Quantum Mechanics: Basic Theory

(preliminary draft updated May 2024)

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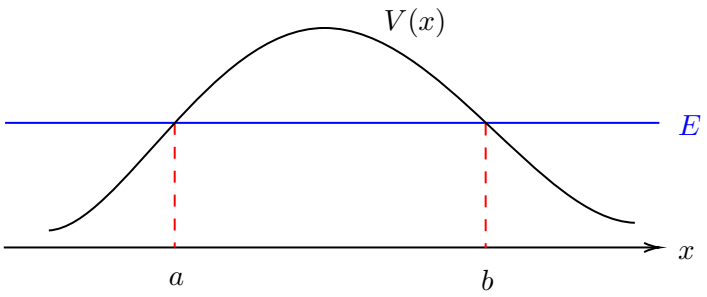
量子隧穿的启示[1]：唯有无惧虚度时间，方能逾越高山险阻。



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

imaginary time (虚时间) for quantum tunneling

Thanks very much for your support of this note! It is greatly appreciated if you are willing to help improve it by sending your comments such as typo, mistake or suggestion at your tea time. You are welcome to submit your comment via either the website

https://www.wjx.cn/vm/OtMinic.aspx

or the barcode below

You can also contact me at sili@mail.tsinghua.edu.cn. The draft will be updated on my homepage: https://sili-math.github.io/. Thank you.

[1]See Section 2.7.3

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Preface

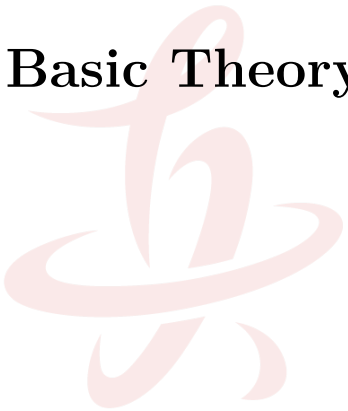
In April 2021, Qiuzhen College (求真书院) was newly established at Tsinghua University under the leadership of Professor Shing-Tung Yau. It homes the distinguished elite mathematics program in China starting in 2021: the "Yau Mathematical Sciences Leaders Program" (丘成桐数学科学领军人才培养计划). This program puts strong 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 Qiuzhen College during the fall semester of 2023. The first part of the note 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. Some useful resources that we consulted in this note are listed at the end of this note.

I greatly appreciate the "*Notes Taker Program*" at Qiuzhen College, which has triggered and supported the production of this note. A preliminary version of this note was typed by Yang Peng (杨鹏) , and I am extremely grateful to his great job. I want to thank the following students 吴越, 郭秀惠, 刘九和 and 王春森 for their help on careful proofreading of this note.

Part I

Basic Theory



Chapter 1 Hilbert Space Formalism

In this chapter, we explains 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

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

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 unitary groups 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.

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, then

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.

1.2.4 Classical Limit

We briefly discuss the algebraic relation between classical and quantum observables.

Definition 1.2.1. A *Poisson algebra* is a commutative algebra P together with a bilinear operation (called the Poisson bracket)

$$\{-,-\} : P \times P \longrightarrow P$$

which satisfies the following properties: $\forall a, b, c \in P$,

- Skew-symmetry:
$$\{a, b\} = -\{b, a\}$$
- Leibniz rule:
$$\{a, bc\} = \{a, b\}c + b\{a, c\}$$
- Jacobi identity:
$$\{\{a, b\}, c\} + \{\{b, c\}, a\} + \{\{c, a\}, b\} = 0$$

Example 1.2.2. Let M be a symplectic manifold. Then

$$(C^\infty(M), \{-,-\})$$

is a Poisson algebra, where $\{-,-\}$ is the standard Poisson bracket associated to the symplectic structure. In other words, classical observables form a Poisson algebra.

In quantum mechanics, the composition of operators are no longer commutative. This quantum effect can be viewed as a deformation.

Definition 1.2.3. Let $\mathbb{V}$ be a vector space. We use $\mathbb{V}[\![\hbar]\!]$ to denote formal power series in $\hbar$ with coefficients in $\mathbb{V}$

$$\mathbb{V}[\![\hbar]\!] = \left\{ \sum_{i=0}^{\infty} a_i \hbar^i \,\middle|\, a_i \in \mathbb{V} \right\}.$$

Definition 1.2.4. Let A be a commutative $\mathbb{C}$-algebra. A *formal deformation* of A is an associative product $*_\hbar$ on $A[\![\hbar]\!]$ such that

① $*_\hbar$ is $\hbar$-bilinear

$$(f(\hbar)a) *_\hbar b = a *_\hbar (f(\hbar)b) = f(\hbar)(a *_\hbar b)$$

for any $a, b \in A[\![\hbar]\!]$, $f(\hbar) \in \mathbb{C}[\![\hbar]\!]$.

② For any $a, b \in A$,

$$a *_\hbar b = a \cdot b + \sum_{k=1}^{\infty} \hbar^k m_k(a, b)$$

where $a \cdot b$ is the commutative product on A, and $m_k : A \times A \to A$ are bilinear mappings.

Note that the associativity of $*_\hbar$ gives strong constraints on the bilinear maps m_k's. We leave it to the readers to express them out. We will discuss one constraint about m_1 below.

Let us take a closer look at the above conditions. Condition ① on the $\hbar$-linearity implies that the information of $*_\hbar$ is completely captured by $\{m_k\}$'s in condition ②. We can view $*_\hbar$ as defining a family of associative products parametrized by $\hbar$. Then condition ② implies

$$\lim_{\hbar \to 0} a *_\hbar b = a \cdot b.$$

In this way, we view $*_\hbar$ as a deformation of the algebra A. It is called formal deformation because we only consider formal power series in $\hbar$ and ignore analytic properties (the analytic property is in fact interesting and important, but irrelevant in the current discussion).

Let $(A[\![\hbar]\!], *_\hbar)$ be a formal deformation. Motivated by our discussion on quantum observables, let us define the quantum bracket

$$[a, b]_\hbar = -\frac{i}{\hbar}(a *_\hbar b - b *_\hbar a) \qquad a, b \in A.$$

Since $(A, \cdot)$ is commutative, we have

$$[-, -]_\hbar : A \times A \longrightarrow A[\![\hbar]\!].$$

Since $*_\hbar$ is associative, $[-, -]_\hbar$ satisfies the Jacobi identity

$$[a, [b, c]_\hbar]_\hbar + [b, [c, a]_\hbar]_\hbar + [c, [a, b]_\hbar]_\hbar = 0.$$

(Check this!)

Therefore $[-, -]_\hbar$ defines a Lie bracket, which measures the noncommutativity of $*_\hbar$.

Let us define $\{-,-\} : A \times A \to A$ by

$$\{a, b\} := \lim_{\hbar \to 0} [a, b]_\hbar.$$

Explicitly, this is

$$\{a, b\} = -i(m_1(a, b) - m_1(b, a)).$$

This can be viewed as the leading order noncommutativity of $*_\hbar$. The associativity of $*_\hbar$ will lead to the following constraint on m_1.

Proposition 1.2.5. $(A, \{-,-\})$ *forms a Poisson algebra.*

Proof: The skew-symmetry is obvious. The Leibniz rule follows from the $\hbar \to 0$ limit of

$$[a, b *_\hbar c]_\hbar = [a, b]_\hbar *_\hbar c + b *_\hbar [a, c]_\hbar.$$

The Jacobi identity follows from the $\hbar \to 0$ limit of

$$[a, [b, c]_\hbar]_\hbar + [b, [c, a]_\hbar]_\hbar + [c, [a, b]_\hbar]_\hbar = 0.$$

□

Now we can summarize the above discussion on the algebraic relationship between classical and quantum observables as

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

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 [1].

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 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:

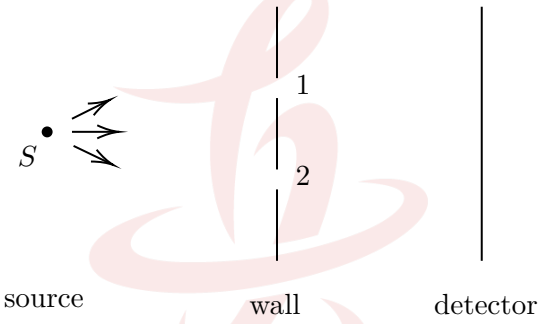
"*If I were forced to sum up in one sentence what the Copenhagen interpretation says to me, it would be 'Shut up and Calculate!'* "

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.



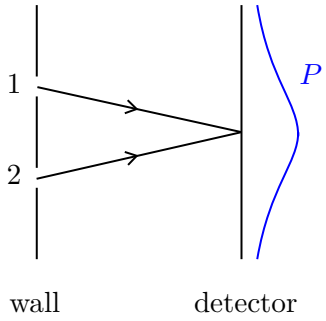
We are looking for the outcome distribution of particle counts on the detector.

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

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

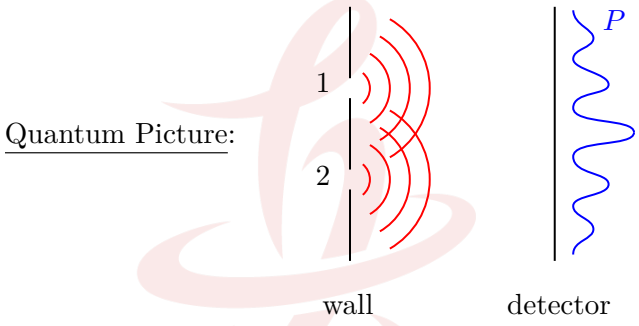
As we have seen, the probability distribution of the measurement is the square of the amplitude

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

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

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

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

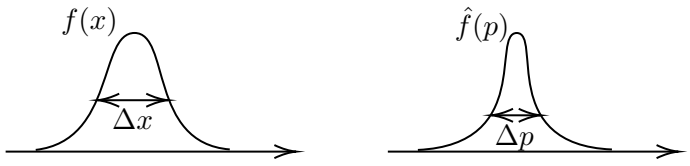
$$\hat{p}_j = -i\hbar \frac{\partial}{\partial x^j}.$$

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 $t = 0$.

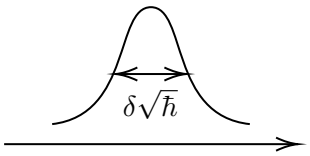
Example 1.6.1 (Gaussian Packet)**.** Consider the one-dimensional case $n = 1$. Let us give the initial wave function at $t = 0$ by

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

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

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

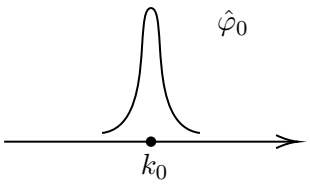
1.6.2 Group Velocity

We would like to understand how a localized wave packet move 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.

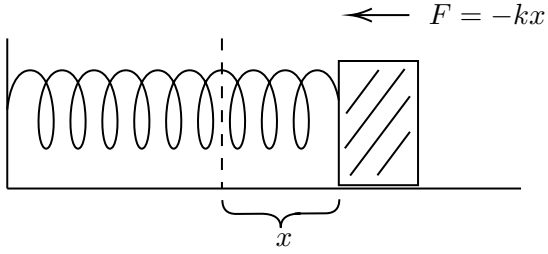
Classically, the particle's motion obeys the Hamilton's equations

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

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 operator 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 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 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 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

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

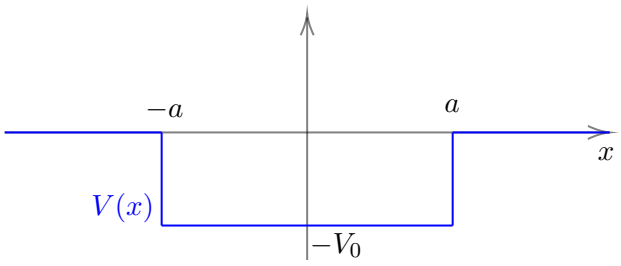
are the *Hermite polynomials*. The first few looks like

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

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

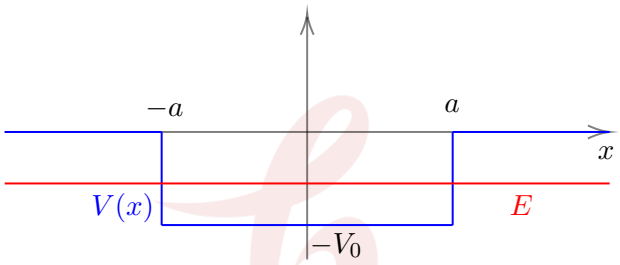
$$\left\langle \psi \middle| -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi \right\rangle = \langle \psi | (E - V(x))\psi \rangle,$$

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 lost 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 normalization. Thus it gives a unique physical state with the corresponding energy E.

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

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

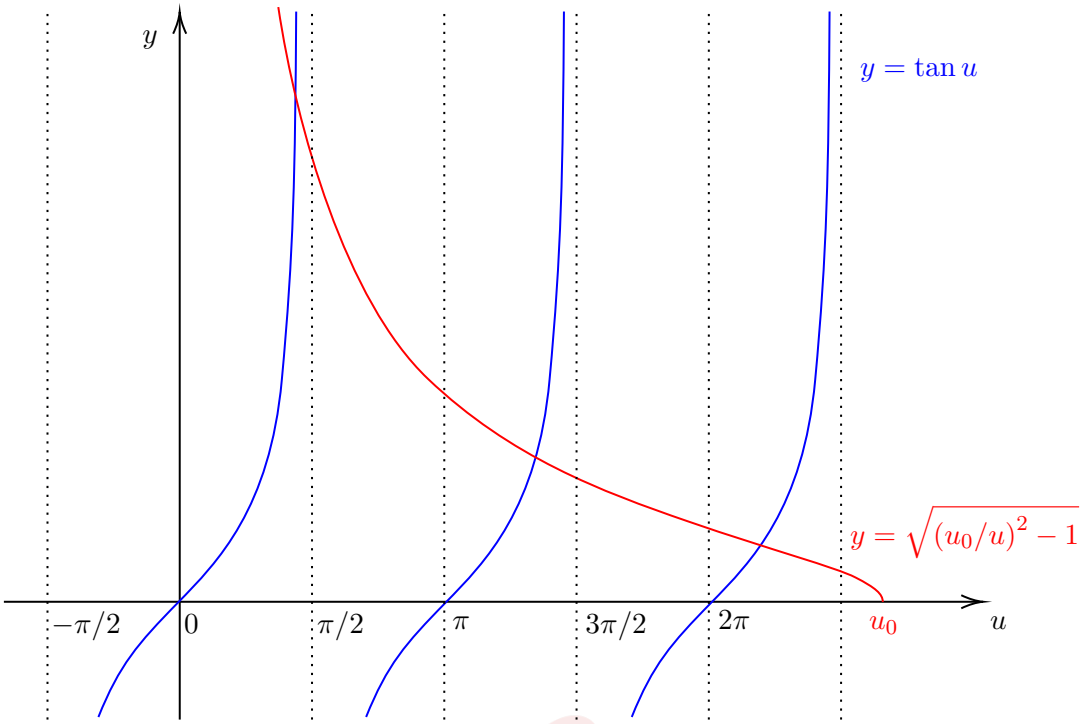
We can express λ, μ in terms of u, u_0

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

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

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

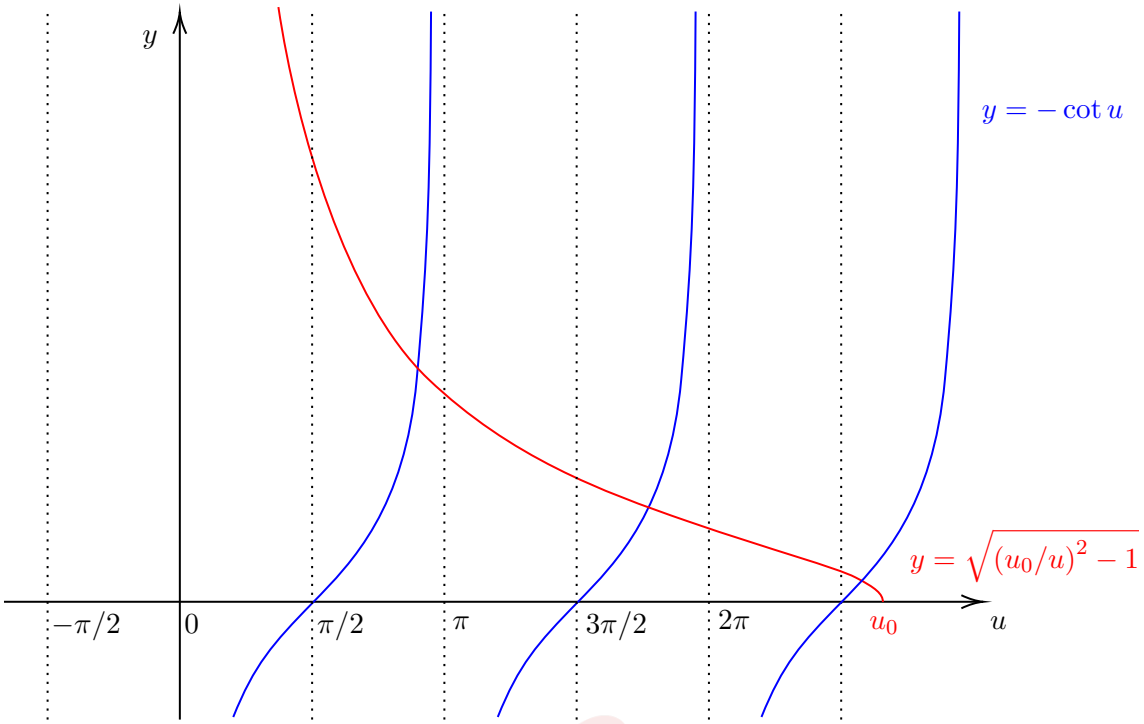
from which we find required relation for E

