Quantum Mechanics

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Chapter 1

Fundamentals of Quantum Mechanics

The mechanical description of a system state in Hamiltonian mechanics is $(q, p) \in$ phase space, where $p = \partial L/\partial q$ is the canonical momentum. The observables are functions of (q, p). Hamiltonian equations describe the evolution of the state

$$\dot{p} = -\frac{\partial H}{\partial q}\ , \quad \dot{q} = \frac{\partial H}{\partial p}. \tag{F.0.1}$$

This description needed to be changed to accommodate experimental results. For example, in Einstein's space-time deformation and geodesic motion, we describe the state by a tensor $g_{\mu\nu}$. In classical field theory, we use electric field, magnetic field, etc., to describe the states.

F.1 States in Quantum Mechanics

In quantum mechanics, we use a ket vector denoted by $|\alpha\rangle$ in a $\mathbb{C}$-Hilbert space denoted by $\mathbb{H}$ to describe a state.

Definition 1. *The inner product in a vector space V, $(-,-) : V \times V \to \mathbb{C}$, satisfies:*

- $(u, v)^* = (v, u)$*, for all* $u, v \in V$*.*
- $(u, c_1 v_1 + c_2 v_2) = c_1(u, v_1) + c_2(u, v_2)$*, for all* $u, v \in V$ *and* $c_1, c_2 \in \mathbb{C}$*.*
- $(u, u) \geq 0$*, for all* $u \in V$*, unless* $u = 0$*.*

Notice that $C\,|\alpha\rangle$, $C \neq 0$, and $|\alpha\rangle$ represent the same physical state. However, $C = |C|e^{i\theta}$ does not imply that the phase has any physical meaning; see more details later on *Berry phase*.

F.2 Observables in Quantum Mechanics

The observables are represented by (Hermitian) operators $A : \mathbb{H} \to \mathbb{H}$. The eigenvalues of the operators are the physical quantities associated with the eigenvectors. For example, the spin operators S_x, S_y, S_z ($S_i = \frac{\hbar}{2}\sigma_i$ in Pauli theory). The operator in the z-direction satisfies

$$S_z \left|+z\right\rangle = \frac{\hbar}{2} \left|+z\right\rangle \ , \quad S_z \left|-z\right\rangle = -\frac{\hbar}{2} \left|-z\right\rangle . \tag{F.2.1}$$

Remark 1. *Let $X, Y, Z : \mathbb{H} \to \mathbb{H}$ be operators. Then:*

- $X = Y$ *if* $X\left|\alpha\right\rangle = Y\left|\alpha\right\rangle$ *for all* $\left|\alpha\right\rangle \in \mathbb{H}$.
- X *is null if* $X\left|\alpha\right\rangle = 0$ *for all* $\left|\alpha\right\rangle \in \mathbb{H}$.
- *Operators are commutative and associative under* $+$*:* $X+Y = Y+X$ *and* $X+(Y+Z) = (X+Y)+Z$.
- $X\left|\alpha\right\rangle \equiv \left|\xi\right\rangle \in \mathbb{H}$ *is dual to the state* $\left\langle\xi\right| \in \mathbb{H}^*$*. We can define an operator* $X^\dagger$ *such that* $\left\langle\xi\right| = \left\langle\alpha\right| X^\dagger$*, where* $X^\dagger$ *is the Hermitian adjoint of* X*.* X *is said to be Hermitian if* $X = X^\dagger$.
- *Operators are associative under* $\cdot$ *(usually omitted):* $(XY)Z = X(YZ) = XYZ$*, but not generally commutative:* $XY \neq YX$ *in general.*
- *The Hermitian adjoint satisfies* $(XY)^\dagger = Y^\dagger X^\dagger$ *and* $\left\langle\beta\right| X \left|\alpha\right\rangle^* = \left\langle\alpha\right| X^\dagger \left|\beta\right\rangle$.

We now discuss some key theorems related to Hermitian operators. The first one is the Hermitian operators in finite-dimensional Hilbert space are always diagonalizable.

Theorem F.2.1. *Spectrum Theorem*
Let $\mathbb{H}$ finite-dimensional Hilbert space. and $A : \mathbb{H} \to \mathbb{H}$ be a Hermitian operator. Then there is a basis for $\mathbb{H}$ consisting entirely of eigenvectors of A.

The proof of this theorem is complicated and therefore skipped. In quantum mechanics, we assume that the Hermitian operators in infinite-dimensional Hilbert space are diagonalizable as well.

Theorem F.2.2. *Let $\mathbb{H}$ finite-dimensional Hilbert space. The eigenvalues of a Hermitian operator $A : \mathbb{H} \to \mathbb{H}$ are real and the eigenvectors of A corresponding to distinct eigenvalues are orthogonal.*

Proof. Let $A : \mathbb{H} \to \mathbb{H}$ be a Hermitian operator, and let $\left|\alpha\right\rangle$ and $\left|\beta\right\rangle$ be eigenvectors of A with eigenvalues α and β, respectively. By definition of a Hermitian operator, we have:

$$A\left|\alpha\right\rangle = \alpha\left|\alpha\right\rangle \quad \text{and} \quad \left\langle\beta\right| A = \beta^* \left\langle\beta\right| . \tag{F.2.2}$$

Taking the inner product of both sides with $\left|\alpha\right\rangle$, we obtain:

$$\left\langle\beta\right| A \left|\alpha\right\rangle = \beta^* \left\langle\beta|\alpha\right\rangle \ . \tag{F.2.3}$$

On the other hand, since $A\left|\alpha\right\rangle = \alpha\left|\alpha\right\rangle$, it follows that:

$$\left\langle\beta\right| A \left|\alpha\right\rangle = \alpha \left\langle\beta|\alpha\right\rangle \ . \tag{F.2.4}$$

Equating the two expressions, we get:

$$\beta^* \left\langle\beta|\alpha\right\rangle = \alpha \left\langle\beta|\alpha\right\rangle \ . \tag{F.2.5}$$

Rearranging, we find:

$$(\beta^* - \alpha) \left\langle\beta|\alpha\right\rangle = 0 \ . \tag{F.2.6}$$

If $\alpha = \beta$, then $\alpha^* - \alpha = 0$, which implies that α is real. Thus, all eigenvalues of A are real. If $\alpha \neq \beta$, then $\left\langle\beta|\alpha\right\rangle = 0$, which shows that $\left|\alpha\right\rangle$ and $\left|\beta\right\rangle$ are orthogonal. $\square$

F.2.1 Matrix Representation

The completeness relation can be expressed in terms of operators. Consider a basis $\{|\alpha\rangle\}_\alpha$ of eigenvectors with corresponding eigenvalues $\{\alpha\}_\alpha$. Then, the completeness relation is given by:

$$\sum_\alpha |\alpha\rangle \langle\alpha| = I \ , \tag{F.2.7}$$

where each projective operator is defined as $P_\alpha \equiv |\alpha\rangle \langle\alpha|$, satisfying:

$$\sum_\alpha P_\alpha = I \ . \tag{F.2.8}$$

For an operator $X : \mathbb{H} \to \mathbb{H}$, we can represent it as:

$$\begin{aligned} X &= 1XI \\ &= \sum_{\alpha,\beta} |\alpha\rangle \langle\alpha| X |\beta\rangle \langle\beta| \\ &= \sum_{\alpha,\beta} |\alpha\rangle \langle\beta| X_{\alpha\beta} \ . \end{aligned} \tag{F.2.9}$$

Here, $X_{\alpha\beta} = \langle\alpha| X |\beta\rangle$ represents the matrix elements of X in the given basis.

In matrix form, the operator X is represented as:

$$X = \begin{pmatrix} \langle 1|X|1\rangle & \langle 1|X|2\rangle & \cdots & \langle 1|X|n\rangle \\ \langle 2|X|1\rangle & \langle 2|X|2\rangle & \cdots & \langle 2|X|n\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle n|X|1\rangle & \langle n|X|2\rangle & \cdots & \langle n|X|n\rangle \end{pmatrix} \ . \tag{F.2.10}$$

In this representation, the bra and ket vectors are expressed in column and row vector forms as:

$$|\alpha\rangle = \begin{pmatrix} \langle 1|\alpha\rangle \\ \langle 2|\alpha\rangle \\ \vdots \\ \langle n|\alpha\rangle \end{pmatrix} \ , \quad \langle\beta| = \begin{pmatrix} \langle\beta|1\rangle & \langle\beta|2\rangle & \cdots & \langle\beta|n\rangle \end{pmatrix} \ . \tag{F.2.11}$$

F.2.2 Physical Observables

Hermitian operators represent physical observables. If Ω denotes an observable and $|\psi_n\rangle$ are its eigenvectors with eigenvalues ω_n, then:

$$\Omega |\psi_n\rangle = \omega_n |\psi_n\rangle \ . \tag{F.2.12}$$

Notice that from the previous theorem, we know that for an arbitrary state, it can be written as:

$$|\psi\rangle = \sum_n C_n |\psi_n\rangle \ , \tag{F.2.13}$$

the values of $|C_n|^2$ determine the probability of the quantum state being measured in state $|\psi_n\rangle$. Therefore, the average of many measurements of Ω is given by:

$$\langle\psi|\Omega|\psi\rangle = \sum_n |C_n|^2 \omega_n. \tag{F.2.14}$$

F.2.3 Dynamics

The dynamics of the quantum states are described by the *time-depenent Schrodinger equation*:

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle \ . \tag{F.2.15}$$

As a consequence, since the operator is Hermitian, the probability is conserved:

$$\frac{d \langle \psi | \psi \rangle}{dt} = 0 \ . \tag{F.2.16}$$

The eigenstates of the Hamiltonian can be obtained from the *time-independent Schrodinger equation*:

$$\frac{\hbar^2}{2m} \nabla^2 |\psi_n\rangle = E_n |\psi_n\rangle \ . \tag{F.2.17}$$

Then the time-dependent state can be obtained by the linear combination of the eigenstates:

$$|\psi\rangle = \sum_n C_n \, \mathrm{e}^{\mathrm{i}\, E_n t/\hbar} |\psi_n\rangle \ . \tag{F.2.18}$$

F.2.4 Uncertainty Principle

Let $A, B : \mathbb{H} \to \mathbb{H}$ be operators. A and B are said to be *compatible* if their commutator is zero and therefore can have the same eigenstates:

$$[A, B] \equiv AB - BA = 0 \ , \tag{F.2.19}$$

and *incompatible* if their commutator is not zero and therefore can not have the same eigenstates:

$$[A, B] \neq 0 \ . \tag{F.2.20}$$

Define a measurement error of the observable A be $\Delta A = A - \langle A \rangle$, then the variation of A is $\langle (\Delta A)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2$ and the standard error is $\sigma_A = \sqrt{\langle (\Delta A)^2 \rangle} = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$.

Let $|\alpha\rangle = \Delta A |\psi\rangle$ and $|\beta\rangle = \Delta B |\psi\rangle$. By Cauchy-Schwarz inequality, we have:

$$\begin{aligned} \langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle &= \langle \alpha | \alpha \rangle \langle \beta | \beta \rangle \\ &\geq |\, \langle \alpha | \beta \rangle \,|^2 = |\, \langle \Delta A \Delta B \rangle \,|^2 \\ &= \frac{1}{4} |\, | \, \langle [\Delta A, \Delta B] \rangle^2 + \frac{1}{4} |\, \langle \{\Delta A, \Delta B\} \rangle \,|^2 \\ &\geq \frac{1}{4} |\, \langle [A, B] \rangle \,|^2 \ . \end{aligned} \tag{F.2.21}$$

Therefore, two observables A and B always satisfy the uncertainty relation:

$$\boxed{\sigma_A \sigma_B \geq \frac{1}{2} |\, \langle [A, B] \rangle \,|} \ . \tag{F.2.22}$$

F.3 Continuous Structures

We discuss the Hilbert space formalism of quantum mechanics so far. However, we only discuss the Hilbert spaces which are finite-dimensional or countably infinite-dimensional. In this section, we discuss some continuous structures important in quantum mechanics.

F.3.1 Position Operator

In quantum mechanics, the position and momentum are operators x and p with eigenstates $|x'\rangle$ and $|p'\rangle$, respectively. The position and momentum operators satisfy the canonical commutation relation:

$$[x, p] = \mathrm{i}\,\hbar \; . \tag{F.3.1}$$

Therefore, we have the Heisenberg uncertainty principle:

$$\sigma_x \sigma_p \geq \frac{\hbar}{2} \; . \tag{F.3.2}$$

Since every particle is at some position x' in the space. We can represent any quantum state in term of $|x'\rangle$:

$$|\alpha\rangle = \sum_{x'} |x'\rangle \langle x'|\alpha\rangle \;\; , \tag{F.3.3}$$

where $\langle x'|\alpha\rangle$ is called the *wavefunction* and $|\langle x'|\alpha\rangle|^2$ is the probability of observing the particle at the position x'.

