

Quantum Mechanics Technology Processing and Conclusions

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1 Quantization

$$\oint p dq = nh + C, \quad n = 1, 2, 3, \dots \quad (1.1)$$

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

2 Heisenberg's Breakthrough

Heisenberg use matrices to represent quantum states.¹

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

With the **Ritz combination law**²

$$\omega_{n,m} = \omega_{n,k} + \omega_{k,m}, \quad (2.2)$$

we can calculate x^2 like

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

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:

$$\ddot{x} + \omega_0^2 x = 0. \quad (2.4)$$

We can deduce that

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

Their's a strange assumption, we may treat³ $\omega_{n,n+1}$ 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

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

in a period can not be zero.⁴ Then we obtain⁵

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

¹Here 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.

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

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

⁴ $\omega_{n,n} = 0$.

⁵Here 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

$$\frac{d\omega}{dk} = v_g = \frac{pc^2}{E} \quad (3.1)$$

and

$$E^2 = p^2 c^2 + m_0^2 c^4 \quad (3.2)$$

with

$$E = \hbar\omega \quad (3.3)$$

to derive that

$$p = \hbar k. \quad (3.4)$$

It is wave-like. The 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

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

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

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

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

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

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 denote¹ the state ψ as $|\psi\rangle$, with its dual form $\langle\psi|$. Each of these vectors contains

¹Clear and simple, its my favorite.

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

$$a|\alpha\rangle + b|\beta\rangle \xrightarrow{DC} a^* \langle\alpha| + b^* \langle\beta|, \quad \forall a, b \in \mathbb{C}. \quad (4.1)$$

Inner product:

$$\langle\alpha|\beta\rangle := \langle\alpha| |\beta\rangle \quad (4.2)$$

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

$$\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^* \quad (4.3)$$

and

$$\langle\alpha|\alpha\rangle \geq 0. \quad (4.4)$$

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

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

4.2 Operator

All the operator¹ 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

$$X|\psi\rangle \xrightarrow{DC} \langle\psi|X^\dagger. \quad (4.5)$$

We say X is **Hermitian** iff.

$$X^\dagger = X. \quad (4.6)$$

Easy to prove:

$$(XY)^\dagger = Y^\dagger X^\dagger, \quad (4.7)$$

$$(|\alpha\rangle\langle\beta|)^\dagger = |\beta\rangle\langle\alpha|, \quad (4.8)$$

$$\langle\beta|X|\alpha\rangle = \langle\alpha|X^\dagger|\beta\rangle^*. \quad (4.9)$$

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

$$A|a_1\rangle = a_1|a_1\rangle, \quad \langle a_2|A = a_2^* \langle a_2|. \quad (4.10)$$

Hence,

$$(a_1 - a_2^*) \langle a_2|a_1\rangle = 0. \quad (4.11)$$

Let $a_2 = a_1$, then we obtain

$$a_1 = a_2^*. \quad (4.12)$$

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

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

$$\langle a_2 | a_1 \rangle = 0. \quad (4.13)$$

i.e. the eigenkets are orthogonal. \square

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

$$\sum_a |a\rangle \langle a| = 1. \quad (4.14)$$

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

$$\Lambda_a = |a\rangle \langle a|. \quad (4.15)$$

If we use (4.14) 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

$$X = \sum_{a,b} |a\rangle \langle a| X |b\rangle \langle b|. \quad (4.16)$$

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

$$X^\dagger = \sum_{a,b} |b\rangle \langle b| X |a\rangle \langle a| = X. \quad (4.17)$$

So X is Hermitian.

5 Commutator and Anticommutator

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

$$[A, B] = AB - BA. \quad (5.1)$$

And the **anticommutator** is

$$\{A, B\} = AB + BA. \quad (5.2)$$

Its easy to check

$$[AB, C] = A[B, C] + [A, C]B, \quad (5.3)$$

$$[A, BC] = [A, B]C + B[A, C], \quad (5.4)$$

$$[A, [B, C]] + [B, [A, C]] + [C, [A, B]] = 0, \quad (5.5)$$

$$[A, B]^\dagger = [B^\dagger, A^\dagger]. \quad (5.6)$$

¹We will explain it soon.

