Quantum Mechanics Technology Processing and Conclusions

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Contents

1   Quantization

$$\oint p \, dq = nh + C, \ n = 1, 2, 3, \ldots \tag{1.1}$$

This is not always right, but it's a good approximation.

2   Heisenberg's Breakthrough

Heisenberg use matrices to represent quantum states.[1]

$$x_{n,m}(t) = x_{n,m} e^{i\omega_{n,m} t}. \tag{2.1}$$

With the **Ritz combination law**[2]

$$\omega_{n,m} = \omega_{n,k} + \omega_{k,m}, \tag{2.2}$$

we can calculate x^2 like

$$\left(x^2\right)_{n,m} e^{i\omega_{n,m} t} = \sum_k x_{n,k}(t) x_{k,m}(t) = \sum_k x_{n,k} x_{k,m} e^{i\omega_{n,m} t}. \tag{2.3}$$

Problem 2.1 (Harmonic Oscillator)

By solving this example, we can get how to deal with the problems in quantum situations. The equation of the harmonic oscillator in the classic mechanics is:

$$\ddot{x} + \omega_0^2 x = 0. \tag{2.4}$$

We can deduce that

$$\left(\omega_0^2 - \omega_{n,m}^2\right) x_{n,m}(t) = 0. \tag{2.5}$$

Their's a strange assumption, we may treat[3] $\omega_{n,n+1}$ as ω_0, then only for those $x_{n,n\pm 1}$ can not be zero. Then we can use (1.1) to obtain other information. (Use t as parameter to do the integration.)

Only when $n = m$, the integration of

$$-m\omega_{n,k}\omega_{k,m} x_{n,k} x_{k,m} e^{i\omega_{n,m} t} \tag{2.6}$$

in a period can not be zero.[4] Then we obtain [5]

$$\frac{\hbar}{2m} = \omega_0 \left[\left|x_{n+1,n}\right|^2 - \left|x_{n,n-1}\right|^2\right]. \tag{2.7}$$

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[1]Here use the similar notation $x(t)$ and x, but they represent different things. In some cases, we will ignore (t) but still represent $x(t)$ for convenience.

[2]You can imagine a electron moving from state m to state n passing state k.

[3]Their must exists a $\omega_{n,m} = \omega_0$, or $x_{n,m} = 0$, or the physics phenomenon can not be detected.

[4]$\omega_{n,n} = 0$.

[5]Here I used f-sum rule exactly. But I think there's some details need to check, about where the $\frac{1}{2}$ comes from. It appear as C in quantization condition.

3 De Broglie's & Schrödinger's Equation

De Broglie use

$$\frac{\mathrm{d}\omega}{\mathrm{d}k} = v_g = \frac{pc^2}{E} \tag{3.1}$$

and

$$E^2 = p^2 c^2 + m_0^2 c^4 \tag{3.2}$$

with

$$E = \hbar\omega \tag{3.3}$$

to derive that

$$p = \hbar k. \tag{3.4}$$

It is wave-like. Debye told to Schrödinger that: If it is a wave, then you can try to get a wave equation to describe it.
If we consider a plane wave, the it take the form of

$$\psi \sim \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(px - Et)}. \tag{3.5}$$

The exponent is similar to S: the action. So we can let $\psi = \mathrm{e}^{\mathrm{i}S/\hbar}$, and try to explore what we can get after plugging it into the Hamilton equation.

$$\frac{\hbar^2}{2m}\left(\nabla\psi\right)^2 + \left(E - V(r)\right)\psi^2 = 0. \tag{3.6}$$

We want a linear equation. Then we let ∇ act on it, and suppose $V(r)$ is smooth at the $\hbar$ scale. Then we get

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\psi = E\psi. \tag{3.7}$$

Born gave ψ a physics meaning: The probability density for the particle that appear at position x.

Problem 3.1 (The relation between image of ψ and E)
We know that, the second order derivative can represent the curvature. So with the energy growing, the image of the wave function will twist and cross the average line more and more.

4 Dirac's Notation

4.1 Bra & Ket

P. A. M Dirac divided the word "bracket" into two parts, one is the bra, and the other is the ket. We call left vector as bra, and right vector as ket. We can denote[1] the state ψ as $|\psi\rangle$, with its dual form $\langle\psi|$. Each of these vectors contains

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[1]Clear and simple, its my favorite.

a complete information about the state. We have to clarify the computation law about the bras and kets.

$$a \left| \alpha \right\rangle + b \left| \beta \right\rangle \xleftrightarrow{DC} a^* \left\langle \alpha \right| + b^* \left\langle \beta \right|, \ \forall a, b \in \mathbb{C}. \tag{4.1}$$

Inner product:

$$\left\langle \alpha | \beta \right\rangle := \left\langle \alpha \right| \ \left| \beta \right\rangle \tag{4.2}$$

is a complex number. Here we postulate two fundamental properties of inner products:

$$\left\langle \alpha | \beta \right\rangle = \left\langle \beta | \alpha \right\rangle^* \tag{4.3}$$

and

$$\left\langle \alpha | \alpha \right\rangle \geq 0. \tag{4.4}$$

The property of the second one is because we can take $\left| \beta \right\rangle = \left| \alpha \right\rangle$ in (4.3), then we can obtain $\left\langle \alpha | \alpha \right\rangle$ is a real number.

In fact, all the states forms a vector space V over $\mathbb{C}$.

4.2 Operator

All the operator[1] forms a unitary ring K, it can be a K-module structure acting on V. If X is an operator, then we define an operator (**Hermitian adjoint**) $X^\dagger$ as[2]

$$X \left| \psi \right\rangle \xleftrightarrow{DC} \left\langle \psi \right| X^\dagger. \tag{4.5}$$

Notation 4.1
Since $X \left| \psi \right\rangle$ is also a ket, we denote it as $\left| X\psi \right\rangle$. And its dual form is $\left\langle X\psi \right|$.

We say X is **Hermitian** iff.

$$X^\dagger = X. \tag{4.6}$$

Easy to prove:

$$(XY)^\dagger = Y^\dagger X^\dagger, \tag{4.7}$$

$$(\left| \alpha \right\rangle \left\langle \beta \right|)^\dagger = \left| \beta \right\rangle \left\langle \alpha \right|, \tag{4.8}$$

$$\tag{4.9}$$

We should tell difference between linear operator and anti-linear operator. They have important difference.
For linear operator A,

$$A(\alpha \left| \psi \right\rangle + \beta \left| \phi \right\rangle) = \alpha A \left| \psi \right\rangle + \beta A \left| \phi \right\rangle. \tag{4.10}$$

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[1]Some where will use hat to distinguish the operator, but not always for convenience.

[2]When define the computing law of a Hermitian adjoint operator, we need to ensure any $\left\langle \psi | \phi \right\rangle = \left\langle \phi | \psi \right\rangle^*$. And if T is an anti-linear operator, we DO NOT define $T^\dagger$. And we'd better understand a expression with right combination.

$$\langle\beta|\,A\,|\alpha\rangle = \langle\alpha|\,A^\dagger\,|\beta\rangle^* . \tag{4.11}$$

But for anti-linear operator T,

$$T(\alpha\,|\psi\rangle + \beta\,|\phi\rangle) = \alpha^*T\,|\psi\rangle + \beta^*T\,|\phi\rangle . \tag{4.12}$$

If we still want to define $T^\dagger$, we should satisfies the conditions in the footnote. Compare the form of the linear case, and let all the operator act on kets but not bras.

$$\langle\beta|T\alpha\rangle = \langle\alpha|T^\dagger\beta\rangle . \tag{4.13}$$

Then $|\alpha\rangle$ and $|\beta\rangle$ still anti-linear in this expression.

Theorem 4.1

The eigenvalues of a Hermitian operator A are real; the eigenkets of A corresponding to different eigenvalues are orthogonal.

Proof. We have

$$A\,|a_1\rangle = a_1\,|a_1\rangle , \quad \langle a_2|\,A = a_2^*\,\langle a_2| . \tag{4.14}$$

Hence,

$$(a_1 - a_2^*)\,\langle a_2|a_1\rangle = 0. \tag{4.15}$$

Let $a_2 = a_1$, then we obtain

$$a_1 = a_2^*. \tag{4.16}$$

So a_1 is real. If $a_1 \neq a_2$, then

$$\langle a_2|a_1\rangle = 0. \tag{4.17}$$

i.e. the eigenkets are orthogonal. $\qquad\qquad\square$

All the observables must be real, so its operator must be Hermitian.[1]
If $\{|a\rangle\}$ is complete, then

$$\sum_a |a\rangle\,\langle a| = 1. \tag{4.18}$$

Let it act on a state, then we can get the state represent as the bases of $\{|a\rangle\}$. And for a particular a, we can define the **projection operator** as

$$\Lambda_a = |a\rangle\,\langle a| . \tag{4.19}$$

If we use (4.18) to act on both left and right of an operator X, then we can make it represent in the matrix form.

We write an observable X as

$$X = \sum_{a,b} |a\rangle\,\langle a|\,X\,|b\rangle\,\langle b| . \tag{4.20}$$

Since $\langle a|\,X\,|b\rangle$ is real,

$$X^\dagger = \sum_{a,b} |b\rangle\,\langle b|\,X\,|a\rangle\,\langle a| = X. \tag{4.21}$$

So X is Hermitian.

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[1] We will explain it soon.

5   Commutator and Anticommutator

For any two operators A and B, we define their **commutator** as

$$[A, B] = AB - BA. \tag{5.1}$$

And the **anticommutator** is

$$\{A, B\} = AB + BA. \tag{5.2}$$

Its easy to check

$$[AB, C] = A[B, C] + [A, C]B, \tag{5.3}$$

$$[A, BC] = [A, B]C + B[A, C], \tag{5.4}$$

$$[A, [B, C]] + [B, [A, C]] + [C, [A, B]] = 0, \tag{5.5}$$

$$[A, B]^\dagger = [B^\dagger, A^\dagger]. \tag{5.6}$$

$$\{AB, C\} = A\{B, C\} - [A, C]B, \tag{5.7}$$

$$\{A, BC\} = \{A, B\}C - B[A, C]. \tag{5.8}$$

Suppose $f(A), g(B)$ are differentiable functions of A and B, let

$$f(A) = \sum_{n=0}^{\infty} a_n A^n, \tag{5.9}$$

we have

$$[A^n, B] = \sum_{k=0}^{n-1} A^{n-k-1}[A, B]A^k. \tag{5.10}$$

If $[A, B]$ is commutable with A, then,

$$[f(A), B] = f'(A)[A, B]. \tag{5.11}$$

Similarly, if $[A, B]$ is commutable with B, then,

$$[A, g(B)] = g'(B)[A, B]. \tag{5.12}$$

6   Compatible Observables

Observables A and B are defined to be **compatible** when the corresponding operators commute,

$$[A, B] = 0. \tag{6.1}$$

Theorem 6.1
Suppose that A and B are compatible observables, and the eigen-values of A are nondegenerate. Then the matrix elements $\langle a''| B |a' \rangle$ are all diagonal.

7   Uncertainty Relation

Define ΔA as

$$\Delta A := A - \langle A \rangle \,, \tag{7.1}$$

where $\langle A \rangle$ is expectation value of A. And the **dispersion** of A is

$$\left\langle (\Delta A)^2 \right\rangle = \left\langle \left(A^2 - 2A \langle A \rangle + \langle A \rangle^2 \right) \right\rangle = \left\langle A^2 \right\rangle - \langle A \rangle^2 \,. \tag{7.2}$$

Theorem 7.1
For any state, we must have the following inequality:

$$\left\langle (\Delta A)^2 \right\rangle \left\langle (\Delta B)^2 \right\rangle \geq \frac{1}{4} \left| \langle [A, B] \rangle \right|^2 \,. \tag{7.3}$$

Proof. The Schwarz inequality[1]:

$$\langle \alpha | \alpha \rangle \langle \beta | \beta \rangle \geq |\langle \alpha | \beta \rangle|^2 \,. \tag{7.4}$$

Take[2]

$$|\alpha\rangle = \Delta A \, |\rangle \,, \quad |\beta\rangle = \Delta B \, |\rangle \,,$$

then,

$$\left\langle (\Delta A)^2 \right\rangle \left\langle (\Delta B)^2 \right\rangle \geq |\langle \Delta A \Delta B \rangle|^2 \,. \tag{7.5}$$

Here we use a trick: Any operator can be divided into Hermitian part and anti-Hermitian part,

$$\Delta A \Delta B = \frac{1}{2} [\Delta A, \Delta B] + \frac{1}{2} \{\Delta A, \Delta B\} \,. \tag{7.6}$$

Easy to prove that the expect value of Hermitian operator is real, and the anti-Hermitian's is purely imaginary. Thus,

$$|\langle \Delta A \Delta B \rangle|^2 = \frac{1}{4} \left| \langle [\Delta A, \Delta B] \rangle \right|^2 + \frac{1}{4} \left| \langle \{\Delta A, \Delta B\} \rangle \right|^2 \,. \tag{7.7}$$

One have $[\Delta A, \Delta B] = [A, B]$ and $|\ldots|^2 \geq 0$, then we get the result. $\qquad\square$

8   Position and Momentum

I will follow J. J. Sakurai's steps to derive some famous results. As continuous spectra, they have following changes [3]:

$$\langle a' | a'' \rangle = \delta_{a', a''} \longrightarrow \langle \xi' | \xi'' \rangle = \delta \left(\xi' - \xi'' \right) \,. \tag{8.1}$$

Where $\delta \left(\xi' - \xi'' \right)$ is the Dirac delta function.

$$\sum_a |a\rangle \langle a| = 1 \longrightarrow \int \mathrm{d}\xi \, |\xi\rangle \langle \xi| = 1 \,. \tag{8.2}$$

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[1]Consider $|\alpha\rangle + \lambda |\beta\rangle$ and take $\lambda = - \langle \beta | \alpha \rangle \langle \beta | \beta \rangle$.
[2]Blank ket $|\rangle$ emphasizes the fact that our consideration may be applied to any ket.
[3]We use ξ to represent a continuous variable.

