf{p} + \mathbb{P}(\theta_m)) \rangle_\gamma^{S^1} \\ :=&e^{i\hbar \sum_{i,j=0}^{m} G(\theta_i,\theta_j) \frac{\partial}{\partial \mathbf{x}^{(i)}} \frac{\partial}{\partial \mathbf{p}^{(j)}}} f_0(\mathbf{x}^{(0)}, \mathbf{p}^{(0)}) \cdots f_m(\mathbf{x}^{(m)}, \mathbf{p}^{(m)}) \Big|_{\substack{\mathbf{x}^{(0)}=\cdots=\mathbf{x}^{(m)}=\mathbf{x} \\ \mathbf{p}^{(0)}=\cdots=\mathbf{p}^{(m)}=\mathbf{p}}}.\end{aligned}$$

It is clear that

$$\lim_{\hbar\to 0} \langle f_0 \otimes f_1 \otimes \cdots \otimes f_m \rangle_{S^1} = f_0 f_1 \cdots f_m m! \int_{\mathrm{Cyc}_{m+1}(S^1)} d\theta_0 d\theta_1 \cdots d\theta_m = f_0 f_1 \cdots f_m$$

which corresponds to the term without propagators. Since f_i's are polynomials, only finite number of propagators can appear. Thus

$$\mathcal{A} \otimes \mathcal{A} \otimes \cdots \otimes \mathcal{A} \xrightarrow{\langle - \rangle_{S^1}} \mathcal{A}[\hbar].$$

Example 3.6.13. *Given two polynomials $f_0, f_1 \in \mathcal{A} = \mathbb{R}[x,p]$,*

$$\begin{aligned}
\langle f_0 \otimes f_1 \rangle_{S^1} &= \int_{\mathrm{Cyc}_2(S^1)} d\theta_0 d\theta_1 \, f_0(x,p) e^{i\hbar G(\theta_0,\theta_1) \frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} + i\hbar G(\theta_1,\theta_0) \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}} f_1(x,p) \\
&= \int_0^1 d\theta \, f_0(x,p) e^{i\hbar g(\theta)\left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)} f_1(x,p) \\
&= \int_0^1 d\theta \, f_0(x,p) e^{i\hbar(\theta - 1/2)\left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)} f_1(x,p) \\
&= \int_{-\frac{1}{2}}^{\frac{1}{2}} d\theta \, f_0(x,p) e^{i\hbar\theta\left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)} f_1(x,p) \\
&= \sum_{m=0}^{\infty} \int_{-\frac{1}{2}}^{\frac{1}{2}} \theta^{2m} d\theta \, \frac{(i\hbar)^{2m}}{(2m)!} f_0(x,p) \left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)^{2m} f_1(x,p) \\
&= \sum_{m=0}^{\infty} \frac{(i\hbar)^{2m}}{(2m+1)2^{2m}(2m)!} f_0(x,p) \left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)^{2m} f_1(x,p).
\end{aligned}$$

For example,

$$\langle x \otimes p \rangle_{S^1} = xp$$
$$\langle x^2 \otimes p^2 \rangle_{S^1} = x^2p^2 - \frac{\hbar^2}{6}$$

Example 3.6.14. *We use Wick's Theorem to compute*

$$\begin{aligned}
\langle x \otimes xp \otimes p \rangle_{S^1} =& x^2p^2 + 2! \int_{\mathrm{Cyc}_3(S^1)} d\theta_0 d\theta_1 d\theta_2 \, i\hbar \left(G(\theta_0,\theta_1) + G(\theta_1,\theta_2) + G(\theta_0,\theta_2)\right) xp \\
&+ 2! \int_{\mathrm{Cyc}_3(S^1)} d\theta_0 d\theta_1 d\theta_2 \, (i\hbar)^2 G(\theta_0,\theta_1) G(\theta_1,\theta_2) \\
=& x^2p^2 + 2xp(i\hbar) \int_{1 \geq \theta_1 \geq \theta_2 \geq 0} d\theta_1 d\theta_2 \, \left(G(1,\theta_1) + G(\theta_1,\theta_2) + G(1,\theta_2)\right) \\
&+ 2(i\hbar)^2 \int_{1 \geq \theta_1 \geq \theta_2 \geq 0} d\theta_1 d\theta_2 \, G(1,\theta_1) G(\theta_1,\theta_2) \\
=& x^2p^2 + 2(i\hbar)xp \int_{1 \geq \theta_1 \geq \theta_2 \geq 0} d\theta_1 d\theta_2 \, \left[\left(\theta_1 - \frac{1}{2}\right) - \left((\theta_1 - \theta_2) - \frac{1}{2}\right) + \left(\theta_2 - \frac{1}{2}\right)\right] \\
&+ 2(i\hbar)^2 \int_{1 \geq \theta_1 \geq \theta_2 \geq 0} d\theta_1 d\theta_2 \, \left(\theta_1 - \frac{1}{2}\right)\left(\frac{1}{2} - (\theta_1 - \theta_2)\right) \\
=& x^2p^2 + \frac{i\hbar}{6} xp.
\end{aligned}$$

3.6.5 Hochschild Homology

As an application of the S^1-correlation function (Definition 3.6.12), we explain how the geometry of S^1 is related to the notion of Hochschild homology and present an explicit construction of a quantum version of the Hochschild-Kostant-Rosenberg (HKR) map. We will apply this quantum HKR map to construction trace map in deformation quantization in Section 4.4.

Hochschild Homology

Let A be an associative algebra over a base field k. We can define a chain complex

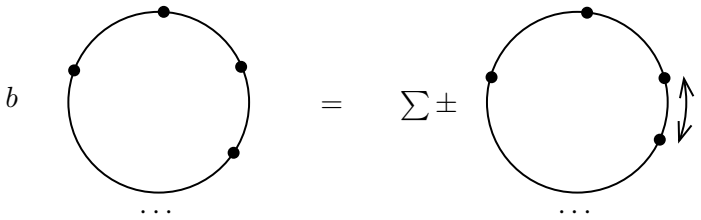
$$\cdots \xrightarrow{b} C_p(A) \xrightarrow{b} C_{p-1}(A) \xrightarrow{b} \cdots \xrightarrow{b} C_1(A) \xrightarrow{b} C_0(A)$$

where

$$C_p(A) = A^{\otimes p+1}, \qquad \text{here } \otimes = \otimes_k.$$

The map b is defined by

$$\begin{aligned} b(a_0 \otimes a_1 \otimes \cdots \otimes a_p) =& a_0a_1 \otimes a_2 \otimes \cdots \otimes a_p - a_0 \otimes a_1a_2 \otimes \cdots \otimes a_p \\ &+ \cdots + (-1)^{p-1} a_0 \otimes a_1 \otimes \cdots \otimes a_{p-1}a_p + (-1)^p a_p a_0 \otimes a_1 \otimes \cdots \otimes a_{p-1}. \end{aligned}$$



Check: $b^2 = 0$.

$$\begin{aligned} & b^2(a_0 \otimes a_1 \otimes \cdots \otimes a_p) \\ =& b\left(a_0a_1 \otimes a_2 \otimes \cdots \otimes a_p - a_0 \otimes a_1a_2 \otimes \cdots \otimes a_p \pm \cdots\right) \\ =& (a_0a_1)a_2 \otimes \cdots \otimes a_p - a_0(a_1a_2) \otimes \cdots \otimes a_p \pm \cdots \\ =& 0 \qquad \text{by associativity.} \end{aligned}$$

The chain complex $(C_\bullet(A), b)$ is called the Hochschild chain complex and

$$HH_\bullet(A) := H_\bullet(C_\bullet(A), b)$$

is called the Hochschild homology.

Example 3.6.15.

$$\begin{aligned} C_2(A) &\longrightarrow C_1(A) \xrightarrow{b} C_0(A) \\ a_0 \otimes a_1 &\longmapsto a_0a_1 - a_1a_0 \end{aligned}$$

So $HH_0(A) = A/[A, A]$ is the abelianization.

Theorem 3.6.16 (Hochschild-Kostant-Rosenberg (HKR))**.** *Let $A = k[y^i]$ be a polynomial ring and $\Omega^\bullet_A = k[y^i, dy^i]$ be the algebraic differential forms. Then*

$$HH_p(A) = \Omega^p_A.$$

Remark 3.6.17. HKR theorem says that on the standard commutative space k^n

$$HH_\bullet = \text{Differential forms.}$$

In general for an associative but non-commutative algebra A, we can view

$$HH_\bullet = \text{Non-commutative differential forms}$$

which is a basic algebraic tool for doing calculus in the noncommutative world.

The HKR isomorphism is realized by

$$\rho : C_\bullet(A) \longrightarrow \Omega_A^\bullet$$
$$f_0 \otimes f_1 \otimes \cdots \otimes f_p \longmapsto f_0\, df_1 \wedge df_2 \wedge \cdots \wedge df_p$$

Check: $\rho(b(-)) = 0$.

$$\begin{aligned}
&\rho(b(f_0 \otimes f_1 \otimes \cdots \otimes f_p)) \\
=&\rho\left(f_0 f_1 \otimes f_2 \otimes \cdots \otimes f_p - f_0 \otimes f_1 f_2 \otimes \cdots \otimes f_p \pm \cdots\right) \\
=&f_0 f_1 df_2 \wedge \cdots \wedge df_p - f_0 d(f_1 f_2) \wedge df_3 \wedge \cdots \wedge df_p \pm \cdots \\
&+ (-1)^{p-1} f_0 df_1 \wedge \cdots \wedge d(f_{p-1} f_p) + (-1)^p f_p f_0 df_1 \wedge \cdots \wedge df_{p-1} \\
=&0.
\end{aligned}$$

Thus ρ defines a map of chain complexes

$$\rho : (C_\bullet(A), b) \longrightarrow (\Omega_A^\bullet, 0).$$

A more precise description of HKR is that the HKR map ρ is a quasi-isomorphism, which induces an isomorphism by passing to homology

$$\rho : HH_\bullet(A) \xrightarrow{\simeq} \Omega_A^\bullet.$$

Quantum HKR

Let $\mathcal{A} = \mathbb{C}[x^i, p_i]$ be the ring of polynomial functions on the phase space $\mathbb{R}^{2n}$. We have a canonical quantization of $\mathcal{A}$ to the associative Weyl algebra

$$\mathcal{A}^\hbar := (\mathcal{A}[\hbar], *)$$

where $*$ is the Moyal product. We will describe a quantum version $\rho^\hbar$ of the HKR map ρ that intertwines the Hochschild chain complex $C_\bullet(\mathcal{A}^\hbar)$ of the Weyl algebra $\mathcal{A}^\hbar$.

Let $f_0, f_1, \cdots, f_m \in \mathcal{A}$. Recall we have the S^1-correlation as in Definition 3.6.12

$$\langle f_0 \otimes f_1 \otimes \cdots \otimes f_m \rangle_{S^1} \in \mathcal{A}[\hbar].$$

To simplify notations, let us denote

$$\mathcal{O}_f(\theta) := f(\mathbf{x} + \mathbb{X}(\theta), \mathbf{p} + \mathbb{P}(\theta)), \qquad \theta \in S^1.$$

By construction

$$\langle f_0 \otimes f_1 \otimes \cdots \otimes f_m \rangle_{S^1} = m! \int_{\mathrm{Cyc}_{m+1}(S^1)} d\theta_0 d\theta_1 \cdots d\theta_m \, \langle \mathcal{O}_{f_0}(\theta_0) \mathcal{O}_{f_1}(\theta_1) \cdots \mathcal{O}_{f_m}(\theta_m) \rangle_\gamma^{S^1}.$$

Given f, its total differential is

$$df = \sum_i \left(\frac{\partial f}{\partial x^i} dx^i + \frac{\partial f}{\partial p_i} dp_i \right).$$

We denote

$$\mathcal{O}_{df}(\theta) := \sum_i \left(\mathcal{O}_{\partial_{x^i} f}(\theta) dx^i + \mathcal{O}_{\partial_{p_i} f}(\theta) dp_i \right).$$

Definition 3.6.18. We define the quantum HKR map

$$\rho^\hbar : \mathcal{A}^{\otimes m+1} \to \Omega_A^m[\hbar]$$

by

$$\rho^\hbar(f_0 \otimes f_1 \otimes \cdots \otimes f_m) := \int_{\mathrm{Cyc}_{m+1}(S^1)} d\theta_0 d\theta_1 \cdots d\theta_m \, \langle \mathcal{O}_{f_0}(\theta_0)\mathcal{O}_{df_1}(\theta_1)\cdots\mathcal{O}_{df_m}(\theta_m)\rangle_\gamma^{S^1}$$

This can be formally written as

$$\rho^\hbar(f_0 \otimes f_1 \otimes \cdots \otimes f_m) = \frac{1}{m!}\langle f_0 \otimes df_1 \otimes \cdots \otimes df_m\rangle_{S^1}$$

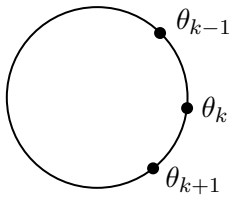
Using Wick's Theorem, we have the explicit formula

$$\begin{aligned}&\rho^\hbar(f_0 \otimes f_1 \otimes \cdots \otimes f_m)\\ &= \int_{\mathrm{Cyc}_{m+1}(S^1)} d\theta_0 d\theta_1 \cdots d\theta_m \, e^{i\hbar \sum_{i,j=0}^{m} G(\theta_i,\theta_j)\frac{\partial}{\partial \mathbf{x}^{(i)}}\frac{\partial}{\partial \mathbf{p}^{(j)}}} f_0(\mathbf{x}^{(0)},\mathbf{p}^{(0)}) df_1(\mathbf{x}^{(1)},\mathbf{p}^{(1)})\cdots df_m(\mathbf{x}^{(m)},\mathbf{p}^{(m)})\Big|_{\substack{\mathbf{x}^{(0)}=\cdots=\mathbf{x}^{(m)}=\mathbf{x}\\ \mathbf{p}^{(0)}=\cdots=\mathbf{p}^{(m)}=\mathbf{p}}}\end{aligned}$$

We next explore algebraic structures of $\rho^\hbar$. Let us consider the following integral

$$\begin{aligned}\int_{\mathrm{Cyc}_{m+1}(S^1)} d\theta_0 d\theta_1 \cdots d\theta_m \, \Big\{ &\frac{\partial}{\partial\theta_1}\langle \mathcal{O}_{f_0}(\theta_0)\mathcal{O}_{f_1}(\theta_1)\cdots\mathcal{O}_{df_m}(\theta_m)\rangle_\gamma^{S^1}\\ &-\frac{\partial}{\partial\theta_2}\langle \mathcal{O}_{f_0}(\theta_0)\mathcal{O}_{df_1}(\theta_1)\mathcal{O}_{f_2}(\theta_2)\cdots\mathcal{O}_{df_m}(\theta_m)\rangle_\gamma^{S^1}\\ &+\cdots\\ &+(-1)^{m-1}\frac{\partial}{\partial\theta_m}\langle \mathcal{O}_{f_0}(\theta_0)\mathcal{O}_{df_1}(\theta_1)\cdots\mathcal{O}_{df_{m-1}}(\theta_{m-1})\mathcal{O}_{f_m}(\theta_m)\rangle_\gamma^{S^1}\Big\} \quad (\dagger)\end{aligned}$$

We compute (†) in two ways. The first is to compute $\int d\theta_k \frac{\partial}{\partial\theta_k}(-)$ as a total derivative. Due to the cyclic ordering



we have

$$\int d\theta_k \frac{\partial}{\partial\theta_k}(-) = \int_{\theta_{k+1}}^{\theta_{k-1}} d\theta_k \frac{\partial}{\partial\theta_k}(-) = (-)\Big|_{\theta_{k+1}}^{\theta_{k-1}}.$$

From Wick's Theorem and the property of S^1-propagator, we find the limit behavior

$$\lim_{\theta_k\to\theta_{k-1}^-}\langle\cdots\mathcal{O}_f(\theta_{k-1})\mathcal{O}_g(\theta_k)\cdots\rangle_\gamma^{S^1} = \langle\cdots\mathcal{O}_{f*g}(\theta_{k-1})\cdots\rangle_\gamma^{S^1}$$

$$\lim_{\theta_k\to\theta_{k+1}^+}\langle\cdots\mathcal{O}_f(\theta_k)\mathcal{O}_g(\theta_{k+1})\cdots\rangle_\gamma^{S^1} = \langle\cdots\mathcal{O}_{f*g}(\theta_{k+1})\cdots\rangle_\gamma^{S^1}$$

Therefore computing (†) in terms of total derivative leads to

$$\begin{aligned}
&\frac{1}{(m-1)!}\langle f_0 * f_1 \otimes df_2 \otimes \cdots \otimes df_m\rangle_{S^1} - \frac{1}{(m-1)!}\langle f_0 \otimes f_1 * df_2 \otimes \cdots \otimes df_m\rangle_{S^1} \\
&-\frac{1}{(m-1)!}\langle f_0 \otimes df_1 * f_2 \otimes df_3 \otimes \cdots \otimes df_m\rangle_{S^1} + \frac{1}{(m-1)!}\langle f_0 \otimes df_1 \otimes f_2 * df_3 \otimes \cdots \otimes df_m\rangle_{S^1} \\
&+\cdots \\
&+(-1)^{m-1}\frac{1}{(m-1)!}\langle f_0 \otimes df_1 \otimes \cdots \otimes df_{m-1} * f_m\rangle_{S^1} - (-1)^{m-1}\frac{1}{(m-1)!}\langle f_m * f_0 \otimes df_1 \otimes \cdots \otimes df_{m-1}\rangle_{S^1}.
\end{aligned}$$

By the Moyal product formula, we have

$$d(f * g) = df * g + f * dg.$$

Here

$$\begin{aligned}
df * g &= \sum_i (\partial_{x^i} f * g)\, dx^i + (\partial_{p_i} f * g)\, dp_i \\
f * dg &= \sum_i (f * \partial_{x^i} g)\, dx^i + (f * \partial_{p_i} g)\, dp_i
\end{aligned}$$

Thus (†) becomes

$$\begin{aligned}
&\frac{1}{(m-1)!}\langle f_0 * f_1 \otimes df_2 \otimes \cdots \otimes df_m\rangle_{S^1} \\
&-\frac{1}{(m-1)!}\langle f_0 \otimes d(f_1 * f_2) \otimes \cdots \otimes df_m\rangle_{S^1} \\
&+\cdots \\
&+(-1)^{m-1}\frac{1}{(m-1)!}\langle f_0 \otimes df_1 \otimes \cdots \otimes d(f_{m-1} * f_m)\rangle_{S^1} \\
&+(-1)^{m}\frac{1}{(m-1)!}\langle f_m * f_0 \otimes df_1 \otimes \cdots \otimes df_{m-1}\rangle_{S^1} \\
=&\rho^{\hbar}(b(f_0 \otimes f_1 \otimes \cdots \otimes f_m)).
\end{aligned}$$

Here b is the Hochschild differential with respect to the Moyal product.