$$\{AB, C\} = A\{B, C\} - [A, C]B, \quad (5.7)$$

$$\{A, BC\} = \{A, B\}C - B[A, C]. \quad (5.8)$$

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

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

we have

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

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

$$[f(A), B] = f'(A)[A, B]. \quad (5.11)$$

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

$$[A, g(B)] = g'(B)[A, B]. \quad (5.12)$$

6 Compatible Observables

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

$$[A, B] = 0. \quad (6.1)$$

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

$$\Delta A := A - \langle A \rangle, \quad (7.1)$$

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

$$\langle (\Delta A)^2 \rangle = \langle (A^2 - 2A \langle A \rangle + \langle A \rangle^2) \rangle = \langle A^2 \rangle - \langle A \rangle^2. \quad (7.2)$$

Theorem 7.1

For any state, we must have the following inequality:

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

Proof. The Schwarz inequality¹:

$$\langle \alpha | \alpha \rangle \langle \beta | \beta \rangle \geq |\langle \alpha | \beta \rangle|^2. \quad (7.4)$$

Take²

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

then,

$$\langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq |\langle \Delta A \Delta B \rangle|^2. \quad (7.5)$$

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

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

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

$$|\langle \Delta A \Delta B \rangle|^2 = \frac{1}{4} |[\Delta A, \Delta B]|^2 + \frac{1}{4} |\{\Delta A, \Delta B\}|^2. \quad (7.7)$$

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

8 Position and Momentum

I will follow J. J. Sakurai's steps to derive some famous results. As continuous spectra, they have following changes³:

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

Where $\delta(\xi' - \xi'')$ is the [Dirac delta function](#).

$$\sum_a |a\rangle \langle a| = 1 \longrightarrow \int d\xi |\xi\rangle \langle \xi| = 1. \quad (8.2)$$

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

$$[\hat{x}_i, \hat{x}_j] = 0. \quad (8.3)$$

$$|\mathbf{x}\rangle = |x, y, z\rangle. \quad (8.4)$$

$$\hat{x} |\mathbf{x}\rangle = x |\mathbf{x}\rangle, \quad \hat{y} |\mathbf{x}\rangle = y |\mathbf{x}\rangle, \quad \hat{z} |\mathbf{x}\rangle = z |\mathbf{x}\rangle. \quad (8.5)$$

We call

$$\psi_\alpha(x) = \langle x | \alpha \rangle \quad (8.6)$$

the wave function.

¹Consider $|\alpha\rangle + \lambda |\beta\rangle$ and take $\lambda = -\langle \beta | \alpha \rangle \langle \beta | \beta \rangle$.

²Blank ket $|\rangle$ emphasizes the fact that our consideration may be applied to any ket.

³We use ξ to represent a continuous variable.

8.2 Translation

Consider an operator $\mathcal{J}(\mathbf{dx})$ satisfying

$$\mathcal{J}(\mathbf{dx})|\mathbf{x}\rangle = |\mathbf{x}\rangle. \quad (8.7)$$

Then

$$\mathcal{J}^\dagger(\mathbf{dx})\mathcal{J}(\mathbf{dx}) = 1 \quad (8.8)$$

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

$$\mathcal{J}(\mathbf{dx}_1 + \mathbf{dx}_2) = \mathcal{J}(\mathbf{dx}_1) + \mathcal{J}(\mathbf{dx}_2). \quad (8.9)$$

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:

$$\mathcal{J}(-\mathbf{dx}) = \mathcal{J}^{-1}(\mathbf{dx}). \quad (8.10)$$

For the fourth property,

$$\lim_{\mathbf{dx} \rightarrow 0} \mathcal{J}(\mathbf{dx}) = 1. \quad (8.11)$$

Consider

$$\mathcal{J}(\mathbf{dx}) = 1 - i\hat{\mathbf{K}} \cdot \mathbf{dx}, \quad (8.12)$$

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

$$[\hat{\mathbf{x}}, \mathcal{J}(\mathbf{dx})] = \mathbf{dx}. \quad (8.13)$$

Plug in (8.12), we obtain

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

8.3 Momentum

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

$$\mathbf{x}_{\text{new}} = \mathbf{x} + \mathbf{dx}, \quad \mathbf{p}_{\text{new}} = \mathbf{p}. \quad (8.15)$$

obtainable from the generating function

$$F(\mathbf{x}, \mathbf{p}) = \mathbf{x} \cdot \mathbf{p}_{\text{new}} + \mathbf{p} \cdot \mathbf{dx}. \quad (8.16)$$