8.1   Position & Wave Function

For position, we can measure its position, which means we can get its components at the same time, they are compatible. So

$$[\hat{x}_i, \hat{x}_j] = 0. \tag{8.3}$$

$$|\mathbf{x}\rangle = |x, y, z\rangle. \tag{8.4}$$

$$\hat{x}|\mathbf{x}\rangle = x|\mathbf{x}\rangle, \ \hat{y}|\mathbf{x}\rangle = y|\mathbf{x}\rangle, \ \hat{z}|\mathbf{x}\rangle = z|\mathbf{x}\rangle. \tag{8.5}$$

We call

$$\psi_\alpha(x) = \langle x|\alpha\rangle \tag{8.6}$$

the wave function.

8.2   Translation

Consider an operator $\mathscr{J}(\mathrm{d}\mathbf{x})$ satisfying

$$\mathscr{J}(\mathrm{d}\mathbf{x})|\mathbf{x}\rangle = |\mathbf{x}\rangle. \tag{8.7}$$

Then

$$\mathscr{J}^\dagger(\mathrm{d}\mathbf{x})\mathscr{J}(\mathrm{d}\mathbf{x}) = 1 \tag{8.8}$$

needs to be guaranteed. We expect the translation does not depend on the trace, which means

$$\mathscr{J}(\mathrm{d}\mathbf{x}_1 + \mathrm{d}\mathbf{x}_2) = \mathscr{J}(\mathrm{d}\mathbf{x}_1) + \mathscr{J}(\mathrm{d}\mathbf{x}_2). \tag{8.9}$$

For the third property,suppose we consider a translation in the opposite direction; we expect the opposite-direction translation to be the same as the inverse of the original translation:

$$\mathscr{J}(-\mathrm{d}\mathbf{x}) = \mathscr{J}^{-1}(\mathrm{d}\mathbf{x}). \tag{8.10}$$

For the fourth property,

$$\lim_{\mathrm{d}\mathbf{x}\to 0} \mathscr{J}(\mathrm{d}\mathbf{x}) = 1. \tag{8.11}$$

Consider

$$\mathscr{J}(\mathrm{d}\mathbf{x}) = 1 - i\hat{\mathbf{K}} \cdot \mathrm{d}\mathbf{x}, \tag{8.12}$$

it let all the properties we want hold, if $\hat{\mathbf{K}}$ is Hermitian. We can check that

$$[\hat{\mathbf{x}}, \mathscr{J}(\mathrm{d}\mathbf{x})] = \mathrm{d}\mathbf{x}. \tag{8.13}$$

Plug in (8.12), we obtain

$$[\hat{x}_i, \hat{K}_j] = i\delta_{ij}. \tag{8.14}$$

8.3 Momentum

An infinitesimal translation in classical mechanics can be regarded as a canonical transformation,

$$\mathbf{x}_{\text{new}} = \mathbf{x} + \mathrm{d}\mathbf{x}, \ \ \mathbf{p}_{\text{new}} = \mathbf{p}. \tag{8.15}$$

obtainable from the generating function

$$F(\mathbf{x}, \mathbf{p}) = \mathbf{x} \cdot \mathbf{p}_{\text{new}} + \mathbf{p} \cdot \mathrm{d}\mathbf{x}. \tag{8.16}$$

This equation has a striking similarity to the infinitesimal translation operator. Let

$$\mathscr{J}(\mathrm{d}\mathbf{x}) = 1 - \mathrm{i}\hat{\mathbf{p}} \cdot \mathrm{d}\mathbf{x}/\hbar. \tag{8.17}$$

The commutation relation (8.14) now becomes

$$[\hat{x}_i, \hat{p}_j] = \mathrm{i}\hbar\delta_{i,j}. \tag{8.18}$$

By (7.3), we obtain the **position-momentum uncertainty relation**:

$$\left\langle (\Delta x)^2 \right\rangle \left\langle (\Delta p)^2 \right\rangle \geq \frac{\hbar^2}{4} \tag{8.19}$$

As for finite position,

$$\mathscr{J}(\Delta\mathbf{x}) = \lim_{N \to \infty} \left(1 - \frac{\mathrm{i}\hat{\mathbf{p}} \cdot \Delta\mathbf{x}}{N\hbar} \right)^N = \exp\left(-\frac{\mathrm{i}\hat{\mathbf{p}} \cdot \Delta\mathbf{x}}{\hbar} \right). \tag{8.20}$$

By computation,

$$[\hat{p}_i, \hat{p}_j] = 0. \tag{8.21}$$

8.4 Momentum Operator in the Position Basis

By computing $\mathscr{J}(\mathrm{d}\mathbf{x})|\alpha\rangle$ in the representation where the position eigenkets are used as base kets, and plug in (8.17), we obtain

$$\hat{\mathbf{p}}|\alpha\rangle = \int \mathrm{d}\mathbf{x} \, |\mathbf{x}\rangle \left(-\mathrm{i}\hbar\nabla \langle\mathbf{x}|\alpha\rangle \right). \tag{8.22}$$

That is also

$$\langle\mathbf{x}|\hat{\mathbf{p}}|\alpha\rangle = -\mathrm{i}\hbar\nabla \langle\mathbf{x}|\alpha\rangle. \tag{8.23}$$

8.5 Momentum-Space Wave Function

The notation $\phi_\alpha(p)$ is often used

$$\langle p|\alpha\rangle = \phi_\alpha(p). \tag{8.24}$$

To transform the bases from position to momentum, we need to calculate $\langle x|p\rangle$. One have

$$\langle x|\hat{p}|p\rangle = p \langle x|p\rangle. \tag{8.25}$$

By (8.23),

$$\langle x | \hat{p} | p \rangle = -i\hbar \frac{\partial}{\partial x} \langle x | p \rangle. \tag{8.26}$$

Thus,

$$\langle x | p \rangle = A \exp\left(\frac{ipx}{\hbar}\right). \tag{8.27}$$

Do the derivation will lose a constant, but integration won't.[1]

$$\delta(x - x') = \int dp \, \langle x | p \rangle \langle p | x' \rangle = 2\pi\hbar A A^* \delta(x - x'). \tag{8.28}$$

For convenience, we take A as a real number, then

$$\langle x | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{ipx}{\hbar}\right). \tag{8.29}$$

For three dimension case,

$$\langle \mathbf{x} | \mathbf{p} \rangle = \left[\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\right] \exp\left(\frac{i\mathbf{p} \cdot \mathbf{x}}{\hbar}\right). \tag{8.30}$$

8.6 Dirac's Corresponding Rule

Replace classical Poission bracket by commutator as follows[2]

$$[\quad,\quad]_{\text{classical}} \longrightarrow \frac{[\quad,\quad]}{i\hbar}. \tag{8.31}$$

9 Schrödinger Equation

Let $\mathscr{U}$ be the time-evolution operator, which means

$$|\psi(t)\rangle = \mathscr{U}(t, t_0) |\psi(t_0)\rangle. \tag{9.1}$$

We want it to satisfy the following conditions:
(1) $\mathscr{U}$ should be linear:

$$\mathscr{U}(t, t_0)\left[c_1 |\psi_1(t_0)\rangle + c_2 |\psi_2(t_0)\rangle\right] = c_1 \mathscr{U}(t, t_0) |\psi_1(t_0)\rangle + c_2 \mathscr{U}(t, t_0) |\psi_2(t_0)\rangle. \tag{9.2}$$

(2) $\mathscr{U}$ should be unitary (to make a state always normalized):

$$\mathscr{U}^\dagger \mathscr{U} = \mathscr{U}\mathscr{U}^\dagger = 1. \tag{9.3}$$

(3) Composition property:

$$\mathscr{U}(t_2, t_1)\mathscr{U}(t_1, t_0) = \mathscr{U}(t_2, t_0). \tag{9.4}$$

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[1]Is it an easy integration?
[2]I think the $i\hbar$ comes from the translation where setting a constant as $i\hbar$.

(4) Continuous and identity:

$$\lim_{\mathrm{d}t \to 0} \mathscr{U}(t_0 + \mathrm{d}t, t_0) = 1. \tag{9.5}$$

Similar to the previous section, we can use a Hermitian operator to construct this operator. And by the classical corresponding rule, we have

$$\mathscr{U}(t_0 + \mathrm{d}t, t_0) = 1 - \frac{\mathrm{i}H\,\mathrm{d}t}{\hbar}. \tag{9.6}$$

Then,

$$\mathscr{U}(t + \mathrm{d}t, t_0) = \mathscr{U}(t + \mathrm{d}t, t)\mathscr{U}(t, t_0) = \left(1 - \frac{\mathrm{i}H\,\mathrm{d}t}{\hbar}\right)\mathscr{U}(t, t_0). \tag{9.7}$$

That is

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\mathscr{U}(t, t_0) = H\mathscr{U}(t, t_0). \tag{9.8}$$

This is the **Schrödinger equation for the time-evolution operator**. Apply this operator to a state $|\alpha, t_0; t\rangle$, we obtain

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\alpha, t_0; t\rangle = H|\alpha, t_0; t\rangle. \tag{9.9}$$

In integration form,

$$\mathscr{U}(t, t_0) = 1 - \frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t_1\,H(t_1)\mathscr{U}(t_1, t_0). \tag{9.10}$$

Then we can induction on n that

$$\mathscr{U}(t, t_0) = \sum_{n=0}^{\infty}\left(\frac{-\mathrm{i}}{\hbar}\right)^n\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\cdots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n\,H(t_1)H(t_2)\ldots H(t_n). \tag{9.11}$$

Now we want to simplify this expression. The bad thing is H at different time may not commute. So we define a time-ordering operator $\mathcal{T}$:

$$\mathcal{T}[A(t_1)B(t_2)] = \begin{cases} B(t_2)A(t_1), & \text{if } t_1 < t_2 \\ A(t_1)B(t_2), & \text{if } t_1 \geq t_2 \end{cases}. \tag{9.12}$$

If we consider the integration is dealing on $[t_0, t]^n$, then it can be divided into $n!$ part, each part has an order of a permutation of $(t_1, \ldots, t_n)$, but it should in order of $(t_1, \ldots, t_n)$. Thus,

$$\begin{aligned}
&\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\cdots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n\,H(t_1)H(t_2)\ldots H(t_n) \\
&= \frac{1}{n!}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t\cdots\int_{t_0}^{t}\mathrm{d}t_n\,\mathcal{T}\left[H(t_1)H(t_2)\ldots H(t_n)\right] \\
&= \frac{1}{n!}\mathcal{T}\left[\left(\int_{t_0}^{t}\mathrm{d}t'\,H(t')\right)^n\right].
\end{aligned} \tag{9.13}$$

Therefore,

$$\mathscr{U}(t, t_0) = \mathcal{T} \exp\left[-\frac{i}{\hbar} \int_{t_0}^{t} dt'\, H(t')\right]. \tag{9.14}$$

In particular, if $H(t)$ is commutable at any different time, then

$$\mathscr{U}(t, t_0) = \exp\left[-\frac{i}{\hbar} \int_{t_0}^{t} dt'\, H(t')\right]. \tag{9.15}$$

Moreover, if H is time-independent, then

$$\mathscr{U}(t, t_0) = \exp\left[-\frac{i}{\hbar} H(t - t_0)\right]. \tag{9.16}$$

10   Probability Density and Probability Current

Let ψ be the wave function, then the probability density is

$$\rho := \psi\psi^*. \tag{10.1}$$

The probability need to be conserved,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0. \tag{10.2}$$

Then we can deduce from Schrödinger equation that

$$\mathbf{j} = \left(\frac{\hbar}{m}\right) \mathrm{Im}(\psi^* \nabla \psi). \tag{10.3}$$

If we write ψ into the form of

$$\psi = \sqrt{\rho}\, e^{\frac{iS}{\hbar}}, \tag{10.4}$$

then[1]

$$\mathbf{j} = \frac{\rho \nabla S}{m}. \tag{10.5}$$

Taking the classical limit, we can see that S is the action.

$$\int \mathbf{j}\, d\mathbf{x} = \frac{\langle \mathbf{p} \rangle}{m}. \tag{10.6}$$

It is some thing like velocity.

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[1] Here is the case with charge.