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

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

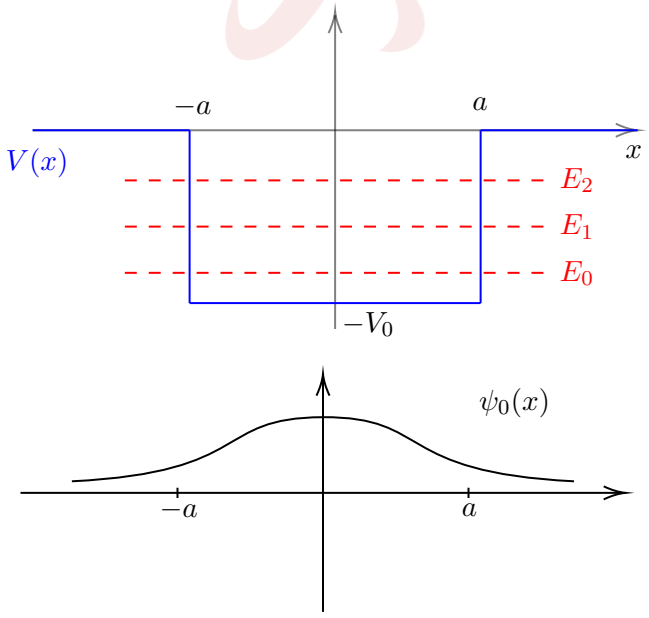
$$\sqrt{\left(\frac{u_0}{u}\right)^2 - 1} = -\cot u.$$

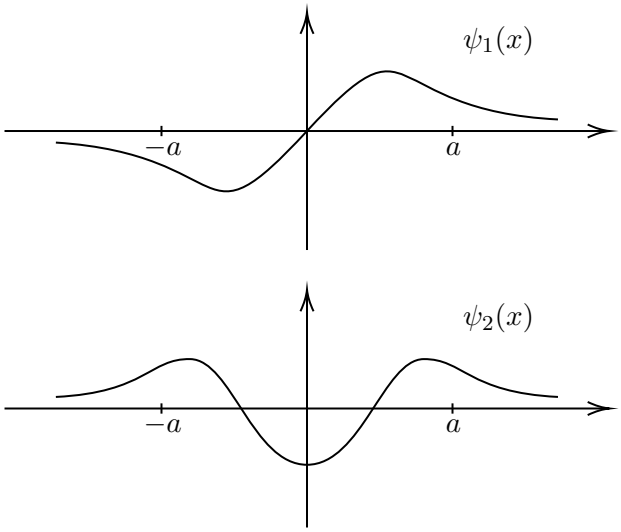
We plot the corresponding curves for $0 < u < u_0$



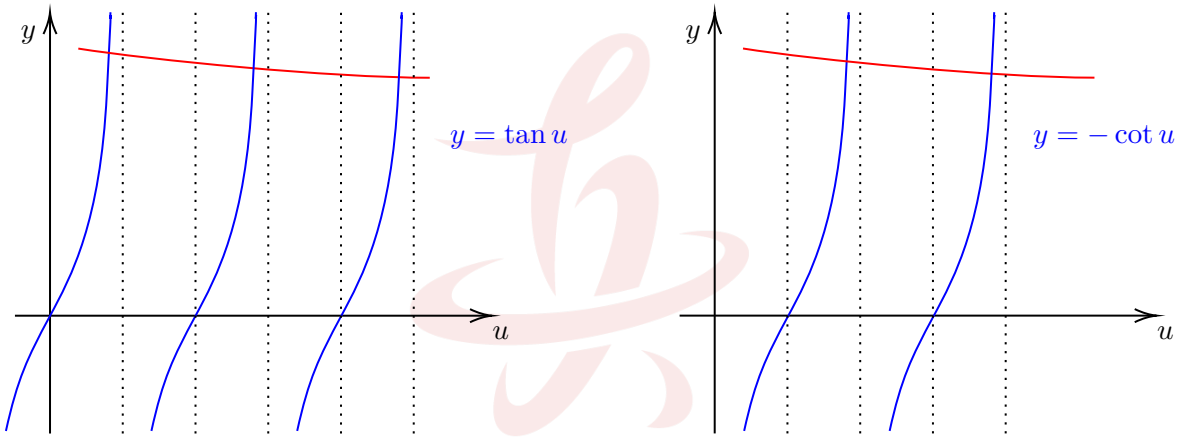
Again, we find only finite number of intersections. The number of odd bound state is bigger for larger u_0, i.e., for wider and deeper well. However, for u_0 sufficiently small, say $u_0 < \pi/2$, there will be no odd bound state.

In summary, we have found 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

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

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

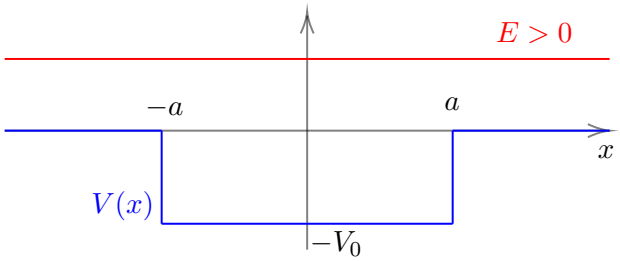
Surprisingly, we will find this formula reappearing for the resonant transmission in the scattering problem as we discuss next.

1.8.3 Scattering States

We have seen that the square well admits a finite number of bounded states. The bounded 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 block 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

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

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

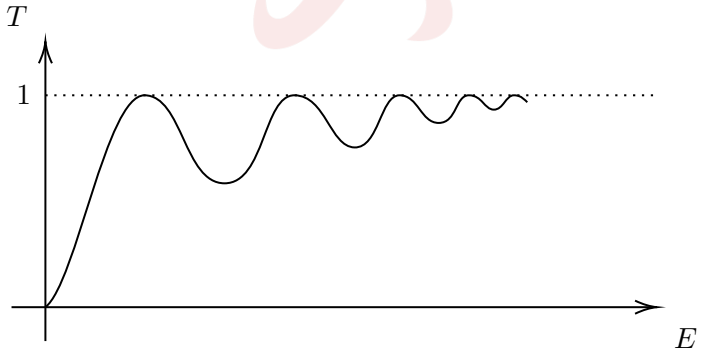
These four equations uniquely determine the five constants A, B, C, D, F up to a total normalization. After a laborious calculation, we find

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

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 form both sides

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

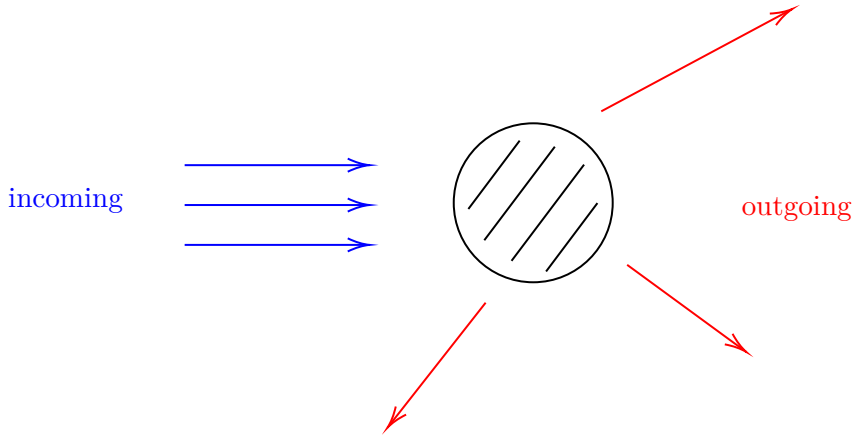
Then A, G represent incoming waves and B, F represent outgoing waves.

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.

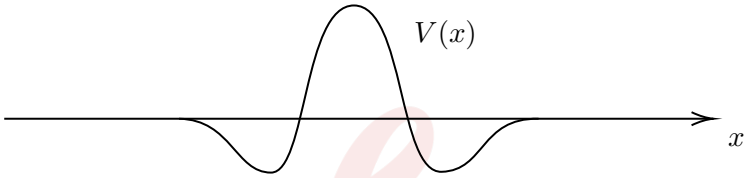
1.9.1 Wave Packet Scattering

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

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

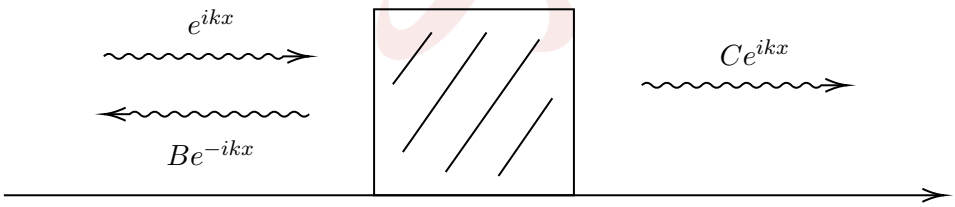
is linear in ψ. This linearity leads to the following strategy. We first look for solutions which are plane waves far away. Then we take the superposition of these asymptotic plane wave solutions with respect to the coefficient $\alpha(k)$ to obtain the physical solution for the scattering.

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 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

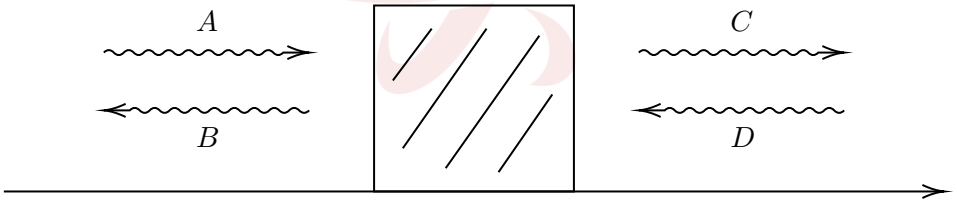
The S-matrix, or the scattering matrix, is about the relation for particle states before and after a scattering process. We illustrate the S-matrix in the one-dimensional scattering process.

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 behavior 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.

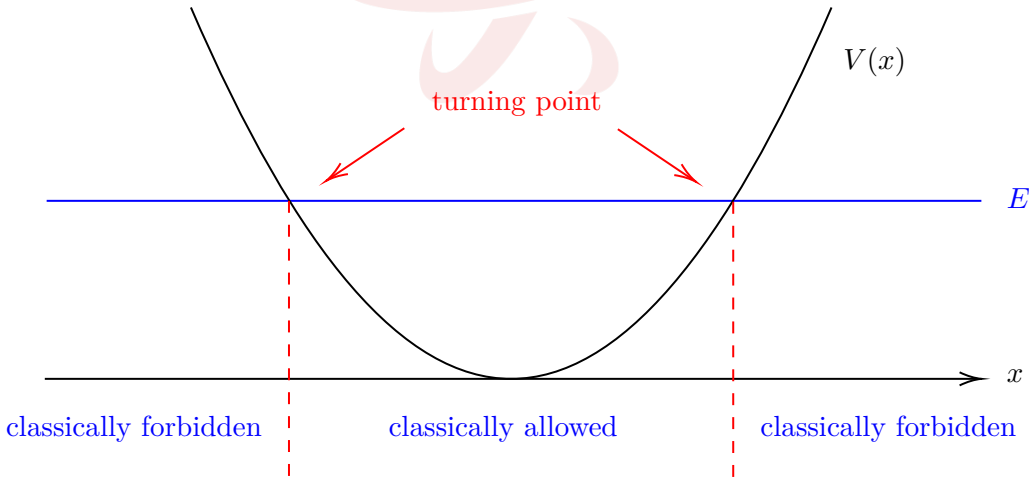
① Classically allowed region. This corresponds to positions where $V(x) < E$. Classically, the energy of motion is

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

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,

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

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

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

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

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

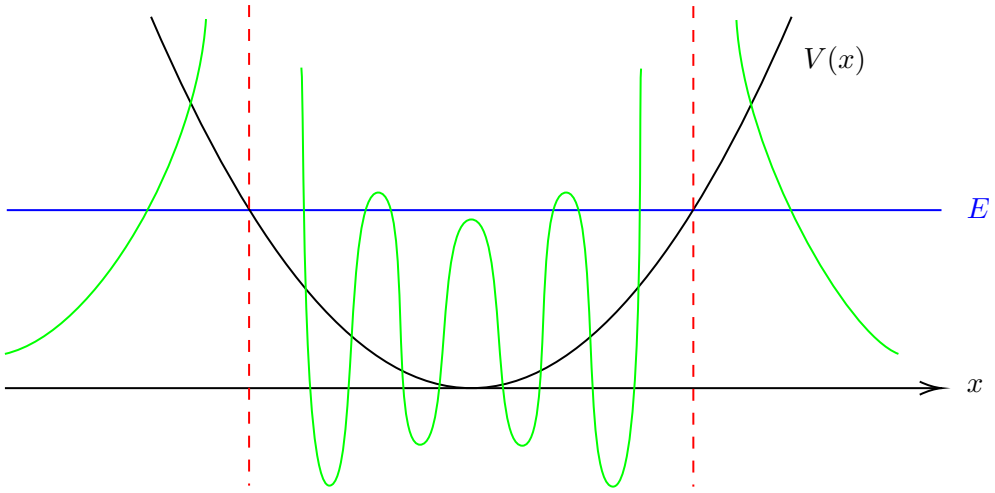
$$\begin{aligned} \psi(x) &= \exp\left(\frac{i}{\hbar}\left(S_0(x) + \hbar S_1(x) + O(\hbar^2)\right)\right) \\ &\simeq e^{\frac{i}{\hbar} S_0(x)} e^{iS_1(x)} \\ &= \frac{A}{(2m(E - V(x)))^{\frac{1}{4}}} e^{\pm \frac{i}{\hbar} \int^x \sqrt{2m(E - V(y))}\, dy} \end{aligned}$$

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 treatment 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

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

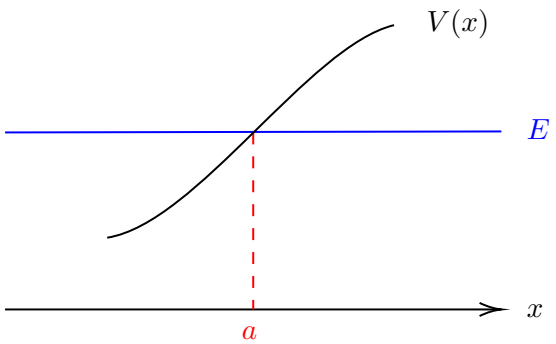
Then the WKB approximated solution takes the form

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

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 behavior

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

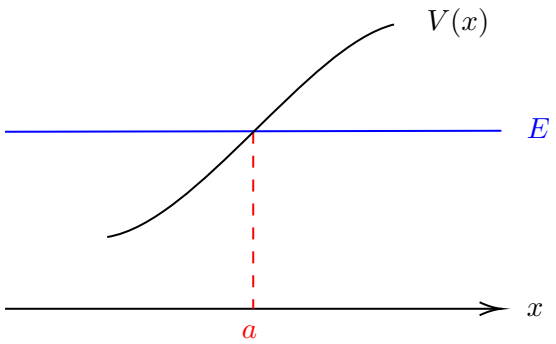
$$\mathrm{Bi}(z) \simeq \begin{cases} \frac{1}{\sqrt{\pi}}|z|^{-\frac{1}{4}}\exp\left(\frac{2}{3}|z|^{\frac{3}{2}}\right) & z \to +\infty \\ -\frac{1}{\sqrt{\pi}}|z|^{-\frac{1}{4}}\sin\left(\frac{2}{3}|z|^{\frac{3}{2}} - \frac{\pi}{4}\right) & z \to -\infty \end{cases}$$

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

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

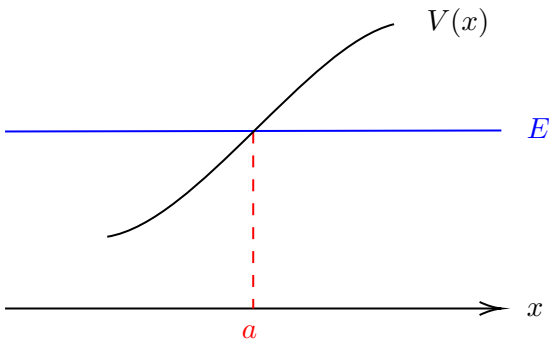
Similarly, if we find the approximate wave function

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

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 $V'(a) > 0$.