However, the spaces are usually continuous except for some discrete spaces, such as lattices. Therefore, we replace the summation notation with integral:

$$|\alpha\rangle = \int_{\text{space}} \mathrm{d}\,x' \, |x'\rangle \langle x'|\alpha\rangle \;\; . \tag{F.3.4}$$

Notice that the Hilbert space for $|x'\rangle$ is uncountably infinite-dimensional. Therefore, if we rewrite the a state $|x'\rangle$ using the integral:

$$|x'\rangle = \int_{\text{space}} \mathrm{d}\,x'' \, |x''\rangle \langle x''|x'\rangle \;\; , \tag{F.3.5}$$

then we can see that:

$$\langle x''|x'\rangle = \delta(x'' - x') \; , \tag{F.3.6}$$

which is called *Dirac orthonormal*. This tells us that the basis $\{|x'\rangle\}$ is not orthonormal but Dirac orthonormal. Therefore, we can obtain the normalizabity of $|\alpha\rangle$ in term of its wave function:

$$\langle\alpha|\alpha\rangle = 1 \iff \int_{\text{space}} \mathrm{d}\,x' |\langle x'|\alpha\rangle|^2 = 1 \; . \tag{F.3.7}$$

Remark 2. *From equation F.3.6, we can immediately know the wavefunction for $|x'\rangle$ is:*

$$\langle x|x'\rangle = \delta(x - x') \ . \tag{F.3.8}$$

This wavefunction is a strange one since it is non-normalizable:

$$\int_{\text{space}} \mathrm{d}\, x \delta(x - x')^2 = \infty \ . \tag{F.3.9}$$

This can be explained as a result of the Heisenberg uncertainty principle since it states that the "perfect measurement" can not exist.

Remark 3. *Although the wavefunctions of $|x'\rangle$ are not really functions, their Dirac orthonormality tells us that a wavefunction of an arbitrary quantum state $\psi(x)$ can be obtained by overlaying them together by integral, that is to say:*

$$\psi(x) = \int_{\text{space}} \mathrm{d}\, x A(x) \delta(x - x') \ . \tag{F.3.10}$$

Just as the Dirac function is not a function but a generalized function that adds an additional structure to the function space, $|x'\rangle$ are not really vectors in a finite-dimensional or countably infinite-dimensional Hilbert space due to its dimension but an additional structure in the Hilbert space.

For an orthonormal eigenbasis $\{|\omega\rangle\}$ of an operator Ω, we can represent it by the wave function as follows:

$$\Omega\, |\omega\rangle = \omega\, |\omega\rangle = \int_{\text{space}} \mathrm{d}\, x' \omega \, \langle x'|\omega\rangle \, |x'\rangle \ \ , \tag{F.3.11}$$

its expectation value is:

$$\begin{aligned} \langle \Omega \rangle &= \langle \omega|\Omega|\omega\rangle \\ &= \int_{\text{space}} \mathrm{d}\, x' \, \mathrm{d}\, x'' \omega \, \langle x''|x'\rangle \, | \, \langle x'|\omega\rangle \, |^2 \\ &= \int_{\text{space}} \mathrm{d}\, x' \omega | \, \langle x'|\omega\rangle \, |^2 \ . \end{aligned} \tag{F.3.12}$$

If we can find an operator Ω_x acting on the wave function such that:

$$\Omega_x \, \langle x'|\omega\rangle = \omega \, \langle x'|\omega\rangle \ \ , \tag{F.3.13}$$

then it is equivalent to the original operator Ω since:

$$\Omega_x \, |\omega\rangle = \int_{\text{space}} \mathrm{d}\, x' \Omega_x \, \langle x'|\omega\rangle \, |x'\rangle = \int_{\text{space}} \mathrm{d}\, x' \omega \, \langle x'|\omega\rangle \, |x'\rangle \ \ . \tag{F.3.14}$$

and the expectation value of Ω is:

$$\int_{\text{space}} \mathrm{d}\, x' \, \langle \omega|x'\rangle \, \Omega_x \, \langle x'|\omega\rangle = \int_{\text{space}} \mathrm{d}\, x' \omega | \, \langle x'|\omega\rangle \, |^2 \ . \tag{F.3.15}$$

Therefore, we can represent the quantum states in terms of the wave functions and use a corresponding operator acting on the wave functions to represent the operator acting on the quantum states. This representation is called *wave function representation*.

F.3.2 Translational Operator and Momentum Operator

The translation operator $T(\mathrm{d}\,x')$ is defined as an operator transforming the quantum states as follows:

$$T(\mathrm{d}\,x')\,|x'\rangle = |T(\mathrm{d}\,x')x'\rangle = |x' + \mathrm{d}\,x'\rangle \ . \tag{F.3.16}$$

Remark 4. *It is easy to check that the collection of all $T(\mathrm{d}\,x')$ is an abelian group under the operation $*$ defined as $T(\mathrm{d}\,x') * T(\mathrm{d}\,x'') = T(\mathrm{d}\,x')T(\mathrm{d}\,x'')$.*

Remark 5. *Since $\{|x'\rangle\}$ is uncountably infinite, we can not represent it in matrix form and therefore:*

$$\langle T(\mathrm{d}\,x')^\dagger x'|x''\rangle \neq \langle x'|\,T(\mathrm{d}\,x')^\dagger\,|x''\rangle \ . \tag{F.3.17}$$

Its adjoint operator can be obtained by considering the wavefunctions:

$$\langle T(\mathrm{d}\,x')^\dagger x''|x'\rangle = \langle x''|T(\mathrm{d}\,x')|x'\rangle = \langle x''|x' + \mathrm{d}\,x'\rangle = \delta(x'' - x' - \mathrm{d}\,x') \,. \tag{F.3.18}$$

Therefore, the adjoint operator of $T(\mathrm{d}\,x')$ is:

$$T(\mathrm{d}\,x')^\dagger\,|x'\rangle = |x' - \mathrm{d}\,x'\rangle \,. \tag{F.3.19}$$

Since $T(\mathrm{d}\,x')$ form a group, we can assume

$$T(\mathrm{d}\,x') = 1 - \mathrm{i}\,k \cdot \mathrm{d}\,x' \ . \tag{F.3.20}$$

Now we need the lemma:

Theorem F.3.1. *The commutator of x and $T(\mathrm{d}\,x')$ is:*

$$[x, T(\mathrm{d}\,x')] = \mathrm{d}\,x' T(\mathrm{d}\,x') \ . \tag{F.3.21}$$

Proof. Compute the commutator directly, we can obtain:

$$\begin{aligned}
[x, T(\mathrm{d}\,x')]\,|x\rangle &= xT(\mathrm{d}\,x')\,|x'\rangle - T(\mathrm{d}\,x')x\,|x'\rangle \\
&= x\,|x' + \mathrm{d}\,x'\rangle - x'T(\mathrm{d}\,x')\,|x'\rangle \\
&= (x' + \mathrm{d}\,x')\,|x' + \mathrm{d}\,x'\rangle - x'\,|x' + \mathrm{d}\,x'\rangle \\
&= \mathrm{d}\,x'\,|x' + \mathrm{d}\,x'\rangle = \mathrm{d}\,x' T(\mathrm{d}\,x')\,|x'\rangle \ .
\end{aligned} \tag{F.3.22}$$

□

By the assumption F.3.20 and theorem F.3.1, we have:

$$\begin{aligned}
[x, T(\mathrm{d}\,x')] &= -\mathrm{i}\,x \cdot k \cdot \mathrm{d}\,x' + \mathrm{i}\,k \cdot \mathrm{d}\,x' \cdot x \\
&= \mathrm{d}\,x'(1 - k \cdot \mathrm{d}\,x') \\
&= \mathrm{d}\,x' + \mathcal{O}(\mathrm{d}\,x'^2) \ .
\end{aligned} \tag{F.3.23}$$

Drop the $\mathcal{O}(\mathrm{d}\,x'^2)$ term, we have:

$$x_i k_j - k_j x_i = \mathrm{i}\,\delta_{ij} \ , \tag{F.3.24}$$

which is naturally analog to the canonical commutation. Therefore, we naturally take:

$$k = \frac{p}{\hbar} \ . \tag{F.3.25}$$

which implies the translational operator is:

$$T(\mathrm{d}\,x') = 1 - \mathrm{i}\,\frac{p \cdot \mathrm{d}\,x'}{\hbar} \ . \tag{F.3.26}$$

Now we can consider the translational operator for ordinary length l, which is:

$$\begin{aligned} T(l) &= T\left(\frac{l}{\mathrm{d}\,x'}\right) \\ &= \left(1 - \mathrm{i}\,\frac{p \cdot l}{(l/\,\mathrm{d}\,x')\hbar}\right)^{l/\,\mathrm{d}\,x'} \\ &\approx \mathrm{e}^{-\mathrm{i}\,p \cdot l/\hbar} \ . \end{aligned} \tag{F.3.27}$$

There is another theorem that gives a similar result. We need a lemma first:

Lemma F.3.2. *Let f be an analytical function. Then:*

$$f(x-a) = \mathrm{e}^{-a\frac{\mathrm{d}}{\mathrm{d}\,x}}\,f(x) \ . \tag{F.3.28}$$

Proof. View $f(x-a)$ as a function of $-a$, then its Taylor expansion near 0 is:

$$\begin{aligned} f(x-a) &= \left(\sum_{k=0}^{\infty} \frac{(-a)^k}{k!}\frac{\mathrm{d}^k}{\mathrm{d}\,x^k}\right) f(x) \\ &= \mathrm{e}^{-a\frac{\mathrm{d}}{\mathrm{d}\,x}}\,f(x) \ . \end{aligned} \tag{F.3.29}$$

□

Theorem F.3.3. *Let $T(l)$ be the translational operator for ordinary length l. Then act $T(l)$ on the quantum state is equivalent to act $\mathrm{e}^{-l\partial_x}$ on the wavefunction.*

Proof. Consider the follows:

$$\begin{aligned} T(l)\left|\alpha\right\rangle &= T(l)\int \mathrm{d}\,x' \left|x'\right\rangle \left\langle x'|\alpha\right\rangle \\ &= \int \mathrm{d}\,x' \left|x'+l\right\rangle \left\langle x'|\alpha\right\rangle \\ &= \int \mathrm{d}\,x' \left|x'+l\right\rangle \left\langle x'|\alpha\right\rangle \\ &= \int \mathrm{d}\,x' \left|x'\right\rangle \left\langle x'-l|\alpha\right\rangle \\ &= \int \mathrm{d}\,x' \left|x'\right\rangle e^{-l\partial_{x'}} \left\langle x'|\alpha\right\rangle \ . \end{aligned} \tag{F.3.30}$$

We know that the quantum state $T(l)\left|\alpha\right\rangle$ has the wavefunction $e^{-l\partial_{x'}}\left\langle x'|\alpha\right\rangle$. Therefore, $T(l)\left|\alpha\right\rangle$ can be equivalently obtained from $e^{-l\partial_{x'}}\left\langle x'|\alpha\right\rangle$. □

Compare the results from theorem F.3.1 and theorem F.3.3, we know that the operator $\mathrm{e}^{-\mathrm{i}\, p\cdot l/\hbar}$ acting on the quantum state is equivalent to the operator $\mathrm{e}^{-l\partial_x}$ acting on wave function.

This relation implies that the momentum operator Now we know that the momentum operator behaves like $-\mathrm{i}\,\hbar\nabla$ in the wavefunction representation.

$$\boxed{\begin{gathered}\textbf{Quantum State Representation} \longleftrightarrow \textbf{Wavefunction Representation}\\ \mathrm{e}^{-\mathrm{i}\, p\cdot l/\hbar} \longleftrightarrow \mathrm{e}^{-l\partial_x}\\ p \longleftrightarrow -\mathrm{i}\,\hbar\partial_x\end{gathered}}$$

The physical meaning of the momentum operator may be not very explicit in this form. Does it still have the same physical meaning as in classical mechanics? We introduce the concept of *classical correspondence pronciple* in the next chapter to solve this problem.

Chapter 2

Classical Correspondence

A new theory is related to an old one in this manner. For example, we have some old theories such as black-body radiation, atomic spectral line, and absence of motion in ether, and some new theories such as mass-energy relation and quantum entanglement. The intersection of the old ones and the new ones is the correspondence.