11 Exponential Operators and Baker-Hausdorff Lemma

If it exists, then we denote[1]

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!}.$$ (11.1)

Easy to check that if $[A, B] = 0$, then

$$\exp(A)\exp(B) = \exp(A + B).$$ (11.2)

Define[2]

$$O(\lambda) = e^{i\lambda G} A e^{-i\lambda G},$$ (11.3)

where A and G are operators, and λ is a complex parameter. Then,

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} O(\lambda) = i e^{i\lambda G} [G, A] e^{-i\lambda G} = i[G, O(\lambda)].$$ (11.4)

Hence,

$$O(\lambda) = O(0) + i \int_0^\lambda \mathrm{d}\lambda_1 \, [G, O(\lambda_1)].$$ (11.5)

We have $O(0) = A$. And we replace $O(\lambda_1)$ similarly, also for $\lambda_2, \lambda_3, \ldots$, then we obtain,

$$O(\lambda) = A + i \int_0^\lambda \mathrm{d}\lambda_1 \, [G, A] + i^2 \int_0^\lambda \mathrm{d}\lambda_1 \int_0^{\lambda_1} \mathrm{d}\lambda_2 \, [G, [G, A]] + \ldots$$ (11.6)

Easy to check

$$\int_0^\lambda \mathrm{d}\lambda_1 \int_0^{\lambda_1} \mathrm{d}\lambda_2 \cdots \int_0^{\lambda_{n-1}} \mathrm{d}\lambda_n = \frac{\lambda^n}{n!}.$$ (11.7)

Therefore[3],

$$\boxed{e^{i\lambda G} A e^{-i\lambda G} = \sum_{n=0}^{\infty} \frac{(i\lambda)^n}{n!} C_G^{(n)}(A)},$$ (11.8)

where[4],

$$C_G(A) = [G, A], \; C_G^{(n)}(A) = [G, C_G^{(n-1)}(A)].$$ (11.9)

Or we can write in the form

$$e^{\Omega} A e^{-\Omega} = e^{\mathrm{Ad}_\Omega}(A).$$ (11.10)

---

[1]Sometimes we denote as $\exp(A)$.

[2]We write extra i because we often use the Hermitian conjugate, and i will give a negative sign to fit the form if G is Hermitian.

[3]It is easy to take the wrong signature, remember it is something like derivative and note the first term, like $[G, A]$, then it won't be wrong.

[4]This notation is not formal, but the following notation "Ad" (get from Deepseek) may be better to use in articles.

Let us consider a special case: $[A, B]$ is commutable with A and B. By Baker-Hausdorff lemma, we have

$$e^A e^B e^{-A} = e^B + [A, e^B] + \dots. \tag{11.11}$$

By (5.4), we can induct on n that

$$[A, [A, B]^{n-1} e^B] = [A, B]^n e^B. \tag{11.12}$$

So,

$$e^A e^B = e^B e^A e^{[A,B]}. \tag{11.13}$$

We also have another more symmetrical form[1]:

Theorem 11.1

$$[A, [A, B]] = [B, [A, B]] = 0 \Rightarrow e^A e^B = e^{A+B} e^{\frac{1}{2}[A,B]}. \tag{11.14}$$

Proof. Let

$$O(\lambda) = e^{\lambda A} e^{\lambda B}, \tag{11.15}$$

then,

$$\frac{\mathrm{d}O}{\mathrm{d}\lambda} = e^{\lambda A} (A + B) e^{\lambda B}. \tag{11.16}$$

We want to get a differential equation of $O(\lambda)$, so we have to take $(A + B)$ to the left of $\exp(\lambda A)$[2].

$$e^{\lambda A} B e^{\lambda B} = e^{\lambda A} B e^{-\lambda A} e^{\lambda A} e^{\lambda B}. \tag{11.17}$$

By Baker-Hausdorff lemma, we obtain

$$\frac{\mathrm{d}O}{\mathrm{d}\lambda} = [(A + B) + \lambda[A, B]] O. \tag{11.18}$$

The solution is

$$O = \exp\left[\lambda(A + B) + \frac{1}{2}\lambda^2[A, B]\right]. \tag{11.19}$$

$\square$

12   Harmonic Oscillator

We discuss the 1D case first. We have the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2. \tag{12.1}$$

---

[1]In fact we do not need any condition, then we can derive a general form, but that is a bit complex and unnecessary.

[2]Trick: If there is not we want, then create one, like $+1 - 1$, here we times 1.

12.1   Method of Analysis (Hermite polynomials)

We solve the wave function in position representation, then we obtain many information. Let $z = \frac{x}{\sqrt{\frac{\hbar}{m\omega}}}$, then

$$\left[-\frac{1}{2}\frac{d^2}{dz^2} + \frac{1}{2}z^2 \right] \psi(z) = \frac{E}{\hbar\omega}\psi(z). \tag{12.2}$$

A must to satisfy is

$$\lim_{z\to\infty} \psi(z) = 0. \tag{12.3}$$

So we first analyze the behavior of $\psi(z)$ at $z \to \pm\infty$. For $\psi'' = z^2\psi$, we try the solution[1] $\psi(z) = e^{S}(z)$

$$\psi' = S'\psi, \ \psi'' = \left(S'' + S'^2 \right)\psi. \tag{12.4}$$

Comparison of two expression yields

$$S'' + S'^2 = z^2. \tag{12.5}$$

The leading order leads to $s' = \pm z$, $s = \pm\frac{1}{2}z^2$. So we can try the solution

$$\psi(z) = e^{-\frac{z^2}{2}}u(z). \tag{12.6}$$

$$\frac{d^2}{dz^2}u(z) - 2z\frac{d}{dz}u(z) - (\lambda - 1)u(z) = 0. \tag{12.7}$$

We consider the series solution, let

$$u(z) = \sum_{k=0}^{+\infty} a_k z^k. \tag{12.8}$$

The we can deduce that

$$\frac{a_{k+2}}{a_k} = \frac{2k + 1 - \lambda}{(k+1)(k+2)}. \tag{12.9}$$

We have $u(\pm\infty) = 1$, so there must exists an $N \in \mathbb{N}$, for any $k > N$,

$$a_k = 0. \tag{12.10}$$

Therefore,

$$\lambda_n = 2n + 1, \ n = 0, 1, 2, \ldots \tag{12.11}$$

which means

$$E_n = \left(n + \frac{1}{2} \right)\hbar\omega. \tag{12.12}$$

---

[1]This may keep the form.

The solution of (12.7) is Hermite polynomials[1] $H_n(z)$.

$$\psi(x) = \mathrm{e}^{-\frac{1}{2}\frac{m\omega x^2}{\hbar}} \sum_{n=0}^{+\infty} \frac{c_n}{n!} H_n\left(x/\sqrt{\frac{\hbar}{m\omega}}\right). \tag{12.13}$$

And for a fixed n, the normalized wavefunction is

$$\psi_n(z) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}} \mathrm{e}^{-\frac{z^2}{2}} H_n(z). \tag{12.14}$$

12.2   Method of Algebra

In usual computing law,

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \frac{1}{2}m\omega^2\left(x - \frac{\mathrm{i}p}{m\omega}\right)\left(x + \frac{\mathrm{i}p}{m\omega}\right). \tag{12.15}$$

Let [2]

$$\hat{a}^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{\mathrm{i}\hat{p}}{m\omega}\right), \ \ \hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{\mathrm{i}\hat{p}}{m\omega}\right). \tag{12.16}$$

Then,

$$[\hat{a}, \hat{a}^{\dagger}] = 1. \tag{12.17}$$

Let

$$\hat{N} = \hat{a}^{\dagger}\hat{a}, \tag{12.18}$$

then,

$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right). \tag{12.19}$$

So $\hat{N}$ is compatible with $\hat{H}$. We denote an energy eigenket of $\hat{N}$ by its eigenvalue[3] n, so

$$\hat{N}\,|n\rangle = n\,|n\rangle, \tag{12.20}$$

$$\hat{H}\,|n\rangle = \left(n + \frac{1}{2}\right)\hbar\omega\,|n\rangle. \tag{12.21}$$

To appreciate the physical significance of $\hat{a}, \hat{a}^{\dagger}$, and $\hat{N}$, let us first note that

$$[\hat{N}, \hat{a}] = -\hat{a}, \ \ [\hat{N}, \hat{a}^{\dagger}] = \hat{a}^{\dagger}. \tag{12.22}$$

As a result, we have

$$\hat{N}\hat{a}^{\dagger}\,|n\rangle = [\hat{N}, \hat{a}^{\dagger}]\,|n\rangle + \hat{a}^{\dagger}\hat{N}\,|n\rangle = (n+1)\,\hat{a}^{\dagger}\,|n\rangle, \tag{12.23}$$

$$\hat{N}\hat{a}\,|n\rangle = [\hat{N}, \hat{a}]\,|n\rangle + \hat{a}\hat{N}\,|n\rangle = (n-1)\,\hat{a}\,|n\rangle. \tag{12.24}$$

---

[1]There's some properties about Hermite polynomial.

[2]If we denote $l = \sqrt{\frac{\hbar}{m\omega}}$, then it will be $a = \frac{1}{\sqrt{2}}\left(\frac{x}{l} + \mathrm{i}\frac{pl}{\hbar}\right)$. $\frac{1}{\sqrt{2}}$ seems like to normalize.

[3]We will later show that n must be a nonnegative integer.

We write

$$\hat{a}\left|n\right\rangle = c\left|n-1\right\rangle, \tag{12.25}$$

then,

$$\left\langle n\right|\hat{N}\left|n\right\rangle = \left\langle n\right|\hat{a}^{\dagger}\hat{a}\left|n\right\rangle = \left|c\right|^{2}. \tag{12.26}$$

Thus,

$$\hat{a}\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle. \tag{12.27}$$

Similarly, it is easy to show that[1]

$$\hat{a}^{\dagger}\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle. \tag{12.28}$$

From (12.26) we know that $n \geq 0$. If we act $\hat{a}$ on a state for many times, we can conclude that the sequence must terminate with $n = 0$, or it won't stop and n will become not real. Use

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}+\hat{a}^{\dagger}\right),\ \hat{p} = \mathrm{i}\sqrt{\frac{m\hbar\omega}{2}}\left(-\hat{a}+\hat{a}^{\dagger}\right), \tag{12.29}$$

we can get more information. To solve the wave function, we can deduce $\left\langle x\right|\hat{a}\left|0\right\rangle = 0$, which leads to a differential equation for the wave function.

12.3 Further Discussion of 1D Case: Coherent State

We have seen that an energy eigenstate does not behave like the classical oscillator—in the sense of oscillating expectation values for x and p—no matter how large n may be. We may logically ask, How can we construct a superposition of energy eigenstates that most closely imitates the classical oscillator? In wave-function language, we want a wave packet that bounces back and forth without spreading in shape. It turns out that a coherent state defined by the eigenvalue equation for the non-Hermitian annihilation operator a,

$$a\left|\lambda\right\rangle = \lambda\left|\lambda\right\rangle,$$

with, in general, a complex eigenvalue λ does the desired job.

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We want it to be related to the states we have known. And the simplest one is $\left|0\right\rangle$. Let $\left|\lambda\right\rangle = A\left|0\right\rangle$. Then what we expect is $aA\left|0\right\rangle = \lambda A\left|0\right\rangle$. Or in another form:

$$(A^{-1}aA - \lambda)\left|0\right\rangle = f(a)\left|0\right\rangle,$$

where f is a arbitrary function. We want to make it easy, let us set $f(a) = a$. Then by the Baker-Hausdorff lemma, the following let what we want holds

$$A = \mathrm{e}^{\lambda a^{\dagger}}. \tag{12.30}$$

---

[1]Memory trick: the square root of a lager one.

use (11.13) to do the normalization[1],

$$\langle 0|e^{\lambda^* a}e^{\lambda a^\dagger}|0\rangle = e^{|\lambda|^2}. \tag{12.31}$$

Therefore[2],

$$|\lambda\rangle = e^{-|\lambda|^2/2}e^{\lambda a^\dagger}|0\rangle = e^{-|\lambda|^2/2}\sum_{n=0}^{\infty}\frac{\lambda^n}{\sqrt{n!}}|n\rangle. \tag{12.32}$$

We have discussed in 8.3 that the operator $e^{-ipl/\hbar}$ is a displacement operator. Let us show we can obtain a coherent state by applying it on $|0\rangle$.

$$e^{-ip\Delta x/\hbar}|0\rangle = e^{\frac{(a^\dagger - a)\Delta x}{\sqrt{2}l}}|0\rangle \sim e^{\frac{a^\dagger \Delta x}{\sqrt{2}l}}|0\rangle. \tag{12.33}$$

12.4   High Dimensional Case

We use the Einstein summation convention. Hamilton in n-dimensional case can be written as

$$H = \frac{p^i p_i}{2m} + \frac{1}{2}m\omega^2 x^i x_i. \tag{12.34}$$

And the creation and annihilation operators are

$$a_i = \frac{1}{\sqrt{2}}\left(\frac{x_i}{l} + \frac{ip_i l}{\hbar}\right), \quad a_i^\dagger = \frac{1}{\sqrt{2}}\left(\frac{x_i}{l} - \frac{ip_i l}{\hbar}\right). \tag{12.35}$$

$$[a_i, a_j] = 0, \quad [a_i, a_j^\dagger] = \delta_{ij}. \tag{12.36}$$

If we denote $a^i a_i^\dagger$ as N, then we can written H as

$$H = \hbar\omega(N + \frac{n}{2}). \tag{12.37}$$

Or H_i^i [3]if we denote $H_i = \hbar\omega(a_i^\dagger a_i + \frac{1}{2})$.

It's easy to check that

$$[a_i^\dagger a_j, H] = 0. \tag{12.38}$$

That means the angular momentum is conserved.