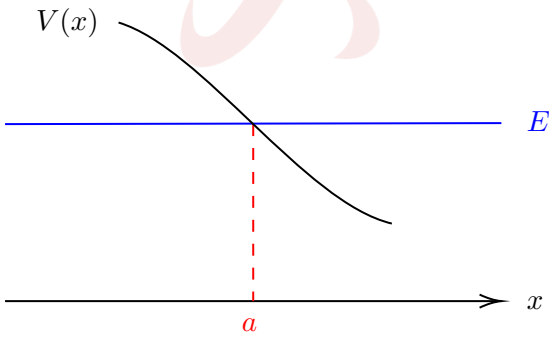


$$\frac{2A}{\sqrt{k(x)}} \cos\left(\int_x^a k(y)\, dy - \frac{\pi}{4}\right) \quad \Longleftarrow \quad \frac{A}{\sqrt{\lambda(x)}} \exp\left(-\int_a^x \lambda(y)\, dy\right)$$

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

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.



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

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

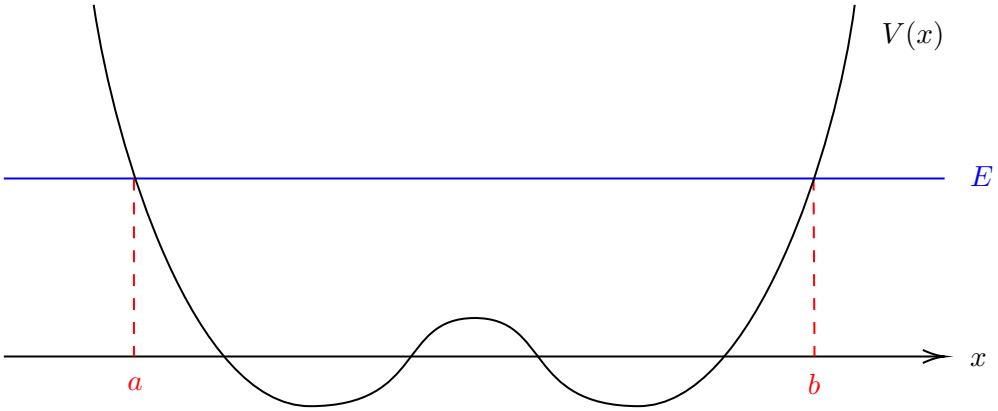
1.10.4 Semi-classical Quantization Rule

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

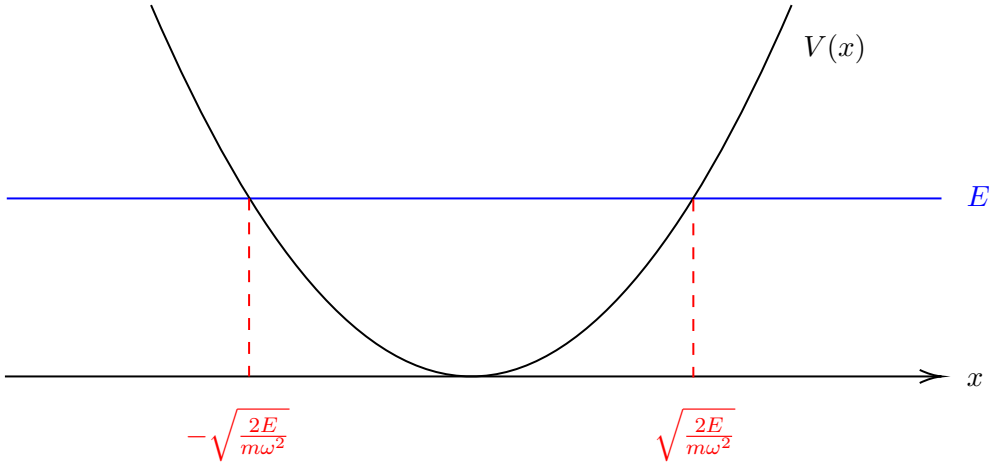
$$\int_a^x k(y)\,dy - \frac{\pi}{4} = -\left(\int_x^b k(y)\,dy - \frac{\pi}{4}\right) + n\pi$$

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

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

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



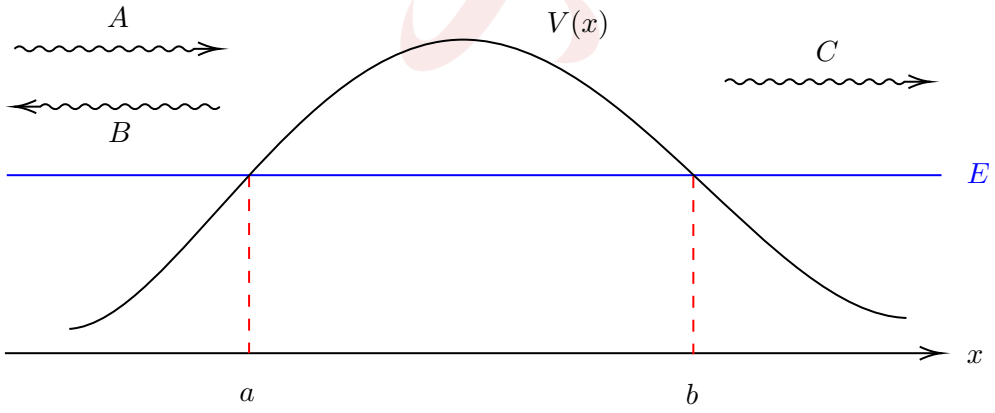
The EBK semi-classical quantization condition asks

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

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 $V(x)\leq E$. 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 $x\to\pm\infty$. Consider 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 $x = b$.

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

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

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

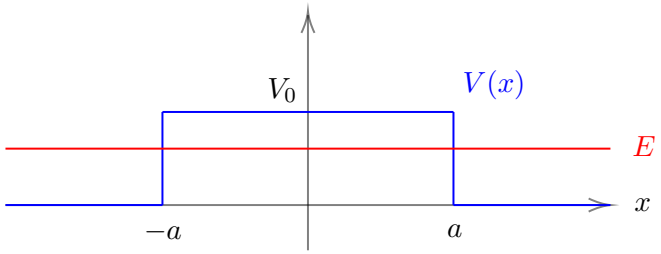
The WKB approximated transmission coefficient is

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

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

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



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

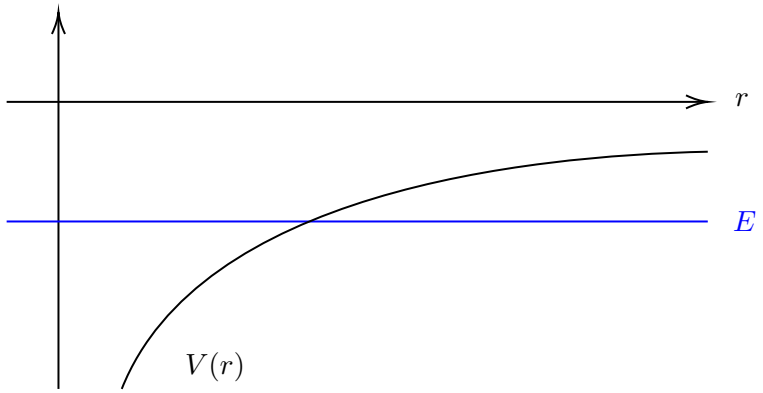
$$\widehat{\mathrm{H}} = \frac{\hat{p}^2}{2m} - \frac{Z}{r}$$

is clearly rotational 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 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 exist 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

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

Assume the classical energy is negative $\mathscr{H} < 0$. Then $A < 1$ and the orbits are ellipses. These are the classical analogue 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 [14] 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

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

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 of so(3)

$$\mathrm{so}(3) = \big\{ A : 3 \times 3 \text{ real matrix} \,\big|\, A^T = -A,\ \mathrm{Tr}\, A = 0 \big\}.$$

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 energy 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

$$\frac{\partial \mathscr{L}}{\partial x_i} - \frac{d}{dt}\left(\frac{\partial \mathscr{L}}{\partial \dot{x}_i}\right) = 0.$$

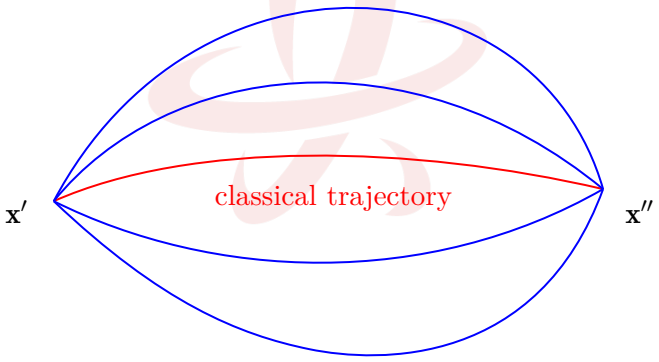
This Lagrangian formulation of classical mechanics is related to the Hamiltonian formulation by the Legendre transform

$$\mathscr{H}(\mathbf{x}, \mathbf{p}) = \mathbf{p} \cdot \dot{\mathbf{x}} - \mathscr{L}(\mathbf{x}, \dot{\mathbf{x}}).$$

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 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

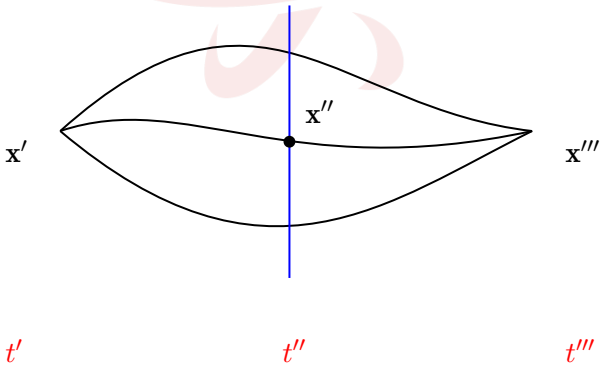
$$\begin{aligned}\left\langle \mathbf{x}'''\middle| e^{-i\,\widehat{\mathrm{H}}(t'''-t')/\hbar}\middle|\mathbf{x}'\right\rangle &= \left\langle \mathbf{x}'''\middle| e^{-i\,\widehat{\mathrm{H}}(t'''-t'')/\hbar} e^{-i\,\widehat{\mathrm{H}}(t''-t')/\hbar}\middle|\mathbf{x}'\right\rangle \\ &= \int d^n\mathbf{x}''\, \left\langle \mathbf{x}'''\middle| e^{-i\,\widehat{\mathrm{H}}(t'''-t'')/\hbar}\middle|\mathbf{x}''\right\rangle \left\langle \mathbf{x}''\middle| e^{-i\,\widehat{\mathrm{H}}(t''-t')/\hbar}\middle|\mathbf{x}'\right\rangle,\end{aligned}$$

i.e.,

$$K(\mathbf{x}''', t'''; \mathbf{x}', t') = \int d^n\mathbf{x}''\, K(\mathbf{x}''', t'''; \mathbf{x}'', t'') K(\mathbf{x}'', t''; \mathbf{x}', t').$$

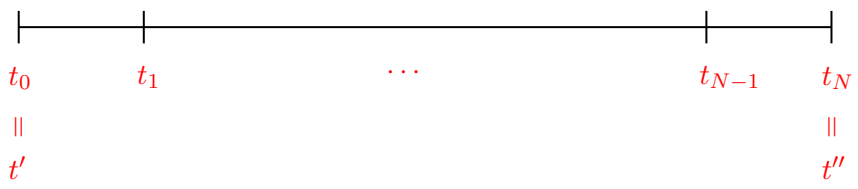
This is the *composition law* for the Feynman kernel K.

Geometrically, this composition law can be illustrated by



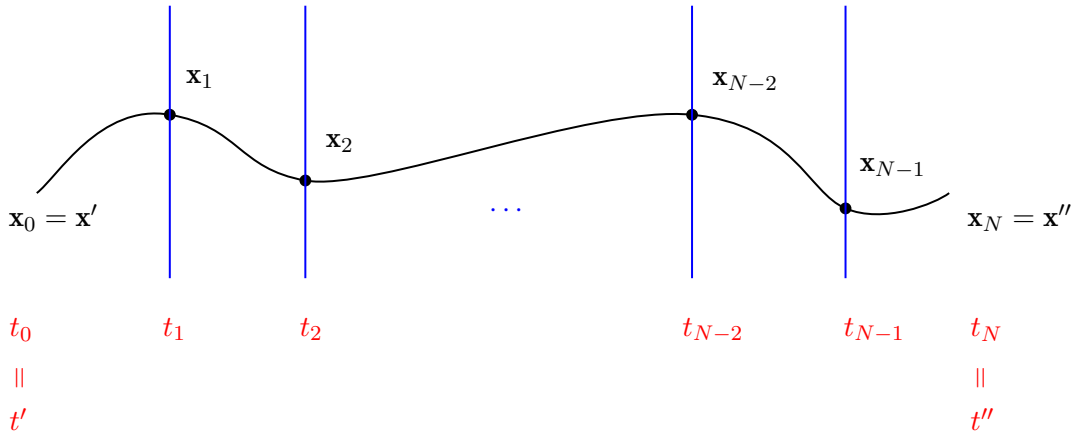
Thinking about $K(\mathbf{x}''', t'''; \mathbf{x}', t')$ as a transition amplitude from $\mathbf{x}'$ at time t' to $\mathbf{x}'''$ at time t''', the composition law says that this transition amplitude is the same as summing over all the transitions at the intermediate time t'' for all possible $\mathbf{x}''$.

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

$$K(\mathbf{x}'',t'';\mathbf{x}',t') = \int \prod_{j=1}^{N-1} d^n\mathbf{x}_j \prod_{j=0}^{N-1} K(\mathbf{x}_{j+1},t_{j+1};\mathbf{x}_j,t_j), \qquad \mathbf{x}_0 = \mathbf{x}',\ \mathbf{x}_N = \mathbf{x}''.$$

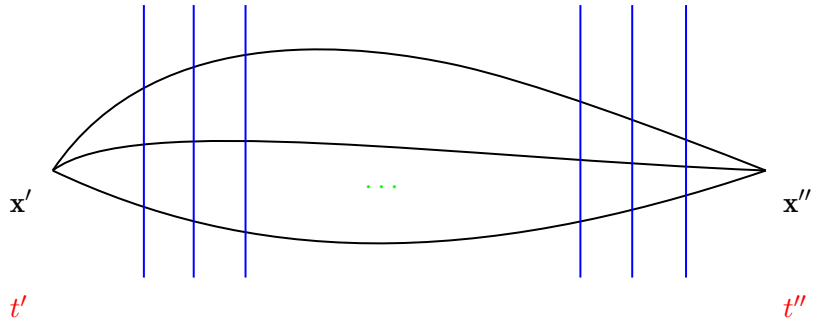
Applying our result for the integral kernel over small time interval, this is approximated by

$$\simeq \left(\frac{m}{2\pi\hbar i\epsilon}\right)^{Nn/2} \int \prod_{j=1}^{N-1} d^n\mathbf{x}_j \, e^{\frac{i}{\hbar}\sum_{j=0}^{N-1}\left[\frac{m}{2}\left(\frac{\mathbf{x}_{j+1}-\mathbf{x}_j}{\epsilon}\right)^2 - V(\mathbf{x}_j)\right]\epsilon}.$$

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 number 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

$$K_0(x'', T; x', 0) = \int_{x(0)=x'}^{x(T)=x''} [Dx(t)]\, e^{\frac{i}{\hbar}\int_0^T \left(\frac{m}{2}\dot{x}^2\right) dt}.$$

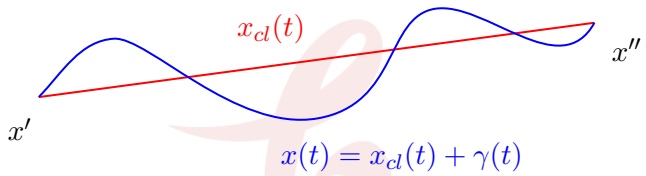
Let $x_{cl}(t)$ denote the classical trajectory from x' at time $t = 0$ to x'' at time $t = T$

$$x_{cl}(t) = x' + \frac{t}{T}(x'' - x').$$

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

$$\ddot{x}_{cl}(t) = -\omega^2 x_{cl}(t), \qquad x_{cl}(0) = x',\ x_{cl}(T) = x''$$

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

$$\prod_{m=1}^{\infty} \left[1 - \left(\frac{z}{m\pi}\right)^2\right] = \frac{\sin z}{z},$$

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 $f'(x_0) = 0$)

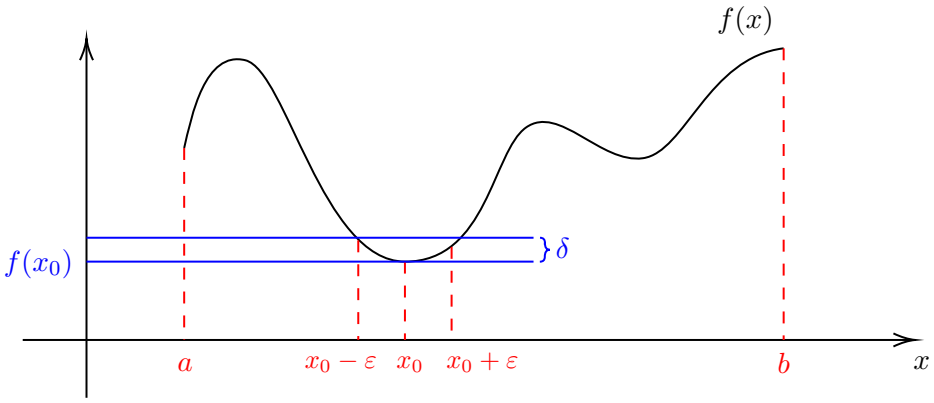
$$f(x) = f(x_0) + \frac{f''(x_0)}{2}(x - x_0)^2 + O((x - x_0)^3)$$

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.