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

$$\mathcal{J}(\mathbf{dx}) = 1 - i\hat{\mathbf{p}} \cdot \mathbf{dx} / \hbar. \quad (8.17)$$

The commutation relation (8.14) now becomes

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{i,j}. \quad (8.18)$$

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

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

As for finite position,

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

By computation,

$$[\hat{p}_i, \hat{p}_j] = 0. \quad (8.21)$$

8.4 Momentum Operator in the Position Basis

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

$$\hat{\mathbf{p}} |\alpha\rangle = \int d\mathbf{x} |\mathbf{x}\rangle (-i\hbar \nabla \langle \mathbf{x} | \alpha \rangle). \quad (8.22)$$

That is also

$$\langle \mathbf{x} | \hat{\mathbf{p}} |\alpha\rangle = -i\hbar \nabla \langle \mathbf{x} | \alpha \rangle. \quad (8.23)$$

8.5 Momentum-Space Wave Function

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

$$\langle p | \alpha \rangle = \phi_\alpha(p). \quad (8.24)$$

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

$$\langle x | \hat{p} | p \rangle = p \langle x | p \rangle. \quad (8.25)$$

By (8.23),

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

Thus,

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

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

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

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

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

¹Is it an easy integration?

For three dimension case,

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

8.6 Dirac's Corresponding Rule

Replace classical Poisson bracket by commutator as follows¹

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

9 Probability Density and Probability Current

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

$$\rho := \psi\psi^*. \quad (9.1)$$

The probability need to be conserved,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0. \quad (9.2)$$

Then we can deduce from Schrödinger equation that

$$\mathbf{j} = \left(\frac{\hbar}{m} \right) \text{Im}(\psi^* \nabla \psi). \quad (9.3)$$

If we write ψ into the form of

$$\psi = \sqrt{\rho} e^{\frac{iS}{\hbar}}, \quad (9.4)$$

then²

$$\mathbf{j} = \frac{\rho \nabla S}{m}. \quad (9.5)$$

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

$$\int \mathbf{j} d\mathbf{x} = \frac{\langle \mathbf{p} \rangle}{m}. \quad (9.6)$$

It is some thing like velocity.

¹I think the $i\hbar$ comes from the translation where setting a constant as $i\hbar$.

²Here is the case with charge.

10 Exponential Operators and Baker-Hausdorff Lemma

If it exists, then we denote¹

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!}. \quad (10.1)$$

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

$$\exp(A) \exp(B) = \exp(A + B). \quad (10.2)$$

Define²

$$O(\lambda) = e^{i\lambda G} A e^{-i\lambda G}, \quad (10.3)$$

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

$$\frac{d}{d\lambda} O(\lambda) = i e^{i\lambda G} [G, A] e^{-i\lambda G} = i [G, O(\lambda)]. \quad (10.4)$$

Hence,

$$O(\lambda) = O(0) + i \int_0^\lambda d\lambda_1 [G, O(\lambda_1)]. \quad (10.5)$$

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

$$O(\lambda) = A + i \int_0^\lambda d\lambda_1 [G, A] + i^2 \int_0^\lambda d\lambda_1 \int_0^{\lambda_1} d\lambda_2 [G, [G, A]] + \dots \quad (10.6)$$

Easy to check

$$\int_0^\lambda d\lambda_1 \int_0^{\lambda_1} d\lambda_2 \dots \int_0^{\lambda_{n-1}} d\lambda_n = \frac{\lambda^n}{n!}. \quad (10.7)$$

Therefore³,

$$\boxed{e^{i\lambda G} A e^{-i\lambda G} = \sum_{n=0}^{\infty} \frac{(i\lambda)^n}{n!} C_G^{(n)}(A)}, \quad (10.8)$$

where⁴,

$$C_G(A) = [G, A], \quad C_G^{(n)}(A) = [G, C_G^{(n-1)}(A)]. \quad (10.9)$$

Or we can write in the form

$$e^\Omega A e^{-\Omega} = e^{\text{Ad}_\Omega}(A). \quad (10.10)$$

¹Sometimes we denote as $\exp(A)$.