13   Gauge Transformations in Electromagnetism

13.1   Gauge Transformations

In Classic mechanics, the Hamiltonian is

$$H = \frac{1}{2m}\left(\mathbf{p} - \frac{q\mathbf{A}}{c}\right)^2 + q\phi. \tag{13.1}$$

---

[1]Expand the series we get $\exp(\lambda a)|0\rangle = |0\rangle$.
[2]A Poission distribution.
[3]It's my own notation means $\sum_i H_i$.

Where $\mathbf{p}$ is the canonical momentum, $\mathbf{A}$ is the vector potential, q is the charge and ϕ is the scalar potential. And now the canonical momentum $\mathbf{p}$ is the e generator of translation. And kinematical (or mechanical) momentum, denoted by:

$$\mathbf{\Pi} := \mathbf{p} - \frac{q\mathbf{A}}{c}. \tag{13.2}$$

Easy to check that

$$[\Pi_i, \Pi_j] = \frac{i\hbar q}{c}\varepsilon_{ijk}B_k. \tag{13.3}$$

The Hamiltonian:

$$H = \frac{\Pi^2}{2m} + q\phi. \tag{13.4}$$

From (13.2) we can use the substitution

$$\mathbf{p} \longrightarrow \mathbf{p} - \frac{q\mathbf{A}}{c} \tag{13.5}$$

In position representation[1],

$$\nabla \longrightarrow \nabla - \left(\frac{iq}{\hbar c}\right)\mathbf{A}. \tag{13.6}$$

to get the expressions of the electromagnetism case. For example, the probability current now is

$$\mathbf{j} = \frac{\rho}{m}\left(\nabla S - \frac{q\mathbf{A}}{c}\right). \tag{13.7}$$

$$\int \mathbf{j}\,\mathrm{d}\mathbf{x} = \frac{\langle \mathbf{\Pi} \rangle}{m}. \tag{13.8}$$

$\mathbf{E}$ and $\mathbf{B}$ are unchanged under

$$\phi \to \phi - \frac{1}{c}\frac{\partial \Lambda}{\partial t}, \quad \mathbf{A} \to \mathbf{A} + \nabla\Lambda. \tag{13.9}$$

We consider the time-independent operator, so in the remaining part of this section, the term *gauge transformation* refers to the case $\frac{\partial \Lambda}{\partial t} = 0$.

Let $|\alpha\rangle, |\tilde{\alpha}\rangle$ be the state ket in the presence of $\mathbf{A}$ and $\tilde{\mathbf{A}}$, where,

$$\tilde{\mathbf{A}} = \mathbf{A} + \nabla\Lambda. \tag{13.10}$$

They must have the same physical situation, at least we need to make sure

$$\langle\alpha|\alpha\rangle = \langle\tilde{\alpha}|\tilde{\alpha}\rangle, \quad \langle\alpha|\mathbf{x}|\alpha\rangle = \langle\tilde{\alpha}|\mathbf{x}|\tilde{\alpha}\rangle, \quad \langle\alpha|\mathbf{\Pi}|\alpha\rangle = \langle\tilde{\alpha}|\tilde{\mathbf{\Pi}}|\tilde{\alpha}\rangle. \tag{13.11}$$

Construct an operator g that relates $|\tilde{\alpha}\rangle$ to $|\alpha\rangle$.

$$|\tilde{\alpha}\rangle = g|\alpha\rangle. \tag{13.12}$$

---

[1]We can use it only when the ∇ comes from $\mathbf{p}$.

By intuition, g is a function of Λ, and it is a function of $\mathbf{x}$, so it is commutable with $\mathbf{x}$, $g^\dagger \mathbf{x} g = \mathbf{x}$. The first and the third conditions give restrictions:

$$g^\dagger g = 1. \tag{13.13}$$

$$g^\dagger \mathbf{p} g = \mathbf{p} + \frac{q \nabla \Lambda}{c}. \tag{13.14}$$

It is easy to find

$$g = \exp\left(\frac{\mathrm{i} q \Lambda}{\hbar c}\right) \tag{13.15}$$

satisfies the above conditions. And we have

$$g^\dagger \tilde{\mathbf{\Pi}}^n g = \prod_{k=1}^n g^\dagger \tilde{\mathbf{\Pi}} g = \mathbf{\Pi}^n. \tag{13.16}$$

So, for any function f,

$$g^\dagger f\left(\tilde{\mathbf{\Pi}}\right) g = f\left(\mathbf{\Pi}\right). \tag{13.17}$$

(13.14) and (13.17) tell us, mechanical momentum is gauge invariant, but the canonical momentum is not.

Form the wave function,

$$S \longrightarrow S + \frac{q \Lambda}{c}. \tag{13.18}$$

This is highly satisfactory because we see that the probability flux given by (13.7) is then gauge invariant.

DO NOT FORGET that when using the gauge transformation, not only the states but also the operators will change. Let's check the Schrödinger equation is still hold under gauge transformation.

$$\tilde{H} \left|\tilde{\alpha}\right\rangle = g g^\dagger \tilde{H} g \left|\alpha\right\rangle = g H \left|\alpha\right\rangle = \mathrm{i}\hbar \frac{\partial}{\partial t} g \left|\alpha\right\rangle = \mathrm{i}\hbar \frac{\partial}{\partial t} \left|\tilde{\alpha}\right\rangle. \tag{13.19}$$

Since t is only a parameter, it does not affect the commutators, so when $\frac{\partial \Lambda}{\partial t} \neq 0$, (13.17) still holds. **BUT**, $\tilde{H} \neq g^\dagger H g$, since ϕ contributes a term. So our notation is not convenient in the Λ is time-dependent case.

13.2   Landau Levels and Quantum Hall Effect

We use IS of units this subsection.

13.2.1   Landau Gauge

Let's consider a simple magnetic field,

$$\mathbf{B} = -B\hat{\mathbf{z}}. \tag{13.20}$$

We take

$$A_x = By, \quad A_y = A_z = 0. \tag{13.21}$$

We just consider 2D case, the Hamiltonian is

$$H = \frac{(p_x - qBy)^2}{2m} + \frac{p_y^2}{2m} = \frac{1}{2}m\omega_c^2\left(y - \frac{p_x l_B^2}{\hbar}\right)^2 + \frac{p_y^2}{2m}, \tag{13.22}$$

where,

$$\omega_c = \frac{qB}{m}, \quad l_B = \sqrt{\frac{\hbar}{qB}}. \tag{13.23}$$

Since $\frac{\partial H}{\partial x} = 0$, we suppose

$$\psi_{n,k_x}(x,y) = e^{ik_x x}\psi(y). \tag{13.24}$$

Then,

$$\left[\frac{p_y^2}{2m} + \frac{1}{2}m\omega_c^2(y - l_B^2 k_x)^2\right]|\psi\rangle = E_n|\psi\rangle. \tag{13.25}$$

It has the same solution as the 1D harmonic oscillator, but with a displacement.

$$E_n = \hbar\omega_c\left(n + \frac{1}{2}\right). \tag{13.26}$$

13.2.2   Symmetrical Gauge

Let

$$l_B = \sqrt{\frac{\hbar}{eB}}, \quad \omega_c = \frac{eB}{m}, \tag{13.27}$$

$$a = \frac{1}{\sqrt{2}}\frac{l_B}{\hbar}\left(\Pi_x + i\Pi_y\right), \; a^\dagger = \frac{1}{\sqrt{2}}\frac{l_B}{\hbar}\left(\Pi_x - i\Pi_y\right). \tag{13.28}$$

Then,

$$[a, a^\dagger] = 1, \; H = \hbar\omega_c\left(a^\dagger a + \frac{1}{2}\right). \tag{13.29}$$

Then we can derivative (13.26) quickly.

To solve the wave function, we need choose a gauge, here we use symmetrical gauge, $(A_x, A_y) = \frac{B}{2}(-y, x)$. Let $w = x + iy$, $\overline{\partial} = \frac{\partial}{\partial\overline{w}} = \frac{1}{2}(\partial_x + i\partial_y)$. Then

$$\langle\mathbf{x}|a|\psi\rangle = -i\sqrt{2}l_B\left(\overline{\partial} + \frac{w}{4l_B^2}\right)\langle\mathbf{x}|\psi\rangle, \langle\mathbf{x}|a^\dagger|\psi\rangle = i\sqrt{2}l_B\left(\partial - \frac{\overline{w}}{4l_B^2}\right)\langle\mathbf{x}|\psi\rangle. \tag{13.30}$$

The wave function of the ground state satisfies

$$\left(\overline{\partial} + \frac{w}{4l_B^2}\right)\psi_0(w,\overline{w}) = 0. \tag{13.31}$$

The solution is

$$\psi_0(w,\overline{w}) = \mathrm{e}^{-\frac{|w|^2}{4l_B^2}} f(w,\overline{w}),\tag{13.32}$$

where f satisfies

$$\overline{\partial} f = 0.\tag{13.33}$$

So, we can write ψ_0 as

$$\psi_0(w,\overline{w}) = f(w)\mathrm{e}^{-\frac{|w|^2}{4l_B^2}}.\tag{13.34}$$

Then

$$\psi_n(w,\overline{w}) = \mathrm{e}^{-\frac{|w|^2}{4l_B^2}} \left(\partial - \frac{\overline{w}}{2l_B^2}\right)^n f(w).\tag{13.35}$$

An arbitrary $f(w)$ makes the states highly degenerate. Expand f in a series,

$$f(w) = \sum_{m\in\mathbb{N}} c_m w^m,\tag{13.36}$$

and denote

$$\psi_{0,m} \sim w^m \mathrm{e}^{-\frac{|w|^2}{4l_B^2}}.\tag{13.37}$$

In fact, $\psi_{0,m}$ is also the eigenstates of $L_z = \hbar(\partial w - \overline{\partial}\overline{w})$, and the eigenvalues are $m\hbar$.

$|\psi_{0,m}|^2$ take the maximum when $|w| = r_m$, where

$$r_m = \sqrt{2m}l_B.\tag{13.38}$$

Easy to note that each state has a area of $2\pi l_B^2$ greater than another.

14 Angular Momentum

14.1 Infinitesimal Rotations in Quantum Mechanics

We want to construct a rotation operator $\mathscr{D}$[1]. The appropriate infinitesimal operators could be written as

$$U_\varepsilon = 1 - \mathrm{i}G\varepsilon\tag{14.1}$$

with a Hermitian operator G. Define the angular-momentum operator J_k in such a way that the operator for an infinitesimal rotation around the kth axis by angle $\mathrm{d}\varphi$ can be obtained by letting

$$G \to \frac{J_k}{\hbar}, \quad \varepsilon \to \mathrm{d}\phi\,.\tag{14.2}$$

---

[1]The symbol $\mathscr{D}$ stems from the German word Drehung, meaning "rotation."

With J_k taken to be Hermitian, the infinitesimal-rotation operator is guaranteed to be unitary and reduces to the identity operator in the limit $\mathrm{d}\phi \to 0$. More generally, we have

$$\mathscr{D}(\hat{\mathbf{n}}, \mathrm{d}\phi) = 1 - \mathrm{i}\left(\frac{\mathbf{J}\cdot\hat{\mathbf{n}}}{\hbar}\right)\mathrm{d}\phi \tag{14.3}$$

for a rotation about the direction characterized by a unit vector $\hat{\mathbf{n}}$ by an infinitesimal angle $\mathrm{d}\phi$. For instance, if we are interested in a finite rotation about the $\hat{\mathbf{n}}$-axis by angle ϕ, we consider

$$\mathscr{D}_{\hat{\mathbf{n}}}(\phi) = \lim_{N\to+\infty}\left[1 - \mathrm{i}\left(\frac{\mathbf{J}\cdot\hat{\mathbf{n}}}{\hbar}\right)\frac{\phi}{N}\right]^N = \exp\left[-\mathrm{i}\left(\frac{\mathbf{J}\cdot\hat{\mathbf{n}}}{\hbar}\right)\phi\right]. \tag{14.4}$$

Taking $\phi = \varepsilon$, the first three term is

$$\mathscr{D}_{\hat{\mathbf{n}}}(\varepsilon) \approx 1 - \mathrm{i}\left(\frac{\mathbf{J}\cdot\hat{\mathbf{n}}}{\hbar}\right)\varepsilon - \frac{1}{2!}\left(\frac{\mathbf{J}\cdot\hat{\mathbf{n}}}{\hbar}\right)^2\varepsilon^2. \tag{14.5}$$

Let $\hat{\mathbf{n}}$ be $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$, by the properties of rotation, $\mathscr{D}$ need to satisfy

$$[\mathscr{D}_x(\varepsilon), \mathscr{D}_y(\varepsilon)] = \mathscr{D}_z(\varepsilon^2) - 1. \tag{14.6}$$

So,

$$[J_x, J_y] = \mathrm{i}\hbar J_z. \tag{14.7}$$

In general,

$$[J_i, J_k] = \mathrm{i}\hbar\varepsilon_{ijk}J_k. \tag{14.8}$$

By the meaning of rotation, we can also know that for any scalar a and vector v_i,

$$[J_i, a] = 0, \quad [J_i, v_j] = \mathrm{i}\hbar\varepsilon_{ijk}v_k. \tag{14.9}$$