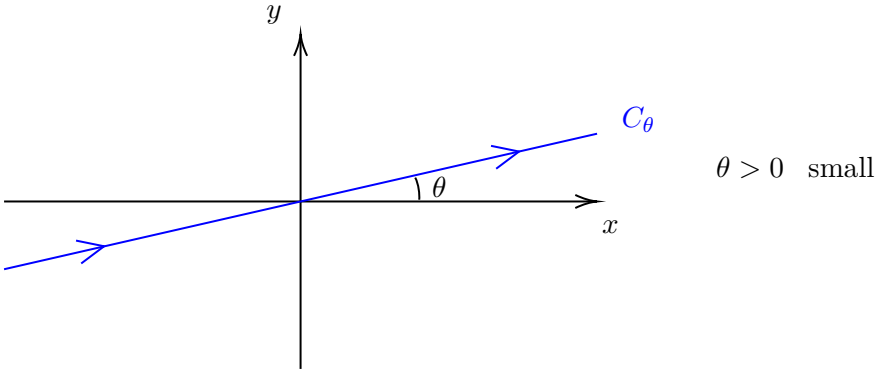
Example 2.5.2. Consider the following integral

$$\int_C e^{ix^2}\, dx.$$

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.

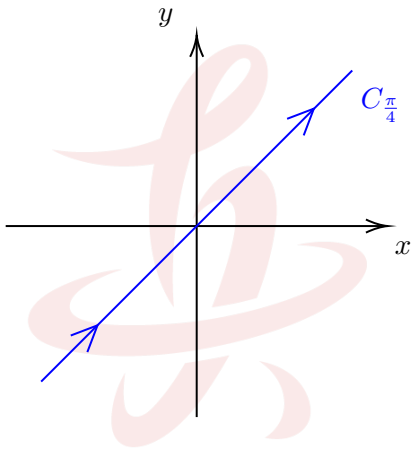
Example 2.5.3. Consider the Gaussian integral

$$\int_C e^{i\lambda z^2}\,dz, \qquad \lambda > 0.$$

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 [28] to illustrate the basic idea in our case. Consider the following flow equation

$$\begin{cases} \dfrac{dz}{du} = -\overline{f'(z)} \\ \lim\limits_{u\to-\infty} z(u) = \text{saddle} \end{cases}$$

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

$$\operatorname{Im} f = 0, \quad \text{and} \quad \operatorname{Re} f \to -\infty \quad \text{along} \quad \partial C.$$

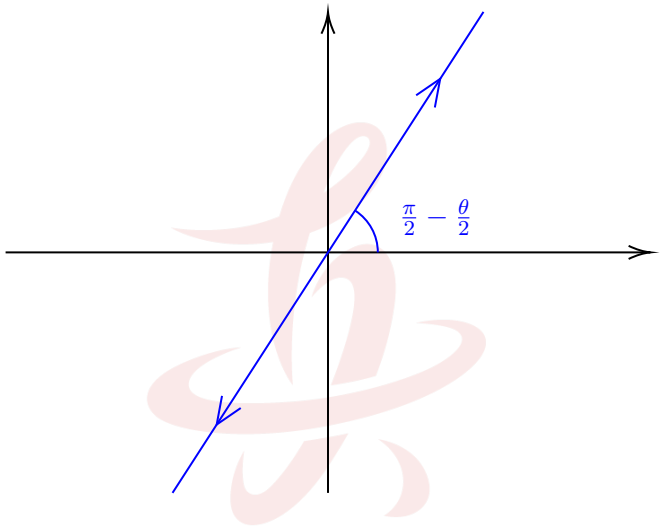
Such curve C can be constructed by solving the flow equation

$$\begin{cases} \dfrac{dz}{du} = -\overline{f'(z)} = -\overline{\alpha z} \\ \lim\limits_{u \to -\infty} z(u) = 0 \end{cases}$$

Let $\alpha = Ae^{i\theta}$, $A > 0$. There are two solutions pointing toward opposite directions

$$z(u) = \pm e^{Au} e^{\frac{i}{2}(\pi - \theta)}.$$

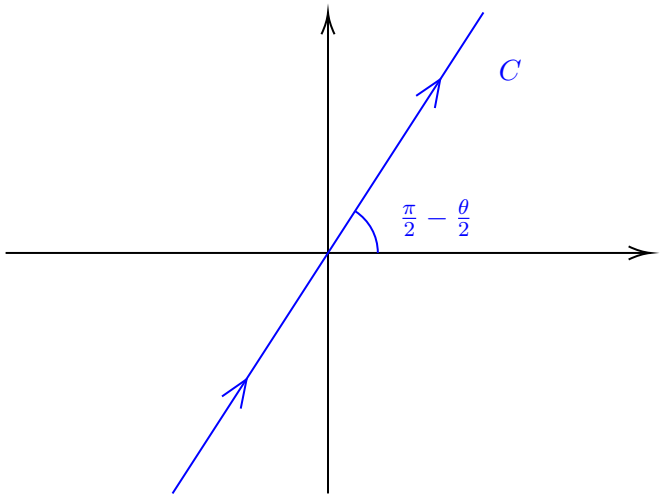
Here is the figure for the corresponding solutions (arrow indicates the flow direction)



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.

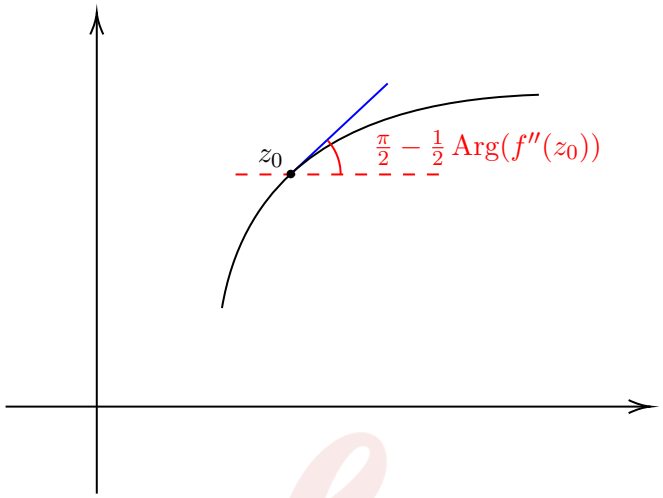


In general, suppose we are to describe the curve of steepest descend for the integral

$$\int_C e^{\lambda f(z)}$$

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 $p_\pm$.

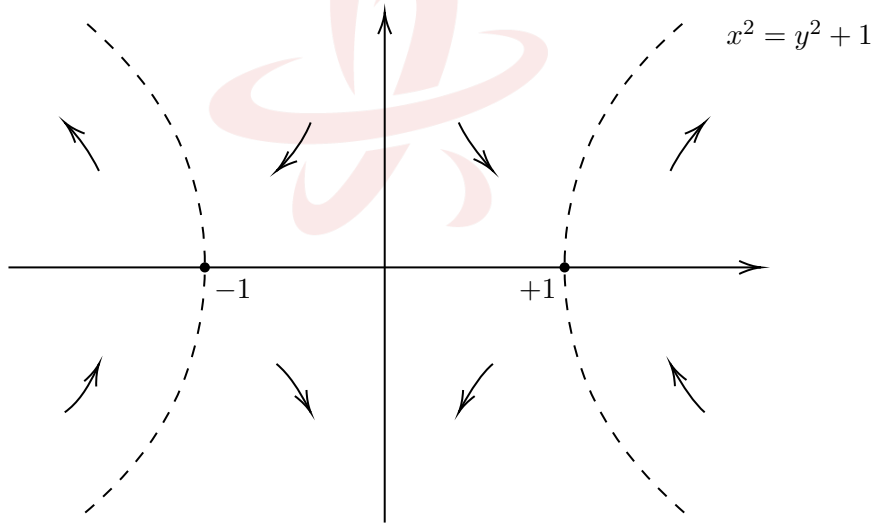
To describe these curves, let us consider the flow equation

$$\frac{dz}{du} = -\overline{f'(z)} = i\lambda(\overline{z}^2 - 1)$$

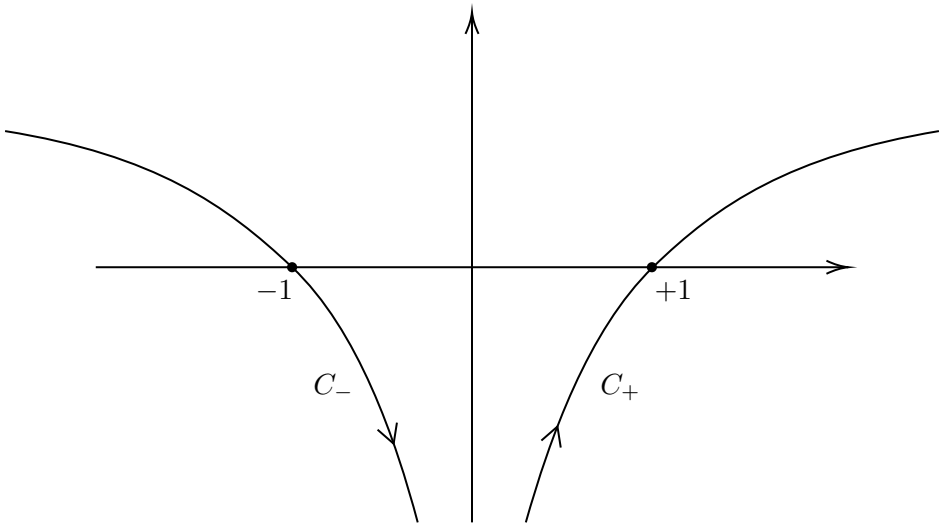
which can be written in real coordinates $z = x + iy$ as

$$\begin{cases} \dfrac{dx}{du} = 2\lambda xy \\ \dfrac{dy}{du} = \lambda(x^2 - y^2 - 1) \end{cases} \qquad (\lambda > 0)$$

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 $C_\pm^\lambda$

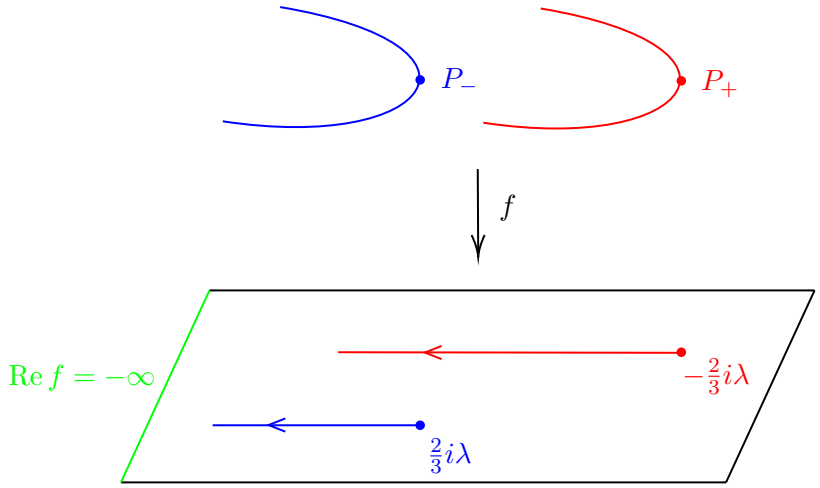
where

$$f = i\lambda\left(\frac{z^3}{3} - z\right).$$

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,

$$\operatorname{Im}(f(p_-)) = \operatorname{Im}(f(p_+))$$

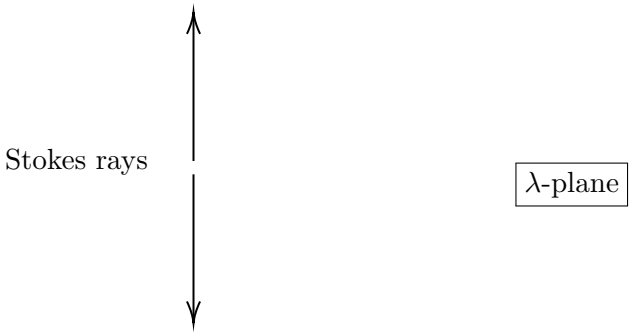
while

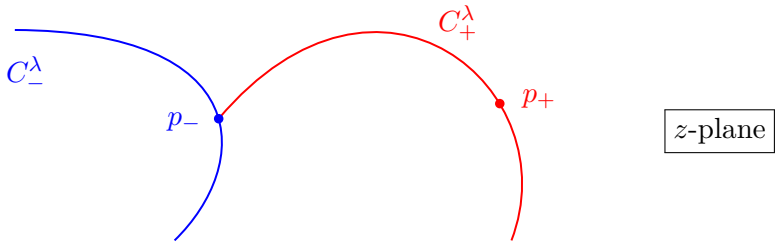
$$\operatorname{Re}(f(p_\pm)) = \pm\frac{2}{3}\operatorname{Im}\lambda.$$

Thus one of the curve of steepest descent connects the two saddle points. The two rays

$$\{\lambda \in i\mathbb{R}_{>0}\} \cup \{\lambda \in i\mathbb{R}_{<0}\}$$

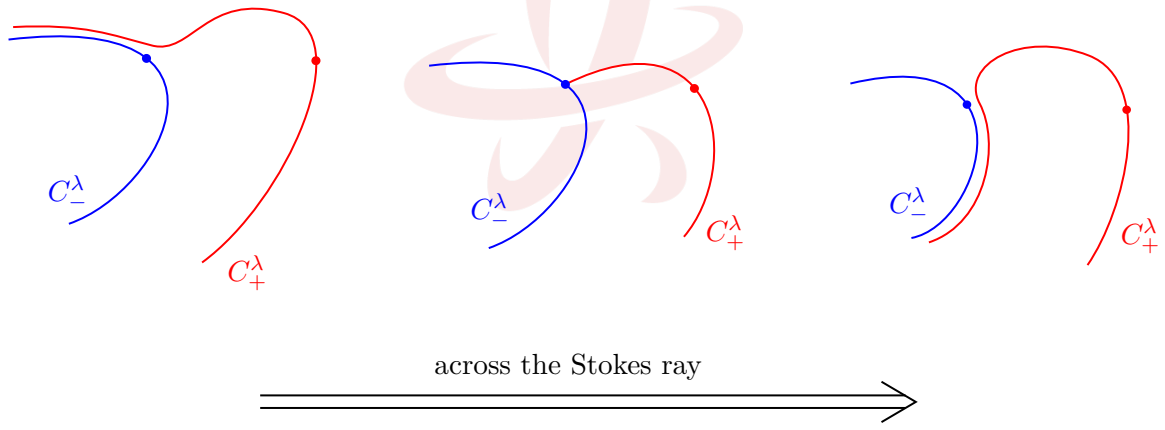
in the λ-plane are called *Stokes rays*.