²We 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.

³It 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.

⁴This 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

$$e^A e^B e^{-A} = e^B + [A, e^B] + \dots \quad (10.11)$$

By (5.4), we can induct on n that

$$[A, [A, B]^{n-1} e^B] = [A, B]^n e^B. \quad (10.12)$$

So,

$$e^A e^B = e^B e^A e^{[A, B]}. \quad (10.13)$$

We also have another more symmetrical form¹:

Theorem 10.1

$$[A, [A, B]] = [B, [A, B]] = 0 \Rightarrow e^A e^B = e^{A+B} e^{\frac{1}{2}[A, B]}. \quad (10.14)$$

Proof. Let

$$O(\lambda) = e^{\lambda A} e^{\lambda B}, \quad (10.15)$$

then,

$$\frac{dO}{d\lambda} = e^{\lambda A} (A + B) e^{\lambda B}. \quad (10.16)$$

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.

$$e^{\lambda A} B e^{\lambda B} = e^{\lambda A} B e^{-\lambda A} e^{\lambda A} e^{\lambda B}. \quad (10.17)$$

By Baker-Hausdorff lemma, we obtain

$$\frac{dO}{d\lambda} = [(A + B) + \lambda[A, B]] O. \quad (10.18)$$

The solution is

$$O = \exp \left[\lambda(A + B) + \frac{1}{2} \lambda^2 [A, B] \right]. \quad (10.19)$$

□

11 Harmonic Oscillator

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

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2. \quad (11.1)$$

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

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

11.1 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

$$\left[-\frac{1}{2} \frac{d^2}{dz^2} + \frac{1}{2} z^2 \right] \psi(z) = \frac{E}{\hbar\omega} \psi(z). \quad (11.2)$$

A must to satisfy is

$$\lim_{z \rightarrow \infty} \psi(z) = 0. \quad (11.3)$$

So we first analyze the behavior of $\psi(z)$ at $z \rightarrow \pm\infty$. For $\psi'' = z^2\psi$, we try the solution¹ $\psi(z) = e^S(z)$

$$\psi' = S' \psi, \quad \psi'' = (S'' + S'^2) \psi. \quad (11.4)$$

Comparison of two expression yields

$$S'' + S'^2 = z^2. \quad (11.5)$$

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

$$\psi(z) = e^{-\frac{z^2}{2}} u(z). \quad (11.6)$$

$$\frac{d^2}{dz^2} u(z) - 2z \frac{d}{dz} u(z) - (\lambda - 1) u(z) = 0. \quad (11.7)$$

We consider the series solution, let

$$u(z) = \sum_{k=0}^{+\infty} a_k z^k. \quad (11.8)$$

The we can deduce that

$$\frac{a_{k+2}}{a_k} = \frac{2k+1-\lambda}{(k+1)(k+2)}. \quad (11.9)$$

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

$$a_k = 0. \quad (11.10)$$

Therefore,

$$\lambda_n = 2n + 1, \quad n = 0, 1, 2, \dots \quad (11.11)$$

which means

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega. \quad (11.12)$$

¹This may keep the form.

The solution of (11.7) is Hermite polynomials¹ $H_n(z)$.

$$\psi(x) = e^{-\frac{1}{2} \frac{m\omega x^2}{\hbar}} \sum_{n=0}^{+\infty} \frac{c_n}{n!} H_n \left(x / \sqrt{\frac{\hbar}{m\omega}} \right). \quad (11.13)$$

And for a fixed n , the normalized wavefunction is

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{-\frac{x^2}{2}} H_n(x). \quad (11.14)$$

11.2 Method of Algebra

In usual computing law,

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 = \frac{1}{2} m \omega^2 \left(x - \frac{ip}{m\omega} \right) \left(x + \frac{ip}{m\omega} \right). \quad (11.15)$$

Let ²

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i\hat{p}}{m\omega} \right), \quad \hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i\hat{p}}{m\omega} \right). \quad (11.16)$$

