

—Chapter 1—

Quantize Variables

1-1 First Quantization

A. LINEAR ALGEBRA OF SCHRÖDINGER WAVE MECHANICS

(1) Review of Schrödinger wave mechanics

I. Time-independent Schrödinger equation

$$\hat{\mathcal{H}}\psi_n(x) = \left[\frac{\hat{p}^2}{2m} + V(x) \right] \psi_n(x) = E_n \psi_n(x)$$

where the Hamiltonian operator $\hat{\mathcal{H}}$ is a Hermitian differential operator,

$$\int \left(\hat{\mathcal{H}}\psi_n(x) \right)^* \psi'_n(x) dx = \int \psi_n^*(x) \left(\hat{\mathcal{H}}\psi'_n(x) \right) dx$$

and the eigenfunctions ψ_n are orthonormal,

$$\int \psi_m^*(x) \psi_n(x) dx = \delta_{mn}$$

Any wavefunction can be written as a linear combination of eigenfunctions $\psi_n(x)$, i.e.,

$$\psi(x) = \sum_n c_n \psi_n(x), \text{ where } c_n = \int \psi_n^*(x) \psi(x) dx$$

II. Born rule and Heisenberg's uncertainty principle

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

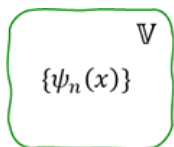
I. Abstract of Schrödinger wave mechanics

1. Vector space $\mathbb{V}$

(A basis is a set of linearly independent wavefunctions that spans the vector space.)

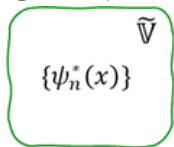
A basis $\{\psi_n(x)\}$ allows any wavefunction $\psi(x)$ to be expanded:

$$\psi(x) = \sum_n c_n \psi_n(x)$$



2. Dual space $\tilde{\mathbb{V}}$

(The dual space is defined automatically for any vector space.)
 The complex conjugate of ψ_n form a basis $\{\psi_n^*(x)\}$ of a vector space $\widehat{V}$, called dual space.



Note: $\psi_n^*(x)$ and $\psi_n(x)$ are independent.

3. Inner product

(A particular mapping between vector space and dual space and is not automatic.)

$$\int_{-\infty}^{\infty} \psi^*(x) \psi'(x) dx = c\text{-number}$$

$$\left(\int_{-\infty}^{\infty} \psi^*(x) \psi'(x) dx \right)^* = \int_{-\infty}^{\infty} \psi'^*(x) \psi(x) dx = c\text{-number}$$

4. Complete

Since

$$\begin{aligned} \psi(x) &= \sum_n c_n \psi_n(x), \text{ where } c_n = \int \psi_n^*(x) \psi(x) dx \\ &= \sum_n \int \psi_n^*(x') \psi(x') dx' \psi_n(x) \\ &= \int \underbrace{\sum_n \psi_n(x) \psi_n^*(x')}_{=\delta(x-x')} \psi(x') dx' \end{aligned}$$

we obtain

$$\sum_n \psi_n(x) \psi_n^*(x') = \delta(x - x') \dots \dots \text{completeness relation}$$

A completeness relation for a set of eigenfunctions is the identity assuring that there is no basis function "missing".

$\Rightarrow$ If the vector space has an appropriate inner product and is complete, we call it a **Hilbert space** $\mathbb{H}_S$.

5. Operator $\hat{\mathcal{H}}$

An operator $\hat{\mathcal{H}}$ is a mapping acting on the vector space.

$$\hat{\mathcal{H}} \psi_n(x) = E_n \psi_n(x) \dots \dots \text{eigenvalue equation}$$

where ψ_n are orthonormal and E_n are real.

II. Abstract of the uncertainty principle

$$\Delta x \Delta p \geq \frac{1}{2} |\langle [\hat{x}, \hat{p}] \rangle| = \frac{\hbar}{2}$$

The Hermitian operators $\hat{x}$ and $\hat{p}$ satisfy the commutation relation,

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

B. DIRAC NOTATION

(1) Algebraic isomorphic Hilbert space

Hilbert space of Schrödinger's mechanics:

uncertainty
principle

$$\Delta x \Delta p \geq \hbar/2 \xrightarrow{\text{abstract}} [\hat{x}, \hat{p}] = i\hbar$$

$$\hat{H}\psi_n(x) = E_n\psi_n(x) \longrightarrow \psi(x) = \sum_n c_n \psi_n(x) \xrightarrow{\text{abstract}} \boxed{\overset{\mathbb{H}_S}{\{\psi_n(x)\}}}$$

Dirac invented a useful alternative notation for the Hilbert space which is now referred to as Dirac notation (or called bra-ket notation).

$$\boxed{\overset{\mathbb{H}_D}{\{|\psi_n\rangle\}}}$$

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

Dirac notation enables us to do calculations in a general Hilbert space without needing to worry about the space's representation.

(2) Hilbert space in Dirac notation

1. Ket space (vector space)

$$\boxed{\overset{\mathbb{V}}{\{|\psi_n\rangle\}}}$$

$|\psi_n\rangle$ are the basis of the ket space.

2. Bra space (dual space)

$$\boxed{\overset{\widehat{\mathbb{V}}}{\{\langle\psi_n|\}}}$$

Note: $\langle \psi_n | \equiv |\psi_n\rangle^\dagger$ and $|\psi_n\rangle$ are independent.

3. Inner product (expectation)

$$\langle \psi_n | \psi \rangle = c\text{-number}$$

4. Completeness relation

Since

$$|\psi\rangle = \sum_n c_n |\psi_n\rangle \cdots \cdots \text{(a)}$$

where c_n is the coefficient and given by

$$\langle \psi_n | \psi \rangle = \sum_m c_m \underbrace{\langle \psi_n | \psi_m \rangle}_{=\delta_{nm}} = c_n \cdots \cdots \text{(b)}$$

Insert equation (b) into equation (a) to obtain

$$|\psi\rangle = \sum_n \langle \psi_n | \psi \rangle |\psi_n\rangle = \sum_n |\psi_n\rangle \langle \psi_n | \psi \rangle \cdots \cdots \text{(c)}$$

Thus, we have

$$\sum_n |\psi_n\rangle \langle \psi_n | = \hat{1}$$

which is also called **the resolution of identity**.