14.2 Orbital Angular Momentum

Orbital angular momentum is defined as

$$\mathbf{L} = \mathbf{x} \times \mathbf{p}. \tag{14.10}$$

Easy to check that $\mathbf{L}$ satisfies (14.7). Expand $\mathbf{L}^2$:

$$\begin{aligned}
\mathbf{L}^2 &= \sum_{ijlmk}\varepsilon_{ijk}x_ip_j\varepsilon_{lmk}x_lp_m \\
&= \sum_{ijlm}(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl})x_ip_jx_lp_m \\
&= \sum_{ijlm}[\delta_{il}\delta_{jm}x_i(x_lp_j - \mathrm{i}\hbar\delta_{jl})p_m - \delta_{im}\delta_{jl}x_ip_j(p_mx_l + \mathrm{i}\hbar\delta_{lm})] \\
&= \mathbf{x}^2\mathbf{p}^2 - \mathrm{i}\hbar\mathbf{x}\cdot\mathbf{p} - \sum_{ijlm}\delta_{im}\delta_{jl}[x_ip_m(x_lp_j - \mathrm{i}\hbar\delta_{jl}) + \mathrm{i}\hbar\delta_{lm}x_ip_j] \\
&= \mathbf{x}^2\mathbf{p}^2 - (\mathbf{x}\cdot\mathbf{p})^2 + \mathrm{i}\hbar\mathbf{x}\cdot\mathbf{p}.
\end{aligned} \tag{14.11}$$

We have

$$[L_i, H] = 0, \quad \left[L^i L_i, H \right] = 0, \quad \left[L^i L_i, L_j \right] = 0. \tag{14.12}$$

So we can get the eigen value of $L_z, \mathbf{L}^2, H$ at the same time.

$$\langle \mathbf{x} | \mathbf{L} | \alpha \rangle = -i\hbar \mathbf{x} \times \nabla \langle \mathbf{x} | \alpha \rangle. \tag{14.13}$$

Under spherical coordinates, the nabla operator can be written as[1]

$$\nabla = \frac{\partial}{\partial r} \hat{\mathbf{r}} + \frac{1}{r} \frac{\partial}{\partial \theta} \hat{\theta} + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \hat{\phi}. \tag{14.14}$$

One has,

$$\mathbf{x} = r\hat{\mathbf{r}}, \tag{14.15}$$

so,

$$\mathbf{x} \times \nabla = \frac{\partial}{\partial \theta} \hat{\phi} - \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \hat{\theta}. \tag{14.16}$$

Then, project on $\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}$, we obtain

$$\langle \mathbf{x} | L_z | \alpha \rangle = -i\hbar \frac{\partial}{\partial \phi} \langle \mathbf{x} | \alpha \rangle, \tag{14.17}$$

$$\langle \mathbf{x} | L_x | \alpha \rangle = -i\hbar \left(-\sin \phi \frac{\partial}{\partial \theta} - \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right) \langle \mathbf{x} | \alpha \rangle, \tag{14.18}$$

$$\langle \mathbf{x} | L_y | \alpha \rangle = -i\hbar \left(\cos \phi \frac{\partial}{\partial \theta} - \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right) \langle \mathbf{x} | \alpha \rangle, \tag{14.19}$$

$$\langle \mathbf{x} | L_\pm | \alpha \rangle = -i\hbar e^{\pm i\phi} \left(\pm i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right) \langle \mathbf{x} | \alpha \rangle. \tag{14.20}$$

Where, $L_\pm = L_x \pm iL_y$. (14.11) gives the fact that

$$\langle \mathbf{x} | \mathbf{L}^2 | \alpha \rangle = -r^2 \hbar^2 \nabla^2_{\theta, \phi} \langle \mathbf{x} | \alpha \rangle. \tag{14.21}$$

$\nabla_{\theta, \phi}$ is the laplacian in spherical coordinates, but without the term[2] of r.

14.3   Eigen Value

We now look for the simultaneous eigenkets of $\mathbf{J}^2$ and J_z. We denote the eigenvalues of $\mathbf{J}^2$ and J_z by a and b, respectively:

$$\mathbf{J}^2 | a, b \rangle = a | a, b \rangle, \quad J_z | a, b \rangle = b | a, b \rangle. \tag{14.22}$$

Consider

$$J_\pm := J_x \pm iJ_y, \tag{14.23}$$

---

[1] $\mathbf{p}$ represent a displacement, it always acts like a gradient.

[2] Term of r is $\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \cdot \right)$. This is equivalent to $\frac{1}{r} \frac{\partial^2}{\partial r^2} (r \cdot)$

then,

$$J_- = J_+^\dagger, \quad \mathbf{J}^2 = J_z^2 + \frac{1}{2}\{J_+, J_-\}. \quad J_-J_+ = \mathbf{J}^2 - J_z^2 - \hbar J_z, \qquad (14.24)$$

$$[J_+, J_-] = 2\hbar J_z, \quad [J_z, J_\pm] = \pm\hbar J_\pm, \quad [\mathbf{J}^2, J_\pm] = 0. \qquad (14.25)$$

$$J_z\left(J_\pm \left|a,b\right\rangle\right) = (b \pm \hbar)\left(J_\pm \left|a,b\right\rangle\right). \qquad (14.26)$$

So, we call $J_\pm$ the **ladder operators**.

$$\mathbf{J}^2\left(J_\pm \left|a,b\right\rangle\right) = J_\pm \mathbf{J}^2 \left|a,b\right\rangle = a\left(J_\pm \left|a,b\right\rangle\right). \qquad (14.27)$$

So,

$$J_\pm \left|a,b\right\rangle = c_\pm \left|a, b \pm \hbar\right\rangle. \qquad (14.28)$$

Then there must exists $b_{\max}$ and $b_{\min}$, such that[1]

$$a = b_{\max}\left(b_{\max} + \hbar\right) = b_{\min}\left(b_{\min} - \hbar\right). \qquad (14.29)$$

We can infer that

$$-b_{\max} = b_{\min}, \qquad (14.30)$$

with $b_{\max}$ is positive, and that the allowed values of b lie within

$$b_{\min} \leq b \leq b_{\max}. \qquad (14.31)$$

$$b_{\max} = \frac{n\hbar}{2} \equiv j\hbar, \qquad (14.32)$$

where j is either an integer or a half-integer[2], then

$$a = \hbar^2 j(j+1). \qquad (14.33)$$

Let us also define m such that

$$b \equiv m\hbar. \qquad (14.34)$$

The allowed m-values for a given j are

$$m = \underbrace{-j, -j+1, \ldots, j-1, j}_{2j+1 \text{ states}}. \qquad (14.35)$$

Instead of $\left|a,b\right\rangle$, it is more convenient to denote a simultaneous eigenket of $\mathbf{J}^2$ and J_z by $\left|j,m\right\rangle$.

$$\mathbf{J}^2\left|j,m\right\rangle = \hbar^2 j(j+1)\left|j,m\right\rangle, \quad J_z\left|j,m\right\rangle = m\hbar\left|j,m\right\rangle. \qquad (14.36)$$

Then we can deduce that

$$J_\pm\left|j,m\right\rangle = \sqrt{(j \mp m)(j \pm m + 1)}\hbar\left|j,m\right\rangle, \qquad (14.37)$$

Important result: If $[K, \mathbf{J}] = 0$, then $K\left|j,m\right\rangle$ is also a eigenket of $\mathbf{J}^2$ and J_z. So,

$$\left\langle j', m'\right| K \left|j,m\right\rangle = \delta_{j'j}\delta_{m'm}f(j,m). \qquad (14.38)$$

By using $\mathbf{J}_\pm$, we can prove that

$$\left\langle j, m+1\right| K \left|j, m+1\right\rangle = \left\langle j,m\right| K \left|j,m\right\rangle. \qquad (14.39)$$

---

[1]By (14.24)

[2]If it represent the orbital angular momentum, we will denote j as l, and l can only take integer number, since the following will show the factor $e^{il\phi}$, and it must admit 2π as a period.

14.4 Representations of the Rotation Operator

If an arbitrary y-axis is rotated around the arbitrary z-axis by α to become y', then for any angle β, then[1]

$$R_{y'}(\beta) = R_z(\alpha)R_y(\beta)R_z^{-1}(\alpha). \tag{14.40}$$

If we use the Euler Rotations[2], then

$$R(\alpha, \beta, \gamma) \equiv R_{z'}(\gamma)R_{y'}(\beta)R_z(\alpha) = R_z(\alpha)R_y(\beta)R_z(\gamma). \tag{14.41}$$
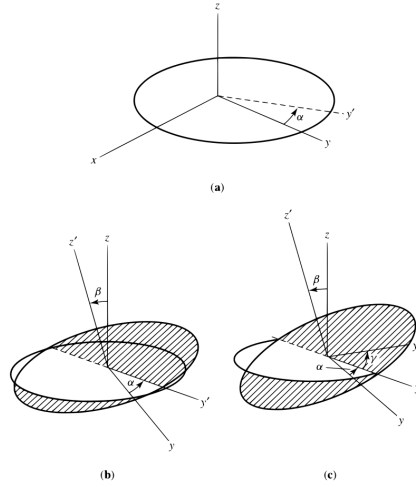
FIGURE 3.4 Euler rotations.

Figure 14.1: Euler Rotations

Having obtained the matrix elements of J_z and $J_\pm$, we are now in a position to study the matrix elements of the rotation operator $\mathscr{D}(R)$. If a rotation R is specified by $\hat{\mathbf{n}}$ and ϕ, we can define its matrix elements by

$$\mathscr{D}^{(j)}_{m'm}(R) = \langle j, m' | \exp\left(\frac{-i\mathbf{J}\cdot\hat{\mathbf{n}}\phi}{\hbar}\right) |j, m\rangle. \tag{14.42}$$

These matrix elements are sometimes called **Wigner functions**. In Euler Rotations, the rotation operator is defined by

$$\begin{aligned}
&\mathscr{D}^{(j)}_{m'm}(\alpha, \beta, \gamma) \\
&= \langle j, m' | \exp\left(\frac{-iJ_z\alpha}{\hbar}\right) \exp\left(\frac{iJ_y\beta}{\hbar}\right) \exp\left(\frac{-iJ_z\gamma}{\hbar}\right) |j, m\rangle \\
&= e^{-i(m'\alpha + m\gamma)} \langle j, m' | \exp\left(\frac{-iJ_y\beta}{\hbar}\right) |j, m\rangle.
\end{aligned} \tag{14.43}$$

---

[1] R also means rotation.
[2] This figure is from *Modern Quantum Mechanics*

We denote nontrivial part as

$$d^{(j)}_{m'm}(\beta) = \langle j, m' | \exp\left(\frac{-\mathrm{i}J_y\beta}{\hbar}\right) | j, m \rangle. \tag{14.44}$$

Since

$$\left[\mathbf{J}^2, \mathscr{D}(R)\right] = 0, \tag{14.45}$$

any state $|j, m\rangle$ after a rotation R is also an eigenket of $\mathbf{J}^2$, and its eigenvalue is still $j(j+1)\hbar^2$.

To find the amplitude for being found in $|j, m\rangle$, we simply expand the rotated state as follows:

$$\mathscr{D}(R)|j, m\rangle = \sum_{m'} |j, m'\rangle \langle j, m'| \mathscr{D}(R) |j, m\rangle = \sum_{m'} |j, m'\rangle \mathscr{D}^{(j)}_{m'm}(R). \tag{14.46}$$

Theorem 14.1 (Wigner)
Given an operator R, if for any state $|\psi\rangle$, $|\phi\rangle$, $|\langle R\psi|R\phi\rangle|$ is held, then R is unitary or anti-unitary.

14.5   Spherical Harmonics

[1] Let us consider a problem with spherical symmetry, we can consider

$$\langle \hat{\mathbf{n}} | l, m \rangle = Y_l^m(\hat{\mathbf{n}}) = Y_l^m(\theta, \phi), \tag{14.47}$$

where we have defined a **direction eigenket $|\hat{\mathbf{n}}\rangle$**.

By (14.36), we have

$$-\mathrm{i}\hbar \frac{\partial}{\partial\phi} Y_l^m(\theta, \phi) = m\hbar Y_l^m(\theta, \phi), \tag{14.48}$$

$$\left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} + l(l+1)\right] Y_l^m = 0. \tag{14.49}$$

By

$$\langle l', m' | l, m \rangle = \delta_{ll'}\delta_{mm'}, \tag{14.50}$$

we obtain,

$$\int_0^{2\pi} \mathrm{d}\phi \int_{-1}^1 \mathrm{d}(\cos\theta)\, Y_{l'}^{m'*}(\theta, \phi)\, Y_l^m(\theta, \phi) = \delta_{ll'}\delta_{mm'}. \tag{14.51}$$

(14.48) implies that the ϕ-independence $Y_l^m(\theta, \phi)$ must behave like $\mathrm{e}^{\mathrm{i}m\phi}$. By (14.20),

$$\left[\mathrm{i}\frac{\partial}{\partial\theta} - \cot\theta \frac{\partial}{\partial\phi}\right] \langle \hat{\mathbf{n}} | l, l \rangle = 0. \tag{14.52}$$

---

[1]Spherical Functions.

So,

$$Y_l^l(\theta, \phi) = c_l \mathrm{e}^{\mathrm{i}l\phi} \sin^l \theta. \tag{14.53}$$

Use (14.51) to normalize,

$$\int_0^\pi \sin^{2l}\theta \sin\theta \,\mathrm{d}\theta = B\left(l+1, \frac{1}{2}\right) = \frac{\Gamma(l+1)\,\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(l+\frac{3}{2}\right)}. \tag{14.54}$$

Then we can use the ladder operator to get Y_l^m. Check details in the reference.