The second way to approach (†) is to compute $\frac{\partial}{\partial\theta_k}\langle\cdots\rangle_\gamma^{S^1}$ explicitly. Observe

$$\frac{\partial}{\partial\theta_k}G(\theta_k,\theta_j) = -1 = -\frac{\partial}{\partial\theta_k}G(\theta_j,\theta_k) \qquad \text{for } \theta_j \neq \theta_k.$$

Thus

$$\begin{aligned}
&\frac{\partial}{\partial\theta_k}\left\langle \mathcal{O}_{f_0}(\theta_0)\mathcal{O}_{df_1}(\theta_1)\cdots\mathcal{O}_{df_{k-1}}(\theta_{k-1})\mathcal{O}_{f_k}(\theta_k)\cdots\mathcal{O}_{df_m}(\theta_m)\right\rangle_\gamma^{S^1} \\
=&i\hbar\sum_i \frac{\partial}{\partial x^i}\left\langle \mathcal{O}_{f_0}(\theta_0)\mathcal{O}_{df_1}(\theta_1)\cdots\mathcal{O}_{df_{k-1}}(\theta_{k-1})\mathcal{O}_{\partial_{p_i}f_k}(\theta_k)\cdots\mathcal{O}_{df_m}(\theta_m)\right\rangle_\gamma^{S^1} \\
&-i\hbar\sum_i \frac{\partial}{\partial p_i}\left\langle \mathcal{O}_{f_0}(\theta_0)\mathcal{O}_{df_1}(\theta_1)\cdots\mathcal{O}_{df_{k-1}}(\theta_{k-1})\mathcal{O}_{\partial_{x^i}f_k}(\theta_k)\cdots\mathcal{O}_{df_m}(\theta_m)\right\rangle_\gamma^{S^1}.
\end{aligned}$$

Introduce the following operator

$$\Delta : \Omega_A^m \longrightarrow \Omega_A^{m-1}, \qquad \Delta = \sum_i \left(\frac{\partial}{\partial x^i}\iota_{\partial_{p_i}} - \frac{\partial}{\partial p_i}\iota_{\partial_{x^i}}\right).$$

Let $\omega^{-1} = \sum_i \frac{\partial}{\partial x^i} \wedge \frac{\partial}{\partial p_i}$ be the Poisson bi-vector. Then Δ is geometrically the Lie derivative

$$\Delta = \mathscr{L}_{\omega^{-1}}.$$

It is clear that $\Delta^2 = 0$. Δ is the prototype of Batalin–Vilkovisky (BV) operator in quantum gauge theory. Then the above computation leads to

$$(\dagger) = i\hbar\Delta\rho^\hbar(f_0 \otimes f_1 \otimes \cdots \otimes f_m).$$

Comparing the two computations, we find

$$\rho^\hbar(b(-)) = i\hbar\Delta(\rho^\hbar(-)).$$

where b is the Hochschild differential with respect to the Moyal product.

We can extend $\rho^\hbar$ $\hbar$-linearly to

$$\rho^\hbar : C_\bullet(\mathcal{A}^\hbar) \longrightarrow \Omega^\bullet_{\mathcal{A}}[\hbar]$$

Then the above calculation shows that $\sigma^\hbar$ is a morphism of chain complexes

$$\rho^\hbar : (C_\bullet(\mathcal{A}^\hbar), b) \longrightarrow (\Omega^\bullet_{\mathcal{A}}[\hbar], i\hbar\Delta).$$

Thus $\rho^\hbar$ provides a quantization of ρ.

Remark 3.6.19. We can further localize $\hbar$ and denote

$$\mathcal{A}^{(\hbar)} := \mathcal{A}^\hbar \otimes_{k[\hbar]} k[\hbar, \hbar^{-1}].$$

The quantum HKR map $\rho^\hbar$ is naturally extended to

$$\rho^\hbar : (C_\bullet(\mathcal{A}^{(\hbar)}), b) \longrightarrow (\Omega^\bullet_{\mathcal{A}}[\hbar, \hbar^{-1}], i\hbar\Delta).$$

Both the Hochschild homology of $\mathcal{A}^{(\hbar)}$ and the homology of $(\Omega^\bullet_{\mathcal{A}}[\hbar, \hbar^{-1}], i\hbar\Delta)$ are concentrated in degree $2n$. Passing to homology, $\rho^\hbar$ gives precisely the Feigin-Felder-Shoikhet trace formula [20] on $HH_{2n}(\mathcal{A}^{(\hbar)})$.

Chapter 4 Deformation Quantization

In this chapter, we discuss the algebraic theory of deformation quantization which deals with the operator of quantum observables as a formal deformation of classical observables. The study of deformation quantization originated from the seminal work by Bayen-Flato-Frönsdal-Lichnerowicz-Sternheimer [3] in 1978. In this theory, the Planck's constant $\hbar$ is treated as a formal variable parametrizing a family of quantum algebras. One remarkable feature is that deformation quantization exists on any Poisson manifold according to a theorem by Kontsevich [34]. This greatly extends the scope of quantization beyond ordinary phase spaces.

4.1 Deformation Quantization

4.1.1 Formal Deformations

We fix a base field, the choice of which in specific case should be clear from the context.

Definition 4.1.1. Let $\mathbb{V}$ be a vector space. We use $\mathbb{V}[[\lambda]]$ to denote formal power series in λ with coefficients in $\mathbb{V}$

$$\mathbb{V}[[\lambda]] := \left\{ \sum_{i=0}^{\infty} a_i \lambda^i \,\middle|\, a_i \in \mathbb{V} \right\}$$

and use $\mathbb{V}((\lambda))$ to denote formal Laurent series

$$\mathbb{V}((\lambda)) := \left\{ \sum_{i=N}^{\infty} a_i \lambda^i \,\middle|\, a_i \in \mathbb{V}, N \in \mathbb{Z} \right\}.$$

When $\mathbb{V} = R$ is a ring, both $R[[\lambda]]$ and $R((\lambda))$ inherit well-defined ring structure by

$$\left(\sum a_i \lambda^i\right)\left(\sum b_j \lambda^j\right) = \sum_k \left(\sum_{i+j=k} a_i b_j \right) \lambda^k.$$

Definition 4.1.2. Let $(A, \cdot)$ be an associative algebra. A formal deformation of A is an associative product $*$ on $A[[\lambda]]$ such that

① $*$ is λ-bilinear

$$(f(\lambda)a) * b = a * (f(\lambda)b) = f(\lambda)(a * b)$$

for any $a, b \in A[[\lambda]]$ and formal power series $f(\lambda)$.

② For any $a, b \in A$,

$$a * b = a \cdot b + \sum_{k=1}^{\infty} \lambda^k \mu_k(a, b)$$

where $a \cdot b$ is the product in A and $\mu_k : A \times A \to A$ are bilinear maps.

Condition ① on λ-linearity implies that $*$ is completely captured by $\{\mu_k\}$ in Condition ②. We can view $*$ as defining a family of associative products parametrized by λ such that

$$\lim_{\lambda \to 0} a * b = a \cdot b.$$

Thus $*$ becomes a formal deformation of the associative product $\cdot$. It is called formal deformation because we only consider formal power series in λ and ignore analytic properties (the analytic property is in fact interesting and important, but irrelevant in the current discussion).

Example 4.1.3. *Consider the ring $C^\infty(\mathbb{R}^{2n})$ of smooth functions on the phase space $\mathbb{R}^{2n}$. Then the Moyal product*

$$f * g = f e^{\frac{\lambda}{2} \sum_i \left(\frac{\overleftarrow{\partial}}{\partial x^i} \frac{\overrightarrow{\partial}}{\partial p_i} - \frac{\overleftarrow{\partial}}{\partial p_i} \frac{\overrightarrow{\partial}}{\partial x^i} \right)} g \qquad (\lambda = i\hbar)$$

defines a formal deformation of $C^\infty(\mathbb{R}^{2n})$. Here

$$\mu_k(f, g) = \frac{1}{k!} \left(\frac{1}{2} \right)^k f \left[\sum_i \left(\frac{\overleftarrow{\partial}}{\partial x^i} \frac{\overrightarrow{\partial}}{\partial p_i} - \frac{\overleftarrow{\partial}}{\partial p_i} \frac{\overrightarrow{\partial}}{\partial x^i} \right) \right]^k g.$$

Example 4.1.4. *The above example extends to the formal power series ring $\mathbb{R}[[x^i, p_i]]$. The same formula via Moyal product*

$$f e^{\frac{\lambda}{2} \sum_i \left(\frac{\overleftarrow{\partial}}{\partial x^i} \frac{\overrightarrow{\partial}}{\partial p_i} - \frac{\overleftarrow{\partial}}{\partial p_i} \frac{\overrightarrow{\partial}}{\partial x^i} \right)} g$$

defines a formal deformation of $\mathbb{R}[[x^i, p_i]]$.

The requirement of associativity of $*$ gives a set of constraints on the bilinear maps $\{\mu_k\}$. For example at first-order in λ

$$\begin{aligned}
&(a * b) * c - a * (b * c) \\
=&(a \cdot b + \mu_1(a, b)\lambda) * c - a * (b \cdot c + \mu_1(b, c)\lambda) + O(\lambda^2) \\
=&(a \cdot b) \cdot c + \lambda(\mu_1(a \cdot b, c) + \mu_1(a, b) \cdot c) - a \cdot (b \cdot c) - \lambda(\mu_1(a, b \cdot c) + a \cdot \mu_1(b, c)) + O(\lambda^2) \\
=&\lambda(\mu_1(a \cdot b, c) + \mu_1(a, b) \cdot c - \mu_1(a, b \cdot c) - a \cdot \mu_1(b, c)) + O(\lambda^2).
\end{aligned}$$

Here in the last step we have used the associativity of the undeformed product $\cdot$. Thus μ_1 has to satisfy the following equation

$$a \cdot \mu_1(b, c) - \mu_1(a \cdot b, c) + \mu_1(a, b \cdot c) - \mu_1(a, b) \cdot c = 0.$$

We remark that this is in fact a cocycle condition in Hochschild cohomology.

4.1.2 Poisson Algebra as Classical Limit

Definition 4.1.5. A Poisson algebra is a commutative algebra P with a bilinear map (called the Poisson bracket)

$$\{-,-\} : P \times P \longrightarrow P$$

satisfying the following properties: for any $a, b, c \in P$,

① Skew-symmetry: $\{a,b\} = -\{b,a\}$

② Leibniz rule: $\{a,bc\} = \{a,b\}\,c + b\,\{a,c\}$

③ Jacobi identity: $\{a,\{b,c\}\} + \{b,\{c,a\}\} + \{c,\{a,b\}\} = 0$

Note that by skew-symmetry, Leibniz rule also holds for the first factor

$$\{ab,c\} = a\,\{b,c\} + \{a,c\}\,b.$$

Example 4.1.6. *Let M be a symplectic manifold. Then*

$$(C^\infty(M), \{-,-\})$$

is a Poisson Algebra. Here $\{-,-\}$ is the Poisson bracket associated to the symplectic structure. In other words, classical observables form a Poisson algebra.

Let $(A,\cdot)$ be a commutative algebra. Let $(A[[\lambda]],*)$ be a formal deformation of A. Let

$$[a,b]_* := a*b - b*a$$

denote the commutator with respect to the product $*$. Since $*$ is associative, $[-,-]_*$ satisfies the Jacobi identity

$$[a,[b,c]_*]_* + [b,[c,a]_*]_* + [c,[a,b]_*]_* = 0$$

(Exercise: Check this.) Therefore $[-,-]_*$ defines a Lie bracket on $A[[\lambda]]$, which measures the noncommutativity of $*$.

By the commutativity of the undeformed algebra $(A,\cdot)$, we have for any $a, b \in A$

$$[a,b]_* = \lambda(\mu_1(a,b) - \mu_1(b,a)) + O(\lambda^2).$$

Let us define $\{-,-\} : A \times A \longrightarrow A$ by

$$\{a,b\} := \mu_1(a,b) - \mu_1(b,a)$$

or written as

$$\{a,b\} = \lim_{\lambda\to 0} \frac{1}{\lambda}\,(a*b - b*a)$$

which captures the first order noncommutativity of $*$.

Proposition 4.1.7. *$(A,\cdot,\{-,-\})$ forms a Poisson algebra.*

Proof: The skew-symmetry is obvious. The Leibniz rule follows from the $\lambda \to 0$ limit of

$$\frac{1}{\lambda}\left([a, b * c]_* - [a, b]_* * c - b * [a, c]_*\right) = 0.$$

The Jacobi identity follows from the $\lambda \to 0$ limit of

$$\frac{1}{\lambda^2}\left([a, [b, c]_*]_* + [b, [c, a]_*]_* + [c, [a, b]_*]_*\right) = 0.$$

□

We can summarize the above discussion as

$$\lambda\text{-family of Associative algebra} \xrightarrow{\lambda \to 0} \text{Poisson algebra}.$$

In mechanical problems, we usually have a classical system with classical observables as a Poisson algebra. The program of deformation quantization asks for constructing a quantized algebra $(A[[\lambda]], *)$ such that its classical limit is the prescribed Poisson algebra ($\lambda = i\hbar$)

$$\text{Poisson algebra} \underset{\text{classical limit}}{\overset{\text{quantization}}{\rightleftarrows}} \text{Associative algebra}$$

Definition 4.1.8. A deformation quantization of a Poisson algebra $(A, \cdot, \{-,-\})$ is a formal deformation $(A[[\lambda]], *)$ such that

$$\{-,-\} = \lim_{\lambda \to 0} \frac{1}{\lambda}[-,-]_*.$$

Given a Poisson algebra, its deformation quantization may not be unique.

Example 4.1.9. *Let $A = C^\infty(\mathbb{R}^2)$ with*

$$\{f, g\} = \frac{\partial f}{\partial x}\frac{\partial g}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial g}{\partial x}.$$

Let $*$ be the standard Moyal product

$$f * g = f e^{\frac{\lambda}{2}\left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)} g.$$

For any $\alpha \in \mathbb{R}$, consider the operator

$$N_\alpha := e^{\frac{\lambda}{2}\alpha \frac{\partial}{\partial x}\frac{\partial}{\partial p}} : A[[\lambda]] \longrightarrow A[[\lambda]].$$

Here $e^{\frac{\lambda}{2}\alpha \frac{\partial}{\partial x}\frac{\partial}{\partial p}}$ is understood via its power series expansion. N_α is invertible and $N_\alpha^{-1} = N_{-\alpha}$.

Let us define

$$f *_\alpha g := N_\alpha^{-1}\left((N_\alpha f) * (N_\alpha g)\right).$$

It is clear that $(A[[\lambda]], *_\alpha)$ defines a formal deformation for any $\alpha \in \mathbb{R}$. Explicitly,

$$f *_\alpha g = f e^{\frac{\lambda}{2}\left[(1-\alpha)\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - (1+\alpha)\frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right]} g.$$

In particular,

$$\{f, g\} = \lim_{\lambda \to 0} \frac{1}{\lambda}(f *_\alpha g - g *_\alpha f)$$

holds for any $\alpha \in \mathbb{R}$. *Thus* $(A[[\lambda]], *_\alpha)$ *is a deformation quantization of* $(A, \cdot, \{-,-\})$ *for any* $\alpha \in \mathbb{R}$. *When* $\alpha = 0$, *we get the Moyal product. When* $\alpha = 1$,

$$f *_1 g = f e^{\left(-\lambda \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)} g$$

is related to the normal ordering by placing the quantum operator $\hat{p} = -\lambda\frac{\partial}{\partial x}$ *to the right of* x

$$x *_1 p = xp$$
$$p *_1 x = xp - \lambda$$

Thus $*_{\alpha=1}$ *captures the composition of differential operators.*

4.2 Geometric Approach on Symplectic Manifolds

Let (M, ω) be a symplectic manifold of dimension $2n$. The classical observables on the phase space M form a Poisson algebra $(C^\infty(M), \{-,-\})$. DeWilde-Lecomte [13] obtained the general existence of deformation quantization on symplectic manifolds via cohomological method in 1983. Independently , Fedosov [18] presented another beautiful approach via differential geometric method in 1985.