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

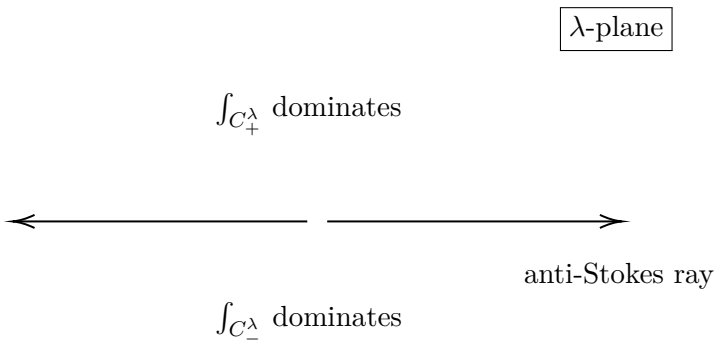
$$\begin{aligned} I(\lambda) &= n_- \int_{C_-^\lambda} e^{i\lambda\left(\frac{z^3}{3} - z\right)} dz + n_+ \int_{C_+^\lambda} e^{i\lambda\left(\frac{z^3}{3} - z\right)} dz \\ &\simeq n_- \sqrt{\frac{\pi}{i\lambda}} e^{\frac{2}{3}i\lambda} + n_+ \sqrt{\frac{\pi}{-i\lambda}} e^{-\frac{2}{3}i\lambda} \qquad \text{as} \quad \lambda \to +\infty e^{i\theta}. \end{aligned}$$

Note that

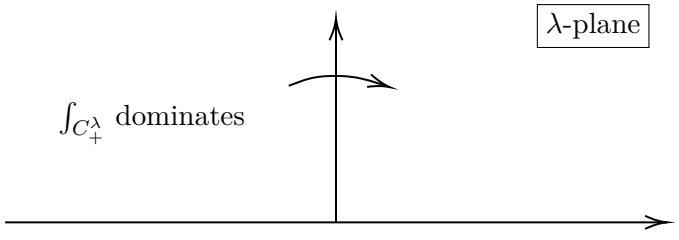
① if $\operatorname{Im}\lambda > 0$, then $\int_{C_+^\lambda}$ dominates

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

$$K_{sc}(x'', t''; x', t') := e^{\frac{i}{\hbar}S[x_{cl}(t)]} \int_{\gamma(t')=0}^{\gamma(t'')=0} [D\gamma(t)]\, e^{\frac{i}{\hbar}\int_{t'}^{t''}\left(\frac{m}{2}\dot{\gamma}^2 - \frac{1}{2}V''(x_{cl})\gamma^2\right)dt}.$$

Apply 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 [5].

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

$$\lim_{\substack{\lambda\to\infty \\ \lambda\notin\mathbb{R}_+}} g(\lambda) = \lim_{\substack{\lambda\to\infty \\ \lambda\notin\mathbb{R}_+}} \frac{\varphi_\lambda^{(0)}(t'')}{\varphi_\lambda^{(0)}(t'')} = 1.$$

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

$$\varphi_0(t) = t - t'.$$

We find

$$c = \frac{\det\tilde{A}}{\tilde{\varphi}_0(t'')} = 2.$$

Thus

$$\det A = 2\varphi_0(t'').$$

We have now 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'.

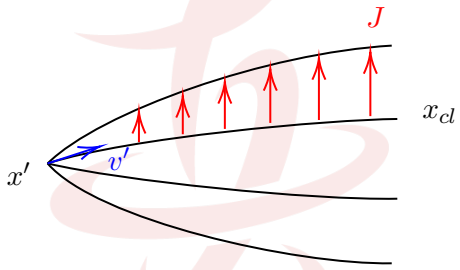
We consider the variation of this family with respect to the parameter v'

$$J(t; v') = \frac{\partial}{\partial v'} x_{cl}(t; v').$$

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

$$\begin{cases} x_{cl}(t'; v') = 0 \\ \dot{x}_{cl}(t'; v') = v' \end{cases} \quad \Longrightarrow \quad \begin{cases} J(t'; v') = 0 \\ \dot{J}(t'; v') = 1 \end{cases}$$

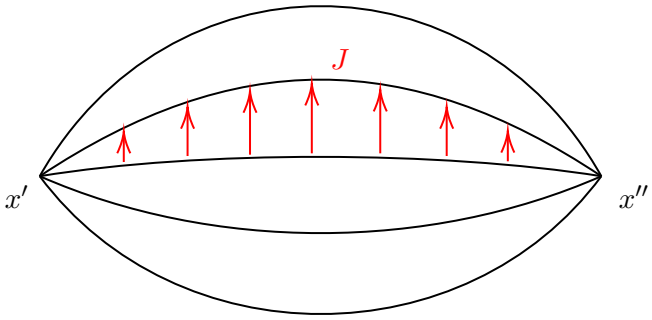
So $J(t; v')$ satisfies the following initial value problem

$$\begin{cases} \left(-\frac{\partial^2}{\partial t^2} - \frac{1}{m} V''(x_{cl}) \right) J = 0 \\ J|_{t=t'} = 0, \qquad \dot{J}|_{t=t'} = 1 \end{cases}$$

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)**.**

$$S[x(t)] = \int_{t'}^{t''} \left(\frac{m}{2}\dot{x}^2 - \frac{m}{2}\omega^2 x^2\right) dt.$$

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: $K_{sc} = K$.

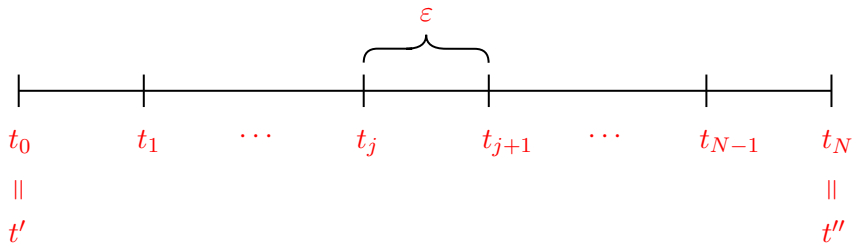
2.6.3 Time-slicing Method

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

$$\widehat{\mathrm{H}}_0 = \frac{\hat{p}^2}{2m}$$

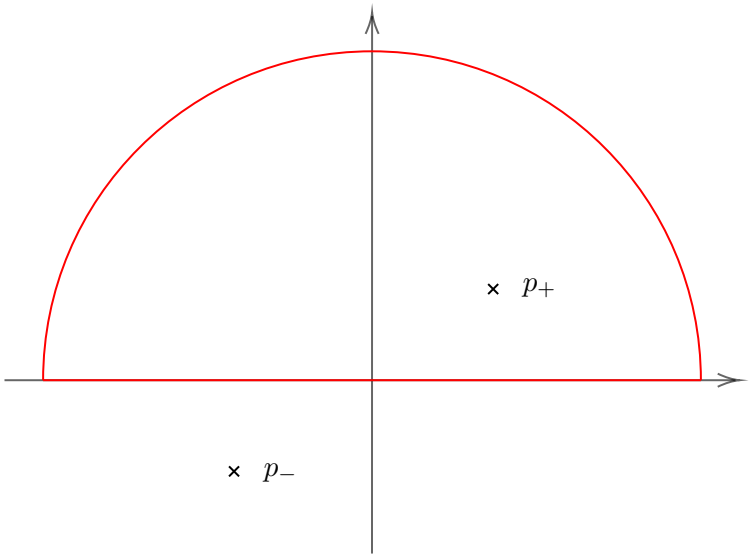
with the free Feynman kernel

$$K_0(x'', T; x', 0) = \Big(\frac{m}{2\pi\hbar i T}\Big)^{\frac{1}{2}} e^{\frac{im(x''-x')^2}{2\hbar T}}.$$

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.,

$$\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-V(x)+E\right)\psi_i(x)=0.$$

Form the following function

$$\xi(x,y;E) := \frac{2m}{\hbar^2 W}\left(\theta(x-y)\psi_1(x)\psi_2(y)+\theta(y-x)\psi_1(y)\psi_2(x)\right)$$

where $W=\psi_1'(x)\psi_2(x)-\psi_2'(x)\psi_1(x)$ 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

$$K(x'', T; x', 0) = \frac{i}{2\pi} \int_{\mathbb{R}} dE\, e^{-iET/\hbar} G(x'', x'; E)$$

which 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

$$G(x'', x'; E) \propto e^{\frac{i}{\hbar}\sqrt{2mE}x''} \qquad \text{as} \quad x'' \to +\infty.$$

Similarly, behavior of an outgoing plane when $x'' \to -\infty$ tells

$$G(x'', x'; E) \propto e^{-\frac{i}{\hbar}\sqrt{2mE}x''} \qquad \text{as} \quad x'' \to -\infty.$$

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., $v(t)$ solves the same equation as J.

Since $v(t)$ 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,

$$\begin{aligned} & T = \int_0^T dt = \int_0^T \frac{dx}{v_{cl}(t)} = \int_{x'}^{x''} \frac{dx}{\sqrt{2(E_{cl} - V(x))/m}} \\ \Longrightarrow \qquad & \frac{dT}{dE_{cl}} = -\frac{1}{m}\int_{x'}^{x''} \frac{dx}{(2(E_{cl} - V(x))/m)^{3/2}} = -\frac{1}{m}\int_{x'}^{x''} \frac{dx}{{v_{cl}}^3} = -\frac{1}{m}\int_0^T \frac{dt}{v_{cl}(t)^2} \\ \Longrightarrow \qquad & \frac{\partial E_{cl}}{\partial T} = -\frac{m}{\int_0^T \frac{dt}{v_{cl}(t)^2}}. \end{aligned}$$

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 $\mathrm{Re}_{\geq 0}$ 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 [4] 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

$$\begin{aligned} \dot{x}_{cl}(0)\dot{x}_{cl}(T_s) &= \left(\frac{x''-x'}{T_s} - \frac{\lambda T_s}{2m}\right)\left(\frac{x''-x'}{T_s} + \frac{\lambda T_s}{2m}\right) \\ &= \frac{(x''-x')^2}{T_s^2} - \frac{\lambda^2}{4m^2}T_s^2 \\ &= \frac{\lambda}{m}(x''+x') - \frac{\lambda^2}{2m^2}T_s^2 \\ &= -\frac{2\lambda}{m}(\pm\sqrt{x''})(\pm\sqrt{x'}). \end{aligned}$$

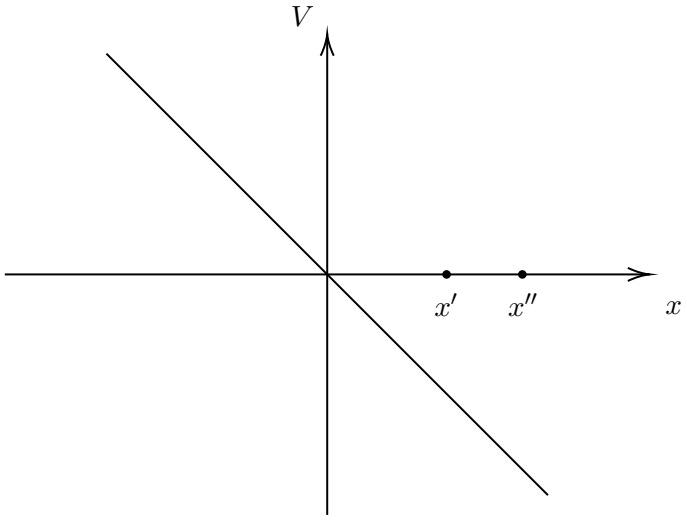
Thus the semi-classical contribution of the saddle (x_{cl}, T_s) to the Green's function is

$$\frac{1}{\hbar}\left(\frac{m}{2\lambda(\pm\sqrt{x''})(\pm\sqrt{x'})}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S_{cl}}.$$

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''.

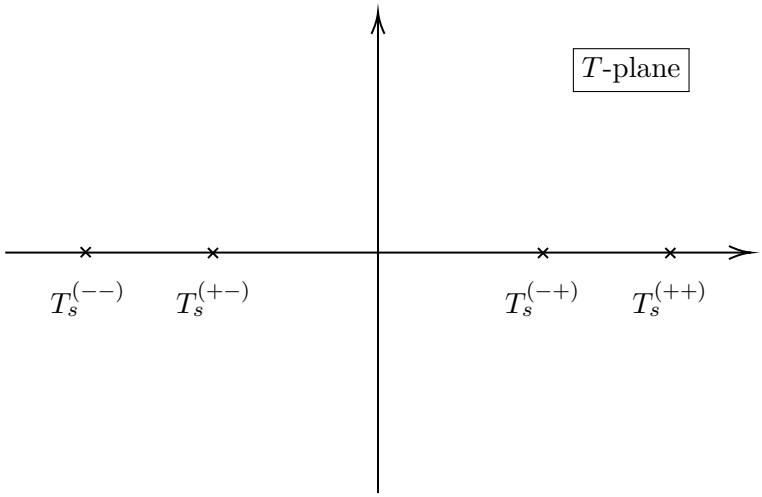
Case $0 < x' < x''$

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 $\lim_{u\to-\infty} T = \text{saddle point}$.

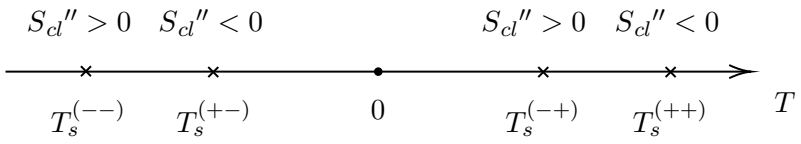
Now let us apply the method in Section 2.5.3 to

$$f(T) = iS_{cl}(T).$$

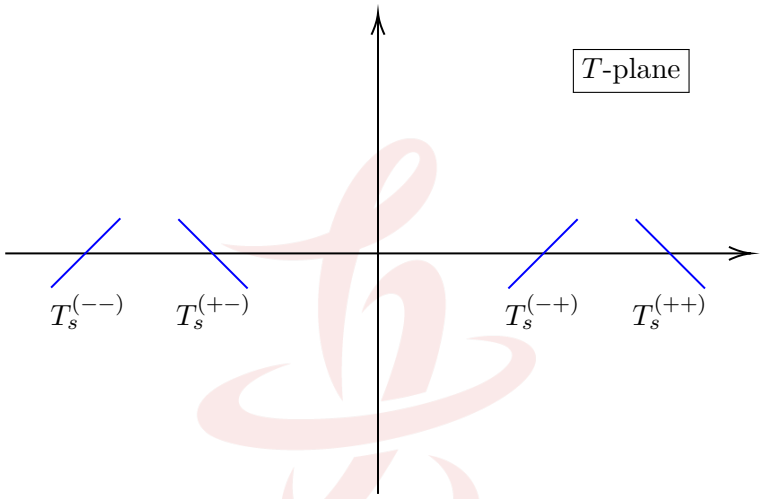
We have

$$S_{cl}{}'(T) = -\frac{\lambda^2}{8mT^2}\left(T - T_s^{(--)}\right)\left(T - T_s^{(+-)}\right)\left(T - T_s^{(-+)}\right)\left(T - T_s^{(++)}\right).$$

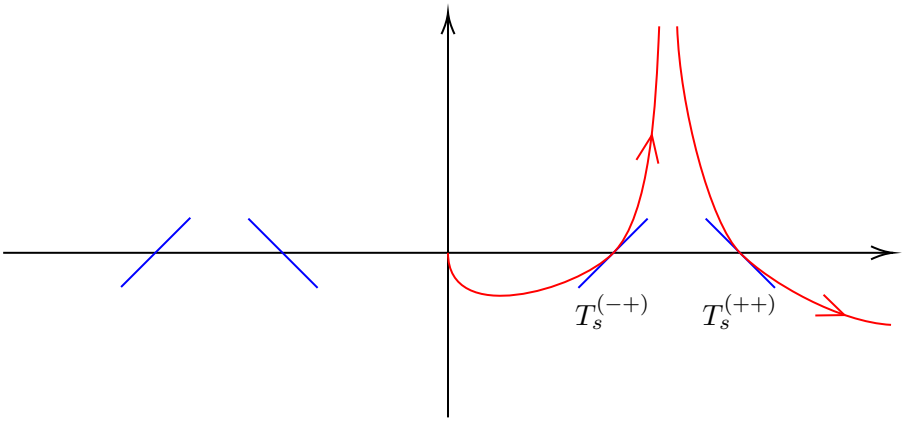
At the four saddle points,



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

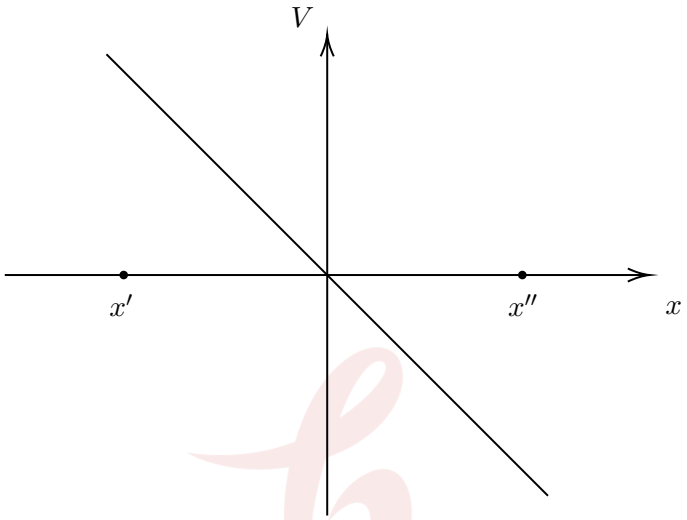
$$T_s^{(-+)} = \left(\frac{2m}{\lambda}\right)^{\frac{1}{2}}\left(-\sqrt{x'} + \sqrt{x''}\right)$$

$$T_s^{(++)} = \left(\frac{2m}{\lambda}\right)^{\frac{1}{2}} \left(\sqrt{x'} + \sqrt{x''}\right).$$

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 $x' < 0 < x''$

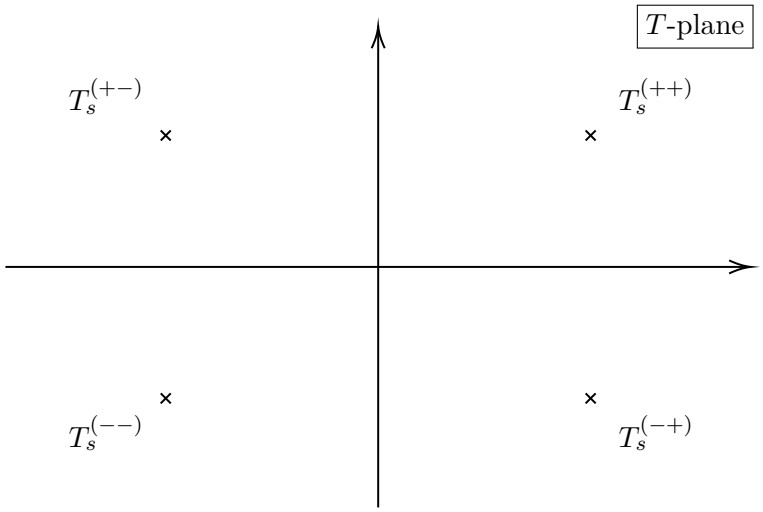
x' lies in the classically forbidden region and x'' lies in the classically allowed region.