14.6   Schwinger's Oscillator Model of Angular Momentum

Consider a 2D harmonic oscillator $H = \hbar\omega(a_1^\dagger a_1 + a_2^\dagger a_2)$ exhibiting the SU(2) symmetry. We define,

$$J_\mu = \frac{1}{2}a_\alpha^\dagger \left(\sigma^\mu\right)^\alpha{}_\beta a^\beta, \tag{14.55}$$

where σ^μ is one of the Pauli matrix with $\mu = 1, 2, 3$, $\{\alpha, \beta\} \subseteq \{1, 2\}$. We can prove that

$$[J_\mu, J_\nu] = \mathrm{i}\varepsilon_{\mu\nu\rho}J_\rho. \tag{14.56}$$

If we let $2J = a_\alpha^\dagger a^\alpha$, then

$$J^\mu J_\mu = J(J+1). \tag{14.57}$$

And the state can be represented as:

$$|j, m\rangle = \frac{(a_1^\dagger)^{j+m}}{\sqrt{(j+m)!}} \frac{(a_2^\dagger)^{j-m}}{\sqrt{(j-m)!}} |0, 0\rangle. \tag{14.58}$$

It satisfies (14.36) and (14.37).

14.7   Addition of Angular Momenta

Consider two independent state $|\alpha\rangle$, $|\beta\rangle$, we can see them as a state $|\alpha, \beta\rangle$[1],

$$|\alpha, \beta\rangle = |\alpha\rangle \otimes |\beta\rangle, \tag{14.59}$$

Consider the rotation

$$\mathscr{D}(R) = \mathscr{D}_1(R) \otimes \mathscr{D}_2(R) = \exp\left(\frac{-\mathrm{i}\mathbf{J}_1 \cdot \hat{\mathbf{n}}\phi}{\hbar}\right) \otimes \exp\left(\frac{-\mathrm{i}\mathbf{J}_2 \cdot \hat{\mathbf{n}}\phi}{\hbar}\right). \tag{14.60}$$

Let $\phi = \varepsilon$, and $\mathscr{D}(R) = \exp(-\mathrm{i}\mathbf{J} \cdot \hat{\mathbf{n}}\phi/\hbar)$ we can get

$$\mathbf{J} = \mathbf{J}_1 \otimes 1 + 1 \otimes \mathbf{J}_2. \tag{14.61}$$

When we are talking about[2]

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2, \tag{14.62}$$

---

[1]The following is tensor product, but in many physics books they mess up with direct product.

[2]The computing law are very similar, so many other places always write like this.

we should understand it as (14.61). Easy to check that (14.62) satisfies the commutation relation of angular momentum. But neither $\mathbf{J}_1 + \mu\mathbf{J}_2$ nor $\lambda(\mathbf{J}_1 + \mathbf{J}_2)$ $(\mu, \lambda \neq 1)$.

Also, we define

$$J_x = J_{1x}\otimes 1 + 1\otimes J_{2x}, \quad J_y = J_{1y}\otimes 1 + 1\otimes J_{2y}, \quad J_z = J_{1z}\otimes 1 + 1\otimes J_{2z}, \quad (14.63)$$

$$J_+ = J_{1+}\otimes 1 + 1\otimes J_{2+}, \quad J_- = J_{1-}\otimes 1 + 1\otimes J_{2-}, \quad (14.64)$$

$$\mathbf{J}^2 = J_x^2 + J_y^2 + J_z^2. \quad (14.65)$$

A calculate example[1]:

$$(A\otimes B)(C\otimes D) = (AC)\otimes(BD). \quad (14.66)$$

$$J_z^2 = J_{1z}^2\otimes 1 + 1\otimes J_{2z}^2 + 2J_{1z}\otimes J_{2z}. \quad (14.67)$$

So we can also write $\mathbf{J}^2$ into the form of

$$\mathbf{J}^2 = \mathbf{J}_1^2\otimes 1 + 1\otimes \mathbf{J}_2^2 + 2J_{1z}\otimes J_{2z} + J_{1+}\otimes J_{2-} + J_{1-}\otimes J_{2+}. \quad (14.68)$$

14.7.1 Clebsch-Gordan Coefficients

As for the choice of base kets, since $[\mathbf{J}^2, J_{1,2z}] \neq 0$, we have two options:

$$|j_1 j_2; jm\rangle \text{ and } |j_1 j_2; m_1 m_2\rangle.$$

We connect them with Clebsch-Gordan coefficients $\langle j_1 j_2 m_1 m_2 | j_1 j_2; jm\rangle$:

$$|j_1 j_2; jm\rangle = \sum_{m_1, m_2} |j_1 j_2; m_1 m_2\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2; jm\rangle. \quad (14.69)$$

We figure out some properties about CG coefficients:
(1) CG coefficients vanish unless

$$m = m_1 + m_2, \quad (14.70)$$

because

$$\begin{aligned}
0 &= \langle j_1 j_2; m_1 m_2 | (J_z - J_{1z} - J_{2z}) | j_1 j_2; jm\rangle \\
&= (m - m_1 - m_2) \langle j_1 j_2; m_1 m_2 | j_1 j_2; jm\rangle.
\end{aligned} \quad (14.71)$$

(2) The coefficients vanish unless

$$|j_1 - j_2| \leq j \leq j_1 + j_2. \quad (14.72)$$

This is based on our choice of base kets, just for convenience, it has already provided a complete bases[2]. In addition, we even choose CG coefficients to be real numbers.
(3) Recursive relations

---

[1]Attention: $A\otimes B + C\otimes D \stackrel{?}{=} (A+C)\otimes(B+D)$. But this is true: $A\otimes C + B\otimes C = (A+B)\otimes C$.
[2]Check the dimension yourself.

15   Discrete Symmetry

15.1   Wigner Theorem

Theorem 15.1 (Wigner)
Given an operator R, if for any state $|\psi\rangle$, $|\phi\rangle$, $|\langle R\psi|R\phi\rangle|$ is held, then R is unitary or anti-unitary[1].

> Let $\mathbb{H}$ denote the Hilbert space describing a system, with its inner product denoted by $\langle \cdot, \cdot \rangle$, and let $\mathbb{PH}$ denote the corresponding projective space (the set of all one-dimensional subspaces of $\mathbb{H}$). The reason for using $\mathbb{PH}$ is that its points correspond bijective to physical states. The inner product $\langle \cdot, \cdot \rangle$ on $\mathbb{H}$ induces a metric d on $\mathbb{PH}$ (the Fubini–Study metric). It is easy to see that a unitary or anti-unitary operator $K : \mathbb{H} \to \mathbb{H}$ (where anti-unitary means $\langle Kv, Kw \rangle = \langle w, v \rangle$) induces a homeomorphism from $\mathbb{PH}$ to $\mathbb{PH}$ that preserves the metric d, meaning $d(Kx, Ky) = d(x, y)$. Wigner's theorem states that any homeomorphism of $\mathbb{PH}$ onto itself that preserves the metric d is necessarily induced by some unitary or anti-unitary operator on $\mathbb{H}$.
>
> **Theorem (Wigner):** If the dimension of $\mathbb{H}$ is greater than or equal to 2, and $U : \mathbb{PH} \to \mathbb{PH}$ is a homeomorphism preserving the metric d, i.e., $d(Ux, Uy) = d(x, y)$, then there exists a unitary or anti-unitary operator $\mathcal{U}$ on $\mathbb{H}$ such that $\mathcal{U}$ induces U. If $\mathcal{V}$ also induces U, then $\mathcal{V} = e^{i\theta}\mathcal{U}$, where $\theta \in \mathbb{R}$.   *—Reference*

15.2   Parity Transformation

Parity operator π will changes a right-handed system into a left-handed system. Somewhere, we denote any ket $|\alpha\rangle$ after action by π as $|\alpha^\pi\rangle$, but in most of my habits, I will just write $|\pi\alpha\rangle$.

$$|\pi\alpha\rangle := \pi \, |\alpha\rangle \tag{15.1}$$

Consider the physical meaning, we require

$$\langle \pi\alpha|\pi\alpha\rangle = \langle \alpha|\alpha\rangle\,, \tag{15.2}$$
$$\langle \pi\alpha|\mathbf{x}|\pi\alpha\rangle = -\langle \alpha|\mathbf{x}|\alpha\rangle\,. \tag{15.3}$$

15.2 implies that π is whether unitary or anti-unitary.

Since the expectation value is a real number, and π keep the module invariant,

$$\langle \pi\alpha|\mathbf{x}|\pi\alpha\rangle = \langle \alpha|\pi^{-1}\mathbf{x}\pi|\alpha\rangle\,. \tag{15.4}$$

Then we will use $\langle \alpha| \pi^{-1}\mathbf{x}\pi \, |\alpha\rangle = -\langle \alpha| \mathbf{x} \, |\alpha\rangle$ to prove $\pi^{-1}\mathbf{x}\pi = -\mathbf{x}$. Since $|\alpha\rangle$ is arbitrary, let $|\alpha\rangle = |\psi\rangle + |\phi\rangle$. Then, we can deduce that

$$\mathrm{Re}\left(\langle \psi| \pi^{-1}\mathbf{x}\pi \, |\phi\rangle\right) = -\mathrm{Re}\left(\langle \psi| \mathbf{x} \, |\phi\rangle\right). \tag{15.5}$$

---

[1]Review 4.2 first.

Let $|\alpha\rangle = |\psi\rangle + \mathrm{i}\,|\phi\rangle$, then,

$$\mathrm{Im}\left(\langle\psi|\,\pi^{-1}\mathbf{x}\pi\,|\phi\rangle\right) = -\mathrm{Im}\left(\langle\psi|\,\mathbf{x}\,|\phi\rangle\right). \tag{15.6}$$

So, for any $|\psi\rangle$, $|\phi\rangle$,

$$\langle\psi|\,\pi^{-1}\mathbf{x}\pi\,|\phi\rangle = -\,\langle\psi|\,\mathbf{x}\,|\phi\rangle. \tag{15.7}$$

Which means

$$\pi^{-1}\mathbf{x}\pi = -\mathbf{x}, \quad \mathbf{x}\pi = -\pi\mathbf{x}. \tag{15.8}$$

Then we derive the effect π act on momentum p. Let us start from position translation. We have

$$\pi\mathscr{T}(\mathrm{d}\mathbf{x}') = \mathscr{T}(-\,\mathrm{d}\mathbf{x}')\pi, \tag{15.9}$$

so,

$$\pi^{-1}\mathbf{p}\pi = -\mathbf{p}, \ \{\pi, \mathbf{p}\} = 0. \tag{15.10}$$

Easy to check that

$$\pi^{-1}\mathrm{i}\hbar\pi = \pi^{-1}[\mathbf{x}, \mathbf{p}]\pi = [\mathbf{x}, \mathbf{p}] = \mathrm{i}\hbar. \tag{15.11}$$

So, π is unitary. Then we can define $\pi^\dagger$, and $\pi^\dagger\pi = 1$.

Note that

$$\mathbf{x}\pi\,|\mathbf{x}'\rangle = -\pi\mathbf{x}\,|\mathbf{x}'\rangle = (-\mathbf{x}')\pi\,|\mathbf{x}'\rangle. \tag{15.12}$$

So $\pi\,|\mathbf{x}'\rangle = \mathrm{e}^{\mathrm{i}\delta}\,|-\mathbf{x}'\rangle$. It is customary to take $\mathrm{e}^{\mathrm{i}\delta} = 1$ by convention. Then $\pi^2 = 1$. Hence,

$$\pi^{-1} = \pi^\dagger = \pi. \tag{15.13}$$

Its eigen-value can only be ± 1.

In geometry, reflection is commutable with rotation. In the language of operators,

$$\pi\mathscr{D}(R) = \mathscr{D}(R)\pi. \tag{15.14}$$

So,

$$\pi^\dagger\mathbf{J}\pi = \mathbf{J}, \ [\pi, \mathbf{J}] = 0. \tag{15.15}$$

Now, we consider the wave-function under parity transformation. For any state $|\psi\rangle$, let the its state after parity transformation be $|\psi'\rangle$, then we have

$$\psi'(\mathbf{x}) = \langle\mathbf{x}|\psi'\rangle = \langle\mathbf{x}|\,\pi\,|\psi\rangle = \langle-\mathbf{x}|\psi\rangle = \psi(-\mathbf{x}). \tag{15.16}$$

If $|\psi\rangle$ is an eigen-state of π, $\pi\,|\psi\rangle = \pm\,|\psi\rangle$, then

$$\psi(\mathbf{x}) = \pm\psi(-\mathbf{x}) \begin{cases} \text{even parity,} \\ \text{odd parity.} \end{cases} \tag{15.17}$$

So for 1D harmonic oscillator,

$$\psi_n(-x) = (-)^n\psi_n(x). \tag{15.18}$$

For angular momentum eigenstates $Y_{l,m}(\hat{\mathbf{n}})$

$$Y_{lm}(-\hat{\mathbf{n}}) = Y_{lm}(\pi - \theta, \pi + \varphi) = (-)^l Y_{lm}(\theta, \varphi). \tag{15.19}$$

Theorem 15.2
Suppose
$$[H, \pi] = 0$$
and $|n\rangle$ is a nondegenerate eigenket of H with eigenvalue E_n:
$$H |n\rangle = E_n |n\rangle \, ;$$
then $|n\rangle$ is also a parity eigenket.