In this section we describe Fedosov's geometric construction of deformation quantization on symplectic manifolds. The basic idea is that locally (M, ω) is modelled on the standard symplectic space $\mathbb{R}^{2n}$ where Weyl quantization is available. Then we can glue such local quantizations into a global one by a consistent parallel transport (i.e. by a flat connection).

4.2.1 Weyl Bundle

Formal Weyl Algebra

Let (V, ω) be a linear symplectic space of dimension $2n$. Denote

$$\widehat{\mathcal{O}}(V) := \prod_{k=0}^{\infty} \mathrm{Sym}^k(V^*), \qquad V^* = \mathrm{Hom}_{\mathbb{R}}(V, \mathbb{R})$$

by the ring of formal power series on V. Let $\{e_1, \cdots, e_{2n}\}$ be a linear basis of V and

$$\omega_{ij} := \omega(e_i, e_j).$$

Let $\left\{y^1, \cdots, y^{2n}\right\}$ be the dual basis of V^*, which can be viewed as a set of linear coordinates on V. Then we can identify

$$\widehat{\mathcal{O}}(V) := \mathbb{R}[[y^i]]$$

and express the symplectic form as

$$\omega = \frac{1}{2}\sum_{i,j=1}^{2n} \omega_{ij} dy^i \wedge dy^j.$$

The Poisson bracket on $\widehat{\mathcal{O}}(V)$ is

$$\{f,g\} = \sum_{i,j} \omega^{ij} \partial_{y^i} f \partial_{y^j} g$$

where ω^{ij} is the inverse matrix of ω_{ij}.

Definition 4.2.1. We define the formal Weyl algebra $\mathcal{W}(V)$ associated to the linear symplectic space (V,ω) by

$$\mathcal{W}(V) = \left(\widehat{\mathcal{O}}(V)[[\lambda]], *\right)$$

where for $f, g \in \widehat{\mathcal{O}}(V)[[\lambda]]$,

$$f * g := f e^{\frac{\lambda}{2}\sum_{i,j}\omega^{ij}\frac{\overleftarrow{\partial}}{\partial y^i}\frac{\overrightarrow{\partial}}{\partial y^j}} g.$$

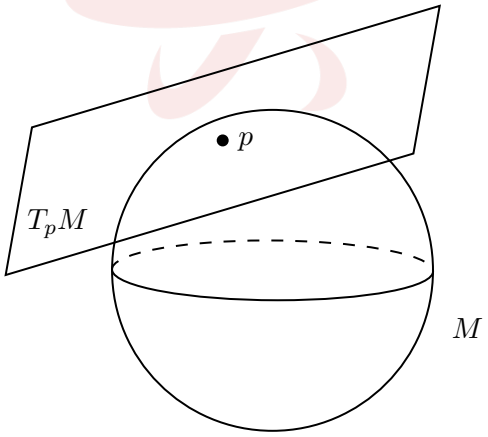
Here we have suppressed the dependence of $\mathcal{W}(V)$ on the linear symplectic form ω for simplicity. The above definition of $*$ does not depend on the choice of linear coordinates. It is clear that $\mathcal{W}(V)$ gives a deformation quantization of $\left(\widehat{\mathcal{O}}(V), \{-,-\}\right)$.

Weyl Bundle

Let (M,ω) be a $2n$-dimensional symplectic manifold. For any $p \in M$,

$$\left(T_pM, \omega|_{T_pM}\right)$$

defines a linear symplectic space.



Let $\mathcal{W}(T_pM)$ be the formal Weyl algebra associated to the linear symplectic space $\left(T_pM, \omega|_{T_pM}\right)$. This can be viewed as a quantization localized near the point $p \in M$.

Definition 4.2.2. The Weyl bundle of (M,ω) is defined to be

$$\mathcal{W}(M) := \prod_{k=0}^{\infty} \mathrm{Sym}^k(T^*M)[[\lambda]].$$

The Weyl bundle has rank of infinity. At each $p \in M$, the fiber of $\mathcal{W}(M)$ at p is

$$\mathcal{W}(M)|_p = \mathcal{W}(T_pM).$$

More precisely, a smooth section s of $\mathcal{W}(M)$ is defined locally by

$$s(\mathbf{x},\mathbf{y},\lambda)=\sum_{\substack{k\geq 0,l\geq 0\\ i_1,\cdots,i_l\geq 0}}\lambda^k a_{k,i_1\cdots i_l}(\mathbf{x})y^{i_1}\cdots y^{i_l}$$

where $\{a_{k,i_1\cdots i_l}(\mathbf{x})\}$ are smooth functions expressed in local coordinates $\left\{x^i\right\}$ of M, and $\left\{y^i\right\}$ are induced fiber coordinates on TM.

For simplicity, we will just write $\mathcal{W}$ for the Weyl bundle $\mathcal{W}(M)$ when the underlying manifold M is clear from the context. We denote

$$\Gamma(U,\mathcal{W})=\{\text{smooth sections of } \mathcal{W} \text{ in the open subset } U\}$$

for smooth sections in U. The Moyal product on each fiber $\mathcal{W}(T_pM)$ defines a fiberwise product on $\mathcal{W}$ which we still denote by $*$. Explicitly, for any two smooth sections s_1, s_2 of $\mathcal{W}$, we have

$$(s_1*s_2)(\mathbf{x},\mathbf{y},\lambda)=s_1(\mathbf{x},\mathbf{y},\lambda)e^{\frac{\lambda}{2}\sum\limits_{i,j}\omega^{ij}(\mathbf{x})\frac{\overleftarrow{\partial}}{\partial y^i}\frac{\overrightarrow{\partial}}{\partial y^j}}s_2(\mathbf{x},\mathbf{y},\lambda)$$

in local coordinates as above. Thus

$$\{\Gamma(U,\mathcal{W}\}\mid U\subset M \text{ open subset}\}$$

form a sheaf of associative algebras on M.

4.2.2 Symplectic Connection

The space $\Gamma(M,\mathcal{W})$ forms an associative algebra, but it is too large for deformation quantization. Our next goal is to construct a flat connection (Fedosov's abelian connection) on $\mathcal{W}$ to cut down the degrees of freedom. Since $\mathcal{W}$ is a bundle built on tensors of the tangent bundle TM, there is an induced connection on $\mathcal{W}$ from any connection on TM. We will start from such a connection , and discuss how Fedosov trivializes the curvature in the next subsection.

Definition 4.2.3. Let (M,ω) be a symplectic manifold. A connection ∇ on the tangent bundle TM is called a symplectic connection if

① ∇ is torsion free

$$\nabla_X Y-\nabla_Y X=[X,Y],\qquad \forall X,Y\in \mathrm{Vect}(M)$$

② ∇ is compatible with ω

$$\nabla\omega=0.$$

Symplectic connection always exists. To see this, let us choose a metric g on M and let ∇^g be the associated Levi-Civita connection. Then ∇^g is torsion-free by construction, but may not be compatible with ω. We look for

$$\nabla=\nabla^g+\alpha,\qquad \alpha\in\Omega^1(M,\mathrm{End}(TM))$$

such that ∇ becomes a symplectic connection. Let us write

$$\nabla_X Y = \nabla^g_X Y + \alpha(X, Y).$$

Torsion-free condition asks

$$\begin{aligned}&\nabla_X Y - \nabla_Y X - [X, Y]\\ =&\nabla^g_X Y + \alpha(X, Y) - \nabla^g_Y X - \alpha(Y, X) - [X, Y]\\ =&\alpha(X, Y) - \alpha(Y, X) = 0\end{aligned}$$

so we need α to satisfy

$$\alpha(X, Y) = \alpha(Y, X).$$

Compatibility with ω asks

$$X\omega(Y, Z) = \omega(\nabla_X Y, Z) + \omega(Y, \nabla_X Z)$$

which is equivalent to

$$\omega(\alpha(X, Y), Z) - \omega(\alpha(X, Z), Y) = X\omega(Y, Z) - \omega(\nabla^g_X Y, Z) - \omega(Y, \nabla^g_X Z).$$

Let ξ be the tensor defined by

$$\xi(X, Y, Z) = X\omega(Y, Z) - \omega(\nabla^g_X Y, Z) - \omega(Y, \nabla^g_X Z).$$

Skew-symmetry of ω implies

$$\xi(X, Y, Z) = -\xi(X, Z, Y).$$

Torsion-freeness of ∇^g and $d\omega = 0$ imply the total skew-symmetrization of ξ vanishes, i.e.

$$\xi(X, Y, Z) + \xi(Y, Z, X) + \xi(Z, X, Y) = 0.$$

We look for α to satisfy

$$\begin{cases}\alpha(X, Y) = \alpha(Y, X)\\ \omega(\alpha(X, Y), Z) - \omega(\alpha(X, Z), Y) = \xi(X, Y, Z)\end{cases}$$

One such α can be found by solving the equation

$$\omega(\alpha(X, Y), Z) = \frac{1}{3}\xi(X, Y, Z) + \frac{1}{3}\xi(Y, X, Z).$$

Non-degeneracy of ω guarantees this equation is uniquely solved. Such determined α clearly satisfies $\alpha(X, Y) = \alpha(Y, X)$ and

$$\begin{aligned}&\omega(\alpha(X, Y), Z) - \omega(\alpha(X, Z), Y)\\ =&\frac{1}{3}\left(\xi(X, Y, Z) + \xi(Y, X, Z) - \xi(X, Z, Y) - \xi(Z, X, Y)\right)\\ =&\frac{1}{3}\left(2\xi(X, Y, Z) - (\xi(Y, Z, X) + \xi(Z, X, Y))\right)\\ =&\frac{1}{3}\left(2\xi(X, Y, Z) + \xi(X, Y, Z)\right)\\ =&\xi(X, Y, Z)\end{aligned}$$

as required.

Unlike the Riemannian case, symplectic connections are not unique.

Theorem 4.2.4. *Symplectic connections on a symplectic manifold always exist. The set of symplectic connections is an affine space modelled on* $\Gamma(M, \mathrm{Sym}^3(T^*M))$.

Proof: We have shown the existence of a symplectic connection above. Let ∇ and ∇' be two symplectic connections and they differ by

$$\nabla'_X Y = \nabla_X Y + \alpha(X, Y).$$

Torsion-freeness requires $\alpha(X, Y) = \alpha(Y, X)$. Compatibility with ω asks $\omega(\alpha(X, Y), Z) = \omega(\alpha(X, Z), Y)$. Let β denote the tensor

$$\beta(X, Y, Z) := \omega(\alpha(X, Y), Z).$$

Then the above two conditions become

$$\begin{cases} \beta(X, Y, Z) = \beta(Y, X, Z) \\ \beta(X, Y, Z) = \beta(X, Z, Y) \end{cases}$$

which is equivalent to the total symmetry of ξ, i.e.

$$\beta \in \Gamma(M, \mathrm{Sym}^3(T^*M)).$$

□

Definition 4.2.5. Let ∇ be a symplectic connection on (M, ω) and R^∇ denote its curvature.

$$R^\nabla(X, Y)Z = \left(\nabla_X \nabla_Y - \nabla_Y \nabla_X - \nabla_{[X,Y]}\right) Z$$

for vector fields X, Y, Z on M. Define the symplectic curvature R^∇_ω by the tensor

$$R^\nabla_\omega(X, Y, Z, T) := \omega(R^\nabla(X, Y)Z, T).$$

Compatibility with ω implies

$$\begin{aligned} & R^\nabla_\omega(X, Y, Z, T) \\ =& \omega(\left(\nabla_X \nabla_Y - \nabla_Y \nabla_X - \nabla_{[X,Y]}\right) Z, T) \\ =& -\omega(Z, \left(\nabla_X \nabla_Y - \nabla_Y \nabla_X - \nabla_{[X,Y]}\right) T) \\ =& -\omega(Z, R^\nabla(X, Y)T) \\ =& \omega(R^\nabla(X, Y)T, Z) \\ =& R^\nabla_\omega(X, Y, T, Z). \end{aligned}$$

Thus R^∇_ω is skew-symmetric in the first two arguments and symmetric in the last two

$$R^\nabla_\omega \in \Gamma(M, \wedge^2(T^*M) \otimes \mathrm{Sym}^2(T^*M)).$$

Since ∇ is torsion-free, R^∇_ω also satisfies the First Bianchi identity

$$R^\nabla_\omega(X, Y, Z, T) + R^\nabla_\omega(Y, Z, X, T) + R^\nabla_\omega(Z, X, Y, T) = 0.$$

4.2.3 Fedosov's Abelian Connection

Let ∇ be a symplectic connection on (M,ω). It naturally induces a connection on all tensor $\mathrm{Sym}^k(T^*M)$ hence a connection on the Weyl bundle

$$\mathcal{W}=\prod_{k=0}^{\infty}\mathrm{Sym}^k(T^*M)[[\lambda]].$$

Let $\left\{x^i\right\}$ be local coordinates on M and

$$\omega=\frac{1}{2}\sum_{i,j}\omega_{ij}(\mathbf{x})dx^i\wedge dx^j,\qquad \omega_{ij}=\omega(\partial_{x^i},\partial_{x^j}).$$

Let $\left\{y^i\right\}$ be the corresponding fiber coordinates on TM. We can represent the symplectic curvature tensor

$$R^{\nabla}_{\omega}\in\Gamma(M,\bigwedge^2(T^*M)\otimes\mathrm{Sym}^2(T^*M))$$

in local coordinates as

$$R^{\nabla}_{\omega}=\frac{1}{4}\sum_{i,j,k,l}R_{ijkl}(\mathbf{x})dx^i\wedge dx^j\otimes y^k y^l$$

where R_{ijkl} is skew-symmetric in the first two (ij)-index and symmetric in the last two (kl)-index. The explicit identification is

$$\omega(\nabla^2(\partial_{x^k}),\partial_{x^l})=\frac{1}{2}\sum_{i,j}R_{ijkl}dx^i\wedge dx^j.$$

Let us see how the curvature of ∇ on the Weyl bundle $\mathcal{W}$ looks like. In local coordinates y^i is dual to ∂_{x^i}, thus

$$0=\nabla^2\left(\sum_k\partial_{x^k}\otimes y^k\right)=\sum_k\nabla^2(\partial_{x^k})\otimes y^k+\partial_{x^k}\otimes\nabla^2 y^k.$$

This implies

$$\sum_k\omega(\partial_{x^k},\partial_{x^l})\nabla^2y^k=-\sum_k\omega(\nabla^2(\partial_{x^k}),\partial_{x^l})\otimes y^k=-\frac{1}{2}\sum_{i,j,k}R_{ijkl}dx^i\wedge dx^j\otimes y^k$$

i.e.

$$\sum_k\omega_{kl}\nabla^2y^k=-\frac{1}{2}\sum_{i,j,k}R_{ijkl}dx^i\wedge dx^j\otimes y^k$$

$$\Longrightarrow\qquad\nabla^2y^m=-\frac{1}{2}\sum_{i,j,k,l}\omega^{lm}R_{ijkl}dx^i\wedge dx^j\otimes y^k.$$

We can write this in terms of the fiberwise Moyal product commutator as

$$\nabla^2y^m=\frac{1}{\lambda}\left[-\frac{1}{4}\sum_{i,j,k,l}R_{ijkl}dx^i\wedge dx^j\otimes y^k y^l,y^m\right]_*=\left[-\frac{1}{\lambda}R^{\nabla}_{\omega},y^m\right]_*.$$

Using the Leibniz rule and Moyal product formula, we find for any section s of $\mathcal{W}$

$$\nabla^2 s=\left[-\frac{1}{\lambda}R^{\nabla}_{\omega},s\right]_*$$

i.e. the curvature of the induced connection ∇ on the Weyl bundle $\mathcal{W}$ is

$$\nabla^2 = \left[-\frac{1}{\lambda}R^{\nabla}_{\omega}, -\right]_*.$$

Another good property of this induced connection ∇ on $\mathcal{W}$ is its compatibility with the fiberwise Moyal product: for any two sections s_1, s_2 of $\mathcal{W}$,

$$\nabla(s_1 * s_2) = (\nabla s_1) * s_2 + s_1 * \nabla s_2$$

i.e., the fiberwise Moyal product $*$ is ∇-parallel. This follows from the fact that $*$ is constructed out of ω which is itself ∇-parallel.