- (3) Hermitian operator (the operator is its own complex conjugate)

$$\hat{A}^\dagger = \hat{A}$$

Its eigenvalue equation is given by:

$$\hat{A} |\psi_n\rangle = \lambda_n |\psi_n\rangle$$

The eigenvalues are real:

$$\lambda_n = \lambda_n^*$$

The eigenkets are orthonormal:

$$\langle \psi_n | \psi_k \rangle = \delta_{nk}, \quad \delta_{nk} = \begin{cases} 1, & n = k \\ 0, & n \neq k \end{cases}$$

Since $|\psi_n\rangle$ are orthonormal, i.e., $|\psi_n\rangle$ are linear independent, thus $|\psi_n\rangle$ form a basis of a Hilbert space $\mathbb{H}$.

- (4) Projection operator

$$\hat{P}_n = \underbrace{|\psi_n\rangle \langle \psi_n|}_{\substack{\text{outer product} \\ \text{of eigenket}}}$$

and $\hat{P}_n$ satisfies the following property:

$$\hat{P}_n^2 = |\psi_n\rangle \underbrace{\langle\psi_n| \cdot |\psi_n\rangle}_{=1} \langle\psi_n| = |\psi_n\rangle \langle\psi_n| = \hat{P}_n$$

(5) Commutator

The Hermitian operators $\hat{x}$ and $\hat{p}$ satisfy the commutation relation,

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

C. UNITARY TRANSFORMATION

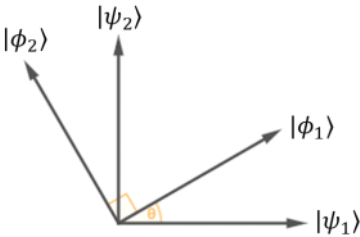
(1) For a Hilbert space $\mathbb{H}$, there are many possible sets of basis as

$$\boxed{\{|\psi_n\rangle\}}^{\mathbb{H}} = \boxed{\{|\psi'_n\rangle\}}^{\mathbb{H}} = \boxed{\{|\phi_n\rangle\}}^{\mathbb{H}}$$

Between any two such sets of basis, there exists a linear transformation that preserves inner product (and hence length), known as a **unitary transformation**.

(2) A unitary transformation is equivalent to a change of basis

Consider two sets of basis $\{|\psi_n\rangle\}$ and $\{|\phi_n\rangle\}$,



where the relationships between two bases are

$$\begin{aligned} |\phi_1\rangle &= a_{11}|\psi_1\rangle + a_{21}|\psi_2\rangle + \cdots + a_{n1}|\psi_n\rangle \\ |\phi_2\rangle &= a_{12}|\psi_1\rangle + a_{22}|\psi_2\rangle + \cdots + a_{n2}|\psi_n\rangle \\ &\vdots \\ |\phi_n\rangle &= a_{1n}|\psi_1\rangle + a_{2n}|\psi_2\rangle + \cdots + a_{nn}|\psi_n\rangle \end{aligned} \quad \text{or} \quad |\phi_n\rangle = \sum_m a_{mn} |\psi_m\rangle$$

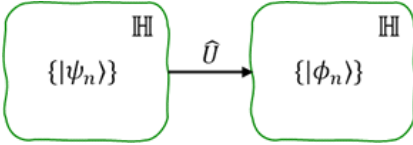
We have, in the matrix form,

$$\begin{pmatrix} |\phi_1\rangle \\ |\phi_2\rangle \\ \vdots \\ |\phi_n\rangle \end{pmatrix} = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{n1} \\ a_{12} & a_{22} & \cdots & a_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1n} & a_{2n} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} |\psi_1\rangle \\ |\psi_2\rangle \\ \vdots \\ |\psi_n\rangle \end{pmatrix}$$

We then write the relationships in the Dirac notation:

$$\begin{pmatrix} |\phi_1\rangle \\ |\phi_2\rangle \\ \vdots \\ |\phi_n\rangle \end{pmatrix} \rightarrow |\Phi\rangle, \begin{pmatrix} |\psi_1\rangle \\ |\psi_2\rangle \\ \vdots \\ |\psi_n\rangle \end{pmatrix} \rightarrow |\Psi\rangle, \text{ and } \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{n1} \\ a_{12} & a_{22} & \cdots & a_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1n} & a_{2n} & \cdots & a_{nn} \end{pmatrix} \rightarrow \hat{U}^\dagger$$

and obtain

$$|\Phi\rangle = \hat{U}^\dagger |\Psi\rangle$$


The diagram shows two green rounded rectangles representing Hilbert spaces $\mathbb{H}$. The left rectangle contains the set $\{|\psi_n\rangle\}$ and the right rectangle contains $\{|\phi_n\rangle\}$. An arrow labeled $\hat{U}$ points from the left rectangle to the right rectangle.

Since

$$\langle \Phi | \Phi \rangle = \langle \Psi | \hat{U} \hat{U}^\dagger | \Psi \rangle = \langle \Psi | \Psi \rangle$$

we obtain

$$\hat{U} \hat{U}^\dagger = \hat{1} \Rightarrow \hat{U}^\dagger = \hat{U}^{-1}$$

Thus, $\hat{U}$ is a unitary operator that maps one basis set to the other.

- (3) A similarity transformation is equivalent to a change of operator

Consider an operator $\hat{A}$ acting on the ket $|\Psi\rangle$ in the basis $\{|\psi_n\rangle\}$,

$$|\Psi'\rangle = \hat{A}|\Psi\rangle$$

Since

$$|\Phi'\rangle = \hat{U}^\dagger |\Psi'\rangle = \hat{U}^\dagger \hat{A} |\Psi\rangle = \hat{U}^\dagger \hat{A} \hat{U} |\Phi\rangle$$

The operator $\hat{A}$ in the basis $\{|\psi_n\rangle\}$ is equal to the operator $\hat{U}^\dagger \hat{A} \hat{U}$ in the basis $\{|\phi_n\rangle\}$.