Proof. Note that $\frac{1}{2}(1 \pm \pi) |n\rangle$ is a parity eigenket with eigenvalues ± 1. But this is also an energy eigenket with eigenvalue E_n, which means it represent the same state as $|n\rangle$. $\qquad\square$

15.3   Time-Reversal Symmetry

First we claim that any anti-unitary operator can be written as
$$\theta = UK, \tag{15.20}$$

where U is a unitary operator, and K is the complex-conjugate operator that forms the complex conjugate of any coefficient that multiplies a ket.

16   Approximation Methods

16.1   Time-independent Perturbation Theory: Non-degenerate Case

Consider
$$H = H_0 + \lambda V, \tag{16.1}$$

where $\lambda \ll 1$, and we have known the eigenvalues and eigenkets of H_0. Then we want to know the eigenvalues and eigenkets of H. Let
$$\Delta_n = E_n - E_n^{(0)}, \tag{16.2}$$

then Schrödinger equation gives
$$(E_n^{(0)} - H_0) |n\rangle = (\lambda V - \Delta_n) |n\rangle \, . \tag{16.3}$$

For convenience, we define the projection operator and an operator like inverse of $(E_n^{(0)} - H_0)$:
$$\phi_n := 1 - |n^{(0)}\rangle \langle n^{(0)}| = \sum_{m \neq n} |m^{(0)}\rangle \langle m^{(0)}| , \tag{16.4}$$

$$\frac{\phi_n}{E_n^{(0)} - H_0} := \sum_{m \neq n} \frac{|m^{(0)}\rangle \langle m^{(0)}|}{E_n^{(0)} - E_m^{(0)}} . \tag{16.5}$$

We define ϕ_n aim at projecting out the component of $|n^{(0)}\rangle$, eliminating the singularity of $(E_n^{(0)} - H_0)^{-1}$.

Now, we have

$$|n\rangle = \frac{\phi_n}{E_n^{(0)} - H_0}(\lambda V - \Delta_n)|n\rangle + |n^{(0)}\rangle \langle n^{(0)}|n\rangle. \tag{16.6}$$

Note that

$$\langle n^{(0)}|(E_n^{(0)} - H_0)|n\rangle = 0. \tag{16.7}$$

So,

$$\Delta_n \langle n^{(0)}|n\rangle = \lambda \langle n^{(0)}|V|n\rangle. \tag{16.8}$$

Since there's just a common multiplicative factor, we can normalize $|n\rangle$ later, and now we let $\langle n^{(0)}|n\rangle = 1$. Then, we can set

$$|n\rangle = |n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \cdots, \tag{16.9}$$

$$\Delta_n = \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots. \tag{16.10}$$

equating the coefficient of various powers of λ, we obtain

$$\Delta_n^{(k)} = \langle n^{(0)}|V|n^{(k-1)}\rangle, \quad k = 1, 2, \ldots, \tag{16.11}$$

Also,

$$|n^{(k)}\rangle = \frac{\phi_n}{E_n^{(0)} - H_0}\left[\left(V - \Delta_n^{(1)}\right)|n^{(k-1)}\rangle - \sum_{j=2}^{k}\Delta_n^{(j)}|n^{(k-j)}\rangle\right], \quad k = 1, 2, \ldots. \tag{16.12}$$

Let

$$V_{nk} := \langle n^{(0)}|V|k^{(0)}\rangle, \tag{16.13}$$

let us simplify the first and second order corrections:

$$\Delta_n^{(1)} = V_{nn}, \tag{16.14}$$

So,

$$|n^{(1)}\rangle = \sum_{m \neq n}\frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}}|m^{(0)}\rangle, \tag{16.15}$$

$$\Delta_n^{(2)} = \sum_{m \neq n}\frac{|V_{mn}|^2}{E_n^{(0)} - E_m^{(0)}}. \tag{16.16}$$

$$|n^{(2)}\rangle = \sum_{m \neq n}\left[\sum_{l \neq n}\frac{V_{ml}V_{ln}}{(E_n^{(0)} - E_m^{(0)})(E_n^{(0)} - E_l^{(0)})} - \frac{V_{nn}V_{mn}}{(E_n^{(0)} - E_m^{(0)})^2}\right]|m^{(0)}\rangle. \tag{16.17}$$

Thus, up to second order in λ, we have

$$E_n \approx E_n^{(0)} + \lambda V_{nn} + \lambda^2 \sum_{m \neq n} \frac{|V_{mn}|^2}{E_n^{(0)} - E_m^{(0)}}, \tag{16.18}$$

$$|n\rangle \approx |n^{(0)}\rangle + \lambda \sum_{m \neq n} \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}} |m^{(0)}\rangle. \tag{16.19}$$

Second order correction of energy at ground state always show minus sign.

It is time to normalize $|n\rangle$. We define

$$|n\rangle_N = Z_n^{1/2} |n\rangle, \; Z_n^{1/2} = \langle n^{(0)} | n\rangle_N. \tag{16.20}$$

Since $\langle n^{(0)} | n^{(k)} \rangle = 0$, if $k \geq 1$,

$$Z_n^{-1} = 1 + \lambda^2 \langle n^{(1)} | n^{(1)} \rangle + \mathcal{O}(\lambda^3) \tag{16.21}$$

$$= 1 + \lambda^2 \sum_{m \neq n} \frac{|V_{mn}|^2}{(E_n^{(0)} - E_m^{(0)})^2} + \mathcal{O}(\lambda^3). \tag{16.22}$$

$$Z_n = 1 - \lambda^2 \sum_{m \neq n} \frac{|V_{mn}|^2}{(E_n^{(0)} - E_m^{(0)})^2} + \mathcal{O}(\lambda^3). \tag{16.23}$$

The second term in (16.23) is to be understood as the probability for "leakage" to states other than $|n^{(0)}\rangle$. Notice that Z_n is less than 1, as expected on the basis of the probability interpretation for Z.

In fact, we have (not only up to second order)

$$Z_n = \frac{\partial E_n}{\partial E_n^{(0)}}. \tag{16.24}$$

16.2   Time-independent Perturbation Theory: Degenerate Case

This is the case where some subtraction of eigenvalues not much greater than perturbation. So we need to deal with the part out of hypothesis in the previous case. We define a projection operator P_0 that project a state to $\{|m^{(0)}\rangle\}$, where the eigen-values are very close such that we do not need to consider their difference while dealing with the perturbation. We denote this subspace as D (Without losing of generality, we concentrate on one subspace.) For convenience, we also define $P_1 := 1 - P_0$. For any ket in D,

$$|l^{(0)}\rangle = \sum_{m \in D} \langle m^{(0)} | l^{(0)} \rangle |m^{(0)}\rangle. \tag{16.25}$$

Different from the reference book, I will estimate the order of difference between eigen-energy in D. And we choose $|n\rangle \in D$.

By projection and orthogonality, it is easy to get

$$(E - H_0 - \lambda P_0 V) P_0 |n\rangle - \lambda P_0 V P_1 |n\rangle = 0. \tag{16.26}$$

$$(E - H_0 - \lambda P_1 V) P_1 \ket{n} - \lambda P_1 V P_0 \ket{n} = 0. \tag{16.27}$$

By (16.27),

$$P_1 \ket{n} = P_1 \frac{\lambda}{E - H_0 - \lambda P_1 V P_1} P_1 V P_0 \ket{n}. \tag{16.28}$$

Let

$$\ket{n} = \ket{n^{(0)}} + \lambda \ket{n^{(1)}} + \mathcal{O}(\lambda^2), \tag{16.29}$$

$$E = E_n^{(0)} + \lambda \Delta_n^{(1)} + \mathcal{O}(\lambda^2), \tag{16.30}$$

Then,

$$P_1 \ket{n^{(1)}} = \sum_{k \notin D} \frac{V_{kl} \ket{k^{(0)}}}{E_n^{(0)} - E_k^{(0)}}. \tag{16.31}$$

Plug (16.28) into (16.26), we obtain (we can call it effect Hamiltonian)

$$(E - H_0 - \lambda P_0 V P_0 - \lambda^2 P_0 V P_1 \frac{1}{E - H_0 - \lambda P_1 V P_0} P_1 V P_0) P_0 \ket{n} = 0. \tag{16.32}$$

The second term:

$$H_0 P_0 \ket{n} = H_0 \ket{n^{(0)}} + \lambda H_0 P_0 \ket{n^{(1)}} + \mathcal{O}(\lambda^2). \tag{16.33}$$

$$\begin{aligned}
H_0 P_0 \ket{n^{(1)}} &= \sum_{k \in D} E_k^{(0)} \bra{k^{(0)}} P_0 \ket{n^{(1)}} \ket{k^{(0)}} \\
&= \sum_{k \in D} (E_D^{(0)} + \varepsilon_k^{(0)}) \bra{k^{(0)}} P_0 \ket{n^{(1)}} \ket{k^{(0)}} \\
&= \sum_{k \in D} \varepsilon_k^{(0)} \bra{k^{(0)}} P_0 \ket{n^{(1)}} \ket{k^{(0)}} + E_D^{(0)} P_0 \ket{n^{(1)}}
\end{aligned} \tag{16.34}$$

$\varepsilon_k^{(0)} := E_k^{(0)} - E_D^{(0)}$ can estimate the difference between eigenvalues in D. I think a good choice is to let

$$\left| \sum_{k \in D} \varepsilon_k^{(0)} \bra{k^{(0)}} P_0 \ket{n^{(1)}} \ket{k^{(0)}} \right|^2 = \sum_{k \in D} \left(\varepsilon_k^{(0)} \right)^2 \left| \bra{k^{(0)}} P_0 \ket{n^{(1)}} \right|^2 \tag{16.35}$$

be possibly the smallest.

Given a shift ε, we want

$$\frac{\partial}{\partial \varepsilon} \sum_{k \in D} \left(\varepsilon_k^{(0)} + \varepsilon \right)^2 \left| \bra{k^{(0)}} P_0 \ket{n^{(1)}} \right|^2 = 0. \tag{16.36}$$

So,

$$\varepsilon = -\frac{\sum \varepsilon_k^{(0)} \left| \bra{k^{(0)}} P_0 \ket{n^{(1)}} \right|^2}{\sum \left| \bra{k^{(0)}} P_0 \ket{n^{(1)}} \right|^2} \tag{16.37}$$

In the following, we assume $\varepsilon_k^{(0)}$ satisfies

$$\sum_{k \in D} \varepsilon_k^{(0)} \left| \langle k^{(0)} | P_0 | n^{(1)} \rangle \right|^2 = 0, \tag{16.38}$$

and

$$\max_{p,q \in D} |\varepsilon_p^{(0)} - \varepsilon_q^{(0)}| = \max_{p,q \in D} |E_p^{(0)} - E_q^{(0)}|. \tag{16.39}$$

If we want to ignore $\varepsilon_k^{(0)}$ in the first λ term, we need

$$\max_{p,q \in D} |E_p^{(0)} - E_q^{(0)}| = o(\lambda) V P_0 | n \rangle. \tag{16.40}$$

The term of λ in (16.32) give us eigen-functions

$$(E - E_D^{(0)} - \lambda P_0 V P_0) | n^{(0)} \rangle = 0. \tag{16.41}$$

That is

$$\det \left(V - \Delta_D^{(1)} I \right) = 0, \tag{16.42}$$

with a stroke of eigenkets $\{ |l^{(0)}\rangle \}$.