On the other hand, we can modify the induced connection ∇ on $\mathcal{W}$ by terms which do not come from a connection on TM. Specifically, for any 1-form valued in the Weyl bundle

$$\gamma \in \Omega^1(M, \mathcal{W})$$

we can define a new connection D on $\mathcal{W}$ by

$$D = \nabla + \frac{1}{\lambda}\left[\gamma, -\right]_*.$$

Such connection is also compatible with the fiberwise Moyal product $*$: for any two sections s_1, s_2 of $\mathcal{W}$,

$$\begin{aligned} D(s_1 * s_2) &= \nabla(s_1 * s_2) + \frac{1}{\lambda}[\gamma, s_1 * s_2]_* \\ &= \nabla s_1 * s_2 + s_1 * \nabla s_2 + \frac{1}{\lambda}[\gamma, s_1]_* * s_2 + \frac{1}{\lambda} s_1 * [\gamma, s_2]_* \\ &= (Ds_1) * s_2 + s_1 * Ds_2. \end{aligned}$$

The upshot is that it is possible to find a γ such that D becomes a flat connection on $\mathcal{W}$. This is Fedosov's key observation which will allow us to construct deformation quantization on symplectic manifolds. To see this, let us first compute the curvature of $D = \nabla + \frac{1}{\lambda}\left[\gamma, -\right]_*$

$$\begin{aligned} D^2 &= \nabla^2 + \frac{1}{\lambda}\left[\nabla\gamma, -\right]_* + \frac{1}{\lambda^2}\left[\gamma, \left[\gamma, -\right]_*\right]_* \\ &= \nabla^2 + \frac{1}{\lambda}\left[\nabla\gamma, -\right]_* + \frac{1}{2\lambda^2}\left[\left[\gamma, \gamma\right]_*, -\right]_* \\ &= \frac{1}{\lambda}\left[-R^{\nabla}_{\omega} + \nabla\gamma + \frac{1}{2\lambda}\left[\gamma, \gamma\right]_*, -\right]_*. \end{aligned}$$

Note that $\frac{1}{2}\left[\gamma, \gamma\right]_* = \gamma * \gamma$ since γ is valued in 1-form. Thus we are looking for $\gamma \in \Omega^1(M, \mathcal{W})$ such that $-R^{\nabla}_{\omega} + \nabla\gamma + \frac{1}{2\lambda}\left[\gamma, \gamma\right]_*$ lies in the center of $\mathcal{W}$, i.e.

$$-R^{\nabla}_{\omega} + \nabla\gamma + \frac{1}{2\lambda}\left[\gamma, \gamma\right]_* \in \Omega^2(M)[[\lambda]].$$

Such a connection is called an abelian connection.

To construct an abelian connection γ, we first consider the operator

$$\delta : \mathcal{W} \longrightarrow \Omega^1(M, \mathcal{W})$$

which is described in local coordinates by

$$\delta = \sum_i dx^i \frac{\partial}{\partial y^i}.$$

Equivalently, if we denote

$$\gamma_0 = \sum_{i,j} \omega_{ij} dx^i y^j \in \Omega^1(M, \mathcal{W})$$

then

$$\delta = \frac{1}{\lambda} [\gamma_0, -]_* .$$

Note that γ_0 is ∇-parallel and

$$\nabla\gamma_0 + \frac{1}{2\lambda}[\gamma_0, \gamma_0]_* = \frac{1}{\lambda}\gamma_0 * \gamma_0 = \frac{1}{2}\sum_{i,j,k,l} \omega_{ik} dx^i \omega^{kl} \omega_{jl} dx^j = -\frac{1}{2}\sum_{i,j} \omega_{ij} dx^i \wedge dx^j = -\omega$$

which is the negative of the symplectic form.

We also consider the adjoint operator

$$\delta^* : \Omega^1(M, \mathcal{W}) \longrightarrow \Gamma(M, \mathcal{W})$$

defined by

$$\delta^* = \sum_i y^i \iota_{\partial_{x^i}}.$$

Both δ and δ^* extend to forms of arbitrary degrees

$$\delta : \Omega^p(M, \mathcal{W}) \longrightarrow \Omega^{p+1}(M, \mathcal{W})$$
$$\delta^* : \Omega^p(M, \mathcal{W}) \longrightarrow \Omega^{p-1}(M, \mathcal{W})$$

and satisfy the following Hodge type relation

$$\delta\delta^* + \delta^*\delta = p + q \qquad \text{on} \quad \Omega^p(M, \mathrm{Sym}^q(T^*M))[[\lambda]].$$

In particular, δ is null-homotopic when $p + q > 0$. This immediately proves the following

Lemma 4.2.6. *The cohomology of* $(\Omega^\bullet(M, \mathcal{W}), \delta)$ *is concentrated in degree* 0 *and*

$$H^\bullet(\Omega^\bullet(M, \mathcal{W}), \delta) = H^0(\Omega^\bullet(M, \mathcal{W}), \delta) = C^\infty(M)[[\lambda]].$$

We define a $\mathbb{Z}$-grading "wt" of weight on the Weyl bundle $\mathcal{W}$ by assigning

$$\mathrm{wt}(y^i) = 1, \qquad \mathrm{wt}(\lambda) = 2.$$

It is clear that the fiberwise Moyal product preserves weights. Such a weight defines a filtration

$$\mathcal{W} = \mathcal{W}_0 \supset \mathcal{W}_1 \supset \cdots \supset \mathcal{W}_m \supset \cdots$$

where $\mathcal{W}_m$ consists of elements of weight $\geq m$.

Theorem 4.2.7 (Fedosov). *Given any sequence $\{\omega_k\}_{k\geq 1}$ of closed 2-forms on M, there exists $\gamma \in \Omega^1(M, \mathcal{W})$ of the form*

$$\gamma = \gamma_0 + \gamma^+, \qquad \gamma^+ \in \Omega^1(M, \mathcal{W}_3)$$

such that

$$-R^\nabla_\omega + \nabla\gamma + \frac{1}{2\lambda}[\gamma, \gamma]_* = \omega_\lambda.$$

Here $\omega_\lambda = -\omega + \sum_{k\geq 1} \lambda^k \omega_k$. In particular, the connection $D = \nabla + \frac{1}{\lambda}[\gamma, -]_*$ is an abelian connection whose curvature on $\mathcal{W}$ is zero.

Proof: Note that $\frac{1}{\lambda}[\gamma_0 + \gamma^+, -]_* = \delta + \frac{1}{\lambda}[\gamma^+, -]_*$ and $\nabla\gamma_0 + \frac{1}{2\lambda}[\gamma_0, \gamma_0]_* = -\omega$. Let us denote

$$\Sigma(\gamma^+) := \delta\gamma^+ + \nabla\gamma^+ + \frac{1}{2\lambda}[\gamma^+, \gamma^+]_* - R^\nabla_\omega - \sum_{k\geq 1} \lambda^k \omega_k.$$

The required equation for γ is $\Sigma(\gamma^+) = 0$.

We decompose γ^+ into

$$\gamma^+ = \gamma^+_3 + \gamma^+_4 + \cdots$$

where γ^+_m is homogeneous of weight m. Observe that both ∇ and $[-,-]_*$ preserve the weights while δ decreases the weight by 1. We will solve $\Sigma(\gamma^+) = 0$ order by order in terms of weight.

The lowest order term in $\Sigma(\gamma^+)$ has weight 2 and we need to solve

$$\delta\gamma^+_3 - R^\nabla_\omega - \lambda\omega_1 = 0.$$

Note that $\delta(R^\nabla_\omega + \lambda\omega_1) = \delta(R^\nabla_\omega) = 0$ by the First Bianchi identity. By Lemma 4.2.6, we know $R^\nabla_\omega + \lambda\omega_1$ must be δ-exact since it lies in cohomology degree 2. Hence γ^+_3 can be solved.

Assume we have found

$$\gamma^+_{\leq m-1} = \gamma^+_3 + \cdots + \gamma^+_{m-1}, \qquad m \geq 4$$

such that

$$\Sigma(\gamma^+_{\leq m-1}) \in \Omega^2(M, \mathcal{W}_{m-1}).$$

We look for γ^+_m such that the following holds

$$\Sigma(\gamma^+_{\leq m}) \in \Omega^2(M, \mathcal{W}_m).$$

First observe that for any γ

$$\left(\nabla + \frac{1}{\lambda}[\gamma, -]_*\right)\left(-R^\nabla_\omega + \nabla\gamma + \frac{1}{2\lambda}[\gamma, \gamma]_*\right) = 0$$

which is essentially the Bianchi identity for the curvature. Let

$$\Sigma(\gamma^+_{\leq m-1}) = \mathcal{O}_{m-1} \qquad \text{modulo} \quad \Omega^2(M, \mathcal{W}_m).$$

where $\mathcal{O}_{m-1}$ has weight $m-1$. Applying the above Bianchi identity to $\gamma_0+\gamma^+_{\leq m-1}$ and using the fact that ω_k's are closed, we find

$$\Longrightarrow \qquad \nabla\Sigma(\gamma^+_{\leq m-1})+\delta\Sigma(\gamma^+_{\leq m-1})+\frac{1}{\lambda}\left[\gamma^+_{\leq m-1},\Sigma(\gamma^+_{\leq m-1})\right]=0.$$

Picking up the leading order in weight, we find

$$\delta\mathcal{O}_{m-1}=0.$$

On the other hand, the leading order in weight of $\Sigma(\gamma^+_{\leq m})$ is

$$\begin{aligned}\Sigma(\gamma^+_{\leq m}) =&\Sigma(\gamma^+_{\leq m-1})+\delta\gamma^+_m \qquad \text{modulo} \quad \Omega^2(M,\mathcal{W}_m)\\ =&\mathcal{O}_{m-1}+\delta\gamma^+_m \qquad \text{modulo} \quad \Omega^2(M,\mathcal{W}_m).\end{aligned}$$

Since $\delta\mathcal{O}_{m-1}=0$ and $\mathcal{O}_{m-1}$ is a 2-form, by Lemma 4.2.6 we know $\mathcal{O}_{m-1}$ must be δ-exact. So we can find γ^+_m such that $\mathcal{O}_{m-1}+\delta\gamma^+_m=0$, i.e., $\Sigma(\gamma^+_{\leq m})\in\Omega^2(M,\mathcal{W}_m)$ holds.

Thus we can recursively construct

$$\gamma=\gamma_0+\gamma^+_3+\gamma^+_4+\cdots+\gamma^+_m+\cdots$$

such that

$$-R^\nabla_\omega+\nabla\gamma+\frac{1}{2\lambda}[\gamma,\gamma]_*=\omega_\lambda$$

holds. In particular, the curvature of $D=\nabla+\frac{1}{\lambda}[\gamma,-]_*$ is

$$D^2=\frac{1}{\lambda}\left[-R^\nabla_\omega+\nabla\gamma+\frac{1}{2\lambda}[\gamma,\gamma]_*,-\right]=\frac{1}{\lambda}[\omega_\lambda,-]=0$$

since ω_λ lies in the center of $\mathcal{W}$. □

4.2.4 Symbol Map

Let $D=\nabla+\frac{1}{\lambda}[\gamma,-]_*$ be Fedosov's abelian connection which gives a flat connection on the Weyl bundle $\mathcal{W}$. It defines a de Rham chain complex

$$(\Omega^\bullet(M,\mathcal{W}),D)$$

with the associated cohomology

$$H^\bullet_D(M,\mathcal{W}):=H^\bullet(\Omega^\bullet(M,\mathcal{W}),D).$$

Proposition 4.2.8. *The cohomology $H^\bullet_D(M,\mathcal{W})$ is*

$$H^p_D(M,\mathcal{W})=\begin{cases}C^\infty(M)[[\lambda]] & p=0\\ 0 & p>0\end{cases}$$

Proof: Consider the following filtration induced by the weight

$$F_m\Omega^p(M,\mathcal{W}) := \Omega^p(M,\mathcal{W}_{m-p}).$$

Here for $k<0$, $\mathcal{W}_k = \mathcal{W}_0 = \mathcal{W}$. This gives a decreasing filtration

$$\Omega^\bullet(M,\mathcal{W}) = F_0\Omega^\bullet(M,\mathcal{W}) \supset F_1\Omega^\bullet(M,\mathcal{W}) \supset \cdots \supset F_m\Omega^\bullet(M,\mathcal{W}) \supset \cdots$$

Fedosov's abelian connection has the form

$$D = \delta + \nabla + \frac{1}{\lambda}\left[\gamma^+, -\right]_*$$

which clearly preserves $F_m\Omega^\bullet(M,\mathcal{W})$. The induced differential on the graded piece is

$$\delta : \mathrm{Gr}_m^F \longrightarrow \mathrm{Gr}_m^F, \qquad \mathrm{Gr}_m^F := \frac{F_m\Omega^\bullet(M,\mathcal{W})}{F_{m+1}\Omega^\bullet(M,\mathcal{W})}.$$

Since $\mathcal{W}$ is built from formal power series, there is a natural vector space isomorphism

$$\widehat{\mathrm{Gr}}^F := \prod_{m\geq 0}\mathrm{Gr}_m^F \xrightarrow{\simeq} \Omega^\bullet(M,\mathcal{W}).$$

It follows from Lemma 4.2.6 that

$$H^\bullet(\widehat{\mathrm{Gr}}^F,\delta) \simeq H^\bullet(\Omega^\bullet(M,\mathcal{W}),\delta) = H^0(\Omega^\bullet(M,\mathcal{W}),\delta) = C^\infty(M)[[\lambda]].$$

So the spectral sequence of the filtration degenerates at E_1-page and the proposition follows. □

Let $\Gamma_D^{flat}(M,\mathcal{W})$ denote the space of flat sections of $\mathcal{W}$

$$\Gamma_D^{flat}(M,\mathcal{W}) := \{s\in\Gamma(M,\mathcal{W}) \,|\, Ds = 0\}.$$

Equivalently, we can identify

$$\Gamma_D^{flat}(M,\mathcal{W}) = H_D^0(M,\mathcal{W}).$$

The above proposition says

$$0 \longrightarrow \Gamma_D^{flat}(M,\mathcal{W}) \longrightarrow \Omega_D^0(M,\mathcal{W}) \xrightarrow{D} \Omega_D^1(M,\mathcal{W}) \xrightarrow{D} \cdots$$

is an exact sequence and

$$\Gamma_D^{flat}(M,\mathcal{W}) \simeq C^\infty(M)[[\lambda]].$$

This isomorphism can be described explicitly as follows.

Definition 4.2.9. Define the symbol map

$$\begin{aligned}\sigma : \Gamma(M,\mathcal{W}) &\longrightarrow C^\infty(M)[[\lambda]]\\ s(\mathbf{x},\mathbf{y},\lambda) &\mapsto s(\mathbf{x},0,\lambda)\end{aligned}$$

which sends all fiber variables y^i to zero.

The above spectral sequence computation shows that

$$\sigma : \Gamma_D^{flat}(M,\mathcal{W}) \xrightarrow{\simeq} C^\infty(M)[[\lambda]]$$

gives the required isomorphism.

4.2.5 Globalization

Fedosov's abelian connection allows us to globalize local Weyl quantization to obtain a deformation quantization on the whole manifold. We explain this construction in this subsection.

The connection $D = \nabla + \frac{1}{\lambda}[\gamma, -]_*$ is compatible with the fiberwise Moyal product

$$D(s_1 * s_2) = Ds_1 * s_2 + s_1 * Ds_2.$$

Thus if s_1, s_2 are flat sections, $Ds_1 = Ds_2 = 0$, then

$$D(s_1 * s_2) = 0$$

so $s_1 * s_2$ is also a flat section. Therefore

$$(\Gamma_D^{flat}(M, \mathcal{W}), *)$$

defines an associative algebra.

In terms of the isomorphism via symbol map

$$\sigma : \Gamma_D^{flat}(M, \mathcal{W}) \xrightarrow{\simeq} C^\infty(M)[[\lambda]]$$

we have an induced associative product $*_D$ on $C^\infty(M)[[\lambda]]$

$$f *_D g := \sigma(\sigma^{-1}(f) * \sigma^{-1}(g))$$

for $f, g \in C^\infty(M)[[\lambda]]$. In other words, the symbol map identifies two associative algebras

$$(\Gamma_D^{flat}(M, \mathcal{W}), *) \xrightarrow{\sigma} (C^\infty(M)[[\lambda]], *_D)$$

Theorem 4.2.10 (Fedosov)**.** *$(C^\infty(M)[[\lambda]], *_D)$ defines a deformation quantization on the symplectic manifold (M, ω).*

Proof: The induced product $*_D$ is clearly λ-linear and associative. Let $f, g \in C^\infty(M)$. By the fiberwise Moyal product

$$f *_D g = \sigma(\sigma^{-1}(f) * \sigma^{-1}(g)) = fg + O(\lambda)$$

so the limit $\lambda \to 0$ of $*_D$ gives the classical product.

We are left to check the first order non-commutativity. Let

$$\sigma^{-1}(f(\mathbf{x})) = f(\mathbf{x}) - \sum_i f_i(\mathbf{x}) y^i \qquad \text{modulo} \quad \mathcal{W}_2.$$

The flatness condition $D(\sigma^{-1}(f)) = 0$ implies

$$df(\mathbf{x}) - \delta\left(\sum_i f_i(\mathbf{x}) y^i\right) = 0 \qquad \Longrightarrow \qquad f_i(\mathbf{x}) = \frac{\partial f}{\partial x^i}.$$

Thus

$$\begin{aligned}\frac{1}{\lambda}[f,g]_{*_D} &= \frac{1}{\lambda}\sigma\left([\sigma^{-1}(f),\sigma^{-1}(g)]_*\right)\\ &= \sigma\left(\sum_{i,j}\omega^{ij}(\mathbf{x})\frac{\partial\sigma^{-1}(f)}{\partial y^i}\frac{\partial\sigma^{-1}(g)}{\partial y^j}+O(\lambda)\right)\\ &= \sum_{i,j}\omega^{ij}(\mathbf{x})f_i(\mathbf{x})f_j(\mathbf{x})+O(\lambda)\\ &= \{f,g\}+O(\lambda)\end{aligned}$$

as required. □

4.3 Poisson Manifold

Functions on a symplectic manifold define a Poisson algebra. However, Poisson algebras can arise in a more general setting on so-called Poisson manifolds. This includes a large class of important examples, such as the dual $\mathfrak{g}^*$ of a Lie algebra $\mathfrak{g}$ whose deformation quantization leads to the universal enveloping algebra $U(\mathfrak{g})$.