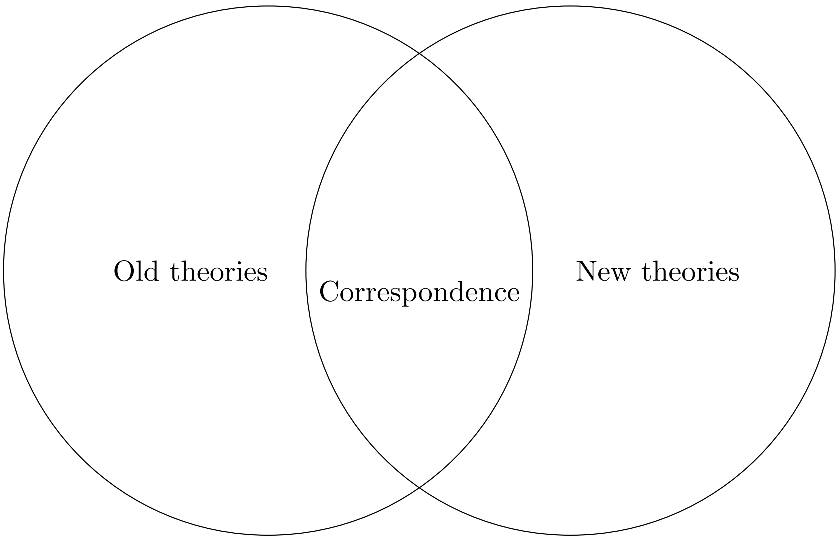

Figure 2.1: Concept of correspondence.

C.1 Ehrenst theorem

There are several different classical correspondences for quantum mechanics. Different in generality. There is an important theorem for the correspondence of classical and quantum mechanics.

Theorem C.1.1. Ehrenst theorem (for position and momentum)
For a single quantum particle in the potential $V(x)$, we have

$$\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}\,t} = \langle p\rangle \ , \quad \frac{\mathrm{d}\langle p\rangle}{\mathrm{d}\,t} = -\langle \nabla V(x)\rangle \ . \tag{C.1.1}$$

Proof. The proof for the position part is

$$\begin{aligned}
\frac{\mathrm{d}\,\langle x\rangle}{\mathrm{d}\,t} &= \frac{\mathrm{d}}{\mathrm{d}\,t}\int \psi^* x\psi \,\mathrm{d}\,x = \int \left(\frac{\partial\psi^*}{\partial t}x\psi + \psi^* x\frac{\partial\psi}{\partial t}\right)\mathrm{d}\,x \\
&= \frac{1}{\mathrm{i}\,\hbar}\int \left\{\psi^* x\left(\frac{\hbar^2}{2m}\nabla^2 + V(x)\right)\psi - \left(\frac{\hbar^2}{2m}\nabla^2 + V(x)\right)\psi^* x\psi\right\}\mathrm{d}\,x \\
&= \frac{\hbar}{2\,\mathrm{i}\,m}\int \left(\psi^* x\nabla^2\psi - \nabla^2\psi^* x\psi\right)\mathrm{d}\,x\ . \qquad \text{(C.1.2)}
\end{aligned}$$

Use the integration by part, this can be simplified to

$$\begin{aligned}
&\frac{\hbar}{2\,\mathrm{i}\,m}\int \left[\nabla(\psi^* x)\nabla\psi - \nabla\psi^*\nabla(x\psi)\right]\mathrm{d}\,x \\
&= \frac{\hbar}{2\,\mathrm{i}\,m}\int \left[\psi^*\nabla x\nabla\psi - \psi\nabla\psi^*\nabla x\right]\mathrm{d}\,x \\
&= \frac{\hbar}{2\,\mathrm{i}\,m}\int \left[\psi^*\left(\frac{\partial\psi}{\partial x} + \frac{\partial\psi}{\partial y} + \frac{\partial\psi}{\partial z}\right) - \psi\left(\frac{\partial\psi^*}{\partial x} + \frac{\partial\psi^*}{\partial y} + \frac{\partial\psi^*}{\partial z}\right)\right]\mathrm{d}\,x \\
&= \frac{1}{2m}\left(2\,\langle p_x\rangle + 2\,\langle p_y\rangle + 2\,\langle p_z\rangle\right) = \frac{1}{m}\,\langle p\rangle\ . \qquad \text{(C.1.3)}
\end{aligned}$$

The proof for the momentum part is

$$\begin{aligned}
\frac{\mathrm{d}\,\langle p\rangle}{\mathrm{d}\,t} &= \frac{\mathrm{d}}{\mathrm{d}\,t}\int \psi^*\left(-\,\mathrm{i}\,\hbar\nabla\right)\psi\,\mathrm{d}\,x = \int \left(\frac{\partial\psi^*}{\partial t}\left(-\,\mathrm{i}\,\hbar\nabla\right)\psi + \psi^*\left(-\,\mathrm{i}\,\hbar\nabla\right)\frac{\partial\psi}{\partial t}\right)\mathrm{d}\,x \\
&= -\,\mathrm{i}\,\hbar\int \left(\frac{\partial\psi^*}{\partial t}\nabla\psi + \psi^*\nabla\frac{\partial\psi}{\partial t}\right)\mathrm{d}\,x \\
&= -\int \left[-\nabla\psi\left(\frac{\hbar^2}{2m}\nabla^2 + V(x)\right)\psi^* + \psi^*\nabla\left(\frac{\hbar^2}{2m}\nabla^2 + V(x)\right)\psi\right]\mathrm{d}\,x\ . \qquad \text{(C.1.4)}
\end{aligned}$$

Use the integration by part twice, and expanse the last term, we can obtain

$$\begin{aligned}
&-\int \left(-V(x)\psi^*\nabla\psi + V(x)\psi^*\nabla\psi + \psi^*\nabla V(x)\psi\right)\mathrm{d}\,x \\
&= -\int \psi^*\nabla V(x)\psi\,\mathrm{d}\,x = \langle -\nabla V(x)\rangle\ . \qquad \text{(C.1.5)}
\end{aligned}$$

□

As we know in Newtonian mechanics the momentum and position have the relation

$$\frac{\mathrm{d}\,x}{\mathrm{d}\,t} = \frac{1}{m}p\ , \qquad \text{(C.1.6)}$$

$$\frac{\mathrm{d}\,p}{\mathrm{d}\,t} = -\nabla V(x)\ , \qquad \text{(C.1.7)}$$

the Ehrenst theorem gives us the classical correspondence of the expectation values of observables. The wave functions and the operators also correspond. We start to observe this from the more generalized version of Ehrenst theorem.

Theorem C.1.2. Ehrenst theorem
Let A be an operator for an observable. Then

$$\frac{\mathrm{d}\,\langle A\rangle}{\mathrm{d}\,t} = \frac{1}{\mathrm{i}\,\hbar}\,\langle [A,H]\rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle \,, \tag{C.1.8}$$

where H is the Hamiltonian operator and $[A,B] = AB - BA$ is the commutator.

Proof.

$$\begin{aligned}\frac{\mathrm{d}\,\langle A\rangle}{\mathrm{d}\,t} &= \frac{\mathrm{d}}{\mathrm{d}\,t}\int \psi^* A\psi \,\mathrm{d}\,x \\ &= \int \frac{\partial \psi^*}{\partial t} A\psi + \psi^* \frac{\partial A}{\partial t}\psi + \psi^* A \frac{\partial \psi}{\partial t} \,\mathrm{d}\,x \\ &= \int \left(\psi^* \frac{1}{\mathrm{i}\,\hbar} AH\psi - \psi^* \frac{1}{\mathrm{i}\,\hbar} HA\psi\right) \mathrm{d}\,x + \left\langle \frac{\partial A}{\partial t} \right\rangle \\ &= \frac{1}{\mathrm{i}\,\hbar}\,\langle [A,H]\rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle \,. \end{aligned} \tag{C.1.9}$$

□

In particular, if the operator A is x or p, then we obtain the relations

$$\frac{\mathrm{d}\,\langle x\rangle}{\mathrm{d}\,t} = \frac{1}{\mathrm{i}\,\hbar}\,\langle [x,H]\rangle \,, \tag{C.1.10}$$

$$\frac{\mathrm{d}\,\langle p\rangle}{\mathrm{d}\,t} = \frac{1}{\mathrm{i}\,\hbar}\,\langle [p,H]\rangle \,. \tag{C.1.11}$$

These relations immediately remind us of the Poisson bracket in classical mechanics. We can construct the correspondence theory for the operators from the Poisson bracket.

C.2 Poisson Bracket

In Hamiltonian mechanics, consider two arbitrary smooth functions f and g on the phase space with canonical coordinate (q,p), we define the Poisson bracket $\{-,-\}$ be a function act on these functions

$$\{f,g\} = \frac{\partial f}{\partial q}\frac{\partial g}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial g}{\partial q} \,. \tag{C.2.1}$$

Generally, we can write

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\,t} f(q,p,t) &= \frac{\partial f}{\partial t} + \frac{\partial f}{\partial q}\frac{\mathrm{d}\,q}{\mathrm{d}\,t} + \frac{\partial f}{\partial p}\frac{\mathrm{d}\,p}{\mathrm{d}\,t} \\ &= \frac{\partial f}{\partial t} + \frac{\partial f}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial H}{\partial q} \\ &= \{f,H\} + \frac{\partial f}{\partial t} \,. \end{aligned} \tag{C.2.2}$$

This is similar to the commutator relation in the previous section. Moreover, the Poisson bracket has an algebraic structure in the following theorem.

Theorem C.2.1. Algebraic structure for the Poisson bracket
Let f, g and h be functions on the phase space. Then

- Skew symmetry: $\{f, g\} = -\{g, f\}$.
- Bilinearity: $\{f, C_1 g + C_2 h\} = C_1\{f, g\} + C_2\{f, h\}$.
- Decomposition: $\{f, gh\} = \{f, g\}h + g\{f, h\}$.
- Jacobi Identity: $\{\{f, g\}, h\} + \{\{h, f\}, g\} + \{\{g, h\}, f\} = 0$.

Notice that the commutator also has this algebraic structure. Therefore, we can expect the correspondence relation

Quantum Mechanics	$\longleftrightarrow$	**Classical Mechanics**
Operators on the Hilbert space	$\longleftrightarrow$	Functions on the phase space
Commutator: $\frac{1}{\mathrm{i}\,\hbar}[-,-]$	$\longleftrightarrow$	Poisson bracket: $\{-,-\}$

Example C.2.1. Consider the quantum operators q^2, p^2 and the commutator of them. Decompose $[q^2, p^2]$ through the algebraic structure, we have

$$\begin{aligned}
[q^2, p^2] &= q[q, p^2] + [q, p^2]q \\
&= q(p[q, p] + [q, p]p) + (p[q, p] + [q, p]p)q \\
&= 2\,\mathrm{i}\,\hbar qp + 2\,\mathrm{i}\,\hbar pq \\
&= 2\,\mathrm{i}\,\hbar(qp + pq - \mathrm{i}\,\hbar) \\
&= 4\,\mathrm{i}\,\hbar qp + 2\hbar^2 \;=\; 4\,\mathrm{i}\,\hbar qp + \mathcal{O}(\hbar^2) \; .
\end{aligned} \tag{C.2.3}$$

Therefore, we have the relation

$$\frac{1}{\mathrm{i}\,\hbar}[q^2, p^2] = 4qp + \mathcal{O}(\hbar) \; . \tag{C.2.4}$$

Consider the classical correspondence for q^2 and p^2. The Poisson bracket for them is

$$\{q^2, p^2\} = \frac{\mathrm{d}\,q^2}{\mathrm{d}\,q}\frac{\mathrm{d}\,p^2}{\mathrm{d}\,p} - \frac{\mathrm{d}\,p^2}{\mathrm{d}\,q}\frac{\mathrm{d}\,q^2}{\mathrm{d}\,p} = 4qp \; . \tag{C.2.5}$$

These results satisfy the correspondence relation under the classical limit $\hbar \to 0$

$$\frac{1}{\mathrm{i}\,\hbar}[-,-] \longleftrightarrow \{-,-\} + \mathcal{O}(\hbar) \; . \tag{C.2.6}$$

Notice that different quantum systems can have the same classical limit due to the non-commutativity, here is an example.