Then we can follow the same procedure as non-degenerate case.

$$\Delta_l^{(1)} = \langle l^{(0)} | V | l^{(0)} \rangle \tag{16.43}$$

$$P_0 | l_i^{(1)} \rangle = \lambda \sum_{j \neq i} \frac{P_0 | l_j^{(0)} \rangle}{\Delta_j^{(1)} - \Delta_i^{(1)}} \langle l_j^{(0)} | \left(V P_1 \frac{1}{E_D^{(0)} - H_0} P_1 V \right) | l_i^{(0)} \rangle \tag{16.44}$$

$$\Delta_l^{(2)} = \sum_{k \notin D} \frac{|V_{kl}|^2}{E_D^{(0)} - E_k^{(0)}}. \tag{16.45}$$

16.3 Time-dependent Potentials: The Interact Picture

Consider a Hamiltonian that can be split into two parts,

$$H = H_0 + V(t), \tag{16.46}$$

where H_0 does not contain time explicitly. The problem $V(t) = 0$ is assumed to be solved in the sense that the energy eigenkets $|n\rangle$ and the energy eigenvalues E_n defined by

$$H_0 | n \rangle = E_n | n \rangle \tag{16.47}$$

are completely known. Suppose that at $t = 0$, the state ket of a physical system is given by

$$|\alpha\rangle = \sum_n c_n(0) | n \rangle. \tag{16.48}$$

We wish to find $c_n(t)$ for $t > 0$ such that

$$|\alpha, t_0; t\rangle = \sum_n c_n(t) e^{-iE_n t/\hbar} |n\rangle. \tag{16.49}$$

We now use interaction picture, define

$$|\alpha, t_0; t\rangle_I = e^{iH_0 t/\hbar} |\alpha, t_0; t\rangle_S. \tag{16.50}$$

Then any operator under interaction picture can be defined as

$$A_I = e^{iH_0 t/\hbar} A_S e^{-iH_0 t/\hbar}. \tag{16.51}$$

And now the Schrödinger equation becomes

$$i\hbar \frac{\partial}{\partial t} |\alpha, t_0; t\rangle_I = V_I |\alpha, t_0; t\rangle_I. \tag{16.52}$$

So we have

$$i\hbar \frac{\partial}{\partial t} \langle n|\alpha, t_0; t\rangle_I = \sum_m \langle n| V_I |m\rangle \langle m|\alpha, t_0; t\rangle_I. \tag{16.53}$$

Using

$$\langle n| e^{iH_0 t/\hbar} V(t) e^{-iH_0 t/\hbar} |m\rangle = V_{nm}(t) e^{i(E_n - E_m)t/\hbar}, \tag{16.54}$$

and

$$c_n = \langle n|\alpha, t_0; t\rangle_I, \tag{16.55}$$

we have

$$i\hbar \frac{d}{dt} c_n = \sum_m V_{nm} e^{i\omega_{nm} t/\hbar} c_m(t), \tag{16.56}$$

where

$$\omega_{nm} = (E_n - E_m)/\hbar. \tag{16.57}$$

Now we deal the case that $V(t) \ll H_0$. Similar to (9.14),

$$U_I(t, t_0) = \mathcal{T} \exp\left[\frac{-i}{\hbar} \int_{t_0}^t dt'\, V_I(t')\right]. \tag{16.58}$$

if we let

$$c_n(t) = c_n^{(0)} + c_n^{(1)} + \ldots, \tag{16.59}$$

then,

$$c_n^{(k)} = \left(\frac{-i}{\hbar}\right)^k \langle n| \mathcal{T} \left[\int_{t_0}^t dt'\, V_I(t')\right]^k |\text{init}\rangle. \tag{16.60}$$

In particular,

$$c_n^{(0)}(t) = \delta_{ni} \tag{16.61}$$

$$c_n^{(1)}(t) = \left(\frac{-i}{\hbar}\right) \int_{t_0}^t dt'\, e^{i\omega_{ni} t'} V_{ni}(t') \tag{16.62}$$

$$c_n^{(2)}(t) = \left(\frac{-i}{\hbar}\right)^2 \sum_m \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2\, e^{i\omega_{nm} t_1} V_{nm}(t_1) e^{i\omega_{mi} t_2} V_{mi}(t_2) \tag{16.63}$$

In most of system in the real world, other atoms will disturb a specific coherent state, thus we can only consider the leaner term, not to worry time too long that can not fit the time condition.

16.4   Adiabatic Evolution and Berry Phase

Consider a parameter dependent Hamiltonian $H(\vec{R})$, and $\vec{R}(t)$ is a slow varying. For each $\vec{R}$, define eigen states:

$$H(\vec{R}) \, |\psi_n(\vec{R})\rangle = E(\vec{R}) \, |\psi_n(\vec{R})\rangle \,. \tag{16.64}$$

We can write

$$|\alpha; t\rangle = \sum_n c_n(t) \mathrm{e}^{\mathrm{i}\theta_n(t)} \, |\psi_n(\vec{R}(t))\rangle \,, \tag{16.65}$$

where

$$\theta_n(t) = -\int_{t_0}^t \mathrm{d}t' \, E_n(t')/\hbar. \tag{16.66}$$

We find

$$\sum_n \mathrm{e}^{\mathrm{i}\theta_n} \left[\dot{c}_n(t) \, |n; t\rangle + c_n(t) \frac{\partial}{\partial t} \, |n; t\rangle \right] = 0. \tag{16.67}$$

So,

$$\dot{c}_m(t) = -\sum_n c_n(t) \mathrm{e}^{\mathrm{i}[\theta_n(t) - \theta_m(t)]} \, \langle m; t| \, \frac{\partial}{\partial t} \, |n; t\rangle \,. \tag{16.68}$$

Since

$$\langle n; t| \, \dot{H} \, |m; t\rangle = [E_n(t) - E_m(t)] \, \langle m; t| \, \frac{\partial}{\partial t} \, |n; t\rangle \,, \tag{16.69}$$

so,

$$\dot{c}_m(t) = -c_m(t) \, \langle m; t| \, \frac{\partial}{\partial t} \, |m; t\rangle - \sum_n c_n(t) \mathrm{e}^{\mathrm{i}(\theta_n - \theta_m)} \frac{\langle m; t| \, \dot{H} \, |n; t\rangle}{E_n - E_m}. \tag{16.70}$$

Now we can apply the adiabatic approximation, which amounts to neglecting the second term in (16.70). Roughly, this means that

$$\frac{\langle m; t| \, \dot{H} \, |n; t\rangle}{E_n - E_m} \ll \langle m; t| \, \frac{\partial}{\partial t} \, |m; t\rangle \sim \frac{E_m}{\hbar}. \tag{16.71}$$

Let

$$c_n(t) = \mathrm{e}^{\mathrm{i}\gamma_n(t)} c_n(0), \ \ \gamma_n(t) = \mathrm{i} \int_0^t \langle n; t'| \frac{\partial}{\partial t'} |n; t'\rangle \, \mathrm{d}t' \,. \tag{16.72}$$

In other words,

$$\dot{\gamma}_n(t) = \mathrm{i} \, \langle n; t| \frac{\partial}{\partial t} |n; t\rangle \,. \tag{16.73}$$

In replace of derivative $R(t)$,

$$\nabla_R \gamma_n = \mathrm{i} \, \langle n; \vec{R}| \nabla_R |n; \vec{R}\rangle = \mathbf{A}(\mathbf{R}). \tag{16.74}$$

We can find that it is independent from time. So we call it geometrical phase. And $\mathbf{A}(\mathbf{R})$ is called Berry connection.

$$\gamma_n = \oint \mathbf{A} \cdot \mathrm{d}\mathbf{R} = \iint_S \mathbf{B} \cdot \mathrm{d}\mathbf{S} . \tag{16.75}$$

Where

$$\mathbf{B} = \nabla_{\mathbf{R}} \times \mathbf{A}. \tag{16.76}$$

We now multiply $|n;t\rangle$ by an arbitrary phase phase factor that changes through $\mathbf{R}$-space:

$$|n;t\rangle \longrightarrow \mathrm{e}^{\mathrm{i}\delta(\mathbf{R})} |n;t\rangle . \tag{16.77}$$

Then

$$\tilde{A}_n(\mathbf{R}) = \mathbf{A}_n(\mathbf{R}) - \nabla_{\mathbf{R}}\delta(\mathbf{R}), \tag{16.78}$$

$$\tilde{\mathbf{B}} = \mathbf{B}. \tag{16.79}$$

For further calculation, we derive another form of $\mathbf{B}_n(\mathbf{R})$.

$$\mathbf{B}_n(\mathbf{R}) = \mathrm{i} \left[\nabla_{\mathbf{R}} \langle n;t| \right] \times \left[\nabla_{\mathbf{R}} |n;t\rangle \right] = \mathrm{i} \sum_{n \neq m} \left[\nabla_{\mathbf{R}} \langle n;t| \right] |m;t\rangle \times \langle m;t| \left[\nabla_{\mathbf{R}} |n;t\rangle \right] . \tag{16.80}$$

Since

$$\langle m;t| \left[\nabla_{\mathbf{R}} |n;t\rangle \right] = \frac{\langle m;t| \left[\nabla_{\mathbf{R}} H \right] |n;t\rangle}{E_n - E_m}, \ n \neq m, \tag{16.81}$$

we have

$$\mathbf{B}_n(\mathbf{R}) = \mathrm{i} \sum_{m \neq n} \frac{\langle n;t| \left[\nabla_{\mathbf{R}} H \right] |m;t\rangle \times \langle m;t| \left[\nabla_{\mathbf{R}} H \right] |n;t\rangle}{(E_n - E_m)^2} \tag{16.82}$$

17   Path Integral

17.1   Propagators

One has

$$\langle \mathbf{x}|\alpha, t_0; t\rangle = \langle \mathbf{x}| \exp\left[\frac{-\mathrm{i}H(t - t_0)}{\hbar} \right] |\alpha, t_0\rangle$$
$$= \int \mathrm{d}\mathbf{x}' \langle \mathbf{x}| \exp\left[\frac{-\mathrm{i}H(t - t_0)}{\hbar} \right] |\mathbf{x}'\rangle \langle \mathbf{x}'|\alpha, t_0\rangle . \tag{17.1}$$

Let

$$K(\mathbf{x}, t; \mathbf{x}', t_0) = \langle \mathbf{x}| \exp\left[\frac{-\mathrm{i}H(t - t_0)}{\hbar} \right] |\mathbf{x}'\rangle , \tag{17.2}$$

then,

$$\psi(\mathbf{x}, t) = \int \mathrm{d}\mathbf{x}' \, K(\mathbf{x}, t; \mathbf{x}', t_0)\psi(\mathbf{x}', t_0). \tag{17.3}$$

We call $K(\mathbf{x}, t; \mathbf{x}', t_0)$ the propagator, it connects the wave functions at t and t_0. It is easy to know that

$$\lim_{t \to t_0} K(\mathbf{x}, t; \mathbf{x}', t_0) = \delta(\mathbf{x} - \mathbf{x}'). \tag{17.4}$$

Let us consider a free particle in one dimension as an example.

$$K(x,t;x',t_0) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \mathrm{d}p' \exp\left[\frac{\mathrm{i}p'(x-x')}{\hbar} - \frac{\mathrm{i}p'^2(t-t_0)}{2m\hbar}\right]. \tag{17.5}$$

The result is[1].

$$K(x,t;x',t_0) = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar(t-t_0)}} \exp\left[\frac{\mathrm{i}m(x-x')^2}{2\hbar(t-t_0)}\right]. \tag{17.6}$$

17.2   Propagator as a Transition Amplitude

In Heisenberg picture, the propagator can also be written as

$$\begin{aligned} K(\mathbf{x},t;\mathbf{x}',t_0) &= \langle\mathbf{x}| \exp\left(\frac{-\mathrm{i}Ht}{\hbar}\right) \exp\left(\frac{\mathrm{i}Ht_0}{\hbar}\right) |\mathbf{x}'\rangle \\ &= \langle\mathbf{x},t|\mathbf{x}',t_0\rangle. \end{aligned} \tag{17.7}$$

It is the amplitude for the particle to go from a space-time point $(\mathbf{x},t)$ to $(\mathbf{x}',t_0)$.

Because at any given time the position kets in the Heisenberg picture form a complete set, it is legitimate to insert the identity operator written as

$$\int \mathrm{d}\mathbf{x}' \, |\mathbf{x}',t'\rangle \, \langle\mathbf{x}',t'| = 1. \tag{17.8}$$

Clearly, we can divide the time interval into as many smaller sub-intervals as we wish.

17.3   Feynman's Formulation

Without loss of generality we restrict ourselves to one-dimensional problems.

$$\begin{aligned} \langle x_N,t_N|x_1,t_1\rangle &= \int \mathrm{d}x_{N-1} \int \mathrm{d}x_{N-2} \cdots \int \mathrm{d}x_2 \, \langle x_N,t_N|x_{N-1},t_{N-1}\rangle \\ &\times \langle x_{N-1},t_{N-1}|x_{N-2},t_{N-2}\rangle \cdots \langle x_2,t_2|x_1,t_1\rangle. \end{aligned} \tag{17.9}$$

Let us make some correspondence between the classical and quantum formalism. We shall know from (17.6) that

$$\exp\left[\mathrm{i}\int_{t_1}^{t_2} \frac{L_{\text{classical}}(x,\dot{x})\,\mathrm{d}t}{\hbar}\right] \sim \langle x_2,t_2|x_1,t_1\rangle. \tag{17.10}$$

Denote

$$S(n,n-1) := \int_{t_{n-1}}^{t_n} L_{\text{classical}}(x,\dot{x})\,\mathrm{d}t. \tag{17.11}$$

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[1]We need to deal with a integral in the form of $\int_{x\in\mathbb{R}} \exp(\pm\mathrm{i}\alpha x^2)\,\mathrm{d}x = \sqrt{\frac{\pi}{\alpha}}\exp(\pm\mathrm{i}\pi/4)$. See Fresnel integral. Usually, it can be written as $\sqrt{\frac{\pi}{\mp\mathrm{i}\alpha}}$.

We multiple this kind of expressions

$$\prod_{i=2}^{N} \exp\left[\frac{\mathrm{i}S(n, n-1)}{\hbar}\right] = \exp\left[\left(\frac{\mathrm{i}}{\hbar}\sum_{n=2} NS(n, n-1)\right)\right] = \exp\left[\frac{\mathrm{i}S(N, 1)}{\hbar}\right].$$
(17.12)

This does not yet give $\langle x_N, t_N | x_1, t_1 \rangle$; rather, this equation is the contribution. We must still integrate over $x_2, x_3, \cdots, x_{N-1}$. At the same time, exploiting the composition property, we let the time interval between t_{n-1} and t_n be infinitesimally small. Thus, we can feel that

$$\langle x_N, t_N | x_1, t_1 \rangle \sim \sum_{\text{all paths}} \exp\left[\frac{\mathrm{i}S(N, 1)}{\hbar}\right].$$
(17.13)