4.3.1 Polyvector Fields

Definition 4.3.1. Let M be a smooth manifold. Denote

$$\mathrm{PV}^\bullet(M)=\bigoplus_k \mathrm{PV}^k(M),\qquad \mathrm{PV}^k(M):=\Gamma(M,\wedge^k TM).$$

Elements of $\mathrm{PV}^k(M)$ are called k-polyvector fields. We denote $|\mu|=k$ for $\mu\in\mathrm{PV}^k(M)$. $\mathrm{PV}^\bullet(M)$ is a graded commutative algebra under the wedge product

$$\alpha\wedge\beta=(-1)^{|\alpha||\beta|}\beta\wedge\alpha.$$

For $k=1$, $\mathrm{PV}^1(M)=\mathrm{Vect}(M)$ are vector fields on M. There is a Lie bracket on $\mathrm{Vect}(M)$

$$[-,-]:\mathrm{Vect}(M)\times\mathrm{Vect}(M)\longrightarrow\mathrm{Vect}(M).$$

This Lie bracket extends to polyvector fields by

$$\begin{aligned}&[X_1\wedge\cdots\wedge X_m,Y_1\wedge\cdots\wedge Y_n]_{\mathrm{SN}}\\ :=&\sum_{i,j}(-1)^{i+j}[X_i,Y_j]\wedge X_1\wedge\cdots\wedge\widehat{X}_i\wedge\cdots\wedge X_m\wedge Y_1\wedge\cdots\wedge\widehat{Y}_j\wedge\cdots\wedge Y_n\end{aligned}$$

and

$$[f,X_1\wedge\cdots\wedge X_m]_{\mathrm{SN}}:=\sum_i(-1)^i X_i(f)X_1\wedge\cdots\wedge\widehat{X}_i\wedge\cdots\wedge X_m$$

for vector fields X_i,Y_j and function f. This bracket

$$[-,-]_{\mathrm{SN}}:\mathrm{PV}^k(M)\times\mathrm{PV}^l(M)\to\mathrm{PV}^{k+l-1}(M)$$

is called the Schouten-Nijenhuis bracket, also known as the Schouten bracket.

Proposition 4.3.2. *The Schouten-Nijenhuis bracket satisfies the following*

- *Skew-symmetry*
$$[\alpha,\beta]_{\mathrm{SN}} = -(-1)^{(|\alpha|-1)(|\beta|-1)}[\beta,\alpha]_{\mathrm{SN}}$$
- *Leibniz rule*
$$[\alpha,\beta\wedge\gamma]_{\mathrm{SN}} = [\alpha,\beta]_{\mathrm{SN}}\wedge\gamma + (-1)^{(|\alpha|-1)|\beta|}\beta\wedge[\alpha,\gamma]_{\mathrm{SN}}$$
- *Jacobi identity*
$$[[\alpha,\beta]_{\mathrm{SN}},\gamma]_{\mathrm{SN}} = [\alpha,[\beta,\gamma]_{\mathrm{SN}}]_{\mathrm{SN}} - (-1)^{(|\alpha|-1)(|\beta|-1)}[\beta,[\alpha,\gamma]_{\mathrm{SN}}]_{\mathrm{SN}}$$

Proof: Direct computation. □

The Jacobi identity can be also written in the symmetric form

$$(-1)^{(|\alpha|-1)(|\gamma|-1)}[\alpha,[\beta,\gamma]_{\mathrm{SN}}]_{\mathrm{SN}}+(-1)^{(|\beta|-1)(|\alpha|-1)}[\beta,[\gamma,\alpha]_{\mathrm{SN}}]_{\mathrm{SN}}+(-1)^{(|\gamma|-1)(|\beta|-1)}[\gamma,[\alpha,\beta]_{\mathrm{SN}}]_{\mathrm{SN}}=0.$$

4.3.2 Poisson Manifold and Poisson Cohomology

Poisson Manifold

Definition 4.3.3. A Poisson bivector on M is a 2-polyvector field $P\in \mathrm{PV}^2(M)$ satisfying

$$[P,P]_{\mathrm{SN}} = 0.$$

A pair (M,P) where P is a Poisson bivector is called a Poisson manifold.

Let (M,P) be a Poisson manifold. We can define a Poisson bracket on $C^\infty(M)$

$$\{-,-\}_P : C^\infty(M)\times C^\infty(M)\longrightarrow C^\infty(M)$$

by

$$\{f,g\}_P := P(df\otimes dg).$$

In local coordinates $\{x^i\}$ on M, let

$$P = \frac{1}{2}\sum_{i,j} P^{ij}(\mathbf{x})\partial_{x^i}\wedge\partial_{x^j}.$$

Then

$$\{f,g\}_P = \sum_{i,j} P^{ij}(\mathbf{x})\partial_{x^i}f\partial_{x^j}g.$$

Proposition 4.3.4. *$(C^\infty(M),\{-,-\}_P)$ defines a Poisson algebra. The Jacobi identity of $\{-,-\}_P$ is equivalent to $[P,P]_{\mathrm{SN}}=0$.*

Proof: Let us check the Jacobi identity of $\{-,-\}_P$.

$$\begin{aligned}
&\{\{f,g\}_P,h\}_P + \text{cyclic permutations}\\
=&\sum P^{ij}\partial_i\left(P^{kl}\partial_k f\partial_l g\right)\partial_j h + \text{cyclic permutations}\\
=&\sum P^{ij}\partial_i P^{kl}\partial_k f\partial_l g\partial_j h + \text{cyclic permutations}\\
=&\left(\frac{1}{2}\sum P^{ij}\partial_i P^{kl}\partial_k\wedge\partial_l\wedge\partial_j\right)(df\otimes dg\otimes dh)\\
=&\left([P,P]_{\mathrm{SN}}\right)(df\otimes dg\otimes dh).
\end{aligned}$$

□

Example 4.3.5. *Let (M,ω) be a symplectic manifold. In local coordinates*

$$\omega = \frac{1}{2}\omega_{ij}dx^i\wedge dx^j.$$

Let ω^{ij} be the inverse of ω_{ij}. Then

$$\omega^{-1} := \frac{1}{2}\sum_{i,j}\omega^{ij}\partial_{x^i}\wedge\partial_{x^j}$$

defines a Poisson bi-vector. The Poisson bracket $\{-,-\}_{\omega^{-1}}$ is precisely the one on the symplectic phase space. In this case

$$d\omega = 0 \qquad\Longleftrightarrow\qquad [\omega^{-1},\omega^{-1}]_{\mathrm{SN}} = 0.$$

Example 4.3.6 (Constant Poisson Structure)**.** *Let $M=\mathbb{R}^n$ and*

$$P = \frac{1}{2}\sum_{i,j}P^{ij}\partial_{x^i}\wedge\partial_{x^j},\qquad P^{ij}\in\mathbb{R}.$$

Since P^{ij}'s are constants, $[P,P]_{\mathrm{SN}}=0$ holds. Such P is called a constant Poisson structure.

Example 4.3.7 (Linear Poisson Structure)**.** *Let $M=\mathbb{R}^n$ and*

$$P = \frac{1}{2}\sum_{i,j}P^{ij}(\mathbf{x})\partial_{x^i}\wedge\partial_{x^j},\qquad P^{ij}(\mathbf{x}) = \sum_k c_k^{ij}x^k.$$

Here $c_k^{ij}\in\mathbb{R}$ are constants, thus $P^{ij}(\mathbf{x})$ is linear in $\mathbf{x}$. The Poisson bracket reads

$$\left\{x^i,x^j\right\}_P = \sum_k c_k^{ij}x^k.$$

It is clear from this expression that the Jacobi identity is equivalent to the condition that c_k^{ij} defines the structure constant of a Lie algebra.

Intrinsically, we can identify $M=\mathfrak{g}^*$ as the linear dual of a Lie algebra $\mathfrak{g}$. The linear coordinates $\left\{x^i\right\}$ can be viewed as a basis of $\mathfrak{g}$, under which the Lie bracket is expressed via the structure constants c_k^{ij}. The linear Poisson structure is also called Lie-Poisson structure.

Poisson Cohomology

Let (M, P) be a Poisson manifold. Define

$$d_P : \mathrm{PV}^\bullet(M) \longrightarrow \mathrm{PV}^{\bullet+1}(M)$$
$$\alpha \longmapsto [P, \alpha]_{\mathrm{SN}}$$

Using the Jacobi identity

$$[[P, P]_{\mathrm{SN}}, -]_{\mathrm{SN}} = 2[P, [P, -]_{\mathrm{SN}}]_{\mathrm{SN}}$$

and the Poisson condition $[P, P]_{\mathrm{SN}} = 0$, we find

$$d_P^2 = 0.$$

Thus $(\mathrm{PV}^\bullet(M), d_P)$ defines a complex

$$0 \longrightarrow \mathrm{PV}^0(M) \xrightarrow{d_P} \mathrm{PV}^1(M) \xrightarrow{d_P} \cdots \xrightarrow{d_P} \mathrm{PV}^n(M) \longrightarrow 0, \qquad n = \dim M$$

which is called the Lichnerowicz complex.

Definition 4.3.8. The cohomology of the Lichnerowicz complex is called the Poisson cohomology, denoted by

$$H_P^k(M) := H^k(\mathrm{PV}^\bullet(M), d_P).$$

Example 4.3.9. *Consider an infinitesimal deformation of the Poisson structure*

$$P \longrightarrow P + \varepsilon Q, \qquad Q \in \mathrm{PV}^2(M)$$

where ε is the infinitesimal parameter. The Poisson condition at leading order

$$[P + \varepsilon Q, P + \varepsilon Q]_{\mathrm{SN}} = 2\varepsilon [P, Q]_{\mathrm{SN}} = 0$$

says Q is d_P-closed. Let X be a vector field. It generates a flow on M which changes

$$P \longrightarrow P + d_P X.$$

So d_P-exact Q corresponds to trivial deformations induced by diffeomorphisms. Thus

$$H_P^2(M) = \frac{\{\textit{first order deformations of } P\}}{\{\textit{trivial deformations}\}}.$$

Example 4.3.10. *Let (M, ω) be a symplectic manifold and P be the Poisson bi-vector $P = \omega^{-1}$. The non-degeneracy of ω induces a bundle isomorphism*

$$\varphi : TM \longrightarrow T^*M$$
$$X \longmapsto -\iota_X \omega$$

In local coordinates $\omega = \frac{1}{2}\omega_{ij} dx^i \wedge dx^j$

$$\varphi(\partial_{x^i}) = -\sum_j \omega_{ij} dx^j.$$

Extending to exterior tensors, φ induces an isomorphism

$$\varphi : \mathrm{PV}^k(M) \longrightarrow \Omega^k(M)$$

between k-polyvector fields and differential k-forms. Observe that

- *for any function f,*

$$\varphi(d_P f) = \varphi\left(\sum_{i,j} \omega^{ij}\partial_{x^j} f \partial_{x^i}\right) = df$$

- *for vector field ∂_{x^k}*

$$\begin{aligned}
\varphi(d_P(\partial_{x^k})) =& \varphi\left(-\frac{1}{2}\sum_{i,j}\partial_k\omega^{ij}\partial_{x^i}\wedge\partial_{x^j}\right)\\
=& -\frac{1}{2}\sum_{i,j,m,l}\partial_k\omega^{ij}\omega_{im}\omega_{jl}dx^m\wedge dx^l\\
=& \frac{1}{2}\sum_{i,j,m,l}\partial_k\omega_{im}\omega^{ij}\omega_{jl}dx^m\wedge dx^l\\
=& \frac{1}{2}\sum_{i,m}\partial_k\omega_{im}dx^m\wedge dx^i\\
\overset{\substack{using\\ d\omega=0}}{=\!=\!=}& -\frac{1}{2}\sum_{i,m}\left(\partial_i\omega_{mk}+\partial_m\omega_{ki}\right)dx^m\wedge dx^i\\
=& -d\left(\sum_i \omega_{ki}dx^i\right)\\
=& d\varphi(\partial_{x^k})
\end{aligned}$$

Using the Leibniz rule, we find φ identifies two complexes

$$(\mathrm{PV}^\bullet(M), d_P) \xrightarrow{\varphi}_{\simeq} (\Omega^\bullet(M), d).$$

In particular, we have

$$H^2_{\omega^{-1}}(M) \overset{\varphi}{\simeq} H^2(M).$$

This says that Poisson deformations of ω^{-1} are parametrized by $H^2(M)$, i.e., are induced from deformations of the symplectic form ω in $H^2(M)$.

4.3.3 Kontsevich's Star Product

Star Product

Definition 4.3.11. Let (M, P) be a Poisson manifold. A star product (or a deformation quantization) on (M, P) is a formal deformation $(C^\infty(M)[[\lambda]], *)$ of $C^\infty(M)$

$$f * g = f \cdot g + \sum_{k=1}^{\infty}\lambda^k\mu_k(f, g)$$

such that

- $\lim_{\lambda\to 0}\frac{1}{\lambda}(f * g - g * f) = \{f, g\}_P$
- Each μ_k is a bi-differential operator.

In other words, a star product on (M,P) is a deformation quantization of the Poisson algebra $(C^\infty(M),\{-,-\}_P)$ such that all μ_k's are "local". We can also replace $C^\infty(M)$ by other appropriate functions (such as polynomials/formal power series, etc) in specific context.

Example 4.3.12. *Let (M,ω) be a symplectic manifold and $P=\omega^{-1}$. Then Fedosov's abelian connection D leads to a star product $*_D$ on (M,ω^{-1}). See Section 4.2.5.*

Example 4.3.13. *Let $M=\mathbb{R}^n$ and*

$$P=\frac{1}{2}\sum_{i,j}P^{ij}\partial_{x^i}\wedge\partial_{x^j},\qquad P^{ij}\in\mathbb{R}$$

be a constant Poisson structure. When $\det(P^{ij})=0$, P does not come from a symplectic structure. Nevertheless, the same formula of Moyal product

$$f*g:=fe^{\frac{\lambda}{2}\sum\limits_{i,j}P^{ij}\frac{\overleftarrow{\partial}}{\partial x^i}\frac{\overrightarrow{\partial}}{\partial x^j}}g$$

defines a star product on $(\mathbb{R}^n,P)$.

Example 4.3.14. *Let $\mathfrak{g}$ be a Lie algebra and $M=\mathfrak{g}^*$ which is equipped with the Lie-Poisson structure $P_{\mathfrak{g}}$. Let*

$$U^\lambda(\mathfrak{g}):=T(\mathfrak{g})[\lambda]/\sim$$

where $T(\mathfrak{g})=\bigoplus\limits_{m\geq 0}\mathfrak{g}^{\otimes m}$ is the tensor algebra of $\mathfrak{g}$ and the quotient relation $\sim$ is

$$x\otimes y-y\otimes x\sim\lambda[x,y].$$

If we specialize to $\lambda=1$, then $U^{\lambda=1}(\mathfrak{g})$ is the universal enveloping algebra of $\mathfrak{g}$. Let

$$\mathrm{Sym}(\mathfrak{g}):=\bigoplus_{m\geq 0}\mathrm{Sym}^m(\mathfrak{g})=\lim_{\lambda\to 0}U^\lambda(\mathfrak{g})$$

denote the ring of polynomial functions on $\mathfrak{g}^*$. We can embed $\mathrm{Sym}(\mathfrak{g})$ into $U^\lambda(\mathfrak{g})$ via the symmetrization map

$$\begin{aligned}\varphi:\mathrm{Sym}(\mathfrak{g})[\lambda]&\longrightarrow U^\lambda(g)\\ x_1x_2\cdots x_m\lambda^l&\longmapsto\frac{\lambda^l}{m!}\sum_{\sigma\in S_m}x_{\sigma(1)}\otimes\cdots\otimes x_{\sigma(m)}\end{aligned}$$

which is a vector space isomorphism by the Poincaré-Birkhoff-Witt Theorem.