Example C.2.2. Consider functions $q^2 p$, pq^2 and p. The Poisson bracket of them is given by

$$\{q^2 p, p\} = \{pq^2, p\} = \frac{\partial q^2 p}{\partial q}\frac{\partial p}{\partial p} - \frac{\partial q^2 p}{\partial p}\frac{\partial p}{\partial q} = 2qp \; . \tag{C.2.7}$$

Consider the quantum operators $q^2p,\ p$. The commutator for them is

$$\begin{aligned}\frac{1}{\mathrm{i}\,\hbar}[q^2p,p] &= q^2\frac{1}{\mathrm{i}\,\hbar}[p,p]p+\frac{1}{\mathrm{i}\,\hbar}[q^2,p]p\\ &= \frac{1}{\mathrm{i}\,\hbar}[q^2,p]p=\frac{1}{\mathrm{i}\,\hbar}(q[q,p]+[q,p]q)p\\ &= 2qp\ .\end{aligned}\tag{C.2.8}$$

However, for the quantum operators $pq^2,\ p$, the commutator for them is

$$\begin{aligned}\frac{1}{\mathrm{i}\,\hbar}[pq^2,p] &= p\frac{1}{\mathrm{i}\,\hbar}[q^2,p]+\frac{1}{\mathrm{i}\,\hbar}[p,p]q^2\\ &= p\frac{1}{\mathrm{i}\,\hbar}[q^2,p]=p\frac{1}{\mathrm{i}\,\hbar}(q[q,p]+[q,p]q)\\ &= 2pq=2qp-2\,\mathrm{i}\,\hbar\ .\end{aligned}\tag{C.2.9}$$

Under the classical limit, two quantum systems are the same. Conversely, the quantization of the classical systems is not unique.

C.3 Hamilton-Jacobi Equation and WKB Approximation

Hamilton-Jacobi equation is a bridge between quantum and classical mechanics and therefore important for the classical correspondence principle in quantum mechanics. In this section, we review the Hamilton-Jacobi equation and its relation to quantum mechanics and WKB approximation.

C.3.1 Hamilton-Jacobi Equation

The classical action is a functional of the path $\vec{x}(t)$ and time t, which is defined as the integral of the Lagrangian over the time interval:

$$S[\vec{x}(t),t]=\int_0^t L(\vec{x}(t),\dot{\vec{x}}(t))\,\mathrm{d}\,t\ .\tag{C.3.1}$$

Then we naturally want to ask how to consider the variation of S with respect to the path $\vec{x}(t)$. We now consider a perturbation of paths $\delta\vec{x}$ satisfying $\delta\vec{x}(0)=0$ but $\delta\vec{x}(t)$ is free as figure 2.2 demonstrates. Then the action becomes:

$$\begin{aligned}\delta S[\vec{x}(t),t] &= \delta\int_0^t L(\vec{x}(t),\dot{\vec{x}}(t))\,\mathrm{d}\,t\\ &= \int_0^t\sum_i\left(\frac{\partial L}{\partial x_i}\delta x_i+\frac{\partial L}{\partial \dot{x}_i}\delta\dot{x}_i\right)\mathrm{d}\,t\\ &= \int_0^t\sum_i\left[\frac{\partial L}{\partial x_i}\delta x_i-\left(\frac{\mathrm{d}}{\mathrm{d}\,t}\frac{\partial L}{\partial \dot{x}_i}\right)\delta x_i\right]\mathrm{d}\,t+\sum_i\frac{\partial L}{\partial \dot{x}_i}\delta x_i\bigg|_0^t\\ &= \int_0^t\sum_i\left(\frac{\partial L}{\partial x_i}-\frac{\mathrm{d}}{\mathrm{d}\,t}\frac{\partial L}{\partial \dot{x}_i}\right)\delta x_i\,\mathrm{d}\,t+\sum_i\frac{\partial L}{\partial \dot{x}_i}\delta x_i(t)=\sum_i p_i\delta x_i(t)\ .\end{aligned}\tag{C.3.2}$$

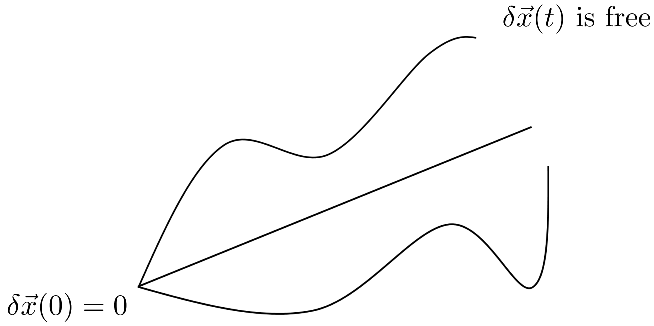

Figure 2.2: The perturbation $\delta\vec{x}(0) = 0$ but $\delta\vec{x}(t)$ is free.

Therefore, we obtain the *first Hamilton-Jacobi equation*, which states that the variation of the action with respect to $x_i(t)$ is:

$$\boxed{\frac{\delta S}{\delta x_i(t)} = p_i} \; . \tag{C.3.3}$$

Now we want to ask, what is the derivative of the action with respect to t, we consider the total derivative of the action:

$$\begin{aligned} L = \frac{\mathrm{d}\, S}{\mathrm{d}\, t} &= \frac{\partial S}{\partial t} + \sum_i \frac{\partial S}{\partial x_i} \dot{x}_i \\ &= \frac{\partial S}{\partial t} + \sum_i p_i \dot{x}_i \; . \end{aligned} \tag{C.3.4}$$

Therefore, the derivative of the action with respect to t is:

$$\frac{\partial S}{\partial t} = L - \sum_i p_i \dot{x}_i \tag{C.3.5}$$

$$\begin{aligned} &= -H\left(\vec{x}, \vec{p}, t\right) \\ &= -H\left(\vec{x}, \frac{\delta S}{\delta \vec{x}(t)}, t\right) \; . \end{aligned} \tag{C.3.6}$$

Therefore, we have the *second Hamilton-Jacobi equation*:

$$\boxed{\frac{\partial S}{\partial t} + H\left(\vec{x}, \frac{\delta S}{\delta \vec{x}(t)}, t\right) = 0} \; . \tag{C.3.7}$$

The variation $\delta S/\delta\vec{x}$ also often be denoted by ∇S or $\partial S/\partial\vec{x}$.

C.3.2 The Semi-Classical Approximation and WKB Approximation

The basic concept of WKB approximation is to assume the solution of the following differential equation:

$$y^{(n)} + \sum_{i=1}^{n-1} a_i(x) y^{(i)} = 0 \tag{C.3.8}$$

be an exponential of asymptotic series:

$$y \approx \exp\left[\frac{1}{\delta}\sum_{i=0}^{\infty}\delta^i S_i(x)\right] , \tag{C.3.9}$$

where $\delta \to 0$.

The wavefunction can be rewritten as the exponential of another function S, which is closely related to the classical action, that is, the wavefunction is:

$$\psi(\vec{x}) = \mathrm{e}^{\mathrm{i}\, S(\vec{x})/\hbar} . \tag{C.3.10}$$

Remark 6. *Notice that the function S here can be complex.*

Substitute the wavefunction in the time-independent Schrodinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{x})\psi = E\psi , \tag{C.3.11}$$

we can obtain:

$$\frac{1}{2m}(\nabla S)^2 + \frac{\hbar}{2m\,\mathrm{i}}\nabla^2 S = E - V . \tag{C.3.12}$$

Notice that under the classical limit $\hbar \to 0$, the function S becomes the classical action, which satisfies the Hamilton-Jacobi equation:

$$(\nabla S)^2 = 2m(E - V) . \tag{C.3.13}$$

In addition, add the time t in ψ and the function S, then we write:

$$S(\vec{x}, t) = \frac{\hbar}{\mathrm{i}}\ln\psi(\vec{x}, t) . \tag{C.3.14}$$

Then using the second Hamilton-Jacobi equation C.3.7, we can obtain:

$$\frac{\partial S(\vec{x}, t)}{\partial t} = -H(\vec{x}, \nabla S, t) = \frac{\hbar}{\mathrm{i}}\frac{\partial_t\psi(\vec{x}, t)}{\psi(\vec{x}, t)} . \tag{C.3.15}$$

Therefore, we obtain the Schrodinger-equation-like equation:

$$\boxed{\mathrm{i}\,\hbar\frac{\partial}{\partial t}\psi(\vec{x}, t) = H(\vec{x}, \vec{p}, t)\psi .} \tag{C.3.16}$$

We can quantize the position and momentum to operators, then we can obtain the Schrodinger equation.

We can now apply the WKB approximation in a one-dimensional system, assuming that the solution for the time-independent Schrodinger equation is $\mathrm{e}^{\mathrm{i}\, S(x)/\hbar}$, where the function S is:

$$S(x) = \sum_{i=0}^{\infty}\left(\frac{\hbar}{\mathrm{i}}\right)^i S_i(x) = S_0(\vec{x}) + \left(\frac{\hbar}{\mathrm{i}}\right) S_1(x) + \left(\frac{\hbar}{\mathrm{i}}\right)^2 S_2(x) + \mathcal{O}(\hbar^3) . \tag{C.3.17}$$

Substitute the series into equation equation C.3.12 and drop the term $\mathcal{O}(\hbar^3)$, then:

$$\frac{1}{2m}\left(S_0'\right)^2+\frac{1}{2m}\left(\frac{\hbar}{\mathrm{i}}\right)\left((S_0')^2+2S_0'S_1'\right) \\ +\frac{1}{2m}\left(\frac{\hbar}{\mathrm{i}}\right)^2\left(2S_0'S_2'+(S_1')^2+S_2''\right)\approx E-V\ . \tag{C.3.18}$$

Assume the only nonzero term is the zeroth order term, that is:

$$S_0'\approx\pm\sqrt{2m(E-V)}\equiv\pm p\ ,\quad S_0=\pm\int^x p(x')\,\mathrm{d}\,x' \tag{C.3.19}$$

Then the first order term implies:

$$S_1'=-\frac{1}{2}\frac{S_0''}{S_0'}=-\frac{1}{2}\frac{p'}{p}\ . \tag{C.3.20}$$

By integrating both sides, we can obtain:

$$S_1=\ln p^{-1/2}+C\ . \tag{C.3.21}$$

Therefore, the wavefunction can be approximated to the $\mathcal{O}(\hbar)$:

$$\psi(x)\approx\frac{C_1}{\sqrt{p}}\exp\left[\frac{\mathrm{i}}{\hbar}\int^x p(x')\,\mathrm{d}\,x'\right]+\frac{C_2}{\sqrt{p}}\exp\left[-\frac{\mathrm{i}}{\hbar}\int^x p(x')\,\mathrm{d}\,x'\right]\ . \tag{C.3.22}$$

This approach approximates the wavefunction to the term $\mathcal{O}(\hbar)$ (or more accurate if needed), this approximation is called *semi-classical approximation*. We can discuss more details about the conditions of the value of p.

Classical Allowed Region

The classical allowed region is the region satisfied $E > V$, that is, the energy is greater than the potential barrier. Therefore, the value of p is a real number. The wavefunction is identical to the equation C.3.22.

Classical Forbidden Region

The classical forbidden region is a region that can not be observed in the classical system. The energy is less than the potential barrier in this region; therefore, the value of p is a purely imaginary number. Let $p=\mathrm{i}\sqrt{2m(V-E)}$, by equation C.3.22, we can obtain the wavefunction is:

$$\psi(x)\approx\frac{C_1'}{\sqrt{k}}\exp\left[-\frac{1}{\hbar}\int^x k(x')\,\mathrm{d}\,x'\right]+\frac{C_2'}{\sqrt{k}}\exp\left[\frac{1}{\hbar}\int^x k(x')\,\mathrm{d}\,x'\right]\ . \tag{C.3.23}$$

Part II

Quantum Particles in Electromagnetic Fields

Chapter 3

Charged Particles in Electromagnetic Fields

E.1 Phase in Quantum Mechanics

From the Stern-Gerlach experiment, we can know that the superposition of quantum states is the heart of quantum mechanics. Naturally, we can choose a phase of the superposition. Then what is its significance? The core reasons are the physical phase and gauge choice.

E.1.1 Physical Phase

In classical mechanics, the electric force is generated by the potential $\vec{F} = -\nabla V$, which is invariant under the transformation $V(x) \mapsto V(x)+V_0$. Is this also true in quantum mechanics?