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.

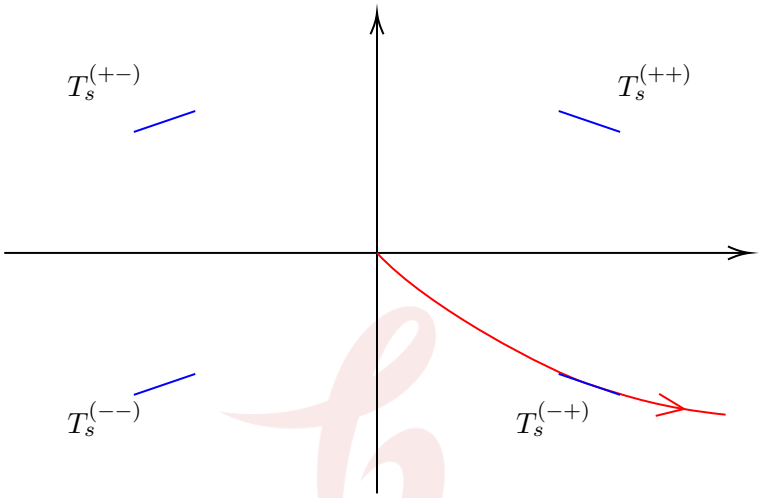


$$S_{cl}{}'(T) = -\frac{\lambda^2}{8mT^2} \left(T - T_s^{(--)}\right) \left(T - T_s^{(+-)}\right) \left(T - T_s^{(-+)}\right) \left(T - T_s^{(++)}\right).$$

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

$$T_s^{(-+)} = \left(\frac{2m}{\lambda}\right)^{\frac{1}{2}}\left(-i\sqrt{|x'|} + \sqrt{x''}\right).$$

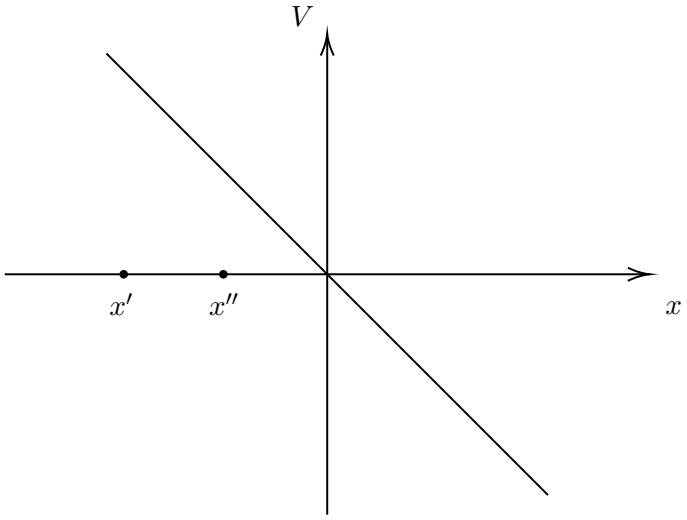
Note that the saddle $T_s^{(-+)}$ has imaginary part. It corresponds to a unique classical path from x' to x'', but has to go through non-real times! This non-real time is due to the fact that the path has to go through a portion of the classically forbidden region. Indeed

$$T = \int_0^T dt = \int_0^T \frac{dx}{\dot{x}} = \int_{x'}^{x''} \frac{dx}{\sqrt{2m(E - V(x))}}.$$

In the classical forbidden region, $E < V(x)$ hence the integration will give rise to imaginary contribution of the travel time.

Case $x' < x'' < 0$

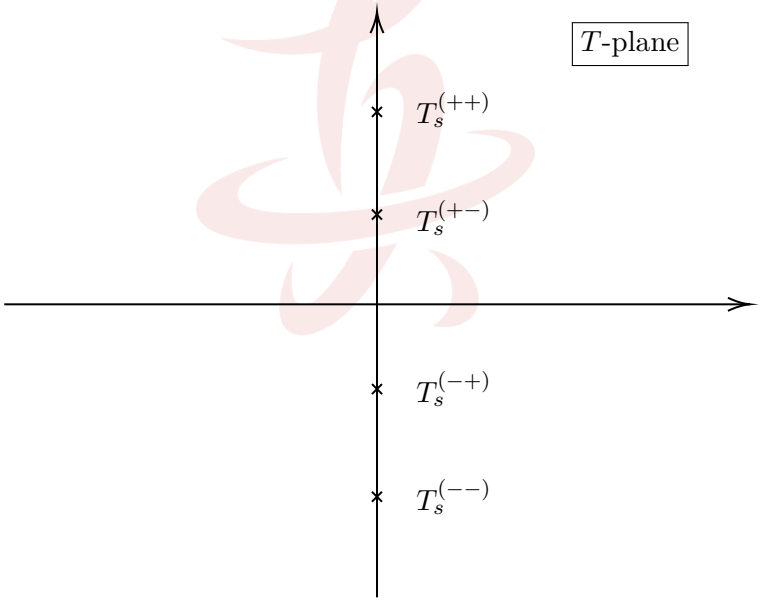
Both x' and x'' lie in the forbidden region.



The four saddle points

$$T_s^{(\pm\pm)} = \left(\frac{2m}{\lambda}\right)^{\frac{1}{2}} \left(\pm i\sqrt{|x'|} \pm i\sqrt{|x''|}\right)$$

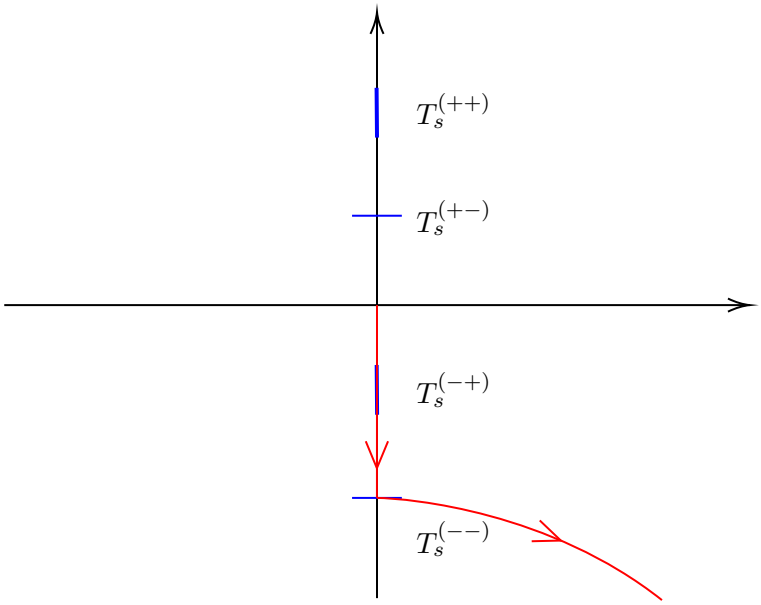
are all imaginary.



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

$$p = m\dot{x} = \sqrt{2m(E - V(x))}$$

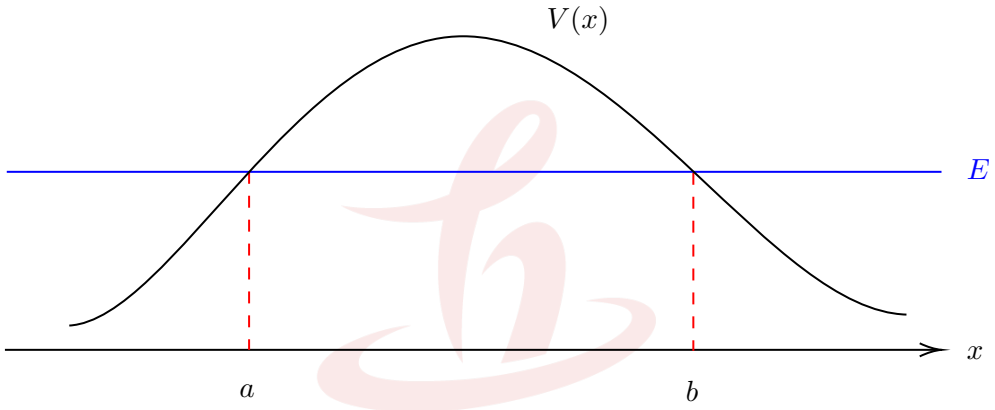
is the classical momentum. Thus semi-classically

$$G(x'', x'; E) \simeq \frac{1}{\hbar} \sum_{(x_{cl}, T_s)} \left(- \frac{1}{\sqrt{\frac{2(E-V(x'))}{m}} \sqrt{\frac{2(E-V(x''))}{m}}} \right)^{\frac{1}{2}} e^{\frac{i}{\hbar} \int_{x'}^{x''} p \, dx}.$$

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 transmission amplitude.

On the other hand, we have a semi-classical asymptotic result

$$G(x'', x'; E) \simeq \sum_{(x_{cl}, T_s)} \frac{1}{\hbar} \left(\frac{1}{-\dot{x}(0)\dot{x}(T_s)} \right)^{\frac{1}{2}} e^{\frac{i}{\hbar} W_{cl}}.$$

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

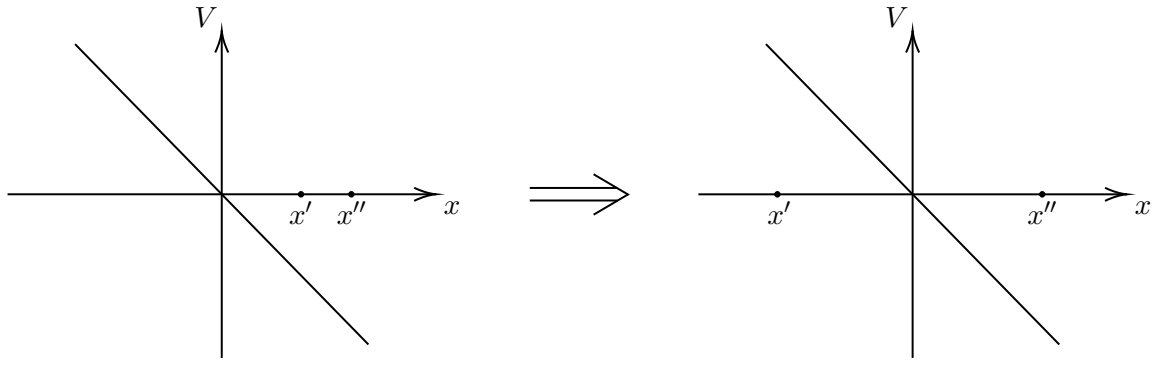
Next we investigate the connection formula of WKB approximation near the turning point where the potential is approximated by a linear potential, say

$$V(x) = -\lambda x, \qquad \lambda > 0.$$

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

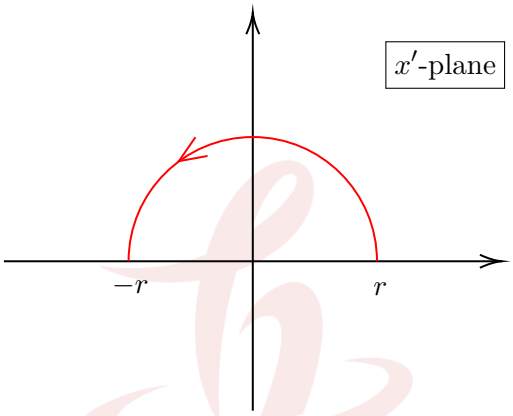
$$\sqrt{\frac{2(E-V)}{m}} = 0 \qquad \text{at} \quad x = 0.$$

So the semi-classical approximation fails and we lose track of the asymptotic information.

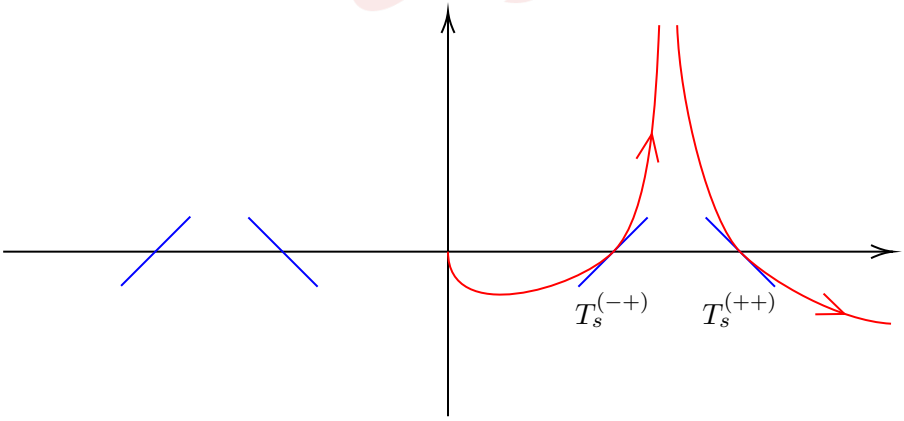
Instead, we can consider the analytic continuation in the complex plane to get around the turning point. For example, we will follow the change

$$x' = re^{i\theta}, \qquad r > 0$$

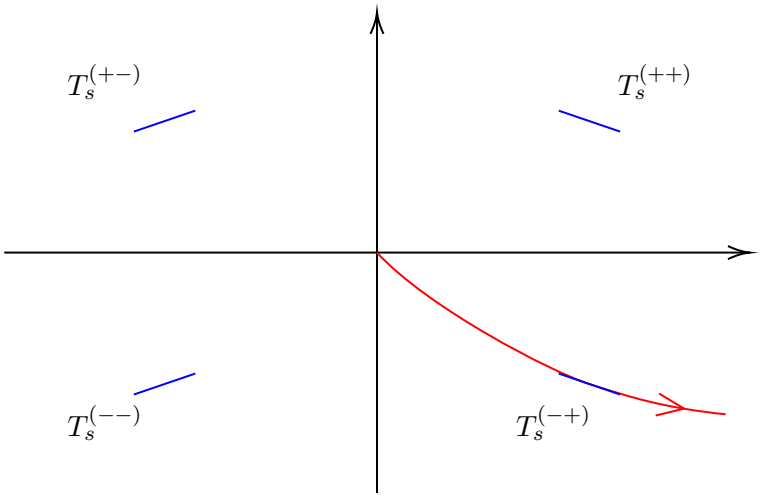
as θ varies from $\theta = 0$ to $\theta = \pi$.