$U^\lambda(\mathfrak{g})$ is an associative algebra with $\otimes$ as the product. This allows us to define a canonical star product $*_{\mathfrak{g}}$ on $\mathrm{Sym}(\mathfrak{g})[\lambda]$ by

$$(f_1*_{\mathfrak{g}}f_2):=\varphi^{-1}(\varphi(f_1)\otimes\varphi(f_2)).$$

For example, if $X,Y\in g$ are linear, then

$$X*_{\mathfrak{g}}Y=\varphi^{-1}(X\otimes Y)=\varphi^{-1}\left(\frac{1}{2}(X\otimes Y+Y\otimes X)+\frac{1}{2}(X\otimes Y-Y\otimes X)\right)=XY+\frac{\lambda}{2}[X,Y].$$

$$
\begin{aligned}
X^2 *_{\mathfrak{g}} Y =& \varphi^{-1}(X \otimes X \otimes Y) \\
=& \varphi^{-1}\left(\frac{1}{3}(X \otimes X \otimes Y + X \otimes Y \otimes X + Y \otimes X \otimes X)\right. \\
&\left. + \frac{2}{3} X \otimes (X \otimes Y - Y \otimes X) + \frac{1}{3}\left((X \otimes Y - Y \otimes X) \otimes X\right)\right) \\
=& X^2 Y + \lambda X[X,Y] + \frac{\lambda^2}{6}[X,[X,Y]].
\end{aligned}
$$

It is worthwhile to point out that the Moyal product formula does not work in this linear Poisson case. The term $\frac{\lambda^2}{6}[X,[X,Y]]$ gives a further correction in the above example. In general, the Moyal product formula

$$
e^{\frac{\lambda}{2}\sum\limits_{i,j} \frac{\overleftarrow{\partial}}{\partial x^i} P^{ij}(\mathbf{x}) \frac{\overrightarrow{\partial}}{\partial x^j}}
$$

fails to be associative when $P^{ij}(\mathbf{x})$ are not constant. This leads to a major difficulty in constructing star product on Poisson manifolds.

Example 4.3.15. *Let $M = \mathbb{R}^2$ and $P = xy\partial_x \wedge \partial_y$. Denote by*

$$
\partial_{\log x} := x\partial_x, \qquad \partial_{\log y} := y\partial_y.
$$

Then we can write P as

$$
P = \partial_{\log x} \wedge \partial_{\log y}.
$$

It follows that

$$
f * g := f e^{\frac{\lambda}{2}\left(\overleftarrow{\partial}_{\log x}\overrightarrow{\partial}_{\log y} - \overleftarrow{\partial}_{\log y}\overrightarrow{\partial}_{\log x}\right)} g
$$

defines a star product on $(\mathbb{R}^2, P)$. In this star product

$$
\begin{aligned}
x * y &= e^{\frac{\lambda}{2}} xy \\
y * x &= e^{-\frac{\lambda}{2}} xy
\end{aligned}
$$

In particular, we find

$$
x * y = e^{\lambda} y * x.
$$

Kontsevich's Star Product

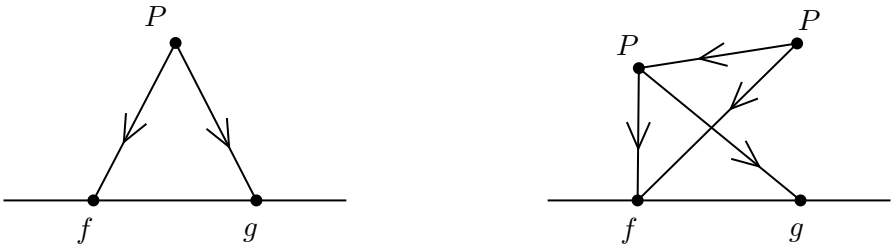
In [34], Kontsevich figured out a remarkable explicit way to correct the Moyal product formula into an associative product using the quantum field theory of two-dimensional Poisson σ-model (as explained later by Cattaneo-Felder [8]).

Theorem 4.3.16 (Kontsevich)**.** *Deformation quantization exists on any Poisson manifold.*

We sketch the basic idea of Kontsevich's construction. Consider the Poisson manifold

$$
(\mathbb{R}^n, P = \frac{1}{2}\sum_{i,j} P^{ij}(\mathbf{x})\partial_{x^i} \wedge \partial_{x^j}).
$$

Let Γ_r be a graph with $r+2$ vertices and $2r$ (directed) edges drawn in the upper half-plane such that two vertices are placed on the real line with only incoming edges and each of the other r vertices is placed in the interior with two out-going edges from it.



From each Γ_r, we can write down a bi-differential operator $C_{\Gamma_r}(f,g)$ by assigning $P = \frac{1}{2}\sum_{i,j} P^{ij}(\mathbf{x})\frac{\partial}{\partial x^i}\otimes\frac{\partial}{\partial x^j}$ to each of the r vertices in the interior where we place the two derivations $\frac{\partial}{\partial x^i}$ and $\frac{\partial}{\partial x^j}$ to its out-going edges. For example, the first graph in the above figure gives

$$\frac{1}{2}\sum_{i,j} P^{ij}(\mathbf{x})\frac{\partial f}{\partial x^i}\otimes\frac{\partial g}{\partial x^j}$$

and the second graph gives

$$\frac{1}{2}\sum_{i,j} P^{ij}\sum_{k,m}\frac{1}{2}\left(\frac{\partial}{\partial x^i}P^{km}\right)\frac{\partial^2 f}{\partial x^k\partial x^j}\frac{\partial g}{\partial x^m}.$$

Then we can construct a star product of the form

$$\mu_r(f,g) = \sum_{\Gamma_r}\omega_{\Gamma_r}C_{\Gamma_r}(f,g)$$

where the coefficients ω_{Γ_r} is obtained from an appropriate Feynman graph integral over the configuration space of the upper half-plane.

The Feynman graph integral arises from the correlation functions in the Poisson σ-model

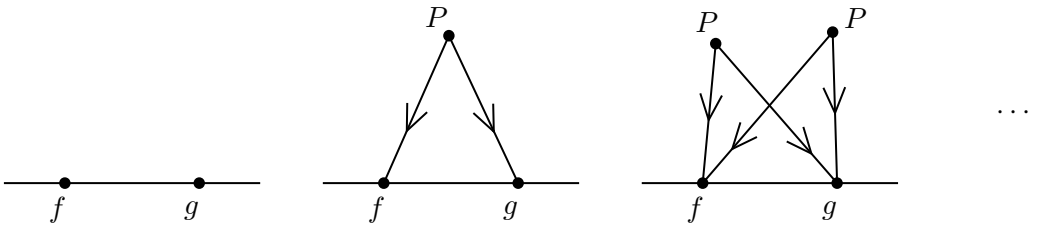
$$S[X,\eta] = \int_H \eta_i dx^i + \frac{1}{2}\int_H P^{ij}(x)\eta_i\wedge\eta_j$$

where $X = (X^i)$ is a bosonic field describing mappings from the upper half-plane H to $\mathbb{R}^n$

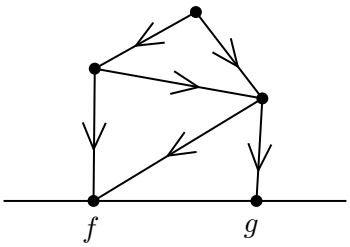
$$X : H \longrightarrow \mathbb{R}^n$$

and $\eta = (\eta_i)$ is a fermionic field valued as a 1-form on H. The associativity of the star product $*$ follows from a version of Stokes Theorem.

The Moyal product formula corresponds to the graphs



Kontsevich's formula gives a manifest correction of the Moyal product by all possible graphs with edges connecting two interior vertices.



4.4 Trace Map

We consider (M,ω) to be a symplectic manifold in this section. Let $(C^\infty(M)[[\lambda]],\star)$ be a deformation quantization. A λ-linear map

$$\mathrm{Tr} : C^\infty(M)[[\lambda]] \to \mathbb{R}((\lambda))$$

is called a trace map if

$$\mathrm{Tr}(f\star g) = \mathrm{Tr}(g\star f) \qquad \text{or equivalently} \qquad \mathrm{Tr}([f,g]_\star) = 0$$

for any $f,g \in C^\infty(M)[[\lambda]]$. Since Tr is λ-linear, it suffices to assume $f,g \in C^\infty(M)$.

The star product $\star$ describes the algebraic structure of quantized operators on the phase space. If there would be a representation of the quantized operators, then the corresponding trace on the representing Hilbert space would annihilate the operator commutators. A trace map defined above precisely models this information without specifying the representation.

It turns out that on a symplectic manifold, there exists a unique nontrivial trace map (up to a coefficient rescaling) on the deformation quantized algebra. In this section, we present an explicit construction of this trace map in terms of the quantum Hochschild-Kostant-Rosenberg (HKR) map in Section 3.6.5 and Fedosov's abelian connection.

4.4.1 Differential Graded Algebra

Differential Graded Algebra (DGA)

Definition 4.4.1. A differential graded algebra (DGA) consists of a graded vector space

$$A = \bigoplus_{n\in\mathbb{Z}} A^n$$

together with an associative product $\cdot$ and a linear map $d : A \to A$ (the differential) such that

① the product $\cdot$ preserves the degree $A^m \cdot A^n \subseteq A^{m+n}$

② the differential d increases the degree by one: $d : A^n \to A^{n+1}$, and satisfies $d^2 = 0$

③ graded Leibniz rule holds: for any $a_1, a_2 \in A$

$$d(a_1\cdot a_2) = d(a_1)\cdot a_2 + (-1)^{|a_1|} a_1 \cdot d(a_2)$$

Here we write $|a|$ for the degree of a, i.e., $|a| = p$ for $a \in A^p$.

For a graded algebra A, we will use $[-,-]$ to denote the graded commutator

$$[a_1, a_2] := a_1 a_2 - (-1)^{|a_1||a_2|} a_2 a_1.$$

If $[a_1, a_2] = 0$ for all $a_1, a_2 \in A$, we say A is graded commutative.

Example 4.4.2. *The de Rham complex $(\Omega^\bullet(M), d)$ on a manifold M is a DGA. The differential d is the de Rham differential. $\Omega^\bullet(M)$ is graded commutative.*

Example 4.4.3. *Let (V, ω) be a linear symplectic space with linear coordinate $\{y^i\}$. Let*

$$\widehat{\Omega}(V) := \mathbb{R}[[y^i, dy^i, \lambda]]$$

denote $\mathbb{R}[[\lambda]]$-valued formal differential forms on V. Let $\hat{d}$ denote the de Rham differential with respect to variables $\{y^i\}$

$$\hat{d} = \sum_i dy^i \frac{\partial}{\partial y^i}$$

The Moyal product $\star$ extends to a product on $\widehat{\Omega}(V)$ by

$$(f_I(y,\lambda) dy^I) \star (g_J(y,\lambda) dy^J) := (f_I(y,\lambda) \star g_J(y,\lambda)) dy^I \wedge dy^J$$

Here I, J are multi-indices. The triple $(\widehat{\Omega}(V), \star, \hat{d})$ defines a DGA, which will be used in Section 4.4.3 to construct the trace map.

Hochschild Chain Complex

In Section 3.6.5, we have discussed the Hochschild chain complex of an associative algebra

$$\cdots \to C_p(A) \xrightarrow{b} C_{p-1}(A) \xrightarrow{b} \cdots \xrightarrow{b} C_1(A) \xrightarrow{b} C_0(A)$$

This generalizes naturally to differential graded algebras. We follow [46].

Let (A, d) be a DGA where d is the differential and

$$C_p(A) = A^{\otimes p+1}.$$

The Hochschild differential b is modified to incorporate with the graded signs

$$\begin{aligned} b(a_0 \otimes a_1 \otimes \cdots \otimes a_p) := &\sum_{k=0}^{p-1} (-1)^{1+\sum_{i=0}^{k}(|a_i|+1)} a_0 \otimes \cdots \otimes a_k a_{k+1} \otimes \cdots \otimes a_p \\ &+ (-1)^{|a_p|+(|a_p|+1)\sum_{i=0}^{p-1}(|a_i|+1)} a_p a_0 \otimes a_1 \otimes \cdots \otimes a_{p-1}. \end{aligned}$$

The differential d induces a differential on Hochschild chains (still called d) by

$$d(a_0 \otimes a_1 \otimes \cdots \otimes a_p) := \sum_{k=0}^{p} (-1)^{\sum_{i=0}^{k-1}(|a_i|+1)} a_0 \otimes \cdots \otimes da_k \otimes \cdots \otimes a_p.$$

It is straight-forward to check that

$$b^2 = d^2 = 0, \qquad bd + db = 0$$

The chain complex $C_\bullet(A)$ is double graded. One grading p is the Hochschild degree $C_p(A)$. There is another internal degree q induced from the tensor of the graded space of A

$$C_p(A)_q = \bigoplus_{j_0+\cdots+j_p=q} A^{j_0} \otimes A^{j_1} \otimes \cdots \otimes A^{j_p}$$

We have

$$b : C_p(A)_q \longrightarrow C_{p-1}(A)_q$$
$$d : C_p(A)_q \longrightarrow C_p(A)_{q+1}$$

The Hochschild chain complex of the DGA (A, d) becomes the total complex of the double complex $C_\bullet(A)$ with differential $d + b$.

It will be useful to introduce the following operations on Hochschild chains.

Definition 4.4.4. Given $a \in A$, we define

$$\mathrm{ad}_a : A \longrightarrow A \quad \text{by} \quad \mathrm{ad}_a(u) := [a, u] = au - (-1)^{|a||u|}ua$$

and extend ad_a to Hochschild chains

$$\mathrm{ad}_a : C_\bullet(A) \longrightarrow C_\bullet(A)$$

by

$$\mathrm{ad}_a(a_0 \otimes a_1 \otimes \cdots \otimes a_p) = \sum_{k=0}^{p} (-1)^{|a| \sum_{i=0}^{k-1} (|a_i|+1)} a_0 \otimes \cdots \otimes \mathrm{ad}_a\, a_k \otimes \cdots \otimes a_p.$$

For example, we have

$$\mathrm{ad}_a(a_0 \otimes a_1) = [a, a_0] \otimes a_1 + (-1)^{|a|(|a_0|+1)} a_0 \otimes [a, a_1].$$

Definition 4.4.5. Given $a \in A$, we define

$$\wedge_a : C_\bullet(A) \longrightarrow C_\bullet(A)$$

by

$$\wedge_a(a_0 \otimes a_1 \otimes \cdots \otimes a_p) := \sum_{k=0}^{p} (-1)^{|a|+(|a|+1)\sum_{i=0}^{k} (|a_i|+1)} a_0 \otimes \cdots \otimes a_k \otimes a \otimes a_{k+1} \otimes \cdots \otimes a_p.$$

For example, we have

$$\wedge_a(a_0 \otimes a_1) = (-1)^{|a|+(|a|+1)(|a_0|+1)} a_0 \otimes a \otimes a_1 + (-1)^{|a|+(|a|+1)(|a_0|+|a_1|+2)} a_0 \otimes a_1 \otimes a.$$

Proposition 4.4.6. *The following relations hold*

$$\begin{aligned}
\mathrm{ad}_{[a,\tilde{a}]} &= \mathrm{ad}_a\, \mathrm{ad}_{\tilde{a}} - (-1)^{|a||\tilde{a}|}\, \mathrm{ad}_{\tilde{a}}\, \mathrm{ad}_a \\
\wedge_a \wedge_{\tilde{a}} &= (-1)^{(|a|+1)(|\tilde{a}|+1)}\, \wedge_{\tilde{a}} \wedge_a \\
\mathrm{ad}_a &= b \wedge_a - (-1)^{|a|+1} \wedge_a b \\
\wedge_{\mathrm{ad}_a \tilde{a}} &= (-1)^{|a|} \left(\mathrm{ad}_a \wedge_{\tilde{a}} - (-1)^{|a|(|\tilde{a}|+1)} \wedge_{\tilde{a}} \mathrm{ad}_a \right) \\
\mathrm{ad}_{da} &= d\, \mathrm{ad}_a - (-1)^{|a|}\, \mathrm{ad}_a\, d \\
\wedge_{da} &= -\left(d \wedge_a - (-1)^{|a|+1} \wedge_a d \right)
\end{aligned}$$

Proof: Direct computation. □

Twisting Construction

Let $a \in A^1$ be a degree 1 element. Consider the twisting of the differential d by

$$d_a := d + \mathrm{ad}_a \,.$$

Such d_a also satisfies the Leibniz rule

$$d_a(a_1 \cdot a_2) = (d_a a_1) \cdot a_2 + (-1)^{|a_1|} a_1 \cdot d_a(a_2).$$

By Proposition 4.4.6, we have

$$d_a^2 = \mathrm{ad}_{da + \frac{1}{2}[a,a]} \,.$$

Definition 4.4.7. A Maurer-Cartan element of (A, d) is a degree 1 element $a \in A^1$ satisfying

$$da + \frac{1}{2}[a, a] = 0.$$

This is also called the Maurer-Cartan equation. Since $|a| = 1$, this is the same as

$$da + a^2 = 0.$$

Thus if a is a Maurer-Cartan element, then (A, d_a) defines a new DGA which will be called the twist of (A, d) by a. The Hochschild chain complex of the twisted DGA is related to the untwisted one by the following proposition.