Let

$$\hat{B} \equiv \hat{U}^\dagger \hat{A} \hat{U} \cdots \text{similarity transformation}$$

- (4) If $\hat{A}$ is diagonalizable, then $\hat{B}$ is diagonalized, i.e., $\hat{B} = \hat{D}$, and then we obtain

$$\hat{D} = \hat{U}^\dagger \hat{A} \hat{U}$$

Recall the basic linear algebra, the matrix $\mathbf{U}$ that diagonalizes $\mathbf{A}$ has the eigenvectors of $\mathbf{v}_n$ as its columns:

$$\mathbf{U} = (\mathbf{v}_1 \quad \mathbf{v}_2 \quad \cdots \quad \mathbf{v}_n)$$

Then we obtain

$$\mathbf{A} = \mathbf{U} \cdot \mathbf{D} \cdot \mathbf{U}^\dagger$$

$$= (\mathbf{v}_1 \quad \mathbf{v}_2 \quad \mathbf{v}_3 \quad \cdots) \begin{pmatrix} \lambda_1 & 0 & 0 & \cdots \\ 0 & \lambda_2 & 0 & \cdots \\ 0 & 0 & \lambda_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \mathbf{v}_1^\dagger \\ \mathbf{v}_2^\dagger \\ \mathbf{v}_3^\dagger \\ \vdots \end{pmatrix}$$

$$= (\mathbf{v}_1 \quad \mathbf{v}_2 \quad \mathbf{v}_3 \quad \cdots) \begin{pmatrix} \lambda_1 \mathbf{v}_1^\dagger \\ \lambda_2 \mathbf{v}_2^\dagger \\ \lambda_3 \mathbf{v}_3^\dagger \\ \vdots \end{pmatrix}$$

$$= \sum_n \lambda_n \mathbf{v}_n \mathbf{v}_n^\dagger$$

In Dirac notation:

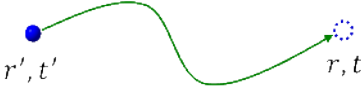
$$\hat{A} = \sum_n \lambda_n |\phi_n\rangle \langle \phi_n|$$

where $|\phi_n\rangle$ are the eigenkets of the Hermitian operator $\hat{A}$. Thus, $\hat{A}$ is expanded in its spectrum λ_n by projection operators $|\phi_n\rangle \langle \phi_n|$, called *spectral representation*.

1-2 Propagation

A. PROPAGATOR

- (1) Consider a particle that is going to move from (r', t') to (r, t)



The probability of finding a particle at position r at time t is

$$|\Psi(r, t)|^2 = |\langle r | \Psi(t) \rangle|^2,$$

where $|\Psi(t)\rangle = \hat{U}(t, t')|\Psi(t')\rangle$ is a state evolving in time and $\hat{U}(t, t')$ is the time evolution operator.

Thus, we obtain

$$\begin{aligned}\Psi(r, t) &= \langle r | \Psi(t) \rangle \\ &= \langle r | \hat{U}(t, t') | \Psi(t') \rangle \\ &= \langle r | \hat{U}(t, t') \underbrace{\int |r'\rangle \langle r' | dr'}_{\hat{1}} | \Psi(t') \rangle \\ &= \int \langle r | \hat{U}(t, t') | r' \rangle \langle r' | \Psi(t') \rangle dr' \\ &= \int K(r, t; r', t') \Psi(r', t') dr'\end{aligned}$$

where $K(r, t; r', t')$ is referred to as the propagator.

- (2) $K(r, t; r', t') = \langle r | \hat{U}(t, t') | r' \rangle$ illustrates that the wavefunction at r and t is determined by the wavefunction at the original time t' , receiving contributions from all r' which are weighted by the amplitude K .

B. TIME-EVOLUTION OPERATOR $\hat{U}(t, t')$

- (1) Assume that time is a continuous parameter

$$\lim_{t \rightarrow t'} |\Psi(t)\rangle = \lim_{t \rightarrow t'} \hat{U}(t, t') |\Psi(t')\rangle = |\Psi(t')\rangle \Rightarrow \hat{U}(t', t') = \hat{1}$$

Since

$$\begin{aligned}|\Psi(t)\rangle &= \hat{U}(t, t') |\Psi(t')\rangle \\ |\Psi(t)\rangle &= \hat{U}(t, t_1) |\Psi(t_1)\rangle = \hat{U}(t, t_1) \hat{U}(t_1, t') |\Psi(t')\rangle\end{aligned}$$

we obtain

$$\hat{U}(t, t') = \hat{U}(t, t_1) \hat{U}(t_1, t'), \text{ for } t > t_1 > t' \dots \dots \text{decomposition}$$

(2) Solve $\hat{U}(t, t')$ from the equation of motion:

$$\frac{\partial}{\partial t} \hat{U}(t, t') = \lim_{\epsilon \rightarrow 0} \frac{\hat{U}(t + \epsilon, t') - \hat{U}(t, t')}{\epsilon}$$

Since $\hat{U}(t + \epsilon, t') = \hat{U}(t + \epsilon, t) \hat{U}(t, t')$,

$$\begin{aligned} \frac{\partial}{\partial t} \hat{U}(t, t') &= \lim_{\epsilon \rightarrow 0} \frac{\hat{U}(t + \epsilon, t) \hat{U}(t, t') - \hat{U}(t, t')}{\epsilon} \\ &= \lim_{\epsilon \rightarrow 0} \frac{[\hat{U}(t + \epsilon, t) - \hat{1}] \hat{U}(t, t')}{\epsilon} \end{aligned}$$

The infinitesimal time evolution of the operator $\hat{U}(t + \epsilon, t)$ describes dynamical evolution under the influence of the Hamiltonian $\hat{H}(t)$ as,

$$\begin{aligned} \hat{U}(t + \epsilon, t) &= \hat{U}(t, t) - \frac{i}{\hbar} \hat{H}(t) \hat{U}(t, t) \epsilon = \hat{1} - \frac{i}{\hbar} \hat{H}(t) \epsilon \\ \Rightarrow \frac{\partial}{\partial t} \hat{U}(t, t') &= \lim_{\epsilon \rightarrow 0} \frac{-\frac{i}{\hbar} \hat{H}(t) \epsilon \hat{U}(t, t')}{\epsilon} = -\frac{i}{\hbar} \hat{H}(t) \hat{U}(t, t') \end{aligned}$$

Integrate with respect to time on both sides

$$\begin{aligned} \int_{t'}^t \frac{\partial}{\partial t_1} \hat{U}(t_1, t') dt_1 &= -\frac{i}{\hbar} \int_{t'}^t \hat{H}(t_1) \hat{U}(t_1, t') dt_1 \\ \hat{U}(t, t') - \hat{1} &= -\frac{i}{\hbar} \int_{t'}^t \hat{H}(t_1) \hat{U}(t_1, t') dt_1 \\ \hat{U}(t, t') &= \hat{1} - \frac{i}{\hbar} \int_{t'}^t \hat{H}(t_1) \hat{U}(t_1, t') dt_1 \end{aligned}$$

Iterate:

$$\begin{aligned} \hat{U}(t, t') &= \hat{1} - \frac{i}{\hbar} \int_{t'}^t \hat{H}(t_1) dt_1 \left[\hat{1} - \frac{i}{\hbar} \int_{t'}^{t_1} \hat{H}(t_2) \hat{U}(t_2, t') dt_2 \right] \\ &= \hat{1} - \frac{i}{\hbar} \int_{t'}^t \hat{H}(t_1) dt_1 + \left(-\frac{i}{\hbar} \right)^2 \int_{t'}^t \hat{H}(t_1) dt_1 \int_{t'}^{t_1} \hat{H}(t_2) \hat{U}(t_2, t') dt_2 \end{aligned}$$

Re-iterate:

$$\hat{U}(t, t') = \hat{1} - \frac{i}{\hbar} \int_{t'}^t \hat{H}(t_1) dt_1 + \left(-\frac{i}{\hbar} \right)^2 \int_{t'}^t \hat{H}(t_1) dt_1 \int_{t'}^{t_1} \hat{H}(t_2) dt_2 + \dots$$

where $t > t_1 > t_2 > \dots > t'$.