The dynamics of quantum mechanics is described by the Schrodinger equation $H\left|\alpha, t\right\rangle = -\mathrm{i}\,\hbar\partial_t \left|\alpha, t\right\rangle$, which leads to

$$\left|\alpha, t\right\rangle = \mathrm{e}^{-\mathrm{i}\int_{t_0}^{t} H(t')\,\mathrm{d}\,t'} \left|\alpha, t_0\right\rangle \ . \tag{E.1.1}$$

Under the same transformation in classical mechanics, the transform is as follows:

$$\begin{aligned} V &\mapsto \tilde{V} = V + V_0 \\ H &\mapsto \tilde{H} = H + V_0 \\ \left|\alpha, t\right\rangle &\mapsto \left|\tilde{\alpha}, t\right\rangle = \mathrm{e}^{-\mathrm{i}(t-t_0)V_0} \left|\alpha, t\right\rangle \ . \end{aligned} \tag{E.1.2}$$

This is an example of gauge transformation in quantum mechanics. More generally, we can consider time-dependent transformation:

$$\begin{aligned} V &\mapsto \tilde{V} = V + V_0(t) \\ H &\mapsto \tilde{H} = H + V_0(t) \\ \left|\alpha, t\right\rangle &\mapsto \left|\tilde{\alpha}, t\right\rangle = \mathrm{e}^{-\mathrm{i}\int_{t_0}^{t} V_0(t')\,\mathrm{d}\,t'} \left|\alpha, t\right\rangle \ . \end{aligned} \tag{E.1.3}$$

These phase differences are detectable, the observables are different in different potential fields. For example, the gravity-induced phase has been detected.

Note that the added term $V_0(t)$ is independent of the position x. Then can we generalize this concept on the electrodynamics, which is position-relevant?

E.1.2 Gauge Symmetry

We know that in classical electrodynamics, the electromagnetic fields have gauge symmetry, but how does this property behave in quantum mechanics? We discuss what the Schrodinger equation looks like in the magnetic field and how the gauge symmetry behaves in quantum mechanics in this section.

Schrodinger Equation in the Magnetic Fields

Consider a particle with mass m and charge q moving in the electromagnetic field, the equation of motion is

$$m\ddot{\vec{x}} = q\left[\vec{E}(x(t),t) + \frac{1}{c}\dot{\vec{x}} \times \vec{B}(x(t),t)\right] - \nabla V(x(t)) \ . \tag{E.1.4}$$

The Lagrangian of the particle is

$$L(\vec{x},\dot{\vec{x}}) = \frac{1}{2}m\dot{x}^2 - q\phi(\vec{x},t) + \frac{q}{c}\dot{\vec{x}}\cdot\vec{A}(\vec{x},t) - V(\vec{x}) \ . \tag{E.1.5}$$

Notice that the canonical momentum and the generalized velocity have the relation

$$\vec{p} = \frac{\partial L}{\partial\dot{\vec{x}}} = m\dot{\vec{x}} - \frac{q}{c}\vec{A}(\vec{x},t) \ , \quad \dot{\vec{x}} = \frac{\vec{p}}{m} - \frac{q}{mc}\vec{A}(\vec{x},t) \ . \tag{E.1.6}$$

So the Hamiltonian of the particle is

$$H(\vec{x},\vec{p}) = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\phi(\vec{x},t) + V(\vec{x}) \ . \tag{E.1.7}$$

We can use the quantization rule to describe the particle quantum mechanically, that is, use the relations

$$[x_i,p_j] = \mathrm{i}\,\hbar\delta_{ij} \ , \quad [x_i,x_j] = [p_i,p_j] = 0 \ . \tag{E.1.8}$$

Replace the momentum by the momentum operator $p \mapsto -\mathrm{i}\,\hbar\nabla$, we have the Schrodinger equation:

$$\begin{aligned}
\mathrm{i}\,\hbar\frac{\partial}{\partial t}\psi &= \left[\frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\phi + V\right]\psi \\
&= \left[\frac{1}{2m}\left(\vec{p}^2 + \frac{q^2}{c^2}\vec{A}^2 - \frac{q}{c}\vec{p}\cdot\vec{A} - \frac{q}{c}\vec{A}\cdot\vec{p}\right) + q\phi + V\right]\psi
\end{aligned} \tag{E.1.9}$$

Notice that as operators $\vec{p}\cdot\vec{A} \neq \vec{A}\cdot\vec{p}$, we need the following relation:

$$\begin{aligned}
\vec{p}\cdot(\vec{A}\psi) &= -\mathrm{i}\,\hbar\nabla\cdot(\vec{A}\psi) \\
&= \vec{A}\cdot(-\mathrm{i}\,\hbar\nabla\psi) - \mathrm{i}\,\hbar\nabla\cdot\vec{A}\psi \\
&= \vec{A}\cdot(\vec{p}\psi) - \mathrm{i}\,\hbar(\nabla\cdot\vec{A})\psi \ ,
\end{aligned} \tag{E.1.10}$$

which implies that as operators:

$$\vec{p}\cdot\vec{A} = \vec{A}\cdot\vec{p} - \mathrm{i}\,\hbar\nabla\cdot\vec{A} \ . \tag{E.1.11}$$

Utilizing eqaution E.1.11 and the gauge $\nabla \cdot \vec{A} = 0$, we can rewrite the equation as:

$$\boxed{\mathrm{i}\,\hbar \frac{\partial}{\partial t}\psi = \left[\frac{1}{2m}\left(\vec{p}^2 + \frac{q^2}{c^2}\vec{A}^2 - \frac{2q}{c}\vec{A}\cdot\vec{p}\right) + q\phi + V\right]\psi} \; . \tag{E.1.12}$$

This is what the Schrodinger equation looks in the magnetic field.

The probability density ρ and current $\vec{J}$ becomes:

$$\rho = |\psi|^2 \; , \quad \vec{J} = \psi^* \frac{1}{2m}\left(-\mathrm{i}\,\hbar\nabla - \frac{q}{c}\vec{A}\right)\psi - \psi\frac{1}{2m}\left(-\mathrm{i}\,\hbar\nabla - \frac{q}{c}\vec{A}\right)\psi^* \; . \tag{E.1.13}$$

Gauge Invariance

In electrodynamics, Maxwell's equations are invariant under the gauge transformation

$$\vec{A} \mapsto \vec{A}' = \vec{A} + \nabla\chi \; , \tag{E.1.14}$$

$$\phi \mapsto \phi' = \phi - \frac{1}{c}\frac{\partial\chi}{\partial t} \; . \tag{E.1.15}$$

Under this transformation, the Lagrangian, action, and Hamiltonian are transformed as follows:

$$L \mapsto L' = L + \frac{q}{c}\frac{\mathrm{d}}{\mathrm{d}\,t}\chi(x(t), t) \; , \tag{E.1.16}$$

$$S \mapsto S' = S \text{ (invariant)} \; , \tag{E.1.17}$$

$$H \mapsto H' = \left[\frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A} - \frac{q}{c}\nabla\chi\right)^2 + q\phi - q\frac{1}{c}\frac{\partial\chi}{\partial t} + V\right] \; . \tag{E.1.18}$$

Consider a unitary operator $\mathrm{e}^{\mathrm{i}\,q\chi/\hbar c}$, which satisfies

$$\begin{aligned}
\exp\left(-\mathrm{i}\,\frac{q\chi}{\hbar c}\right)\vec{p}\exp\left(\mathrm{i}\,\frac{q\chi}{\hbar c}\right) &= \exp\left(-\mathrm{i}\,\frac{q\chi}{\hbar c}\right)\left[\vec{p}\exp\left(\mathrm{i}\,\frac{q\chi}{\hbar c}\right) - \exp\left(\mathrm{i}\,\frac{q\chi}{\hbar c}\right)\vec{p}\right] + \vec{p} \\
&= \exp\left(-\mathrm{i}\,\frac{q\chi}{\hbar c}\right)\left[\vec{p}, \exp\left(\mathrm{i}\,\frac{q\chi}{\hbar c}\right)\right] + \vec{p} \\
&= \exp\left(-\mathrm{i}\,\frac{q\chi}{\hbar c}\right)\left(-\mathrm{i}\,\hbar\exp\left(\mathrm{i}\,\frac{q\chi}{\hbar c}\right)\mathrm{i}\,\frac{q\nabla\chi}{\hbar c}\right) + \vec{p} \\
&= \exp\left(-\mathrm{i}\,\frac{q\chi}{\hbar c}\right)\left(\exp\left(\mathrm{i}\,\frac{q\chi}{\hbar c}\right)\frac{q\nabla\chi}{c}\right) + \vec{p} \\
&= \vec{p} + \frac{q\nabla\chi}{c} \; .
\end{aligned} \tag{E.1.19}$$

Substitute this into the transformation of the Hamiltonian, one can represent the transformation as

$$H \mapsto H' = \mathrm{e}^{\mathrm{i}\,q\chi/\hbar c}\,H\,\mathrm{e}^{-\mathrm{i}\,q\chi/\hbar c} \tag{E.1.20}$$

Another Hamiltonian $H - \mathrm{i}\,\hbar\partial_t$ satisfies the transformation as well:

$$H - \mathrm{i}\,\hbar\partial_t \mapsto \mathrm{e}^{\mathrm{i}\,q\chi/\hbar c}(H - \mathrm{i}\,\hbar\partial_t)\,\mathrm{e}^{-\mathrm{i}\,q\chi/\hbar c} \; . \tag{E.1.21}$$

Utilize this relation, one can obtain the Schrodinger equation under the transformation:

$$(H - \mathrm{i}\,\hbar\partial_t)\psi = 0 \mapsto eu^{\mathrm{i}\,q\chi/\hbar c}(H - \mathrm{i}\,\hbar\partial_t)\,\mathrm{e}^{-\mathrm{i}\,q\chi/\hbar c}\,\psi = 0\,. \tag{E.1.22}$$

Reduce the equation to the original form:

$$\begin{aligned}
&\mathrm{e}^{\mathrm{i}\,q\chi/\hbar c}(H - \mathrm{i}\,\hbar\partial_t)\,\mathrm{e}^{-\mathrm{i}\,q\chi/\hbar c}\,\psi = 0\\
&\implies \mathrm{e}^{\mathrm{i}\,q\chi/\hbar c}\,H\,\mathrm{e}^{-\mathrm{i}\,q\chi/\hbar c}\,\psi = \mathrm{e}^{\mathrm{i}\,q\chi/\hbar c}\,\mathrm{i}\,\hbar\partial_t\,\mathrm{e}^{-\mathrm{i}\,q\chi/\hbar c}\,\psi\\
&\implies H\,\mathrm{e}^{-\mathrm{i}\,q\chi/\hbar c}\,\psi = \mathrm{i}\,\hbar\partial_t\,\mathrm{e}^{-\mathrm{i}\,q\chi/\hbar c}\,\psi
\end{aligned} \tag{E.1.23}$$

Once the transformation of the Schrodinger equation is obtained, so is the solution:

$$\psi \mapsto \psi' = \mathrm{e}^{\mathrm{i}\,q\chi/\hbar c}\,\psi\,. \tag{E.1.24}$$

This transformation satisfies

$$\begin{aligned}
\left(\vec{p} - \frac{q}{c}\vec{A} - \frac{q}{c}\nabla\chi\right)\psi' &= -\mathrm{i}\,\hbar\left(\frac{\mathrm{i}\,q\nabla\chi}{\hbar c}\psi' + \mathrm{e}^{\mathrm{i}\,q\chi/\hbar c}\,\nabla\psi\right) - \left(\frac{q}{c}\vec{A} + \frac{q}{c}\nabla\chi\right)\psi'\\
&= \mathrm{e}^{\mathrm{i}\,q\chi/\hbar c}\,\vec{p}\psi - \frac{q}{c}\vec{A}\psi' = \mathrm{e}^{\mathrm{i}\,q\chi/\hbar c}\left(\vec{p} - \frac{q}{c}\vec{A}\right)\psi\,,
\end{aligned} \tag{E.1.25}$$

Remark 7. *Notice that by the gauge invariance discussed previously, the equation E.1.12 is form invariant under the gauge transformation:*

$$\begin{aligned}
&\mathrm{i}\,\hbar\frac{\partial}{\partial t}\psi = \left[\frac{1}{2m}\left(\vec{p}^2 + \frac{q^2}{c^2}\vec{A}^2 - \frac{2q}{c}\vec{A}\cdot\vec{p}\right) + q\phi + V\right]\psi\\
&\mapsto \mathrm{i}\,\hbar\frac{\partial}{\partial t}\psi' = \left[\frac{1}{2m}\left(\vec{p}^2 + \frac{q^2}{c^2}\vec{A}'^2 - \frac{2q}{c}\vec{A}'\cdot\vec{p}\right) + q\phi' + V\right]\psi'\,.
\end{aligned} \tag{E.1.26}$$

Remark 8. *We derive the Schrodinger equation in the magnetic field from the classical equation of motion E.1.4. Conversely, we can derive equation E.1.4 from the ordinary Schrodinger equation by requiring that the Schrodinger equation is invariant under the transformation $\psi \mapsto \psi\,\mathrm{e}^{\mathrm{i}\,q\chi/\hbar c}$.*

Under this transformation the Schrodinger equation is transformed as follows:

$$\mathrm{i}\,\hbar\frac{\partial}{\partial t}\psi = \frac{\vec{p}^2}{2m}\psi \mapsto \left(\mathrm{i}\,\hbar\frac{\partial}{\partial t} - \frac{q}{c}\frac{\partial\chi}{\partial t}\right)\psi' = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\nabla\chi\right)^2\psi'\,. \tag{E.1.27}$$

Use the gauge transformation E.1.14, we can obtain:

$$\mathrm{i}\,\hbar\frac{\partial}{\partial t}\psi = \frac{1}{2m}\left[\left(\vec{p} - \frac{q\vec{A}}{c}\right)^2 + q\phi\right]\psi\,. \tag{E.1.28}$$

Replace the quantum mechanical operators with classical quantities, we can reproduce the classical equation of motion E.1.4.