Proposition 4.4.8. *For any degree* 1 *element* $a \in A^1$*, we have*

$$e^{-\wedge_a}(d + b)e^{\wedge_a} = d + b + \mathrm{ad}_a - \wedge_{da+a^2} \,.$$

In particular if a *is a Maurer-Cartan element, then the operator* $e^{\wedge_a}$ *intertwines the Hochschild chain complex of the twisted* (A, d_a) *with the untwisted* (A, d) *in the following sense*

$$(d + b)e^{\wedge_a} = e^{\wedge_a}(d + \mathrm{ad}_a + b).$$

Proof: By Proposition 4.4.6,

$$\begin{aligned} [d, \wedge_a] &= -\wedge_{da} \\ [b, \wedge_a] &= \mathrm{ad}_a \\ [\mathrm{ad}_a, \wedge_a] &= -\wedge_{\mathrm{ad}_a(a)} = -2\wedge_{a^2} \end{aligned}$$

It follows that

$$e^{-\wedge_a}(d + b)e^{\wedge_a} = (d + b) + [d + b, \wedge_a] + \frac{1}{2}\left[[d + b, \wedge_a], \wedge_a\right] = d + b + \mathrm{ad}_a - \wedge_{da} - \wedge_{a^2} \,.$$

□

4.4.2 Quantum HKR Map

In Section 3.6.5, we have explained how S^1-correlation on the phase space $\mathbb{R}^{2n}$ leads to a quantum HKR map. We reformulate this construction on the formal Weyl algebra and explain how to glue it to the Weyl bundle on a symplectic manifold.

Local Case

Recall the S^1-propagator in Section 3.6.4

$$G(\theta_1,\theta_2)=g(\theta_2-\theta_1)=\sum_{n\in\mathbb{Z}\setminus\{0\}}\frac{i}{2\pi n}e^{2\pi i n(\theta_2-\theta_1)}.$$

The periodic function $g(\theta)$ is explicitly given by

$$g(\theta)=\begin{cases}0 & \theta=0\\ \theta-\dfrac{1}{2} & 0<\theta<1\end{cases}$$

Let (V,ω) be a linear symplectic space with

$$\omega=\frac{1}{2}\sum_{i,j}\omega_{ij}dy^i\wedge dy^j.$$

The associated formal Weyl algebra is

$$\widehat{\mathcal{W}}(V)=(\mathcal{O}(V)[[\lambda]],*)=(\mathbb{R}[[y^i,\lambda]],*).$$

The following definition is a reformulation of Definition 3.6.12 into the current setting.

Definition 4.4.9. We define the S^1-correlation map

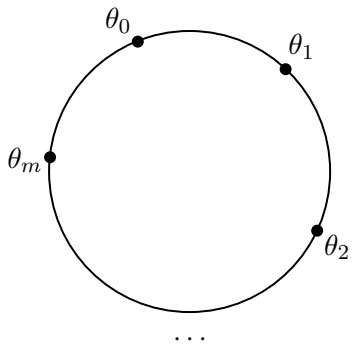
$$\langle-\rangle_{S^1}:\widehat{\mathcal{W}}(V)\otimes\cdots\otimes\widehat{\mathcal{W}}(V)\longrightarrow\widehat{\mathcal{W}}(V)$$

by

$$\begin{aligned}&\langle f_0\otimes f_1\otimes\cdots\otimes f_m\rangle_{S^1}\\ :=\ & m!\int_{\mathrm{Cyc}_{m+1}(S^1)}d\theta_0d\theta_1\cdots d\theta_m e^{\frac{\lambda}{2}\sum\limits_{i,j,\alpha,\beta}\omega^{ij}G(\theta_\alpha,\theta_\beta)\frac{\partial}{\partial y_i^{(\alpha)}}\frac{\partial}{\partial y_j^{(\beta)}}}f_0(\mathbf{y}^{(0)},\lambda)\cdots f_m(\mathbf{y}^{(m)},\lambda)\Big|_{y_i^{(\alpha)}=y^i}.\end{aligned}$$

Here

$$\mathrm{Cyc}_{m+1}(S^1)=\left\{(\theta_0,\theta_1,\cdots,\theta_m)\in(S^1)^{m+1}\,|\,\theta_0,\theta_1,\cdots,\theta_m\text{ are distinct in clockwise cyclic order}\right\}.$$



The following lemma will be useful when we discuss gluing the S^1-correlation map on general symplectic manifolds.

Lemma 4.4.10. *Assume $h(y)$ is a constant or linear in y. Then for any $f_i \in \widehat{\mathcal{W}}(V)$*

$$\sum_{i=0}^{m-1} \langle f_0 \otimes \cdots \otimes f_i \otimes h \otimes f_{i+1} \otimes \cdots \otimes f_m \rangle_{S^1} + \langle f_0 \otimes \cdots \otimes f_m \otimes h \rangle_{S^1} = h \langle f_0 \otimes \cdots \otimes f_m \rangle_{S^1}$$

Proof: This is clearly true when h = constant. Assume h is linear in y. Using the explicit formula in Definition 4.4.9,

$$\begin{aligned} &\sum_{i=0}^{m-1} \langle f_0 \otimes \cdots \otimes f_i \otimes h \otimes f_{i+1} \otimes \cdots \otimes f_m \rangle_{S^1} + \langle f_0 \otimes \cdots \otimes f_m \otimes h \rangle_{S^1} \\ &\qquad = h \langle f_0 \otimes \cdots \otimes f_m \rangle_{S^1} + \text{terms involving } \int_0^1 d\theta_i G(\theta_i, \theta_j). \end{aligned}$$

The proposition follows by observing that

$$\int_0^1 d\theta_i G(\theta_i, \theta_j) = \int_0^1 d\theta \left(\theta - \frac{1}{2}\right) = 0.$$

□

Let us denote

$$\widehat{\Omega}(V) := \mathbb{R}[[y^i, dy^i, \lambda]]$$

which represents $\mathbb{R}[[\lambda]]$-valued formal differential forms on V. Let

$$\widehat{d} = \sum_i dy^i \frac{\partial}{\partial y^i}$$

denote the de Rham differential in $\{y^i\}$'s.

Definition 4.4.11. We define the quantum HKR map

$$\rho^\lambda : \widehat{\mathcal{W}}(V) \otimes \cdots \otimes \widehat{\mathcal{W}}(V) \longrightarrow \widehat{\Omega}(V)$$

by

$$\rho^\lambda (f_0 \otimes f_1 \otimes \cdots \otimes f_m) = \frac{1}{m!} \left\langle f_0 \otimes \widehat{d} f_1 \otimes \cdots \otimes \widehat{d} f_m \right\rangle_{S^1}.$$

Here $\widehat{d} f = \sum_i \partial_{y^i} f dy^i$ and

$$\left\langle f_0 \otimes \widehat{d} f_1 \otimes \cdots \otimes \widehat{d} f_m \right\rangle_{S^1} := \sum_{i_1, \cdots, i_m} \langle f_0 \otimes \partial_{y^{i_1}} f_1 \otimes \cdots \otimes \partial_{y^{i_m}} f_m \rangle_{S^1} \, dy^{i_1} \wedge \cdots \wedge dy^{i_m}.$$

Proposition 4.4.12. *The quantum HKR map is a chain map*

$$\rho^\lambda : (C_\bullet(\widehat{\mathcal{W}}(V)), b) \longrightarrow (\widehat{\Omega}^\bullet(V), \lambda \Delta).$$

Here $\Delta = \sum_{i,j} \omega^{ij} \frac{\partial}{\partial y^i} \iota_{\partial_{y^j}}$ is the Lie derivative with respect to the Poisson bi-vector ω^{-1}.

Proof: The proof is the same as in Section 3.6.5.

□

Global Case

Let (M,ω) be a symplectic manifold and ∇ be a symplectic connection. Let $\mathcal{W}=\mathcal{W}(M)$ be the Weyl bundle and we define similarly the bundle of formal differential forms on TM

$$\widehat{\Omega}=\widehat{\Omega}(TM):=\prod_{k=0}^{\infty}\mathrm{Sym}^k(T^*M)\otimes\wedge^\bullet T^*M[[\lambda]].$$

We also define the bundle $C_\bullet(\mathcal{W})$ of Hochschild chains of $\mathcal{W}$ whose fiber over $p\in M$ is the Hochschild chains of $\widehat{\mathcal{W}}(T_pM)$, i.e.

$$C_p(\mathcal{W}):=\left(\prod_{k=0}^{\infty}\mathrm{Sym}^k(T^*M)[[\lambda]]\right)^{\otimes p+1}.$$

The Hochschild differential b defines bundle maps

$$b:C_p(\mathcal{W})\longrightarrow C_{p-1}(\mathcal{W})$$

and $(C_\bullet(\mathcal{W}),b)$ forms a chain complex of bundles.

The fiberwise quantum HKR map leads to a chain map of complexes of bundles

$$\rho^\lambda:(C_\bullet(\mathcal{W}),b)\longrightarrow(\widehat{\Omega}^\bullet,\lambda\Delta).$$

Here Δ is the fiberwise BV operator, which in local coordinates is

$$\Delta=\sum_{i,j}\omega^{ij}(\mathbf{x})\frac{\partial}{\partial y^i}\iota_{\partial_{y^j}}.$$

As bundle maps, all b,Δ and ρ^λ are $C^\infty(M)$-linear.

The symplectic connection ∇ also induces a connection (still called ∇) on $\widehat{\Omega}$ via the tensor construction. Since ω is ∇-parallel, both b and Δ are ∇-parallel

$$\nabla(b)=\nabla(\Delta)=0.$$

Since ρ^λ is constructed out of ω and the S^1-propagator $G(\theta_1,\theta_2)$, we know ρ^λ is also ∇-parallel. Thus we have a commutative diagram

$$\begin{array}{ccc} C_p(\mathcal{W}) & \xrightarrow{\rho^\lambda} & \widehat{\Omega}^p \\ \downarrow{\scriptstyle b} & & \downarrow{\scriptstyle \lambda\Delta} \\ C_{p-1}(\mathcal{W}) & \xrightarrow{\rho^\lambda} & \widehat{\Omega}^{p-1} \end{array}$$

where all maps in this diagram are ∇-parallel bundle maps.

4.4.3 Twisting by Fedosov's Abelian Connection

Let $D=\nabla+\frac{1}{\lambda}[\gamma,-]_*$ be a Fedosov's abelian connection as in Theorem 4.2.7. It gives a flat connection on $\mathcal{W}$ and extends to

$$D:\Omega^\bullet(M,\mathcal{W})\to\Omega^{\bullet+1}(M,\mathcal{W})$$

via the following Leibniz rule

$$D(\alpha \otimes s) = d\alpha \otimes s + (-1)^{|p|}\alpha \wedge \nabla s, \qquad \alpha \in \Omega^p(M), s \in \mathcal{W}.$$

The flatness of D implies $D^2 = 0$ on $\Omega^\bullet(M, \mathcal{W})$. Thus we have a complex

$$(\Omega^\bullet(M, \mathcal{W}), D)$$

which is called the de Rham complex with values in $\mathcal{W}$.

Since D is compatible with the fiberwise Moyal product, $(\Omega^\bullet(M, \mathcal{W}), D)$ becomes a DGA with $\Omega^p(M, \mathcal{W})$ the degree p piece. We denote this DGA as

$$\Omega(M, \mathcal{W}) := (\Omega^\bullet(M, \mathcal{W}), D)$$

Thus we have the Hochschild chain complex as in Section 4.4.1

$$C_\bullet(\Omega(M, \mathcal{W}), D + b).$$

Let

$$\widehat{d} : \widehat{\Omega}^\bullet \longrightarrow \widehat{\Omega}^{\bullet+1}$$

denote the fiberwise de Rham differential. In local coordinates

$$\widehat{d} = \sum_i dy^i \frac{\partial}{\partial y^i}.$$

This $\widehat{d}$ is a bundle map and compatible with the fiberwise Moyal product:

$$\widehat{d}(s_1 * s_2) = \widehat{d}(s_1) * s_2 + s_1 * (\widehat{d}s_2), \qquad \forall s_1, s_2 \in \mathcal{W}.$$

We extend $\widehat{d}$ to a $C^\infty(M)$-linear map

$$\widehat{d} : \Omega^\bullet(M, \widehat{\Omega}^\bullet) \longrightarrow \Omega^\bullet(M, \widehat{\Omega}^{\bullet+1})$$

by

$$\widehat{d}(\alpha \otimes u) = (-1)^p \alpha \otimes \widehat{d}u, \qquad \alpha \in \Omega^p(M), u \in \widehat{\Omega}^\bullet.$$

Let

$$\nabla : \Omega^\bullet(M, \widehat{\Omega}^\bullet) \longrightarrow \Omega^{\bullet+1}(M, \widehat{\Omega}^\bullet)$$

be the map induced on tensors from the symplectic connection ∇. Let $\{x^i\}$ be local coordinates on M and $\{y^i\}$ be the induced fiberwise coordinates on TM. Assume the connection ∇ acts as

$$\nabla y^i = \sum_j \alpha^i_j(\mathbf{x}) y^j,$$

then

$$\nabla dy^i = \sum_j \alpha^i_j(\mathbf{x}) dy^j = -\widehat{d}\left(\sum_j \alpha^i_j(\mathbf{x}) y^j\right) = -\widehat{d}\nabla y^i.$$

A slight generalization of this computation shows

$$\nabla\widehat{d} + \widehat{d}\nabla = 0 \qquad \text{on} \quad \Omega^\bullet(M, \widehat{\Omega}^\bullet).$$

which simply says $\widehat{d}$ is ∇-parallel.

Similarly we extend the BV operator Δ to

$$\Delta : \Omega^\bullet(M, \widehat{\Omega}^\bullet) \to \Omega^\bullet(M, \widehat{\Omega}^{\bullet-1})$$

by

$$\Delta(\alpha \otimes u) = (-1)^{|p|}\alpha \otimes \Delta U, \qquad \alpha \in \Omega^p(M), u \in \widehat{\Omega}^\bullet.$$

Then Δ is compatible with the symplectic connection ∇ in the sense

$$\nabla\Delta + \Delta\nabla = 0 \qquad \text{on} \quad \Omega^\bullet(M, \widehat{\Omega}^\bullet).$$

We also extend the quantum HKR map $\rho^\lambda : C_\bullet(\mathcal{W}) \longrightarrow \widehat{\Omega}^\bullet$ to be valued in $\Omega^\bullet(M)$

$$\rho^\lambda : C_\bullet(\Omega(M, \mathcal{W})) \longrightarrow \Omega(M, \widehat{\Omega}^\bullet)$$

by

$$\rho^\lambda\left(\alpha_0 u_0 \otimes \alpha_1 u_1 \otimes \cdots \otimes \alpha_m u_m\right) := (-1)^{\sum_{k=1}^{m-1} k|\alpha_k|}\left(\alpha_0 \wedge \cdots \wedge \alpha_m\right)\rho^\lambda\left(u_0 \otimes \cdots \otimes u_m\right).$$

Here $\alpha_i \in \Omega^{|\alpha_i|}(M)$ and $u_i \in \mathcal{W}$. The following diagram commutes

$$\begin{array}{ccc} C_\bullet(\Omega(M, \mathcal{W})) & \xrightarrow{\rho^\lambda} & \Omega(M, \widehat{\Omega}^\bullet) \\ \downarrow{\scriptstyle b} & & \downarrow{\scriptstyle \lambda\Delta} \\ C_\bullet(\Omega(M, \mathcal{W})) & \xrightarrow{\rho^\lambda} & \Omega(M, \widehat{\Omega}^\bullet) \end{array}$$

Now we are ready to incorporate Fedosov's abelian connection $D = \nabla + \frac{1}{\lambda}[\gamma, -]_*$. Let us consider the twisting of Hochschild chains by $\gamma \in \Omega^1(M, \mathcal{W})$

$$e^{\wedge_{\gamma/\lambda}} : C_\bullet(\Omega(M, \mathcal{W})) \longrightarrow C_\bullet(\Omega(M, \mathcal{W})[\lambda^{-1}]).$$

Here $[\lambda^{-1}]$ means localizing λ

$$(-)[\lambda^{-1}] := (-) \otimes_{\mathbb{R}[[\lambda]]} \mathbb{R}((\lambda)).$$

By the same computation as in Proposition 4.4.8

$$e^{-\wedge_{\gamma/\lambda}}(\nabla + b)e^{\wedge_{\gamma/\lambda}} = \nabla + b + \mathrm{ad}_{\gamma/\lambda} - \wedge_{\nabla(\gamma/\lambda)+\gamma/\lambda*\gamma/\lambda} = D + b - \frac{1}{\lambda}\wedge_{R^\nabla_\omega + \omega_\lambda}.$$

Here we have used $\nabla\gamma + \frac{1}{2\lambda}[\gamma, \gamma]_* = R^\nabla_\omega + \omega_\lambda$ in Theorem 4.2.7. Thus

$$e^{\wedge_{\gamma/\lambda}}(D + b) = \left(\nabla + b + \frac{1}{\lambda}\wedge_{R^\nabla_\omega + \omega_\lambda}\right)e^{\wedge_{\gamma/\lambda}}.$$

Definition 4.4.13. We define the Fedosov-twisted quantum HKR map by

$$\rho_D^\lambda := \rho^\lambda \circ e^{\wedge_{\gamma/\lambda}} : C_\bullet(\Omega(M,\mathcal{W})) \longrightarrow \Omega(M,\widehat{\Omega}^\bullet)[\lambda^{-1}].$$

The following proposition is a reformulation of the BV quantization result in [23] [28].