Then,

$$[\hat{a}, \hat{a}^\dagger] = 1. \quad (11.17)$$

Let

$$\hat{N} = \hat{a}^\dagger \hat{a}, \quad (11.18)$$

then,

$$\hat{H} = \hbar\omega \left(\hat{N} + \frac{1}{2} \right). \quad (11.19)$$

So \hat{N} is compatible with \hat{H} . We denote an energy eigenket of \hat{N} by its eigenvalue³ n , so

$$\hat{N} |n\rangle = n |n\rangle, \quad (11.20)$$

$$\hat{H} |n\rangle = \left(n + \frac{1}{2} \right) \hbar\omega |n\rangle. \quad (11.21)$$

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

$$[\hat{N}, \hat{a}] = -\hat{a}, \quad [\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger. \quad (11.22)$$

As a result, we have

$$\hat{N} \hat{a}^\dagger |n\rangle = [\hat{N}, \hat{a}^\dagger] |n\rangle + \hat{a}^\dagger \hat{N} |n\rangle = (n+1) \hat{a}^\dagger |n\rangle, \quad (11.23)$$

$$\hat{N} \hat{a} |n\rangle = [\hat{N}, \hat{a}] |n\rangle + \hat{a} \hat{N} |n\rangle = (n-1) \hat{a} |n\rangle. \quad (11.24)$$

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

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

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

We write

$$\hat{a} |n\rangle = c |n-1\rangle, \quad (11.25)$$

then,

$$\langle n | \hat{N} | n \rangle = \langle n | \hat{a}^\dagger \hat{a} | n \rangle = |c|^2. \quad (11.26)$$

Thus,

$$\hat{a} |n\rangle = \sqrt{n} |n-1\rangle. \quad (11.27)$$

Similarly, it is easy to show that¹

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle. \quad (11.28)$$

From (11.26) 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

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^\dagger), \quad \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}} (-\hat{a} + \hat{a}^\dagger), \quad (11.29)$$

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

11.3 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 ,

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

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

—*Modern Quantum Mechanics*

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

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

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

$$A = e^{\lambda a^\dagger}. \quad (11.30)$$

¹Memory trick: the square root of a larger one.

use (10.13) to do the normalization¹,

$$\langle 0 | e^{\lambda^* a} e^{\lambda a^\dagger} | 0 \rangle = e^{|\lambda|^2}. \quad (11.31)$$

Therefore²,

$$|\lambda\rangle = e^{-|\lambda|^2/2} e^{\lambda a^\dagger} |0\rangle = e^{-|\lambda|^2/2} \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}} |n\rangle. \quad (11.32)$$

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 $|0\rangle$.

$$e^{-ip\Delta x/\hbar} |0\rangle = e^{\frac{(a^\dagger - a)\Delta x}{\sqrt{2}i}} |0\rangle \sim e^{\frac{a^\dagger \Delta x}{\sqrt{2}i}} |0\rangle. \quad (11.33)$$

11.4 High Dimensional Case

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

$$H = \frac{p^i p_i}{2m} + \frac{1}{2} m \omega^2 x^i x_i. \quad (11.34)$$

And the creation and annihilation operators are

$$a_i = \frac{1}{\sqrt{2}} \left(\frac{x_i}{l} + \frac{ip_i l}{\hbar} \right), \quad a_i^\dagger = \frac{1}{\sqrt{2}} \left(\frac{x_i}{l} - \frac{ip_i l}{\hbar} \right). \quad (11.35)$$

$$[a_i, a_j] = 0, \quad [a_i, a_j^\dagger] = \delta_{ij}. \quad (11.36)$$

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

$$H = \hbar \omega \left(N + \frac{n}{2} \right). \quad (11.37)$$

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

$$[a_i^\dagger a_j, H] = 0. \quad (11.38)$$

That means the angular momentum is conserved.

12 Gauge Transformations in Electromagnetism

12.1 Gauge Transformations

In Classic mechanics, the Hamiltonian is

$$H = \frac{1}{2m} \left(\mathbf{p} - \frac{q\mathbf{A}}{c} \right)^2 + q\phi. \quad (12.1)$$

¹Expand the series we get $\exp(\lambda a) |0\rangle = |0\rangle$.

²A Poission distribution.