Considering the dummy variables t_1 and t_2 , the integral can be rewritten into a compact form

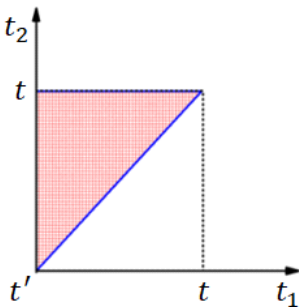
$$\begin{aligned}
& \int_{t'}^t \hat{H}(t_1) dt_1 \int_{t'}^{t_1} \hat{H}(t_2) dt_2 \\
&= \frac{1}{2} \int_{t'}^t \hat{H}(t_1) dt_1 \int_{t'}^{t_1} \hat{H}(t_2) dt_2 + \frac{1}{2} \int_{t'}^t \hat{H}(t_2) dt_2 \int_{t'}^{t_2} \hat{H}(t_1) dt_1 \\
&= \frac{1}{2} \int_{t'}^t \int_{t'}^t \hat{H}(t_1) \hat{H}(t_2) dt_1 dt_2 \Theta(t_1 - t_2) \\
&\quad + \frac{1}{2} \int_{t'}^t \int_{t'}^t \hat{H}(t_2) \hat{H}(t_1) dt_2 dt_1 \Theta(t_2 - t_1)
\end{aligned}$$

where $\Theta(t_1 - t_2) = \begin{cases} 1, & t_1 \geq t_2 \\ 0, & t_1 < t_2 \end{cases}$

Let $\hat{T}$ be the time ordering operator,

$$\begin{aligned}
\hat{T}[\hat{H}(t_1)\hat{H}(t_2)] &= \begin{cases} \hat{H}(t_1)\hat{H}(t_2), & \text{if } t_1 > t_2 \\ \hat{H}(t_2)\hat{H}(t_1), & \text{if } t_2 > t_1 \end{cases} \\
\int_{t'}^t \hat{H}(t_1) dt_1 \int_{t'}^{t_1} \hat{H}(t_2) dt_2 &= \frac{1}{2} \int_{t'}^t \int_{t'}^t \hat{T}[\hat{H}(t_1)\hat{H}(t_2)] dt_1 dt_2
\end{aligned}$$

Pictorially, the area of integration is



Thus, we obtain

$$\begin{aligned}
\int_{t'}^t \int_{t'}^{t_1} dt_1 dt_2 &= \frac{1}{2} \int_{t'}^t \int_{t'}^t \hat{T}[\dots] dt_1 dt_2 = \frac{1}{2!} \int_{t'}^t \int_{t'}^t \hat{T}[\dots] dt_1 dt_2 \\
\int_{t'}^t \int_{t'}^{t_1} \int_{t'}^{t_2} dt_1 dt_2 dt_3 &= \frac{1}{6} \int_{t'}^t \int_{t'}^t \int_{t'}^t \hat{T}[\dots] dt_1 dt_2 dt_3 \\
&= \frac{1}{3!} \int_{t'}^t \int_{t'}^t \int_{t'}^t \hat{T}[\dots] dt_1 dt_2 dt_3 \\
&\vdots \\
\int_{t'}^t \int_{t'}^{t_1} \dots \int_{t'}^{t_N} dt_1 \dots dt_N &= \frac{1}{N!} \int_{t'}^t \int_{t'}^t \dots \int_{t'}^t \hat{T}[\dots] dt_1 \dots dt_N
\end{aligned}$$

$$\begin{aligned}\hat{U}(t, t') &= \hat{1} - \frac{i}{\hbar} \int_{t'}^t \hat{H}(t_1) dt_1 + \frac{1}{2!} \left(-\frac{i}{\hbar} \right)^2 \int_{t'}^t \int_{t'}^t \hat{T}[\hat{H}(t_1) \hat{H}(t_2)] dt_1 dt_2 + \dots \\ &= \hat{T} \left[\exp \left(-\frac{i}{\hbar} \int_{t'}^t \hat{H}(t_1) dt_1 \right) \right]\end{aligned}$$

C. SCHRÖDINGER PICTURE AND HEISENBERG PICTURE

- (1) Properties of the time-evolution operator $\hat{U}(t, t')$

Since

$$\hat{U}(t, t') \hat{U}(t', t) = \hat{U}(t, t) = \hat{1}$$

we obtain

$$\hat{U}^{-1}(t, t') = \hat{U}(t', t) \dots \text{time-reversal}$$

Since

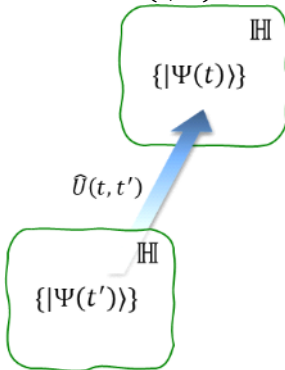
$$\langle \Psi(t) | \Psi(t) \rangle = \langle \Psi(t') | \hat{U}^\dagger(t, t') \hat{U}(t, t') | \Psi(t') \rangle = \langle \Psi(t') | \Psi(t') \rangle$$

we obtain

$$\hat{U}^\dagger(t, t') \hat{U}(t, t') = \hat{1}$$

$$\Rightarrow \hat{U}^{-1}(t, t') = \hat{U}^\dagger(t, t') \dots \text{unitary}$$

$$\Rightarrow \hat{U}^\dagger(t, t') = \hat{U}^{-1}(t, t') = \hat{U}(t', t)$$



- (2) The time evolution of the expectation value is preserved by similarity transformation when a change of basis is made (unitary transformation).

$$\underbrace{\langle \Psi(t) | \hat{A} | \Psi(t) \rangle}_{\text{Schrödinger picture}} = \langle \Psi(0) | \hat{U}^\dagger(t) \hat{A} \hat{U}(t) | \Psi(0) \rangle = \underbrace{\langle \Psi(0) | \hat{A}(t) | \Psi(0) \rangle}_{\text{Heisenberg picture}}$$