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

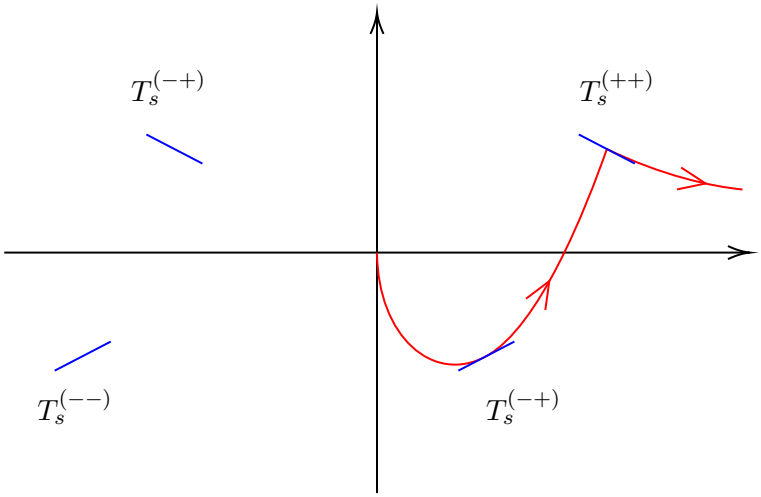
$$S_{cl}\left(T_s^{(-+)}\right) = \frac{2}{3}(2m\lambda)^{\frac{1}{2}} \left(-e^{\frac{3}{2}i\theta}\sqrt{r}^3 + \sqrt{x''}^3\right)$$

$$S_{cl}\left(T_s^{(++)}\right) = \frac{2}{3}(2m\lambda)^{\frac{1}{2}} \left(e^{\frac{3}{2}i\theta}\sqrt{r}^3 + \sqrt{x''}^3\right).$$

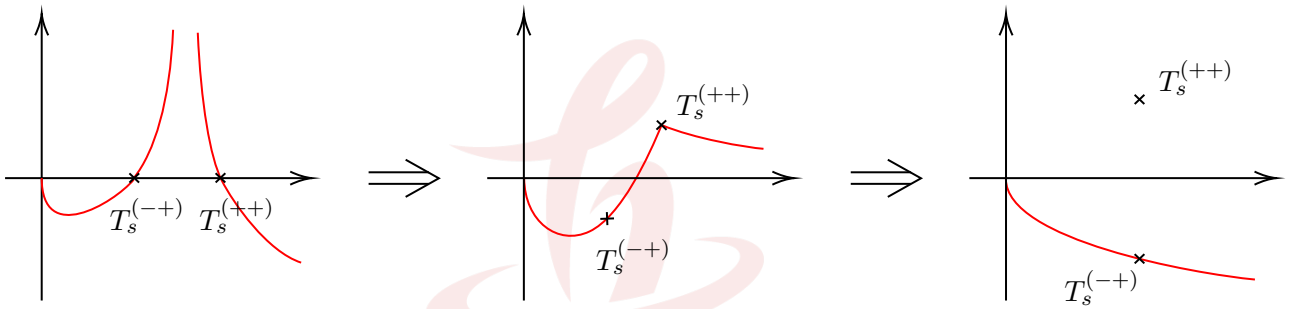
As we vary θ, the saddle contributions to the asymptotic behavior may jump by Stokes phenomenon, where one of the curve of steepest descent may hit another saddle point. The Stokes phenomenon happens when

$$\mathrm{Re}\left(S_{cl}\left(T_s^{(-+)}\right)\right) = \mathrm{Re}\left(S_{cl}\left(T_s^{(++)}\right)\right)$$

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

$$e^{\frac{i}{\hbar}S_{cl}(T_s^{(-+)})} = e^{\frac{i}{\hbar}\frac{2}{3}(2m\lambda)^{\frac{1}{2}}(-\sqrt{x'}^3+\sqrt{x''}^3)}$$

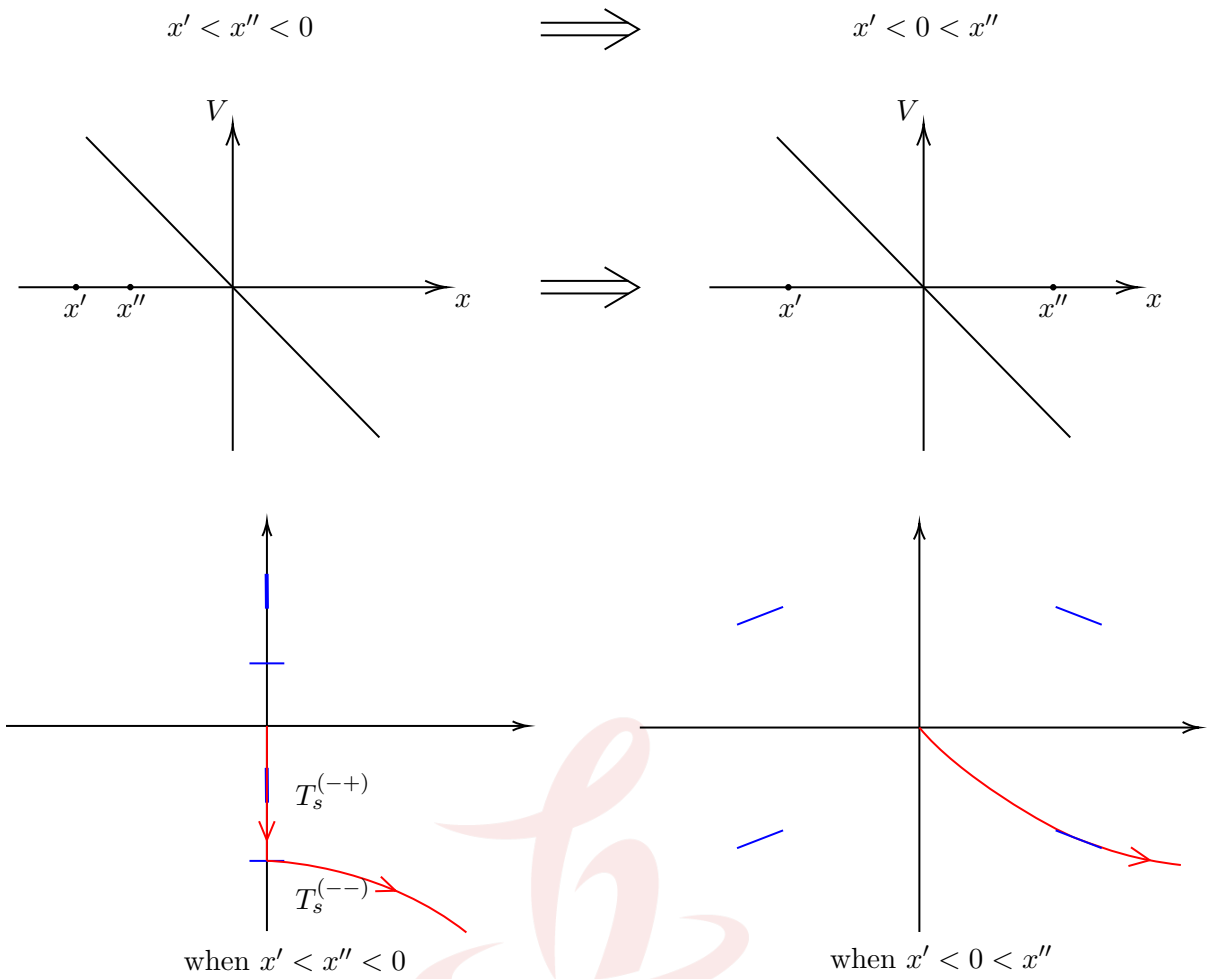
$$e^{\frac{i}{\hbar}S_{cl}(T_s^{(++)})} = e^{\frac{i}{\hbar}\frac{2}{3}(2m\lambda)^{\frac{1}{2}}(\sqrt{x'}^3+\sqrt{x''}^3)}.$$

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''

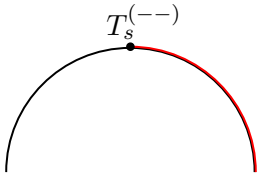


When $x' < x'' < 0$, we have two saddle contributions from $T_s^{(-+)}$ and $T_s^{(--)}$ with

$$e^{\frac{i}{\hbar}S_{cl}(T_s^{(-+)})} = e^{\frac{1}{\hbar}\frac{2}{3}(2m\lambda)^{\frac{1}{2}}(-\sqrt{-x'}^3+\sqrt{-x''}^3)}$$
$$e^{\frac{i}{\hbar}S_{cl}(T_s^{(--)})} = e^{\frac{1}{\hbar}\frac{2}{3}(2m\lambda)^{\frac{1}{2}}(-\sqrt{-x'}^3-\sqrt{-x''}^3)}.$$

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 [4]).

2.8 Phase Space

2.8.1 Path Integral in Phase Space

Recall the Feynman kernel

$$K(\mathbf{x}'', t''; \mathbf{x}', t') = \big\langle \mathbf{x}'' \big| e^{-i\,\widehat{\mathrm{H}}(t''-t')/\hbar} \big| \mathbf{x}' \big\rangle.$$

We can also write this as a path integral in the phase space by

$$K(\mathbf{x}'', t''; \mathbf{x}', t') = \int_{\mathbf{x}(t')=\mathbf{x}'}^{\mathbf{x}(t'')=\mathbf{x}''} [D\mathbf{x}(t) D\mathbf{p}(t)] e^{\frac{i}{\hbar}\int_{t'}^{t''} (\mathbf{p}\cdot\dot{\mathbf{x}}(t) - \mathscr{H}(\mathbf{x},\mathbf{p}))\,dt}$$

where the integral is on the space of paths $(\mathbf{x}(t), \mathbf{p}(t))$ in the phase space with $\mathbf{x}(t') = \mathbf{x}'$ and $\mathbf{x}(t'') = \mathbf{x}''$. The argument toward this phase space path integral is similar as before, by subdividing the interval and inserting both (see Section 2.1.2 for our convention)

$$1 = \int d^n\mathbf{x}\, |\mathbf{x}\rangle\langle\mathbf{x}|, \qquad 1 = \frac{1}{(2\pi\hbar)^n} \int d^n\mathbf{p}^n\, |\mathbf{p}\rangle\langle\mathbf{p}|$$

at the intermediate points, and finally take the short time limit for the subdivision. Here for simplicity, we again work with time-independent Hamiltonian.

In general, there is a delicate issue in obtaining the expression $\mathscr{H}(\mathbf{x}, \mathbf{p})$ due to the ordering of the quantum operators $\hat{\mathbf{x}}, \hat{\mathbf{p}}$ in expressing the quantum Hamiltonian. As a result, the function $\mathscr{H}(\mathbf{x}, \mathbf{p})$ on the phase space may have terms with $\hbar$-dependence such that

$$\lim_{\hbar\to 0} \mathscr{H}(\mathbf{x}, \mathbf{p}) = \text{classical Hamiltonian}.$$

We will not dive much into this issue. Instead, we discuss briefly the Weyl ordering in the next.

2.8.2 Weyl Quantization and Wigner Map

Weyl Quantization

The Weyl quantization (or Weyl transform) associates an operator $\mathrm{Op}[f]$ on the Hilbert space from a function f on the phase space. Precisely, let

$$\tilde{f}(\boldsymbol{\xi}, \mathbf{y}) = \int d^n\mathbf{x} d^n\mathbf{p}\, e^{-\frac{i}{\hbar}[\boldsymbol{\xi}\cdot\mathbf{x} + \mathbf{y}\cdot\mathbf{p}]} f(\mathbf{x}, \mathbf{p})$$

denote the Fourier transform of f. Then $\mathrm{Op}[f]$ is the operator defined by

$$\mathrm{Op}[f] := \frac{1}{(2\pi\hbar)^{2n}} \int d^n\boldsymbol{\xi} d^n\mathbf{y}\, e^{\frac{i}{\hbar}[\boldsymbol{\xi}\cdot\hat{\mathbf{x}} + \mathbf{y}\cdot\hat{\mathbf{p}}]} \tilde{f}(\boldsymbol{\xi}, \mathbf{y}),$$

where $\hat{\mathbf{x}}, \hat{\mathbf{p}}$ are the quantized operators on the Hilbert space satisfying the canonical commutation relations. Combining the above two formulae, we have

$$\mathrm{Op}[f] = \frac{1}{(2\pi\hbar)^{2n}} \int d^n\boldsymbol{\xi} d^n\mathbf{y} d^n\mathbf{x} d^n\mathbf{p}\, e^{\frac{i}{\hbar}[\boldsymbol{\xi}\cdot(\hat{\mathbf{x}}-\mathbf{x}) + \mathbf{y}\cdot(\hat{\mathbf{p}}-\mathbf{p})]} f(\mathbf{x}, \mathbf{p}).$$

Example 2.8.1. Consider the case $n = 1$. Let

$$f(x,p) = e^{iax+ibp}.$$

Then

$$\begin{aligned}
\mathrm{Op}[f] &= \frac{1}{(2\pi\hbar)^2}\int d\xi dy dx dp\, e^{\frac{i}{\hbar}\xi(\hat{x}-x)+y(\hat{p}-p)}e^{iax+ibp} \\
&= \frac{1}{(2\pi\hbar)^2}\int d\xi dy\, e^{\frac{i}{\hbar}(\xi\hat{x}+y\hat{p})}\int dx dp\, e^{-\frac{i}{\hbar}x(\xi-\hbar a)}e^{-\frac{i}{\hbar}p(y-\hbar b)} \\
&= \int d\xi dy\, e^{\frac{i}{\hbar}(\xi\hat{x}+y\hat{p})}\delta(\xi-\hbar a)\delta(y-\hbar b) \\
&= e^{ia\hat{x}+ib\hat{p}}.
\end{aligned}$$

Thus

$$\mathrm{Op}[e^{iax+ibp}] = e^{ia\hat{x}+ib\hat{p}}.$$

Expanding in power of a and b, we find

$$\mathrm{Op}[x^m p^n] = \mathrm{Sym}(\hat{x}^m\hat{p}^n)$$

where $\mathrm{Sym}(-)$ is the symmetrized order average. For example

$$\begin{aligned}
\mathrm{Op}[xp] =& \frac{1}{2}(\hat{x}\hat{p}+\hat{p}\hat{x}) \\
\mathrm{Op}[x^2p] =& \frac{1}{3}(\hat{x}^2\hat{p}+\hat{x}\hat{p}\hat{x}+\hat{p}\hat{x}^2) \\
\mathrm{Op}[x^2p^2] =& \frac{1}{6}(\hat{x}^2\hat{p}^2+\hat{p}^2\hat{x}^2+\hat{x}\hat{p}\hat{x}\hat{p}+\hat{x}\hat{p}^2\hat{x}+\hat{p}\hat{x}\hat{p}\hat{x}+\hat{p}\hat{x}^2\hat{p}).
\end{aligned}$$

This symmetrized ordering is also called the *Weyl ordering*. Operators expressed in a different ordering are all related by the canonical commutation relation. For example

$$\mathrm{Op}[xp] = \hat{p}\hat{x} + \frac{i}{2}\hbar.$$

We give another useful integral kernel description of $\mathrm{Op}[f]$ as follows. Using the Baker-Campbell-Hausdorff formula and the canonical commutation relation, we have

$$e^{\frac{i}{\hbar}(\mathbf{a}\cdot\hat{\mathbf{x}}+\mathbf{b}\cdot\hat{\mathbf{p}})} = e^{\frac{i}{2\hbar}\mathbf{a}\cdot\mathbf{b}}e^{\frac{i}{\hbar}\mathbf{a}\cdot\hat{\mathbf{x}}}e^{\frac{i}{\hbar}\mathbf{b}\cdot\hat{\mathbf{p}}}.$$

Here $\mathbf{a}, \mathbf{b}$ are constant vectors.

Let us apply this to compute the matrix element of $\mathrm{Op}[f]$ in the position representation

$$\big\langle \mathbf{x}''\big|\,\mathrm{Op}[f]\,\big|\mathbf{x}'\big\rangle.$$

Observe that $e^{\frac{i}{\hbar}\mathbf{b}\cdot\hat{\mathbf{p}}} = e^{\mathbf{b}\cdot\nabla}$ is the translation by $\mathbf{b}$, thus on any state $|\psi\rangle$ with wave function $\psi(\mathbf{x})$

$$\langle\mathbf{x}|e^{\frac{i}{\hbar}\mathbf{b}\cdot\hat{\mathbf{p}}}|\psi\rangle = e^{\mathbf{b}\cdot\vec{\nabla}}\psi(\mathbf{x}) = \psi(\mathbf{x}+\mathbf{b}).$$

Applying this to $|\psi\rangle = |\mathbf{x}'\rangle$ whose wave function is $\psi(\mathbf{x}) = \delta(\mathbf{x}-\mathbf{x}')$

$$\Longrightarrow \qquad e^{\frac{i}{\hbar}\mathbf{b}\cdot\hat{\mathbf{p}}}\big|\mathbf{x}'\big\rangle = \big|\mathbf{x}'-\mathbf{b}\big\rangle.$$

Let us use this to compute

$$\langle \mathbf{x}''| \operatorname{Op}[f] |\mathbf{x}'\rangle = \frac{1}{(2\pi\hbar)^{2n}} \int d^n\mathbf{x} d^n\mathbf{p} d^n\boldsymbol{\xi} d^n\mathbf{y} f(\mathbf{x},\mathbf{p}) \langle \mathbf{x}''| e^{\frac{i}{\hbar}[\boldsymbol{\xi}\cdot(\hat{\mathbf{x}}-\mathbf{x})+\mathbf{y}\cdot(\hat{\mathbf{p}}-\mathbf{p})]} |\mathbf{x}'\rangle.$$

We find

$$\begin{aligned}
&\langle \mathbf{x}''| e^{\frac{i}{\hbar}[\boldsymbol{\xi}\cdot(\hat{\mathbf{x}}-\mathbf{x})+\mathbf{y}\cdot(\hat{\mathbf{p}}-\mathbf{p})]} |\mathbf{x}'\rangle \\
=&e^{-\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\mathbf{x}+\mathbf{y}\cdot\mathbf{p})} e^{\frac{i}{2\hbar}\boldsymbol{\xi}\cdot\mathbf{y}} \langle \mathbf{x}''| e^{\frac{i}{\hbar}\boldsymbol{\xi}\cdot\hat{\mathbf{x}}} e^{\frac{i}{\hbar}\mathbf{y}\cdot\hat{\mathbf{p}}} |\mathbf{x}'\rangle \\
=&e^{-\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\mathbf{x}+\mathbf{y}\cdot\mathbf{p})} e^{\frac{i}{2\hbar}\boldsymbol{\xi}\cdot\mathbf{y}} e^{\frac{i}{\hbar}\boldsymbol{\xi}\cdot\hat{\mathbf{x}}''} \langle \mathbf{x}''| \mathbf{x}'-\mathbf{y}\rangle \\
=&e^{-\frac{i}{\hbar}\boldsymbol{\xi}\cdot(\mathbf{x}-\frac{1}{2}\mathbf{y}-\mathbf{x}'')-\frac{i}{\hbar}\mathbf{y}\cdot\mathbf{p}} \delta(\mathbf{x}''-\mathbf{x}'+\mathbf{y}) \\
=&e^{-\frac{i}{\hbar}\boldsymbol{\xi}\cdot(\mathbf{x}-\frac{1}{2}(\mathbf{x}'+\mathbf{x}''))+\frac{i}{\hbar}(\mathbf{x}''-\mathbf{x}')\cdot\mathbf{p}} \delta(\mathbf{x}''-\mathbf{x}'+\mathbf{y}).
\end{aligned}$$

It follows that

$$\langle \mathbf{x}''| \operatorname{Op}[f] |\mathbf{x}'\rangle = \frac{1}{(2\pi\hbar)^n} \int d^n\mathbf{p}\, e^{i\mathbf{p}\cdot(\mathbf{x}''-\mathbf{x}')/\hbar} f\left(\frac{\mathbf{x}'+\mathbf{x}''}{2},\mathbf{p}\right).$$

This gives the explicit formula for the integral kernel of $\operatorname{Op}[f]$.