E.2 Charged Particle in the Magnetic Field

We have derived the quantum mechanical equation for *non-relativistic* and *spinless* charged particles in the electromagnetic fields. Now consider a charged particle moving in a constant magnetic field:

$$A_x = -\frac{1}{2}By\ , \quad A_y = \frac{1}{2}Bx\ , \quad A_z = 0\ . \tag{E.2.1}$$

The Hamiltonian of the particle is:

$$\begin{aligned} H &= \frac{1}{2m}\left[\left(p_x + \frac{1}{2c}Byq\right)^2 + \left(p_y - \frac{1}{2c}Bxq\right)^2 + p_z^2\right] && \text{(E.2.2)} \\ &= \frac{1}{2m}\left[(p_x^2 + p_y^2) + \frac{B^2q^2}{4c^2}(x^2+y^2) + \frac{Bq}{c}(p_x y - p_y x) + p_z^2\right]\ . && \text{(E.2.3)} \end{aligned}$$

Define the following variables:

$$\begin{aligned} &\vec{p}_{x,y} = p_x + p_y \text{ (motion in } x,y\text{-plane)}\ , \quad \frac{Bq}{2mc} = \omega_L \text{ (Oscillation Frequency)}\ , \\ &p_x y - p_y x = l_z \text{ (Angular momentum in } z\text{- direction)}\ . \end{aligned} \tag{E.2.4}$$

The Hamiltonian can be rewritten in the following form, each term leads to a corresponding physical phenomenon:

$$\boxed{H = \frac{\vec{p}^{\,2}_{x,y}}{2m} + \underbrace{\frac{1}{2}m\omega_L^2(x^2+y^2)}_{\text{Zeeman effect}} + \underbrace{\omega_L l_z}_{\text{Landau levels}} + \underbrace{\frac{p_z^2}{2m}}_{\text{Free motion}}}\ . \tag{E.2.5}$$

E.2.1 Zeeman Effect

We now move our focus on the electron in the hydrogen atom, that is, the charge $q = -e$.

Consider the hydrogen atom is in a weak magnetic field, that is, $\mathcal{O}(B^2)$ can be dropped. Then the Hamiltonian becomes

$$H = \frac{\vec{p}^{\,2}_{x,y}}{2m} + \omega_L l_z + V(r)\ , \tag{E.2.6}$$

here $V(r) = -e^2/r$ is the electric potential due to the nuclear, only dependent on the distance to the nuclear r.

The algebra for the angular momentum is

$$[l_i, l_j] = \mathrm{i}\,\epsilon_{ijk} l_k\ , \tag{E.2.7}$$

here $l_1 = l_x,\ l_2 = l_y,\ l_3 = l_z$. Using this algebraic structure, we can obtain the following commutation relation

$$[l_i, l^2] = 0\ , \quad [H, l^2] = 0\ , \quad [H, l_i] = 0\ . \tag{E.2.8}$$

Therefore, in an ordinary hydrogen atom (without the magnetic field), the set $\{H, l_z, l^2\}$ forms a complete set of commuting observables. The eigenstates of these operators are $\{|E_n, l, m\rangle\}_{n,l,m}$, which have the eigenvalues for each operator:

$$H\,|E_n, l, m\rangle = E_n\,|E_n, l, m\rangle \ , \tag{E.2.9}$$

$$l^2\,|E_n, l, m\rangle = l(l+1)\hbar^2\,|E_n, l, m\rangle \ , \tag{E.2.10}$$

$$l_z\,|E_n, l, m\rangle = m\hbar\,|E_n, l, m\rangle \ . \tag{E.2.11}$$

Due to the spherical symmetry of the atomes, the corresponding wave functions can be expressed as two parts which are dependent on n, l and l, m respectively, which can be expressed as follows:

$$\psi_{nlm} = R_{nl}(r) Y_l^m(\theta, \phi) \ , \tag{E.2.12}$$

where $Y_l^m(\theta, \phi)$ is the spherical harmonic function.

Similarly, in the hydrogen atom in the magnetic field, the complete set of commuting observables is:

$$\left\{ H = \frac{\vec{p}_{x,y}^{\,2}}{2m} + \omega_L l_z + V(r) \ , \quad l \ , \quad l^2 \right\} . \tag{E.2.13}$$

But the eigenstates and their eigenvalues now are:

$$H\,|E_n, l, m\rangle = (E_n + \omega_L m\hbar)\,|E_n, l, m\rangle \ , \tag{E.2.14}$$

$$l^2\,|E_n, l, m\rangle = l(l+1)\hbar^2\,|E_n, l, m\rangle \ , \tag{E.2.15}$$

$$l_z\,|E_n, l, m\rangle = m\hbar\,|E_n, l, m\rangle \ . \tag{E.2.16}$$

The degenerate spectra of the atom will split into $2l+1$ levels. For example, if the energy difference of 3p and 3s orbitals is ΔE, consider the Zeeman effect, the spectra split into $\Delta E - \omega_L$, ΔE, $\Delta E + \omega_L$.

E.2.2 Landau Levels

The Zeeman effect only considers the weak magnetic field and drops the $\mathcal{O}(B^2)$ term. Now we include the $\mathcal{O}(B^2)$ term.

Similarly, the wave function can be expressed as several different parts. Notice that the system does not have spherical symmetry but cylindrical symmetry. Hence, the wave function can be expressed as three parts in cylindrical coordinates:

$$\psi(\rho, \phi, z) = \chi(\rho)\, \mathrm{e}^{\mathrm{i}\, m\phi}\, \mathrm{e}^{\mathrm{i}\, kz} \ , \tag{E.2.17}$$

where $m = 0, \pm 1, \pm 2, \cdots$ and k is the conserved momentum in the z-direction.

We now first solve the solution of the equation, and express the operators in spherical coordinates, we can obtain a one-variable equation:

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{m^2}{\rho^2}\right) + \frac{1}{2}\mu\omega_L^2\rho^2\right]\chi(\rho) = \left[E - m\hbar\omega_L - \frac{\hbar^2k^2}{2\mu}\right]\chi(\rho) \ , \tag{E.2.18}$$

where the last term is the total energy minus the energy from the terms $\omega_L l_z$ and $p_z^2/(2m)$, we now denote it by E'. Rewrite it into a homogeneous equation form:

$$\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{m^2}{\rho^2}-\frac{\mu^2\omega_L^2}{\hbar^2}\rho^2+\frac{2\mu E'}{\hbar^2}\right)\chi(\rho)=0\ . \tag{E.2.19}$$

Define $\alpha\equiv\mu\omega_L/\hbar$, $E'=\hbar\omega_L\epsilon$, and $\xi\equiv\alpha\rho$ then it becomes:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\,\xi^2}+\frac{1}{\xi}\frac{\mathrm{d}}{\mathrm{d}\,\xi}-\frac{m^2}{\xi^2}-\xi^2+2\xi\right)\xi(\xi)=0\ . \tag{E.2.20}$$

Consider the boundary condition $\xi\to 0$, the equation becomes:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\,\xi^2}+\frac{1}{\xi}\frac{\mathrm{d}}{\mathrm{d}\,\xi}-\frac{m^2}{\xi^2}\right)\xi(\xi)=0\ , \tag{E.2.21}$$

which has the solution $\chi=\xi^\beta$, where $\beta=|m|$.

For the boundary condition $\xi\to\infty$, the equation becomes:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\,\xi^2}-\xi^2\right)\xi(\xi)=0\ , \tag{E.2.22}$$

which has the solution $\chi=\mathrm{e}^{\pm\xi^2/2}$.

With the ansatz $\chi(\xi)=\xi^\beta\,\mathrm{e}^{\pm\xi^2/2}\,u(\xi)$. Substitute it in the equation, we obtain:

$$u''+\left(\frac{2\beta-1}{\xi}-2\xi\right)u'+[2\epsilon-2(\beta+1)]u=0\ . \tag{E.2.23}$$

Now define $\zeta\equiv\xi^2$ and therefore $\mathrm{d}\,u/\,\mathrm{d}\,\xi=2\zeta\,\mathrm{d}\,u/\,\mathrm{d}\,\zeta$, substitute them in the equation, we can obtain:

$$\zeta u''+(\beta+1-\zeta)u'-\left(\frac{\beta+1}{2}-\frac{\epsilon}{2}\right)\left(\frac{\beta+1}{2}-\frac{\epsilon}{2}\right)u=0\ , \tag{E.2.24}$$

which is a hypergeometric equation:

$$\zeta f''+(\gamma-\zeta)f'-\alpha f=0\ , \tag{E.2.25}$$

with $\alpha=\left(\frac{\beta+1}{2}-\frac{\epsilon}{2}\right)$ and $\gamma=\beta+1$. The solution is an unusual special function *hypergeometric function* $F(\alpha,\beta,\zeta)$, which is defined as

$$F(\alpha,\gamma,\zeta)=\sum_{n=0}^{\infty}\frac{(\alpha)_n}{n!(\gamma)_n}\zeta^n\ , \tag{E.2.26}$$

where

$$\frac{(\alpha)_n}{(\gamma)_n}=\frac{\alpha}{\gamma}\frac{\alpha+1}{\gamma+1}\cdots\frac{\alpha+b}{\gamma+b}\ . \tag{E.2.27}$$

Therefore, we ultimately obtain:

$$\chi(\rho)=\mathrm{e}^{-(\alpha\rho)^2/2}(\alpha\rho)^\beta F(\alpha,\gamma,\alpha^2\rho^2)\ . \tag{E.2.28}$$

Consider the boundary condition $\rho \to \infty$, then $\chi(\rho)$ diverges unless $F(\alpha, \beta, \alpha^2\rho^2)$ is finite. Then we require $(\alpha)_n = 0$. Therefore, $\alpha = n_\rho \in \mathbb{N}$. Hence, $\epsilon = 2n_\rho + |m| + 1$.

We ultimately obtain the spectrum and the wave function:

$$E'_{n_\rho m} = \hbar\omega_L(2n_\rho + |m| + 1) \,, \tag{E.2.29}$$

$$\psi_{n_\rho m k}(\rho, \phi, z) = \mathrm{e}^{\mathrm{i}\, m\phi}\, \mathrm{e}^{\mathrm{i}\, kz}\, \mathrm{e}^{-(\alpha\rho)^2/2}(\alpha\rho)^{|m|} F(\alpha, \gamma, \alpha^2\rho^2) \,. \tag{E.2.30}$$

The total energy is:

$$\begin{aligned} E &= E'_{n_\rho m} + m\hbar\omega_L + \frac{\hbar^2 k^2}{2\mu} \\ &= \hbar\omega_L(2n_\rho + |m| + 1 + m) + \frac{\hbar^2 k^2}{2\mu} \,. \end{aligned} \tag{E.2.31}$$

Notice that E can be rewritten as:

$$E = \mu_z B_z + \frac{\hbar^2 k^2}{2\mu} \,, \tag{E.2.32}$$

where $\mu_z = -\frac{e\hbar}{2\mu c}(2n_\rho + |m| + 1 + m)$.

Therefore, the term μ_z is actually the quantum-induced dipole moment for free electrons in the magnetic field.

E.2.3 Superconductivity (Phenomenological Description)

Superconductivity is a phenomenon of zero resistance in the conductor, that is, there is no potential barrier in the conductor and the electrons in the superconductor are free. In this section, we discuss some phenomena originating from this property.

Meissner Effect

Meissner effect is a phenomenon that which the magnetic field vanishes in the superconductor as figure 3.1. This phenomenon can not be explained by classical electromagnetism. We discuss the quantum mechanics description of this phenomenon in this section.

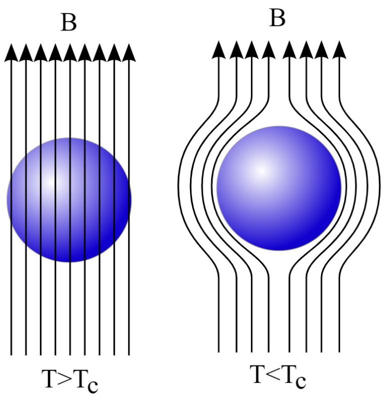

Figure 3.1: Meissner effect, the magnetic field is expelled outside the superconductor.