COMMENTS:

The time evolution of the expectation value

$$\underbrace{\langle \Psi(t) | \hat{A} | \Psi(t) \rangle}_{\text{Schrödinger picture}} = \underbrace{\langle \Psi(0) | \hat{A}(t) | \Psi(0) \rangle}_{\text{Heisenberg picture}}$$

Schrödinger picture:

The time-dependent state is given by the unitary transformation.

$$|\Psi(t)\rangle = \hat{U}(t) |\Psi(0)\rangle$$

Heisenberg picture:

The time-dependent operator is given by the similarity transformation.

$$\hat{A}(t) = \hat{U}^\dagger(t) \hat{A} \hat{U}(t)$$

EXAMPLES:

1. Harmonic oscillator

$$\hat{H} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right)$$

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar}$$

$$\frac{d}{dt} \hat{a}(t) = -\frac{i}{\hbar} [\hat{a}(t), \hat{H}] = -\frac{i}{\hbar} e^{i\hat{H}t/\hbar} [\hat{a}, \hat{H}] e^{-i\hat{H}t/\hbar}$$

$$\frac{d}{dt} \hat{a}^\dagger(t) = -\frac{i}{\hbar} [\hat{a}^\dagger(t), \hat{H}] = -\frac{i}{\hbar} e^{i\hat{H}t/\hbar} [\hat{a}^\dagger, \hat{H}] e^{-i\hat{H}t/\hbar}$$

Since $[\hat{a}, \hat{H}] = \hbar\omega \hat{a}$ and $[\hat{a}^\dagger, \hat{H}] = -\hbar\omega \hat{a}^\dagger$

$$\frac{d}{dt} \hat{a}(t) = -i\omega e^{i\hat{H}t/\hbar} \hat{a} e^{-i\hat{H}t/\hbar} = -i\omega \hat{a}(t) \Rightarrow \hat{a}(t) = e^{-i\omega t} \hat{a}$$

$$\frac{d}{dt} \hat{a}^\dagger(t) = i\omega e^{i\hat{H}t/\hbar} \hat{a}^\dagger e^{-i\hat{H}t/\hbar} = i\omega \hat{a}^\dagger(t) \Rightarrow \hat{a}^\dagger(t) = e^{i\omega t} \hat{a}^\dagger$$

$$\hat{x}(t) = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^\dagger(t) + \hat{a}(t))$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \left(\frac{e^{i\omega t}}{\sqrt{2m\hbar\omega}} (m\omega \hat{x} - i\hat{p}) + \frac{e^{-i\omega t}}{\sqrt{2m\hbar\omega}} (m\omega \hat{x} + i\hat{p}) \right)$$

$$= \left(\frac{e^{i\omega t} + e^{-i\omega t}}{2} \hat{x} + \frac{e^{i\omega t} - e^{-i\omega t}}{2i} \frac{\hat{p}}{m\omega} \right)$$

$$= \hat{x} \cos \omega t + \frac{\hat{p}}{m\omega} \sin \omega t$$

$$\hat{p}(t) = i \sqrt{\frac{m\omega\hbar}{2}} (\hat{a}^\dagger(t) - \hat{a}(t)) = \hat{p} \cos \omega t - m\omega \hat{x} \sin \omega t$$

1-3 Feynman Path Integral

A. PATH INTEGRALS IN QUANTUM MECHANICS

- (1) The propagation of a free particle from (x', t') to (x, t)

$$\begin{aligned}
 \hat{U}(t, t') &= e^{-\frac{i}{\hbar} \int_{t'}^t \hat{H} dt_1} = e^{-i \frac{\hat{H} \cdot (t-t')}{\hbar}} = e^{-i \frac{\hat{p}^2 \cdot (t-t')}{2m\hbar}} \\
 K(x, t; x', t') &= \langle x | \hat{U}(t, t') | x' \rangle \\
 &= \langle x | e^{-i \frac{\hat{p}^2 \cdot (t-t')}{2m\hbar}} | x' \rangle \\
 &= \langle x | e^{-i \frac{\hat{p}^2 \cdot (t-t')}{2m\hbar}} \underbrace{\int |p\rangle \langle p| dp}_{\hat{1}} | x' \rangle \\
 &= \int e^{-i \frac{p^2 \cdot (t-t')}{2m\hbar}} \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \frac{e^{-ipx'/\hbar}}{\sqrt{2\pi\hbar}} dp \\
 &= \frac{1}{2\pi\hbar} \int e^{-\frac{i(t-t')}{2m\hbar} p^2 + \frac{i(x-x')}{\hbar} p} dp
 \end{aligned}$$

Using the Gauss integral

$$\int_{-\infty}^{\infty} e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}} e^{b^2/4a}$$

we obtain

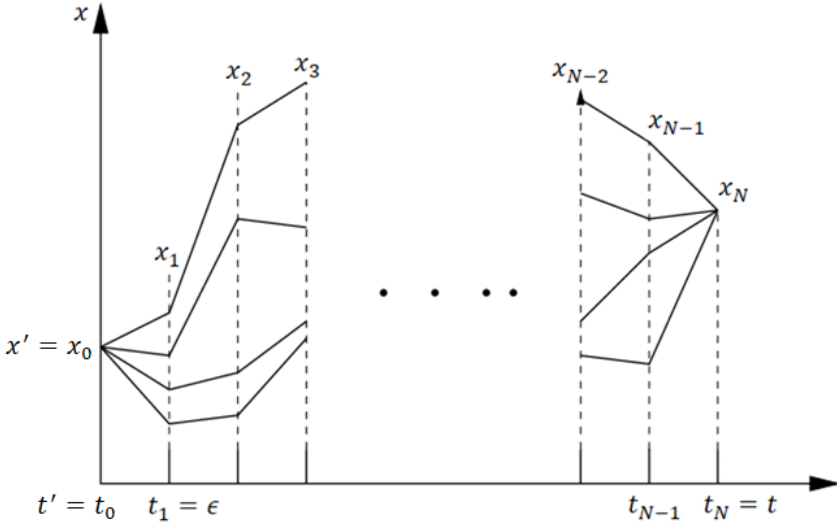
$$\begin{aligned}
 K(x, t; x', t') &= \frac{1}{2\pi\hbar} \sqrt{\frac{\pi}{i(t-t')/2m\hbar}} e^{\left(\frac{i(x-x')}{\hbar}\right)^2 / 4 \left(\frac{i(t-t')}{2m\hbar}\right)} \\
 &= \sqrt{\frac{m}{2\pi i\hbar(t-t')}} e^{\frac{im(x-x')^2}{2\hbar(t-t')}}
 \end{aligned}$$