Wigner Map

The inverse of the Weyl quantization is called the *Wigner map*, which takes an operator back to a phase space function. Using the integral kernel formula of $\operatorname{Op}[f]$, we have

$$\left\langle \mathbf{x}+\frac{1}{2}\mathbf{y}\right| \operatorname{Op}[f] \left|\mathbf{x}-\frac{1}{2}\mathbf{y}\right\rangle = \frac{1}{(2\pi\hbar)^n} \int d^n\mathbf{p}\, e^{i\mathbf{p}\cdot\mathbf{y}/\hbar} f(\mathbf{x},\mathbf{p}).$$

Applying the inverse Fourier transform leads to

$$f(\mathbf{x},\mathbf{p}) = \int d^n\mathbf{y}\, e^{-i\mathbf{p}\cdot\mathbf{y}/\hbar} \left\langle \mathbf{x}+\frac{1}{2}\mathbf{y}\right| \operatorname{Op}[f] \left|\mathbf{x}-\frac{1}{2}\mathbf{y}\right\rangle.$$

This formula illustrates the Wigner map $W[\hat{\Theta}]$ of an operator $\hat{\Theta}$ on the Hilbert space by

$$W[\hat{\Theta}](\mathbf{x},\mathbf{p}) := \int d^n\mathbf{y}\, e^{-i\mathbf{p}\cdot\mathbf{y}/\hbar} \left\langle \mathbf{x}+\frac{1}{2}\mathbf{y}\right| \hat{\Theta} \left|\mathbf{x}-\frac{1}{2}\mathbf{y}\right\rangle.$$

One remarkable aspect of Wigner map is that it allows us to study the noncommutative world of quantum operators through the commutative world of phase space.

2.8.3 Moyal Product

Operators on the Hilbert space have naturally a noncommutative associative product given by compositions. Under the Weyl-Wigner correspondence, we will have a product defined for functions on the phase space. Such product is known as the *Moyal product* $*$. Explicitly, given two functions $f(\mathbf{x},\mathbf{p})$ and $g(\mathbf{x},\mathbf{p})$ on the phase space, their Moyal product is defined to be

$$f * g := f e^{\frac{i}{2}\hbar \sum_{i=1}^n \left(\frac{\overleftarrow{\partial}}{\partial x_i}\frac{\overrightarrow{\partial}}{\partial p_i} - \frac{\overleftarrow{\partial}}{\partial p_i}\frac{\overrightarrow{\partial}}{\partial x_i}\right)} g.$$

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.

As an example, let us consider the Moyal product of x_i and p_i. The above formula gives

$$x_i * p_i = x_i p_i + \frac{i}{2}\hbar.$$

Under the Weyl quantization

$$\mathrm{Op}[x_i * p_i] = \mathrm{Op}[x_i p_i] + \frac{i}{2}\hbar = \frac{1}{2}(\hat{x}_i\hat{p}_i + \hat{p}_i\hat{x}_i) + \frac{i}{2}\hbar = \hat{x}_i\hat{p}_i = \mathrm{Op}[x_i]\,\mathrm{Op}[p_i]$$

as expected. In general, we have the identity

$$\mathrm{Op}[f * g] = \mathrm{Op}[f]\,\mathrm{Op}[g].$$

To see this, let us rewrite the Moyal product as follows.

$$\begin{aligned}
(f*g)(\mathbf{x},\mathbf{p}) &= \int d^n\tilde{\mathbf{x}}d^n\tilde{\mathbf{p}}\delta(\tilde{\mathbf{x}}-\mathbf{x})\delta(\tilde{\mathbf{p}}-\mathbf{p})e^{\frac{i}{2}\hbar\sum_{i=1}^{n}\frac{\partial}{\partial x_i}\frac{\partial}{\partial\tilde{p}_i}-\frac{\partial}{\partial p_i}\frac{\partial}{\partial\tilde{x}_i}} f(\mathbf{x},\mathbf{p})g(\tilde{\mathbf{x}},\tilde{\mathbf{p}}) \\
&= \frac{1}{(2\pi\hbar)^{4n}}\int d^n\boldsymbol{\xi}d^n\mathbf{y}\int d^n\tilde{\boldsymbol{\xi}}d^n\tilde{\mathbf{y}}\int d^n\tilde{\mathbf{x}}d^n\tilde{\mathbf{p}}\delta(\tilde{\mathbf{x}}-\mathbf{x})\delta(\tilde{\mathbf{p}}-\mathbf{p}) \\
&\quad e^{\frac{i}{2}\hbar\sum_{i=1}^{n}\frac{\partial}{\partial x_i}\frac{\partial}{\partial\tilde{p}_i}-\frac{\partial}{\partial p_i}\frac{\partial}{\partial\tilde{x}_i}}\left(e^{\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\mathbf{x}+\mathbf{y}\cdot\mathbf{p})}e^{\frac{i}{\hbar}(\tilde{\boldsymbol{\xi}}\cdot\tilde{\mathbf{x}}+\tilde{\mathbf{y}}\cdot\tilde{\mathbf{p}})}\tilde{f}(\boldsymbol{\xi},\mathbf{y})g(\tilde{\boldsymbol{\xi}},\tilde{\mathbf{y}})\right) \\
&= \frac{1}{(2\pi\hbar)^{4n}}\int d^n\boldsymbol{\xi}d^n\mathbf{y}\int d^n\tilde{\boldsymbol{\xi}}d^n\tilde{\mathbf{y}}\int d^n\tilde{\mathbf{x}}d^n\tilde{\mathbf{p}}\delta(\tilde{\mathbf{x}}-\mathbf{x})\delta(\tilde{\mathbf{p}}-\mathbf{p}) \\
&\quad e^{\frac{i}{2\hbar}(\tilde{\boldsymbol{\xi}}\cdot\mathbf{y}-\boldsymbol{\xi}\cdot\tilde{\mathbf{y}})}e^{\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\mathbf{x}+\mathbf{y}\cdot\mathbf{p})}e^{\frac{i}{\hbar}(\tilde{\boldsymbol{\xi}}\cdot\tilde{\mathbf{x}}+\tilde{\mathbf{y}}\cdot\tilde{\mathbf{p}})}\tilde{f}(\boldsymbol{\xi},\mathbf{y})g(\tilde{\boldsymbol{\xi}},\tilde{\mathbf{y}}) \\
&= \frac{1}{(2\pi\hbar)^{4n}}\int d^n\boldsymbol{\xi}d^n\mathbf{y}\int d^n\tilde{\boldsymbol{\xi}}d^n\tilde{\mathbf{y}}\,e^{\frac{i}{2\hbar}(\tilde{\boldsymbol{\xi}}\cdot\mathbf{y}-\boldsymbol{\xi}\cdot\tilde{\mathbf{y}})}e^{\frac{i}{\hbar}((\boldsymbol{\xi}+\tilde{\boldsymbol{\xi}})\cdot\mathbf{x}+(\mathbf{y}+\tilde{\mathbf{y}})\cdot\mathbf{p})}\tilde{f}(\boldsymbol{\xi},\mathbf{y})g(\tilde{\boldsymbol{\xi}},\tilde{\mathbf{y}})
\end{aligned}$$

Therefore

$$\begin{aligned}
\mathrm{Op}[f*g](\hat{\mathbf{x}},\hat{\mathbf{p}}) &= \frac{1}{(2\pi\hbar)^{4n}}\int d^n\boldsymbol{\xi}d^n\mathbf{y}\int d^n\tilde{\boldsymbol{\xi}}d^n\tilde{\mathbf{y}}\,e^{\frac{i}{2\hbar}(\tilde{\boldsymbol{\xi}}\cdot\mathbf{y}-\boldsymbol{\xi}\cdot\tilde{\mathbf{y}})}e^{\frac{i}{\hbar}((\boldsymbol{\xi}+\tilde{\boldsymbol{\xi}})\cdot\hat{\mathbf{x}}+(\mathbf{y}+\tilde{\mathbf{y}})\cdot\hat{\mathbf{p}})}\tilde{f}(\boldsymbol{\xi},\mathbf{y})g(\tilde{\boldsymbol{\xi}},\tilde{\mathbf{y}}) \\
&= \frac{1}{(2\pi\hbar)^{4n}}\int d^n\boldsymbol{\xi}d^n\mathbf{y}\int d^n\tilde{\boldsymbol{\xi}}d^n\tilde{\mathbf{y}}\,e^{\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\hat{\mathbf{x}}+\mathbf{y}\cdot\hat{\mathbf{p}})}e^{\frac{i}{\hbar}(\tilde{\boldsymbol{\xi}}\cdot\hat{\mathbf{x}}+\tilde{\mathbf{y}}\cdot\hat{\mathbf{p}})}\tilde{f}(\boldsymbol{\xi},\mathbf{y})g(\tilde{\boldsymbol{\xi}},\tilde{\mathbf{y}}) \\
&= \frac{1}{(2\pi\hbar)^{2n}}\int d^n\boldsymbol{\xi}d^n\mathbf{y}e^{\frac{i}{\hbar}(\boldsymbol{\xi}\cdot\hat{\mathbf{x}}+\mathbf{y}\cdot\hat{\mathbf{p}})}\tilde{f}(\boldsymbol{\xi},\mathbf{y})\;\frac{1}{(2\pi\hbar)^{2n}}\int d^n\tilde{\boldsymbol{\xi}}d^n\tilde{\mathbf{y}}\,e^{\frac{i}{\hbar}(\tilde{\boldsymbol{\xi}}\cdot\hat{\mathbf{x}}+\tilde{\mathbf{y}}\cdot\hat{\mathbf{p}})}g(\tilde{\boldsymbol{\xi}},\tilde{\mathbf{y}}) \\
&= \mathrm{Op}[f](\hat{\mathbf{x}},\hat{\mathbf{p}})\;\;\mathrm{Op}[g](\hat{\mathbf{x}},\hat{\mathbf{p}}).
\end{aligned}$$

Here in the second line, we have used the Baker-Campbell-Hausdorff formula and the canonical commutation relation for the operators $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}$.

Now let us consider the Feynman kernel

$$\left\langle \mathbf{x}'' \middle| e^{-i\,\widehat{\mathrm{H}}\,T/\hbar} \middle| \mathbf{x}' \right\rangle.$$

Let $H = W[\widehat{\mathrm{H}}]$ be the phase space function obtained via Wigner map such that

$$\mathrm{Op}[H] = \widehat{\mathrm{H}}\,.$$

Since Op intertwines the operator composition with the Moyal product, we have

$$e^{-i\,\widehat{\mathrm{H}}\,T/\hbar} = \mathrm{Op}\left[\exp^*\left(-iHT/\hbar\right)\right].$$

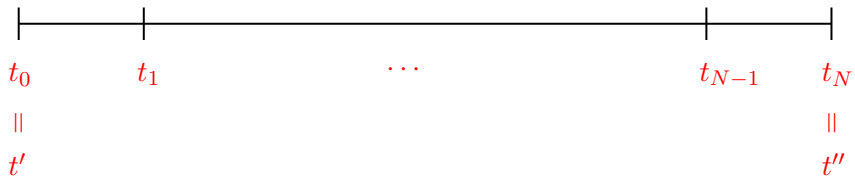
Here $\exp^*$ denotes the Moyal product exp

$$\exp^*(f) := \sum_{n=0}^{\infty} \frac{1}{n!} \underbrace{f * \cdots * f}_{n}.$$

Thus the Feynman kernel can be expressed via the Weyl quantization formula as

$$\begin{aligned}\left\langle \mathbf{x}'' \middle| e^{-i\,\widehat{\mathrm{H}}\,T/\hbar} \middle| \mathbf{x}' \right\rangle &= \left\langle \mathbf{x}'' \right| \mathrm{Op}\left[\exp^*\left(-iHT/\hbar\right)\right] \left| \mathbf{x}' \right\rangle \\ &= \frac{1}{(2\pi\hbar)^n} \int d^n\mathbf{p}\, e^{i\mathbf{p}\cdot(\mathbf{x}''-\mathbf{x}')} \exp^*\left(-iHT/\hbar\right) \left(\frac{\mathbf{x}'+\mathbf{x}''}{2}, \mathbf{p}\right).\end{aligned}$$

This formula can be used to understood the phase space path integral [22]. Let us subdivide the time interval into small pieces



By the above formula, the path integral from t_i to t_{i+1} contributes to

$$\langle \mathbf{x}_{i+1} | e^{-i\,\widehat{\mathrm{H}}(t_{i+1}-t_i)} | \mathbf{x}_i \rangle \simeq \frac{1}{(2\pi\hbar)^n} \int d^n\mathbf{p}\, e^{\frac{i}{\hbar}\left(\mathbf{p}_i(\mathbf{x}_{i+1}-\mathbf{x}_i) - H\left(\frac{\mathbf{x}_{i+1}+\mathbf{x}_i}{2}, \mathbf{p}_i\right)(t_{i+1}-t_i)\right)}.$$

Then if we sum up all the intermediate x_i and p_i, and in the continuum limit, we find

$$e^{\frac{i}{\hbar}\int_0^T (\mathbf{p}\cdot\dot{\mathbf{x}} - \mathscr{H})\,dt}$$

for the phase space path integral (careful reader could see where we cheat about the ordering).

Example 2.8.2 (Harmonic Oscillator)**.**

$$H(x,p) = \frac{1}{2}p^2 + \frac{1}{2}x^2.$$

Consider $f(H)$ an arbitrary function of H. A straight-forward computation of Moyal product shows

$$H * f(H) = Hf(H) - \frac{\hbar^2}{4}f'(H) - \frac{\hbar^2}{4}Hf''(H).$$

This implies $\exp^*\left(-iHT/\hbar\right)$ is again a function of H. Moreover it satisfies the equation

$$i\hbar\frac{\partial}{\partial T}\exp^*\left(-iHT/\hbar\right) = \left(H - \frac{\hbar^2}{4}\frac{\partial}{\partial H} - \frac{\hbar^2}{4}H\frac{\partial^2}{\partial H^2}\right)\exp^*\left(-iHT/\hbar\right).$$

This equation is solved by

$$\exp^*\left(-iHT/\hbar\right) = \frac{e^{\frac{2H}{i\hbar}\tan\left(\frac{T}{2}\right)}}{\cos\left(\frac{T}{2}\right)}.$$

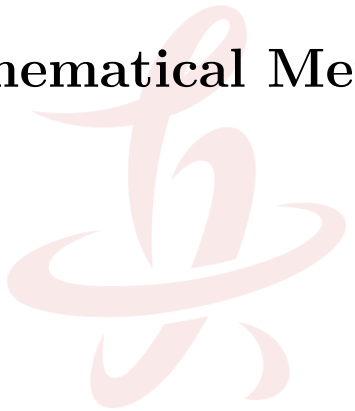
Substituting this expression into the Feynman kernel, we find

$$\left\langle x'' \middle| e^{-i\,\widehat{\mathrm{H}}\,T/\hbar} \middle| x' \right\rangle = \left(\frac{1}{2\pi i\hbar\sin T}\right)^{\frac{1}{2}} e^{\frac{i}{2\hbar\sin T}\left[\left((x'')^2+(x')^2\right)\cos T - 2x'x''\right]}$$

which is precisely the formula we found in Section 2.4 (with unit mass and frequency).

Part II

Mathematical Methods



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