Proposition 4.4.14. *The following diagram commutes*

$$\begin{array}{ccc} C_\bullet(\Omega(M,\mathcal{W})) & \xrightarrow{\rho_D^\lambda} & \Omega(M,\widehat{\Omega}^\bullet)[\lambda^{-1}] \\ \downarrow{\scriptstyle D+b} & & \downarrow{\scriptstyle \nabla+\lambda\Delta+\frac{1}{\lambda}\widehat{d}R_\omega^\nabla} \\ C_\bullet(\Omega(M,\mathcal{W})) & \xrightarrow{\rho_D^\lambda} & \Omega(M,\widehat{\Omega}^\bullet)[\lambda^{-1}] \end{array}$$

Equivalently, ρ_D^λ gives a chain map of complexes

$$\rho_D^\lambda : (C_\bullet(\Omega(M,\mathcal{W})), D+b) \longrightarrow \left(\Omega(M,\widehat{\Omega}^\bullet)[\lambda^{-1}], \nabla+\lambda\Delta+\frac{1}{\lambda}\widehat{d}R_\omega^\nabla\right).$$

Proof: Observe

$$\widehat{d}(R_\omega^\nabla+\omega_\lambda) = \widehat{d}R_\omega^\nabla$$

which is linear in y. It follows from the defintion of ρ^λ and Lemma 4.4.10 that

$$\rho^\lambda \circ \wedge_{R_\omega^\nabla+\omega_\lambda}(-) = \widehat{d}R_\omega^\nabla \cdot \rho^\lambda(-).$$

Thus

$$\begin{aligned} \rho_D^\lambda \circ (D+b) &= \rho^\lambda \circ e^{\wedge_{\gamma/\lambda}} \circ (D+b) \\ &= \rho^\lambda \circ \left(\nabla + b + \frac{1}{\lambda}\wedge_{R_\omega^\nabla+\omega_\lambda}\right) \circ e^{\wedge_{\gamma/\lambda}} \\ &= \left(\nabla+\lambda\Delta+\frac{1}{\lambda}\widehat{d}R_\omega^\nabla\right) \circ \rho^\lambda \circ e^{\wedge_{\gamma/\lambda}} \\ &= \left(\nabla+\lambda\Delta+\frac{1}{\lambda}\widehat{d}R_\omega^\nabla\right) \circ \rho_D^\lambda. \end{aligned}$$

□

4.4.4 Trace Map and Index

Definition 4.4.15. We define the bundle map (here $\dim M = 2n$)

$$\int_{\mathrm{Ber}} : \Omega(M,\widehat{\Omega}^\bullet)[\lambda^{-1}] \longrightarrow \Omega(M)((\lambda))$$

by

$$\int_{\mathrm{Ber}} s(\mathbf{x},\mathbf{y},\lambda) := \frac{1}{n!}\left(\frac{1}{2}\sum_{i,j}\omega^{ij}(\mathbf{x})\iota_{\partial_{y^i}}\iota_{\partial_{y^j}}\right)^n s\Big|_{\substack{y^i=0\\ dy^i=0}}.$$

Remark 4.4.16. The map $\int_{\mathrm{Ber}}$ is a version of Berezin integral on Grassmann variables.

Note that $\int_{\text{Ber}} s = 0$ unless $s \in \Omega(M, \widehat{\Omega}^{2n})$. Let us denote

$$\hat{\omega} := \frac{1}{2} \sum_{i,j} \omega_{ij}(\mathbf{x}) dy^i \wedge dy^j$$

Then for any $\alpha \in \Omega(M)$, we have

$$\int_{\text{Ber}} \alpha \frac{\hat{\omega}^n}{n!} = \alpha.$$

Proposition 4.4.17. *$\int_{\text{Ber}}$ is a chain map intertwining*

$$\int_{\text{Ber}} : \left(\Omega(M, \widehat{\Omega}^\bullet)[\lambda^{-1}], \nabla + \lambda\Delta + \frac{1}{\lambda} \widehat{d} R_\omega^\nabla \right) \longrightarrow (\Omega(M)((\lambda)), d).$$

Here d is the de Rham differential on M.

Proof: For any $s \in \Omega(M, \widehat{\Omega}^\bullet)$.

$$\int_{\text{Ber}} \Delta(s) = 0 \quad \text{and} \quad \int_{\text{Ber}} \widehat{d} R_\omega^\nabla \wedge s = 0$$

since $\Delta(s)$ can not lie in $\widehat{\Omega}^{2n}$ while $\widehat{d} R_\omega^\nabla$ contains y which goes to zero under $\int_{\text{Ber}}$.

Let us assume s is of the form $s = \alpha \frac{\hat{\omega}^n}{n!}$ where $\alpha \in \Omega(M)$. Since ∇ is a sympletic connection, $\nabla \hat{\omega} = 0$. Thus

$$\int_{\text{Ber}} \nabla \left(\alpha \frac{\hat{\omega}^n}{n!} \right) = \int_{\text{Ber}} d\alpha \frac{\hat{\omega}^n}{n!} = d\alpha = d \int_{\text{Ber}} \alpha \frac{\hat{\omega}^n}{n!}$$

This proves the proposition. □

Proposition 4.4.18. *The composition of the Fedosov-twisted quantum HKR map with $\int_{\text{Ber}}$ gives a chain map*

$$\int_{\text{Ber}} \circ \rho_D^\lambda : (C_\bullet(\Omega^\bullet(M, \mathcal{W})), D + b) \longrightarrow (\Omega^\bullet(M)((\lambda)), d).$$

Proof: This follows from Proposition 4.4.14 and Proposition 4.4.17.

□

Recall that the space $\Gamma_D^{flat}(M, \mathcal{W})$ of flat sections of $\mathcal{W}$ defines a deformation quantization. Restricting $\int_{\text{Ber}} \circ \rho_D^\lambda$ to $\Gamma_D^{flat}(M, \mathcal{W})$, we obtain a chain map

$$\int_{\text{Ber}} \circ \rho_D^\lambda : (C_\bullet(\Gamma_D^{flat}(M, \mathcal{W})), b) \longrightarrow (\Omega^\bullet(M)((\lambda)), d).$$

Definition 4.4.19. Define the trace map on the deformation quantized algebra $\Gamma_D^{flat}(M, \mathcal{W})$

$$\text{Tr} : \Gamma_D^{flat}(M, \mathcal{W}) \to \mathbb{R}((\lambda))$$

by

$$\text{Tr}(s) := \int_M \int_{\text{Ber}} \rho_D^\lambda(s) = \int_M \int_{\text{Ber}} \rho^\lambda(e^{\wedge_{\gamma/\lambda}}(s)).$$

Remark 4.4.20. This approach to trace in Definition 4.4.19 is equivalent to [23, Definition 2.41].

Theorem 4.4.21. *The trace map* Tr *satisfies the following properties*

① *For* $f \in C^\infty(M)$,

$$\mathrm{Tr}\,\sigma^{-1}(f) = \frac{(-1)^n}{n!\lambda^n}\left(\int_M f\frac{\omega^n}{n!} + O(\lambda)\right).$$

② *For any* $s_1, s_2 \in \Gamma_D^{flat}(M, \mathcal{W})$ *which are compactly supported on* M,

$$\mathrm{Tr}(s_1 * s_2) = \mathrm{Tr}(s_2 * s_1).$$

Proof: For ①, the leading λ-order contribution of $\mathrm{Tr}\,\sigma^{-1}(f)$ comes from

$$\begin{aligned}
&\int_M \int_{\mathrm{Ber}} \rho^\lambda(f \otimes (\gamma_0/\lambda)^{\otimes 2n}) \\
=&\int_M \int_{\mathrm{Ber}} \frac{1}{(2n)!\lambda^{2n}} \left\langle f \otimes \underbrace{\widehat{d}\gamma_0 \otimes \cdots \otimes \widehat{d}\gamma_0}_{2n} \right\rangle_{S^1} \\
=&\frac{1}{(2n)!\lambda^{2n}} \int_M \int_{\mathrm{Ber}} \left(f(\widehat{d}\gamma_0)^{2n} + O(\lambda)\right)
\end{aligned}$$

Here $\gamma_0 = \sum_{i,j} \omega_{ij} dx^i y^j \in \Omega^1(M, \mathcal{W})$, and $\hat{d}\gamma_0 = -\sum_{i,j} \omega_{ij} dx^i dy^j$.

Using a Darboux coordinate, it is straight-foward to compute

$$\frac{1}{(2n)!}(\widehat{d}\gamma_0)^{2n} = (-1)^n \frac{\omega^n}{n!}\frac{\hat{\omega}^n}{n!}.$$

Then ① follows from

$$\frac{1}{(2n)!}\int_M \int_{\mathrm{Ber}} f(\widehat{d}\gamma_0)^{2n} = \int_M \int_{\mathrm{Ber}} (-1)^n f \frac{\omega^n}{n!}\frac{\hat{\omega}^n}{n!} = (-1)^n \int_M f\frac{\omega^n}{n!}.$$

For ②, by Proposition 4.4.18 we have

$$\begin{aligned}
&\mathrm{Tr}(s_1 * s_2 - s_2 * s_1) \\
=&\,\mathrm{Tr}(b(s_1 \otimes s_2)) \\
=&\int_M \int_{\mathrm{Ber}} \rho_D^\lambda(b(s_1 \otimes s_2)) \\
=&\int_M d \int_{\mathrm{Ber}} \rho_D^\lambda(s_1 \otimes s_2) = 0.
\end{aligned}$$

□

One remarkable property of the trace map is

$$\mathrm{Tr}(1) = \int_M e^{-\omega_\lambda/\lambda}\hat{A}(M)$$

Here ω_λ appears in Theorem 4.2.7 which parametrizes the deformation quantization. This formula is called the Algebraic Index Theorem which was established by Fedosov [19] and Nest-Tsygan [40] as the algebraic analogue of Atiyah-Singer Index theorem. One geometric approach to compute the algebraic index is to use the explicit trace map (Definition 4.4.19) and reduce it to an exact semi-classical calculation in terms of Feynman diagrams. This is explained in [23] [28], and $\hat{A}(M)$ appears as the one-loop contribution.

Bibliography

[1] Arnol' d, Vladimir I., Alexander B. Givental, Sergei P. Novikov. *Symplectic Geometry.* In: Arnold, V.I., Novikov, S.P. (eds) Dynamical Systems IV. Encyclopaedia of Mathematical Sciences, vol 4. Springer, Berlin, Heidelberg. (2001)

[2] Bates, Sean, and Alan Weinstein. *Lectures on the Geometry of Quantization.* Vol. 8. American Mathematical Soc., 1997.

[3] Bayen, François, Moshé Flato, Christian Fronsdal, André Lichnerowicz, and Daniel Sternheimer. *Deformation theory and quantization. I. Deformations of symplectic structures.* Annals of Physics 111, no. 1 (1978): 61-110. *Deformation theory and quantization. II. Physical applications.* Annals of Physics 111, no. 1 (1978): 111-151.

[4] Berezin, Felix Aleksandrovich. *Feynman path integrals in a phase space.* Soviet Physics Uspekhi 23.11 (1980): 763.

[5] Bordemann, Martin. *Deformation quantization: a survey.* Journal of Physics: Conference Series. Vol. 103. No. 1. IOP Publishing, 2008.

[6] Born, Max. *Statistical interpretation of quantum mechanics.* Science 122.3172 (1955): 675-679.

[7] Brylinski, Jean-Luc. *Loop spaces, characteristic classes and geometric quantization.* Springer Science & Business Media, 2009.

[8] Cattaneo, Alberto S., and Giovanni Felder. *Poisson sigma models and deformation quantization.* Modern Physics Letters A 16.04n06 (2001): 179-189.

[9] Carlitz, Robert D., and Denis A. Nicole. *Classical paths and quantum mechanics.* Annals of Physics 164.2 (1985): 411-462.

[10] Coleman, Sidney. *Aspects of symmetry: selected Erice lectures.* Cambridge University Press, 1988.

[11] Curtright, Thomas L., and Cosmas K. Zachos. *Quantum mechanics in phase space.* Asia Pacific Physics Newsletter 1.01 (2012): 37-46.

[12] De Gosson, Maurice A. *Symplectic geometry and quantum mechanics.* Vol. 166. Springer Science & Business Media, 2006.

[13] De Wilde, Marc, and Pierre BA Lecomte. *Existence of star-products and of formal deformations of the Poisson Lie algebra of arbitrary symplectic manifolds.* Letters in Mathematical Physics 7 (1983): 487-496.

[14] Dirac, Paul Adrien Maurice. *The principles of quantum mechanics*. No. 27. Oxford University Press, 1981.

[15] Faddeev, Ljudvig D., and Oleg Aleksandrovich IAkubovskiĭ. *Lectures on quantum mechanics for mathematics students*. Vol. 47. American Mathematical Soc., 2009.

[16] Feynman, Richard P., Albert R. Hibbs, and Daniel F. Styer. *Quantum mechanics and path integrals*. Courier Corporation, 2010.

[17] Feynman, Richard Phillips, and Laurie M. Brown. *Feynman's thesis: a new approach to quantum theory*. World Scientific, 2005.

[18] Fedosov, Boris V. *A simple geometrical construction of deformation quantization.* Journal of differential geometry 40.2 (1994): 213-238.

[19] Fedosov, Boris V. *Deformation quantization and index theory.* Mathematical topics 9 (1996).

[20] Feigin, Boris, Giovanni Felder, and Boris Shoikhet. *Hochschild cohomology of the Weyl algebra and traces in deformation quantization.* Duke Mathematical Journal 127 (3) 487 - 517, (2005)

[21] Folland, Gerald B. *Harmonic analysis in phase space.* No. 122. Princeton university press, 1989.

[22] Gel'fand, Israel M., and Akiva M. Yaglom. *Integration in functional spaces and its applications in quantum physics*. Journal of Mathematical Physics 1.1 (1960): 48-69.

[23] Grady, Ryan E., Qin Li, and Si Li. *Batalin–Vilkovisky quantization and the algebraic index.* Advances in Mathematics 317 (2017): 575-639.

[24] Ginzburg, Victor. *Lectures on noncommutative geometry.* arXiv:math/0506603 (2005).

[25] Griffiths, David J., and Darrell F. Schroeter. *Introduction to quantum mechanics*. Cambridge University Press, 2018.

[26] Grosche, Christian, Frank Steiner, and Frank Steiner. *Handbook of Feynman path integrals*. Vol. 145. Berlin: Springer, 1998.

[27] Guillemin, Victor, and Shlomo Sternberg. *Semi-classical analysis.* Boston, MA: International Press, 2013.

[28] Gui, Zhengping, Si Li, and Kai Xu. *Geometry of localized effective theories, exact semi-classical approximation and the algebraic index.* Communications in Mathematical Physics 382.1 (2021): 441-483.

[29] Hall, Brian C. *Holomorphic methods in analysis and mathematical physics.* Contemporary Mathematics 260 (2000): 1-60.

[30] Hall, Brian C. *Quantum theory for mathematicians.* Springer Publication, 2013.

[31] Hislop, Peter D., and Israel Michael Sigal. *Introduction to spectral theory: With applications to Schrödinger operators.* Vol. 113. Springer Science & Business Media, 2012.

[32] Holstein, Barry R., and Arthur R. Swift. *Path integrals and the WKB approximation.* American Journal of Physics 50.9 (1982): 829-832.

[33] Kaiser, David. *History: Shut up and calculate!.* Nature 505.7482 (2014): 153-155.

[34] Kontsevich, Maxim. *Deformation quantization of Poisson manifolds.* Letters in Mathematical Physics 66 (2003): 157-216.

[35] Landau, Lev Davidovich, and Evgenii Mikhailovich Lifshitz. *Quantum mechanics: non-relativistic theory.* Vol. 3. Elsevier, 2013.

[36] Li, Si. *Classical Mechanics and Geometry.* Boston, MA: International Press of Boston, 2023.

[37] Li, Si. *Electromagnetism and Geometry.* Boston, MA: International Press of Boston, 2023.

[38] Littlejohn, Robert G. *The semiclassical evolution of wave packets.* Physics reports 138.4-5 (1986): 193-291.

[39] Loday, Jean-Louis. *Cyclic homology.* Vol. 301. Springer Science & Business Media, 2013.

[40] Nest, Ryszard, and Boris Tsygan. *Algebraic index theorem.* Communications in Mathematical Physics 172, 223-262 (1995)

[41] Shankar, Ramamurti. *Principles of quantum mechanics.* Springer Science & Business Media, 2012.

[42] Sharan, Pankaj. *Star-product representation of path integrals.* Physical Review D 20.2 (1979): 414.

[43] Susskind, Leonard, and Art Friedman. *Quantum mechanics: the theoretical minimum.* Basic Books, 2014.

[44] Takhtadzhian, Leon Armenovich. *Quantum mechanics for mathematicians.* Vol. 95. American Mathematical Soc., 2008.

[45] Teschl, Gerald. *Mathematical methods in quantum mechanics*. Vol. 157. American Mathematical Soc., 2014.

[46] Tsygan, Boris. *Cyclic homology*. Cyclic homology in non-commutative geometry. Vol. 121, 73-113. Springer Science & Business Media (2003)

[47] Von Neumann, John. *Mathematical foundations of quantum mechanics: New edition*. Vol. 53. Princeton University Press, 2018.

[48] Weinberg, Steven. *Lectures on quantum mechanics*. Cambridge University Press, 2015.

[49] Witten, Edward. *Analytic continuation of Chern-Simons theory*. AMS/IP Stud. Adv. Math 50 (2011): 347.

[50] Woodhouse, Nicholas Michael John. *Geometric quantization*. Oxford university press, 1992.

[51] Zinn-Justin, Jean. *Path integrals in quantum mechanics*. OUP Oxford, 2004.