- (2) Alternatively, the propagator of a single particle can be decomposed by dividing the time interval $t - t'$ into N infinitesimal pieces, i.e.,

$$K(x, t; x', t') = \langle x | \hat{U}(t, t_{N-1}) \hat{U}(t_{N-1}, t_{N-2}) \cdots \hat{U}(t_1, t') | x' \rangle$$

Insert $N - 1$ resolutions of identity

$$\begin{aligned}
K(x, t; x', t') &= \langle x | \hat{U}(t, t_{N-1}) \underbrace{\int |x_{N-1}\rangle \langle x_{N-1}| dx_{N-1}}_{\hat{1}} \hat{U}(t_{N-1}, t_{N-2}) \cdots \\
&\quad \times \hat{U}(t_2, t_1) \underbrace{\int |x_1\rangle \langle x_1| dx_1}_{\hat{1}} \hat{U}(t_1, t') |x'\rangle \\
&= \int dx_{N-1} \cdots dx_1 \langle x | \hat{U}(t, t_{N-1}) |x_{N-1}\rangle \cdots \langle x_1 | \hat{U}(t_1, t') |x'\rangle \\
&= \int dx_{N-1} \cdots dx_1 K(x, t; x_{N-1}, t_{N-1}) \cdots K(x_1, t_1; x', t')
\end{aligned}$$



The propagation from (x', t') to (x, t) can be viewed as the sum of all paths that go through intermediate states on each time slice.

(3) The propagator on each time slice:

Let $t' = t_0$ and $t = t_N$

In the infinitesimal time interval,

$$\frac{t_N - t_0}{N} = \epsilon, \quad t_i - t_{i-1} = \epsilon$$

the Hamiltonian can be considered as time-independent

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

$$\hat{U}(t_i, t_{i-1}) = e^{-\frac{i\hat{H} \cdot (t_i - t_{i-1})}{\hbar}} = e^{-\frac{i\epsilon\hat{H}}{\hbar}}$$

$$\begin{aligned}
K(x_i, t_i; x_{i-1}, t_{i-1}) &= \langle x_i | e^{-\frac{i\epsilon \hat{H}}{\hbar}} | x_{i-1} \rangle \\
&= \langle x_i | \left(1 - \frac{i\epsilon \hat{H}}{\hbar} + O(\epsilon^2) \right) | x_{i-1} \rangle \\
&= \langle x_i | x_{i-1} \rangle - \frac{i\epsilon}{\hbar} \langle x_i | \hat{H} | x_{i-1} \rangle + O(\epsilon^2)
\end{aligned}$$

Here

$$\begin{aligned}
\langle x_i | x_{i-1} \rangle &= \delta(x_i - x_{i-1}) = \int e^{\frac{ip_i(x_i - x_{i-1})}{\hbar}} \frac{dp_i}{2\pi\hbar} \\
-\frac{i\epsilon}{\hbar} \langle x_i | \hat{H} | x_{i-1} \rangle &= -\frac{i\epsilon}{\hbar} \langle x_i | \left(\frac{\hat{p}^2}{2m} + V(\hat{x}) \right) \underbrace{\int |p_i\rangle \langle p_i| dp_i}_{\hat{1}} | x_{i-1} \rangle \\
&= -\frac{i\epsilon}{\hbar} \int \left(\frac{p_i^2}{2m} + V(x_i) \right) \langle x_i | p_i \rangle \langle p_i | x_{i-1} \rangle dp_i \\
&= -\frac{i\epsilon}{\hbar} \int \left(\frac{p_i^2}{2m} + V(x_i) \right) \frac{e^{\frac{ip_i x_i}{\hbar}}}{\sqrt{2\pi\hbar}} \frac{e^{-\frac{ip_i x_{i-1}}{\hbar}}}{\sqrt{2\pi\hbar}} dp_i \\
&= -\frac{i\epsilon}{\hbar} \int \left(\frac{p_i^2}{2m} + V(x_i) \right) e^{\frac{ip_i(x_i - x_{i-1})}{\hbar}} \frac{dp_i}{2\pi\hbar} \\
K(x_i, t_i; x_{i-1}, t_{i-1}) &= \int \left[1 - \frac{i\epsilon}{\hbar} \left(\frac{p_i^2}{2m} + V(x_i) \right) + O(\epsilon^2) \right] e^{\frac{ip_i(x_i - x_{i-1})}{\hbar}} \frac{dp_i}{2\pi\hbar}
\end{aligned}$$

Since $1 - \frac{i\epsilon}{\hbar} \left(\frac{p_i^2}{2m} + V(x_i) \right) + O(\epsilon^2) = e^{-i\epsilon \left(\frac{p_i^2}{2m} + V(x_i) \right) / \hbar}$

we obtain

$$K(x_i, t_i; x_{i-1}, t_{i-1}) = \frac{1}{2\pi\hbar} \int e^{-\frac{i\epsilon}{\hbar} \left(\frac{p_i^2}{2m} + V(x_i) \right)} e^{\frac{ip_i(x_i - x_{i-1})}{\hbar}} dp_i$$

Since $e^{\frac{ip_i(x_i - x_{i-1})}{\hbar}} = e^{\frac{i\epsilon p_i}{\hbar} \frac{(x_i - x_{i-1})}{\epsilon}} = e^{\frac{i\epsilon p_i \dot{x}_i}{\hbar}}$

we obtain

$$\begin{aligned}
K(x_i, t_i; x_{i-1}, t_{i-1}) &= \frac{1}{2\pi\hbar} \int e^{-\frac{i\epsilon}{\hbar} \left(\frac{p_i^2}{2m} + V(x_i) - p_i \dot{x}_i \right)} dp_i \\
&= \frac{1}{2\pi\hbar} \sqrt{\frac{\pi}{i\epsilon/2m\hbar}} e^{\frac{i\epsilon m \dot{x}_i^2}{\hbar}} e^{-\frac{i\epsilon}{\hbar} V(x_i)} \\
&= \sqrt{\frac{m}{2\pi i \hbar \epsilon}} e^{\frac{i}{\hbar} \left(\frac{m \dot{x}_i^2}{2} - V(x_i) \right) \epsilon}
\end{aligned}$$

Let $L(x_i, \dot{x}_i) = \frac{m\dot{x}_i^2}{2} - V(x_i)$ Lagrangian

$$K(x_i, t_i; x_{i-1}, t_{i-1}) = \sqrt{\frac{m}{2\pi i \hbar \epsilon}} e^{\frac{i}{\hbar} L(x_i, \dot{x}_i) \epsilon}$$