Quantum mechanics provides a description of the charge carriers in the superconductor as:

$$\mathrm{i}\,\hbar\frac{\partial}{\partial t}\psi = \frac{1}{2\mu}\left[\left(-\mathrm{i}\,\hbar\nabla - \frac{q}{c}\vec{A}\right)^2 + q\phi\right]\psi\ , \tag{E.2.33}$$

take $\psi = \sqrt{\rho}\,\mathrm{e}^{\mathrm{i}\,\theta}$, where $\theta = S(t)/\hbar$. Then since $-\mathrm{i}\,\hbar\nabla \mapsto (-\mathrm{i}\,\hbar\nabla - q\vec{A}/c)$, we have

$$\mu\vec{v} = \hbar\nabla\theta - \frac{q\vec{A}}{c}\ . \tag{E.2.34}$$

Then we have the continuity equation:

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\vec{v}) = \frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0\ , \tag{E.2.35}$$

$$\vec{j} = \frac{\rho}{\mu}\left(\hbar\nabla\theta - \frac{q}{c}\vec{A}\right)\ . \tag{E.2.36}$$

Notice that since the second equation is the probability current, it gives rise to a quantum current density:

$$\vec{J} = \frac{q\rho}{\mu}\left(\hbar\nabla\theta - \frac{q}{c}\vec{A}\right)\ . \tag{E.2.37}$$

We can perform the gauge transformation to make it become:

$$\boxed{\vec{J} = -\frac{q^2\rho}{\mu c}\vec{A}}\ , \tag{E.2.38}$$

This is called *London equation*.

Another equation is the incompressible-fluid-like equation, known as the Bernoulli equation:

$$\frac{\mu}{2}\vec{v}^2 + q\phi + \underbrace{\hbar\frac{\partial\theta}{\partial t} - \frac{\hbar^2}{2\mu}\frac{1}{\sqrt{\rho}}\nabla^2\sqrt{\rho}}_{\text{quantum effects}} = 0\ . \tag{E.2.39}$$

This equation states that the quantum current density behaves like the incompressible fluid.

Remark 9. *Take the gradient of the equation, we can obtain:*

$$\begin{aligned}0 &= \frac{\mu}{2}\nabla\vec{v}^2 - q\vec{E} + \hbar\frac{\partial}{\partial t}(\nabla\theta) - \frac{\hbar^2}{2\mu}\nabla\left(\frac{1}{\sqrt{\rho}}\nabla^2\sqrt{\rho}\right)\\ &= \mu[\vec{v}\times(\nabla\times\vec{v}) + (\vec{v}\cdot\nabla)\vec{v}] - q\vec{E} + \frac{\partial}{\partial t}\left(\mu\vec{v} + \frac{q\vec{A}}{c}\right) - \frac{\hbar^2}{2\mu}\nabla\left(\frac{1}{\sqrt{\rho}}\nabla^2\sqrt{\rho}\right)\ .\end{aligned} \tag{E.2.40}$$

Utilize the relations:

$$\nabla\times\vec{v} = -\frac{q}{\mu c}\nabla\times\vec{A} = -\frac{q}{\mu c}\vec{B}\ , \tag{E.2.41}$$

$$\frac{\mathrm{d}\,\vec{v}}{\mathrm{d}\,t} = \frac{\partial\vec{v}}{\partial t} + v_x\frac{\partial\vec{v}}{\partial x} + v_y\frac{\partial\vec{v}}{\partial y} + v_z\frac{\partial\vec{v}}{\partial z} = (\vec{v}\cdot\nabla)\vec{v}\ . \tag{E.2.42}$$

We can obtain the equation of motion:

$$\mu\frac{\mathrm{d}\,\vec{v}}{\mathrm{d}\,t} = q(\vec{E} + \frac{1}{c}\vec{v}\times\vec{B}) + \frac{\hbar^2}{2\mu}\left(\frac{1}{\sqrt{\rho}}\nabla^2\sqrt{\rho}\right) \ . \tag{E.2.43}$$

This tells us that the last term can be interpreted as the quantum-induced potential. We can denote it as

$$-V_{\text{quantum}} = \frac{\hbar^2}{2\mu}\left(\frac{1}{\sqrt{\rho}}\nabla^2\sqrt{\rho}\right) \ . \tag{E.2.44}$$

Back to the quantum current density, employ the Maxwell's equation:

$$\nabla\times\vec{B} = \frac{4\pi}{c}\vec{J} + \frac{1}{c}\frac{\partial\vec{E}}{\partial t} \ , \tag{E.2.45}$$

assume the electric field is steady, we can obtain:

$$\begin{aligned}\nabla\times(\nabla\times\vec{B}) &= \frac{4\pi}{c}\nabla\times\vec{J} \\ &= -\frac{4\pi}{c}\frac{q^2\rho}{\mu c}\nabla\times\vec{A} \\ &= -\frac{4\pi q^2\rho}{\mu c^2}\vec{B} \ .\end{aligned} \tag{E.2.46}$$

Apply the Maxwell's equation and the vector identity:

$$\nabla\cdot\vec{B} = 0 \ , \tag{E.2.47}$$

$$\nabla\times(\nabla\times\vec{B}) = \nabla(\nabla\cdot\vec{B}) - \nabla^2\vec{B} \ . \tag{E.2.48}$$

Define $\lambda = \sqrt{4\pi\rho q^2/(\mu c^2)}$. We ultimately obtain the equation:

$$\boxed{\nabla^2\vec{B} = \lambda^2\vec{B}} \ . \tag{E.2.49}$$

Notice that $\lambda \approx 10^3\,\mathrm{m}$. Therefore, according to the differential equation, we know that the magnetic field exponential decay in the material rapidly:

$$\boxed{B_i \propto \mathrm{e}^{-\lambda x}} \ . \tag{E.2.50}$$

This is the Meissner effect.

Flux Quantization

Define the magnetic flux for a surface $\mathbb{S}$ as

$$\Phi = \int_{\mathbb{S}} \vec{B}\cdot\mathrm{d}\,\vec{s} \ . \tag{E.2.51}$$

Due to the Meissner effect, we can know that:

$$\hbar\nabla\theta = \frac{q\vec{A}}{c} \ . \tag{E.2.52}$$

Consider the integral over a curve. It is easy to obtain the relation:

$$\begin{aligned}\oint_{\partial\mathbb{S}} \hbar\nabla\theta \cdot \mathrm{d}\,\vec{l} &= \frac{q}{c}\oint_{\partial\mathbb{S}} \vec{A}\cdot\mathrm{d}\,\vec{l} \\ &= \frac{q}{c}\int_{\mathbb{S}} \vec{B}\cdot\mathrm{d}\,\vec{s} = \frac{q}{c}\Phi\ .\end{aligned} \tag{E.2.53}$$

Since $\sqrt{\rho}\,\mathrm{e}^{\mathrm{i}\,\theta}$ should be invariant when the curve integral goes back to the same point, that is, $\theta \in \mathbb{R}/\sim$, where $\sim$ is an equivalent relation defined by $a \sim b$ if and only if $0 \sim 2\pi$. Therefore, the integral becomes:

$$\oint_{\partial\mathbb{S}} \nabla\theta \cdot \mathrm{d}\,\vec{l} = 0 \in \mathbb{R}/\sim\ . \tag{E.2.54}$$

If we view $\oint_{\partial\mathbb{S}} \nabla\theta \cdot \mathrm{d}\,\vec{l}$ on $\mathbb{R}$, then

$$\oint_{\partial\mathbb{S}} \nabla\theta \cdot \mathrm{d}\,\vec{l} = 2\pi n,\ n \in \mathbb{Z}\ . \tag{E.2.55}$$

Therefore, we obtain the magnetic flux satisfies:

$$\Phi = \frac{2n\hbar\pi c}{q} \equiv n\Phi_0\ , \tag{E.2.56}$$

where Φ_0 is the flux quantum. In superconductors, the copper pairs have charges $q = -2e$, then the flux quantum is:

$$\Phi_0 = \frac{\pi\hbar c}{e} \approx 2\times 10^{-7}\,\mathrm{Gauss}\cdot\mathrm{cm}^2\ . \tag{E.2.57}$$

E.2.4 Aharonov–Bohm effect

Aharonov–Bohm effect is a quantum mechanics phenomenon stating a charged particle is affected by an electromagnetic field even though the particle is in the region without any electromagnetic field.

Consider a device that particles are emitted at the A side and collected at the B side, the particles can pass through two paths I and II as figure 3.2 demonstrates.

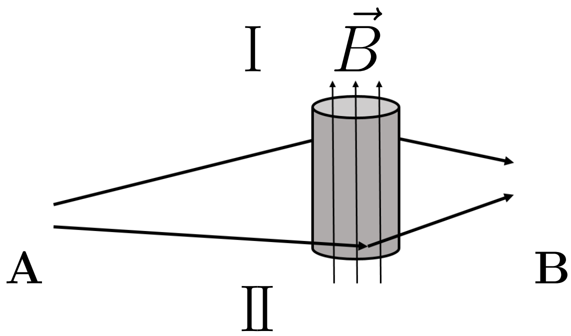

Figure 3.2: Device for the Aharonov–Bohm effect experiment.

The wave function at the B side can be written as path integral form:

$$\psi(\vec{x}) = \int_{\mathrm{I}} \mathcal{D}[\vec{x}(t)]\, \mathrm{e}^{\mathrm{i}\, S[\vec{x}(t),t]/\hbar} + \int_{\mathrm{II}} \mathcal{D}[\vec{x}(t)]\, \mathrm{e}^{\mathrm{i}\, S[\vec{x}(t),t]/\hbar} \; . \tag{E.2.58}$$

The Lagrangian and the action are:

$$L(\vec{x}(t), \dot{\vec{x}}(t)) = L_0(\vec{x}(t), \dot{\vec{x}}(t)) + \frac{q\vec{A}\cdot\dot{\vec{x}}(t)}{c} \; , \tag{E.2.59}$$

$$\begin{aligned} S(\vec{x}(t), t) &= \int_{t_0}^{t} L_0(\vec{x}(t'), \dot{\vec{x}}(t'))\, \mathrm{d}\, t' + \int_{t_0}^{t} \frac{q\vec{A}\cdot\dot{\vec{x}}(t')}{c}\, \mathrm{d}\, t' \\ &= S_0[\vec{x}(t), t] + \frac{q}{c}\int_{\vec{x}([t_0,t])} \vec{A}\cdot \mathrm{d}\,\vec{x}' \; . \end{aligned} \tag{E.2.60}$$

Therefore, the wavefunction becomes:

$$\begin{aligned} \psi(\vec{x}) = &\left(\int_{\mathrm{I}} \mathcal{D}[\vec{x}(t)]\, \mathrm{e}^{\mathrm{i}\, S_0[\vec{x}(t),t]/\hbar}\right) \times \exp\left[\frac{\mathrm{i}\, q}{\hbar c}\int_{\vec{x}\in \mathrm{I}} \vec{A}\cdot \mathrm{d}\,\vec{x}'\right] \\ &+ \left(\int_{\mathrm{II}} \mathcal{D}[\vec{x}(t)]\, \mathrm{e}^{\mathrm{i}\, S_0[\vec{x}(t),t]/\hbar}\right) \times \exp\left[\frac{\mathrm{i}\, q}{\hbar c}\int_{\vec{x}\in \mathrm{II}} \vec{A}\cdot \mathrm{d}\,\vec{x}'\right] \; . \end{aligned} \tag{E.2.61}$$

Define the path integral terms in the equation E.2.61 be R_1 and R_2 and the exponential terms in the equation E.2.61 be $\mathrm{e}^{\mathrm{i}\,\theta_1}$ and $\mathrm{e}^{\mathrm{i}\,\theta_2}$. The wavefunction can be rewritten as:

$$\begin{aligned} \psi &= R_1\, \mathrm{e}^{\mathrm{i}\,\theta_1} + R_2\, \mathrm{e}^{\mathrm{i}\,\theta_2} \\ &= R_1\, \mathrm{e}^{\mathrm{i}\,\theta_1}\left(1 + \frac{R_2}{R_1}\, \mathrm{e}^{\mathrm{i}(\theta_2-\theta_1)}\right) \; . \end{aligned} \tag{E.2.62}$$

Notice the definition of θ_1 and θ_2, we can view it as a closed curve integral as follows:

$$\begin{aligned} \theta_2 - \theta_1 &= \frac{q}{\hbar c}\int_{\vec{x}\in \mathrm{I}} \vec{A}\cdot \mathrm{d}\,\vec{x}' - \frac{q}{\hbar c}\int_{\vec{x}\in \mathrm{II}} \vec{A}\cdot \mathrm{d}\,\vec{x}' \\ &= \frac{q}{\hbar c}\oint \vec{A}\cdot \mathrm{d}\,\vec{x}' = \frac{q}{\hbar c}\int \vec{B}\cdot \mathrm{d}\,\vec{x}' = 2\pi\frac{\Phi}{\Phi_0} \; . \end{aligned} \tag{E.2.63}$$

Therefore, we can see that the phase factor of the wave function can be affected by the magnetic field. This phenomenon is called *Aharonov–Bohm effect*, which is a purely quantum mechanical phenomenon.