³It'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 generator of translation. And kinematical (or mechanical) momentum, denoted by:

$$\mathbf{\Pi} := \mathbf{p} - \frac{q\mathbf{A}}{c}. \quad (12.2)$$

Easy to check that

$$[\Pi_i, \Pi_j] = \frac{i\hbar q}{c} \varepsilon_{ijk} B_k. \quad (12.3)$$

The Hamiltonian:

$$H = \frac{\Pi^2}{2m} + q\phi. \quad (12.4)$$

From (12.2) we can use the substitution

$$\mathbf{p} \longrightarrow \mathbf{p} - \frac{q\mathbf{A}}{c} \quad (12.5)$$

In position representation¹,

$$\nabla \longrightarrow \nabla - \left(\frac{iq}{\hbar c} \right) \mathbf{A}. \quad (12.6)$$

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

$$\mathbf{j} = \frac{\rho}{m} \left(\nabla S - \frac{q\mathbf{A}}{c} \right). \quad (12.7)$$

$$\int \mathbf{j} d\mathbf{x} = \frac{\langle \mathbf{\Pi} \rangle}{m}. \quad (12.8)$$

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

$$\phi \rightarrow \phi - \frac{1}{c} \frac{\partial \Lambda}{\partial t}, \quad \mathbf{A} \rightarrow \mathbf{A} + \nabla \Lambda. \quad (12.9)$$

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,

$$\tilde{\mathbf{A}} = \mathbf{A} + \nabla \Lambda. \quad (12.10)$$

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

$$\langle \alpha | \alpha \rangle = \langle \tilde{\alpha} | \tilde{\alpha} \rangle, \quad \langle \alpha | \mathbf{x} | \alpha \rangle = \langle \tilde{\alpha} | \mathbf{x} | \tilde{\alpha} \rangle, \quad \langle \alpha | \mathbf{\Pi} | \alpha \rangle = \langle \tilde{\alpha} | \tilde{\mathbf{\Pi}} | \tilde{\alpha} \rangle. \quad (12.11)$$

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

$$|\tilde{\alpha}\rangle = g |\alpha\rangle. \quad (12.12)$$

¹We 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:

$$g^\dagger g = 1. \quad (12.13)$$

$$g^\dagger \mathbf{p} g = \mathbf{p} + \frac{q \nabla \Lambda}{c}. \quad (12.14)$$

It is easy to find

$$g = \exp \left(\frac{iq\Lambda}{\hbar c} \right) \quad (12.15)$$

satisfies the above conditions. And we have

$$g^\dagger \tilde{\Pi}^n g = \prod_{k=1}^n g^\dagger \tilde{\Pi} g = \Pi^n. \quad (12.16)$$

So, for any function f ,

$$g^\dagger f(\tilde{\Pi}) g = f(\Pi). \quad (12.17)$$

(12.14) and (12.17) tell us, mechanical momentum is gauge invariant, but the canonical momentum is not.

Form the wave function,

$$S \longrightarrow S + \frac{q\Lambda}{c}. \quad (12.18)$$

This is highly satisfactory because we see that the probability flux given by (12.7) 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.

$$\tilde{H} |\tilde{\alpha}\rangle = g g^\dagger \tilde{H} g |\alpha\rangle = g H |\alpha\rangle = i\hbar \frac{\partial}{\partial t} g |\alpha\rangle = i\hbar \frac{\partial}{\partial t} |\tilde{\alpha}\rangle. \quad (12.19)$$

Since t is only a parameter, it does not affect the commutators, so when $\frac{\partial \Lambda}{\partial t} \neq 0$, (12.17) 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.

12.2 Landau Levels and Quantum Hall Effect

¹ Let's consider a simple magnetic field,

$$\mathbf{B} = -B\hat{\mathbf{z}}. \quad (12.20)$$

We take

$$A_x = By, \quad A_y = A_z = 0. \quad (12.21)$$

¹We use IS of units this subsection.