(4) The propagator for one "path"

$$K_{\text{path}} = \prod_{i=1}^N K(x_i, t_i; x_{i-1}, t_{i-1}) = \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{N/2} e^{\frac{i}{\hbar} \sum_{i=1}^N L(x_i, \dot{x}_i) \epsilon}$$

In the limit $N \rightarrow \infty, \epsilon \rightarrow 0$, the summation goes over to an integral

$$\sum_{i=1}^N L(x_i, \dot{x}_i) \epsilon \rightarrow \int_{t_0}^t L(x, \dot{x}) dt'$$

$$K_{\text{path}} = \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{N/2} e^{\frac{i}{\hbar} \int_{t_0}^t L(x, \dot{x}) dt'}$$

(5) Summing over all " N -legged" paths

$$K(x, t; x_0, t_0) = \int \prod_{i=1}^{N-1} dx_i K_{\text{path}}$$

$$= \int \prod_{i=1}^{N-1} dx_i \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{N/2} e^{\frac{i}{\hbar} \int_{t_0}^t L(x, \dot{x}) dt'}$$

Let $D[x(t)] = \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{N/2} \prod_{i=1}^{N-1} dx_i$ called measure

Since the action of a single particle system is

$$S[x(t)] = \int_{t_0}^t L(x, \dot{x}) dt'$$

we obtain

$$K(x, t; x_0, t_0) = \int D[x(t)] e^{\frac{i}{\hbar} S[x(t)]}$$

Feynman's conjecture: The propagator is the sum of all paths connecting x_0 and x . Each path is assigned a weight $e^{\frac{i}{\hbar} S[x(t)]}$.

B. PATH INTEGRALS IN STATISTICAL MECHANICS

(1) The partition function of one-particle system is given by

$$Z = \text{Tr } e^{-\beta \hat{H}} = \sum_n \langle n | e^{-\beta \hat{H}} | n \rangle$$

where $|n\rangle$ are bases in the Hilbert space.

Inserting the resolution of identity

$$\begin{aligned} Z &= \sum_n \langle n | \underbrace{\int |x\rangle \langle x| dx}_{\hat{1}} e^{-\beta \hat{H}} | n \rangle \\ &= \int \langle x | e^{-\beta \hat{H}} \underbrace{\sum_n |n\rangle \langle n|}_{\hat{1}} | x \rangle dx \\ &= \int \langle x | e^{-\beta \hat{H}} | x \rangle dx \end{aligned}$$

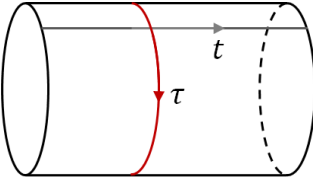
(2) Path integral representation in imaginary time $\tau = it$

$$d\tau = idt \Rightarrow \begin{cases} \frac{dt}{d\tau} = -i \\ \frac{dx}{d\tau} = \frac{dx}{dt} \frac{dt}{d\tau} = -i \frac{dx}{dt} \Rightarrow \left(\frac{dx}{d\tau} \right)^2 = - \left(\frac{dx}{dt} \right)^2 \end{cases}$$

Thus, the imaginary time evolution operator is

$$\hat{U}(t, 0) = e^{-i\hat{H}t/\hbar} \Rightarrow \hat{U}(\tau, 0) = e^{-\hat{H}\tau/\hbar}$$

Since the propagation of a free particle from (x, t) to (x, t) , τ is periodic with period $\beta\hbar$ on the interval $\tau \in (0, \beta\hbar)$ in the imaginary time axis.



Thus, we have

$$\begin{aligned}
i \int_{t_0}^t L(x, \dot{x}) dt' &= i \int_{t_0}^t \left[\frac{m}{2} \left(\frac{\partial x}{\partial t'} \right)^2 - V(x(t')) \right] dt' \\
&= i \int_0^{\beta \hbar} \left[-\frac{m}{2} \left(\frac{\partial x}{\partial \tau'} \right)^2 - V(x(\tau')) \right] (-id\tau') \\
&= - \int_0^{\beta \hbar} \left[\frac{m}{2} \left(\frac{\partial x}{\partial \tau'} \right)^2 + V(x(\tau')) \right] d\tau' \\
D[x(\tau)] &= \left(\frac{m}{2\pi\beta\hbar^2} \right)^{N/2} \prod_{k=1}^{N-1} dx_k \\
\langle x | e^{-\beta \hat{H}} | x \rangle &= \int_{x(0)}^{x(\beta\hbar)} D[x(\tau)] e^{-\frac{1}{\hbar} \int_0^{\beta\hbar} \left[\frac{m}{2} \left(\frac{\partial x}{\partial \tau'} \right)^2 + V(x(\tau')) \right] d\tau'}
\end{aligned}$$

Let the action in the imaginary time as

$$S[x(t)] = \int_0^{\beta \hbar} \left[\frac{m}{2} \left(\frac{\partial x}{\partial \tau'} \right)^2 + V(x(\tau')) \right] d\tau'$$

We can obtain

$$Z = \int \int_{x(0)}^{x(\beta\hbar)} D[x(\tau)] e^{-S[x(t)]/\hbar} dx = \oint_{x(0)}^{x(\beta\hbar)} D[x(\tau)] e^{-S[x(t)]/\hbar}$$

The symbol indicates the periodic boundary condition $x(\beta\hbar) = x(0)$, i.e., the partition function is thus a sum over all closed paths.

(3) The action of a harmonic oscillator in imaginary time

$$\begin{aligned}
V(x) &= \frac{1}{2} m \omega^2 x^2 \\
S[x(t)] &= \int_0^{\beta \hbar} L(x, \dot{x}) d\tau' = \int_0^{\beta \hbar} \left[\frac{m}{2} \left(\frac{\partial x}{\partial \tau'} \right)^2 + \frac{m \omega^2 x^2}{2} \right] d\tau'
\end{aligned}$$