We just consider 2D case, the Hamiltonian is

$$H = \frac{(p_x - qBy)^2}{2m} + \frac{p_y^2}{2m} = \frac{1}{2}m\omega_c^2 \left(y - \frac{p_x l_B^2}{\hbar} \right)^2 + \frac{p_y^2}{2m}, \quad (12.22)$$

where,

$$\omega_c = \frac{qB}{m}, \quad l_B = \sqrt{\frac{\hbar}{qB}}. \quad (12.23)$$

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

$$\psi_{n,k_x}(x, y) = e^{ik_x x} \psi(y). \quad (12.24)$$

Then,

$$\left[\frac{p_y^2}{2m} + \frac{1}{2}m\omega_c^2 (y - l_B^2 k_x)^2 \right] |\psi\rangle = E_n |\psi\rangle. \quad (12.25)$$

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

$$E_n = \hbar\omega_c \left(n + \frac{1}{2} \right). \quad (12.26)$$

13 Angular Momentum

13.1 Infinitesimal Rotations in Quantum Mechanics

We want to construct a rotation operator \mathcal{D}^1 . The appropriate infinitesimal operators could be written as

$$U_\varepsilon = 1 - iG\varepsilon \quad (13.1)$$

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 k th axis by angle $d\varphi$ can be obtained by letting

$$G \rightarrow \frac{J_k}{\hbar}, \quad \varepsilon \rightarrow d\phi. \quad (13.2)$$

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 $d\phi \rightarrow 0$. More generally, we have

$$\mathcal{D}(\hat{\mathbf{n}}, d\phi) = 1 - i \left(\frac{\mathbf{J} \cdot \hat{\mathbf{n}}}{\hbar} \right) d\phi \quad (13.3)$$

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

$$\mathcal{D}_{\hat{\mathbf{n}}}(\phi) = \lim_{N \rightarrow +\infty} \left[1 - i \left(\frac{\mathbf{J} \cdot \hat{\mathbf{n}}}{\hbar} \right) \frac{\phi}{N} \right]^N = \exp \left[-i \left(\frac{\mathbf{J} \cdot \hat{\mathbf{n}}}{\hbar} \right) \phi \right]. \quad (13.4)$$

¹The symbol \mathcal{D} stems from the German word *Drehung*, meaning “rotation.”

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

$$\mathcal{D}_{\hat{\mathbf{n}}}(\varepsilon) \approx 1 - i \left(\frac{\mathbf{J} \cdot \hat{\mathbf{n}}}{\hbar} \right) \varepsilon - \frac{1}{2!} \left(\frac{\mathbf{J} \cdot \hat{\mathbf{n}}}{\hbar} \right)^2 \varepsilon^2. \quad (13.5)$$

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

$$[\mathcal{D}_x(\varepsilon), \mathcal{D}_y(\varepsilon)] = \mathcal{D}_z(\varepsilon^2) - 1. \quad (13.6)$$

So,

$$[J_x, J_y] = i\hbar J_z. \quad (13.7)$$

In general,

$$[J_i, J_k] = i\hbar \varepsilon_{ijk} J_k. \quad (13.8)$$

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

$$[J_i, a] = 0, \quad [J_i, v_j] = i\hbar \varepsilon_{ijk} v_k. \quad (13.9)$$

13.2 Orbital Angular Momentum

Orbital angular momentum is defined as

$$\mathbf{L} = \mathbf{x} \times \mathbf{p}. \quad (13.10)$$

Easy to check that \mathbf{L} satisfies (13.7). Expand \mathbf{L}^2 :

$$\begin{aligned} \mathbf{L}^2 &= \sum_{ijklmk} \varepsilon_{ijk} x_i p_j \varepsilon_{lmk} x_l p_m \\ &= \sum_{ijlm} (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) x_i p_j x_l p_m \\ &= \sum_{ijlm} [\delta_{il} \delta_{jm} x_i (x_l p_j - i\hbar \delta_{jl}) p_m - \delta_{im} \delta_{jl} x_i p_j (p_m x_l + i\hbar \delta_{lm})] \\ &= \mathbf{x}^2 \mathbf{p}^2 - i\hbar \mathbf{x} \cdot \mathbf{p} - \sum_{ijlm} \delta_{im} \delta_{jl} [x_i p_m (x_l p_j - i\hbar \delta_{jl}) + i\hbar \delta_{lm} x_i p_j] \\ &= \mathbf{x}^2 \mathbf{p}^2 - (\mathbf{x} \cdot \mathbf{p})^2 + i\hbar \mathbf{x} \cdot \mathbf{p}. \end{aligned} \quad (13.11)$$