Since all possible paths satisfy the periodic boundary condition $x(\beta\hbar) = x(0)$, thus $x(\tau)$ can be expanded in Fourier series as

$$x(\tau) = a_0 + \sum_{n=1}^{\infty} (a_n \cos v_n \tau + b_n \sin v_n \tau), \quad v_n = \frac{2\pi n}{\beta \hbar}$$

$$\begin{aligned}
& \frac{m}{2} \left(\frac{\partial x}{\partial \tau'} \right)^2 + \frac{m\omega^2 x^2}{2} \\
&= \frac{m}{2} \sum_{n=1}^{\infty} v_n^2 \left[a_n^2 \sin^2 v_n \tau + b_n^2 \cos^2 v_n \tau - 2a_n b_n \sin v_n \tau \cos v_n \tau \right] \\
&\quad + \frac{1}{2} m\omega^2 \left(a_0^2 + \sum_{n=1}^{\infty} a_n^2 \cos^2 v_n \tau + \sum_{n=1}^{\infty} b_n^2 \sin^2 v_n \tau \right. \\
&\quad + 2a_0 \sum_{n=1}^{\infty} a_n \cos v_n \tau + 2a_0 \sum_{n=1}^{\infty} b_n \sin v_n \tau \\
&\quad \left. + 2 \sum_{n=1}^{\infty} a_n b_n \sin v_n \tau \cos v_n \tau \right) \\
S &= \int_0^{\beta \hbar} \left[\frac{m}{2} \left(\frac{\partial x}{\partial \tau'} \right)^2 + \frac{m\omega^2 x^2}{2} \right] d\tau' \\
&= \frac{m}{2} \sum_{n=1}^{\infty} v_n^2 \left(a_n^2 \frac{\beta \hbar}{2} + b_n^2 \frac{\beta \hbar}{2} \right) + \frac{1}{2} m\omega^2 \left[a_0^2 \beta \hbar + \sum_{n=1}^{\infty} \left(a_n^2 \frac{\beta \hbar}{2} + b_n^2 \frac{\beta \hbar}{2} \right) \right] \\
&= \frac{\beta \hbar m}{2} \left[\omega^2 a_0^2 + \frac{1}{2} \sum_{n=1}^{\infty} (v_n^2 + \omega^2) (a_n^2 + b_n^2) \right]
\end{aligned}$$

The partition function is

$$\begin{aligned}
Z &= \oint_{x(0)}^{x(\beta \hbar)} D[x(\tau)] e^{-S[x(t)]/\hbar} \\
&= \oint_{x(0)}^{x(\beta \hbar)} D[x(\tau)] e^{-\frac{\beta m}{2} \left[\omega^2 a_0^2 + \frac{1}{2} \sum_{n=1}^{\infty} (v_n^2 + \omega^2) (a_n^2 + b_n^2) \right]}
\end{aligned}$$

The integration over all possible paths can be done by integrating over the Fourier coefficients a_n and b_n .

$$\begin{aligned}
D[x(\tau)] &= \sqrt{\frac{m}{2\pi\beta\hbar^2}} \prod_{k=1}^{N-1} \left(\frac{m}{2\pi\beta\hbar^2} \right)^{\frac{N-1}{2}} dx_k \\
&= \sqrt{\frac{m}{2\pi\beta\hbar^2}} da_0 \prod_{n=1}^{\infty} J_n da_n db_n
\end{aligned}$$

where J_n is the Jacobian.

The partition function becomes

$$Z = \sqrt{\frac{m}{2\pi\beta\hbar^2}} \oint da_0 \prod_{n=1}^{\infty} J_n da_n db_n e^{-\frac{\beta m}{2} \left[\omega^2 a_0^2 + \frac{1}{2} \sum_{n=1}^{\infty} (v_n^2 + \omega^2)(a_n^2 + b_n^2) \right]}$$

In principle, we need to know the Jacobi determinant of the transformation from the path integral to the integral over the Fourier coefficients. Since this Jacobi determinant is independent of the oscillator frequency ω , we may also compare with the free particle.

First, we put $\omega = 0$ to obtain the partition function of a free particle.

$$Z_{\text{free}} = \sqrt{\frac{m}{2\pi\beta\hbar^2}} \oint da_0 \prod_{n=1}^{\infty} J_n da_n db_n e^{-\frac{\beta m}{4} \left[\sum_{n=1}^{\infty} v_n^2 (a_n^2 + b_n^2) \right]}$$

$$= \sqrt{\frac{m}{2\pi\beta\hbar^2}} \prod_{n=1}^{\infty} J_n \frac{4\pi}{\beta m} \frac{1}{v_n^2}$$

$$\text{Since } Z_{\text{free}} = \sqrt{\frac{m}{2\pi\beta\hbar^2}}$$

this leads the value of J_n to be

$$J_n = \frac{\beta m v_n^2}{4\pi}$$

The partition function of a harmonic oscillator can be rewritten as follows:

$$\begin{aligned} Z &= \sqrt{\frac{m}{2\pi\beta\hbar^2}} \oint da_0 \prod_{n=1}^{\infty} \frac{\beta m v_n^2}{4\pi} da_n db_n e^{-\frac{\beta m}{2} \left[\omega^2 a_0^2 + \frac{1}{2} \sum_{n=1}^{\infty} (v_n^2 + \omega^2)(a_n^2 + b_n^2) \right]} \\ &= \sqrt{\frac{m}{2\pi\beta\hbar^2}} \sqrt{\frac{2\pi}{\beta m \omega^2}} \oint \prod_{n=1}^{\infty} \frac{\beta m v_n^2}{4\pi} da_n db_n e^{-\frac{\beta m}{4} \left[\sum_{n=1}^{\infty} (v_n^2 + \omega^2)(a_n^2 + b_n^2) \right]} \\ &= \frac{1}{\beta\hbar\omega} \prod_{n=1}^{\infty} \frac{\beta m v_n^2}{4\pi} \frac{4\pi}{\beta m} \frac{1}{v_n^2 + \omega^2} \\ &= \frac{1}{\beta\hbar\omega} \prod_{n=1}^{\infty} \frac{v_n^2}{v_n^2 + \omega^2} \\ &= \frac{1}{\beta\hbar\omega} \prod_{n=1}^{\infty} \frac{1}{1 + \frac{(\beta\hbar\omega/2\pi)^2}{n^2}} \end{aligned}$$

Using the infinite product representation of the hyperbolic function

$$\prod_{n=1}^{\infty} \left(1 + \frac{x^2}{n^2}\right) = \frac{\sinh \pi x}{\pi x}$$

we obtain

$$\begin{aligned} Z &= \frac{1}{\beta \hbar \omega} \frac{\pi \times \frac{\beta \hbar \omega}{2\pi}}{\sinh \left(\pi \times \frac{\beta \hbar \omega}{2\pi} \right)} \\ &= \frac{1}{2 \sinh \left(\frac{\beta \hbar \omega}{2} \right)} \\ &= \frac{e^{-\beta \hbar \omega / 2}}{1 - e^{-\beta \hbar \omega}} \\ &= \sum_{n=0}^{\infty} e^{-\beta \left(n + \frac{1}{2} \right) \hbar \omega} \end{aligned}$$