We have

$$[L_i, H] = 0, \quad [L^i L_i, H] = 0, \quad [L^i L_i, L_j] = 0. \quad (13.12)$$

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

$$\langle \mathbf{x} | \mathbf{L} | \alpha \rangle = -i\hbar \mathbf{x} \times \nabla \langle \mathbf{x} | \alpha \rangle. \quad (13.13)$$

Under spherical coordinates, the nabla operator can be written as¹

$$\nabla = \frac{\partial}{\partial r} \hat{\mathbf{r}} + \frac{1}{r} \frac{\partial}{\partial \theta} \hat{\boldsymbol{\theta}} + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \hat{\boldsymbol{\phi}}. \quad (13.14)$$

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

One has,

$$\mathbf{x} = r\hat{\mathbf{r}}, \quad (13.15)$$

so,

$$\mathbf{x} \times \nabla = \frac{\partial}{\partial \theta} \hat{\phi} - \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \hat{\theta}. \quad (13.16)$$

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

$$\langle \mathbf{x} | L_z | \alpha \rangle = -i\hbar \frac{\partial}{\partial \phi} \langle \mathbf{x} | \alpha \rangle, \quad (13.17)$$

$$\langle \mathbf{x} | L_x | \alpha \rangle = -i\hbar \left(-\sin \phi \frac{\partial}{\partial \theta} - \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right) \langle \mathbf{x} | \alpha \rangle, \quad (13.18)$$

$$\langle \mathbf{x} | L_y | \alpha \rangle = -i\hbar \left(\cos \phi \frac{\partial}{\partial \theta} - \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right) \langle \mathbf{x} | \alpha \rangle. \quad (13.19)$$

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:

$$\mathbf{J}^2 |a, b\rangle = a |a, b\rangle, \quad J_z |a, b\rangle = b |a, b\rangle. \quad (13.20)$$

Consider

$$J_{\pm} := J_x \pm iJ_y, \quad (13.21)$$

then,

$$J_- = J_+^\dagger, \quad \mathbf{J}^2 = J_z^2 + \frac{1}{2}\{J_+, J_-\}. \quad J_- J_+ = \mathbf{J}^2 - J_z^2 - \hbar J_z, \quad (13.22)$$

$$[J_+, J_-] = 2\hbar J_z, \quad [J_z, J_{\pm}] = \pm \hbar J_{\pm}, \quad [\mathbf{J}^2, J_{\pm}] = 0. \quad (13.23)$$

$$J_z (J_{\pm} |a, b\rangle) = (b \pm \hbar) (J_{\pm} |a, b\rangle). \quad (13.24)$$

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

$$\mathbf{J}^2 (J_{\pm} |a, b\rangle) = J_{\pm} \mathbf{J}^2 |a, b\rangle = a (J_{\pm} |a, b\rangle). \quad (13.25)$$

So,

$$J_{\pm} |a, b\rangle = c_{\pm} |a, b \pm \hbar\rangle. \quad (13.26)$$

Then there must exist b_{\max} and b_{\min} , such that¹

$$a = b_{\max} (b_{\max} + \hbar) = b_{\min} (b_{\min} - \hbar). \quad (13.27)$$

We can infer that

$$-b_{\max} = b_{\min}, \quad (13.28)$$

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

$$b_{\min} \leq b \leq b_{\max}. \quad (13.29)$$

¹By (13.22)

$$b_{\max} = \frac{n\hbar}{2} \equiv j\hbar, \quad (13.30)$$

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

$$a = \hbar^2 j(j+1). \quad (13.31)$$

Let us also define m such that

$$b \equiv m\hbar. \quad (13.32)$$

The allowed m -values for a given j are

$$m = \underbrace{-j, -j+1, \dots, j-1, j}_{2j+1 \text{ states}}. \quad (13.33)$$

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

$$\mathbf{J}^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle, \quad J_z |j, m\rangle = m\hbar |j, m\rangle. \quad (13.34)$$

Then we can deduce that

$$J_{\pm} |j, m\rangle = \sqrt{(j \mp m)(j \pm m + 1)} \hbar |j, m\rangle, \quad (13.35)$$