In addition, there is a similar phenomenon called *Aharonov–Casher effect* stating that the magnetic dipole moment μ displays a similar effect in the presence of an electric field, that is, the figure 3.2 becomes figure 3.3.

The Lagrangian can be derived from the Dirac equation, which is:

$$L = L_0 - (\vec{E}\times\vec{\mu})\cdot\dot{\vec{x}} \; . \tag{E.2.64}$$

By a similar trick, we can obtain the same form of the wavefunction with the only difference being $q\vec{A}/c \mapsto -\vec{E}\times\vec{\mu}$. Therefore, the phase factor difference becomes:

$$\theta_2 - \theta_1 = -\frac{1}{\hbar}\int_{\vec{x}\in \mathrm{I}} (\vec{E}\times\vec{\mu})\cdot \mathrm{d}\,\vec{x}' + \frac{1}{\hbar}\int_{\vec{x}\in \mathrm{II}} (\vec{E}\times\vec{\mu})\cdot \mathrm{d}\,\vec{x}'$$

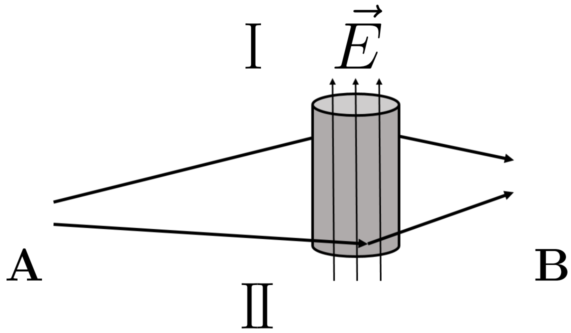

Figure 3.3: Device for the Aharonov–Casher effect experiment.

$$
\begin{aligned}
&= -\frac{1}{\hbar}\oint (\vec{E}\times\vec{\mu})\cdot \mathrm{d}\,\vec{x}' = -\frac{1}{\hbar}\oint \nabla\times(\vec{E}\times\vec{\mu})\cdot \mathrm{d}\,\vec{s}' \\
&= -\frac{1}{\hbar}\oint (\vec{\mu}\cdot\nabla)\vec{E}\cdot \mathrm{d}\,\vec{s}' + \frac{1}{\hbar}\oint (\nabla\cdot\vec{E})\vec{\mu}\cdot \mathrm{d}\,\vec{s}' \\
&= -\frac{1}{\hbar}\oint (\vec{\mu}\cdot\nabla)\vec{E}\cdot \mathrm{d}\,\vec{s}' + \frac{1}{\hbar}\oint \rho\vec{\mu}\cdot \mathrm{d}\,\vec{s}'\ . \qquad \text{(E.2.65)}
\end{aligned}
$$

Chapter 4

Electron Spin and Angular Momentum

Spin is a purely quantum phenomenon proposed to solve the problems of the atomic spectrum. The first problem is *sodium atomic spectrum*, usually, sodium atom spectrum has a yellow line with wavelength about 5893 Å. However, under high resolution, it actually consists of 2 lines with wavelength 5896, Å and 5890, Å. Another one is *anomalous Zeeman effect*. The normal Zeeman effect states that the spectrum line splits into $2l+1$ lines in the magnetic field. However, sometimes the spectrum line splits into an even number of lines, this is called the *anomalous Zeeman effect*. We need to introduce the concept of *spin* to explain these phenomena. The spin has the properties that the spin angular momentum of magnitude $\hbar/2$ and projection on the z-direction can take only two values $\pm\hbar/2$. The magnetic dipole moment is $e\hbar/(4mc)$.

S.1 Pauli Theory

The original mechanical model of spin describes that the spin is due to the rotation of electrons. However, it requires the velocity of the surface of the spin to be about $137c$, which makes no sense. Now, we use the *Pauli theory* to describe the spin.

The Pauli theory states that the spin S and the spin magnetic moment μ are new intrinsic properties of electrons. Assume that the spin obeys the angular momentum algebra

$$[S_i, S_j] = \mathrm{i}\,\hbar \sum_{k=1}^{3} \epsilon_{ijk} S_k \; . \tag{S.1.1}$$

Instead of assuming that they are mechanical, we assume that, like other quantum observables, they can be described as operators and quantum states.

The simplest spin structure is in two-dimensional Hilbert space:

$$\mathcal{H} = \{\, |\uparrow\rangle \,,\; |\downarrow\rangle \,\} \,, \tag{S.1.2}$$

which satisfies $S_z\,|\uparrow\rangle = \hbar/2,\ S_z\,|\downarrow\rangle = -\hbar/2$. We can represent it as matrices by introducing the *Pauli matrices*, which are defined by:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \,, \quad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \,, \quad \sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \; . \tag{S.1.3}$$

Alternatively, we can write three Pauli matrices as one matrix:

$$\sigma_i = \begin{pmatrix} \delta_{i3} & \delta_{i1} - \mathrm{i}\,\delta_{i2} \\ \delta_{i1} + \mathrm{i}\,\delta_{i2} & -\delta_{i3} \end{pmatrix} \tag{S.1.4}$$

These Hermitian matrices follow similar algebra as the spin operators, the commutator and the anti-commutator for the Pauli matrices are:

$$[\sigma_i, \sigma_j] = 2\,\mathrm{i} \sum_{k=1}^{3} \epsilon_{ijk}\sigma_k \ , \quad \{\sigma_i, \sigma_j\} = 2\delta_{ij} I \ . \tag{S.1.5}$$

Combine the commutator and the anti-commutator together, we can obtain the product of two Pauli matrices:

$$\begin{aligned} \sigma_i\sigma_j &= \frac{1}{2}[\sigma_i, \sigma_j] + \frac{1}{2}\{\sigma_i, \sigma_j\} \\ &= \mathrm{i} \sum_{k=1}^{3} \epsilon_{ijk}\sigma_k + \delta_{ij} I \ . \end{aligned} \tag{S.1.6}$$

Consider two vectors $\vec{a} = (a_x, a_y, a_z)$ and $\vec{b} = (v_x, v_y, v_z)$, then

$$\sum_{i=1}^{3}\sum_{j=1}^{3}(a_i\sigma_i)(b_j\sigma_j) = \sum_{i=1}^{3}\sum_{j=1}^{3}\left(\mathrm{i}\sum_{k=1}^{3}\epsilon_{ijk}a_ib_j\sigma_k + \delta_{ij}a_ib_jI\right) \ . \tag{S.1.7}$$

We can rewrite this relationship in outer product and inner product form:

$$(\vec{a}\cdot\vec{\sigma})(\vec{b}\cdot\vec{\sigma}) = \mathrm{i}(\vec{a}\times\vec{b})\cdot\vec{\sigma} + (\vec{a}\cdot\vec{b})I \ . \tag{S.1.8}$$

The spin operations and the quantum states can be represented as:

$$S_i = \frac{\hbar}{2}\sigma_i \ , \quad |{\uparrow}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \quad |{\downarrow}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \ . \tag{S.1.9}$$

S.2 Intrinsic Magnetic Dipole Moment

The algebra of the angular momentum and the spin are very similar. The magnetic dipole moments from these properties are similar as well. However, their original properties clearly differ. We will discuss the difference between these two properties.

S.2.1 Magnetic Moment from Angular Momentum

We now are interested in the interaction between the magnetic field and the electrons. Assume the magnetic field is uniform, then the Hamiltonian is:

$$H = \frac{1}{2\mu}\left(\vec{p}^2 + \frac{e\vec{A}}{c}\right)^2 = \frac{\vec{p}^2}{2\mu} + \frac{e\vec{A}\cdot\vec{p}}{\mu c} + \frac{e^2\vec{A}^2}{2\mu c^2} \ . \tag{S.2.1}$$

We assume the uniform magnetic field here; therefore

$$\vec{A} = \frac{1}{2}\vec{B} \times \vec{r}\,. \tag{S.2.2}$$

The Hamiltonian becomes:

$$\begin{aligned} H &= \frac{\vec{p}^2}{2\mu} + \frac{e\vec{A}\cdot\vec{p}}{\mu c} + \frac{e^2\vec{A}^2}{2\mu c^2} \\ &= \frac{\vec{p}^2}{2\mu} + \frac{e\vec{p}\cdot(\vec{B}\times\vec{r})}{2\mu c} + \frac{e^2\vec{A}^2}{2\mu c^2} \\ &= \frac{\vec{p}^2}{2\mu} + \frac{e\vec{B}\cdot(\vec{r}\times\vec{p})}{2\mu c} + \frac{e^2\vec{A}^2}{2\mu c^2} \\ &= \frac{\vec{p}^2}{2\mu} + \frac{e\vec{B}\cdot\vec{l}}{2\mu c} + \frac{e^2\vec{A}^2}{2\mu c^2} = \frac{\vec{p}^2}{2\mu} + \frac{e^2\vec{A}^2}{2\mu c^2} - \vec{\mu}_l\cdot\vec{B}\,, \end{aligned} \tag{S.2.3}$$

where $\vec{\mu}_l = e\vec{l}/(2\mu c)$ is the magnetic moment due to the orbital angular momentum. Notice that this is not intrinsic since it originates from the orbital angular momentum $\vec{l}$.

S.2.2 Magnetic Moment from Orbital Spin

The spin differs from the angular momentum, the magnetic moment due to the spin is a kind of intrinsic property. We start our discussion with the free spin particle.

Since the wave functions for the spin particles are $\psi(\vec{r}, S_z) = (\psi_+(\vec{r}), \psi_-(\vec{r0}))^T$, the momentum operator in the spinor space is:

$$\vec{\sigma}\cdot = \sigma_x p_x + \sigma_y p_y + \sigma_z p_z\,, \tag{S.2.4}$$

which can be imaged as the projection of the momentum operator on each of the spin states. Therefore, the Hamiltonian for the spin particle in the magnetic field is:

$$H = \frac{[\vec{\sigma}\cdot(\vec{p} + e\vec{A}/c)]^2}{2\mu}\,. \tag{S.2.5}$$

Utilize the relationship:

$$(\vec{a}\cdot\vec{\sigma})(\vec{b}\cdot\vec{\sigma}) = \mathrm{i}(\vec{a}\times\vec{b})\cdot\vec{\sigma} + (\vec{a}\cdot\vec{b})\,. \tag{S.2.6}$$

The Hamiltonian becomes:

$$\begin{aligned} H &= \frac{\mathrm{i}(\vec{p} + e\vec{A}/c)\times(\vec{p} + e\vec{A}/c)\cdot\vec{\sigma}}{2\mu} + \frac{(\vec{p} + e\vec{A}/c)^2}{2\mu} \\ &= \frac{\mathrm{i}\,e}{2\mu c}(\vec{p}\times\vec{A} + \vec{A}\times\vec{p})\cdot\vec{\sigma} + \frac{(\vec{p} + e\vec{A}/c)^2}{2\mu}\,. \end{aligned} \tag{S.2.7}$$

Notice that the term $\vec{p}\times\vec{A} + \vec{A}\times\vec{p}$ here is an operator; therefore, we need the relation:

$$\begin{aligned} \left[\vec{p}\times(\vec{A}\psi) + \vec{A}\times(\vec{p}\psi)\right] &= -\mathrm{i}\,\hbar\left[\nabla\times(\vec{A}\psi) + \vec{A}\times(\nabla\psi)\right] \\ &= -\mathrm{i}\,\hbar\left[\left(\nabla\times\vec{A}\right)\psi + (\nabla\psi)\times\vec{A} + \vec{A}\times(\nabla\psi)\right] \end{aligned}$$

$$= -\mathrm{i}\,\hbar\left(\nabla \times \vec{A}\right)\psi = -\mathrm{i}\,\hbar\vec{B}\psi\ . \tag{S.2.8}$$

This relationship means that as an operator $\vec{p}\times\vec{A}+\vec{A}\times\vec{p} = -\mathrm{i}\,\hbar\vec{B}$, then the Hamiltonian becomes:

$$\begin{aligned} H &= \frac{e\hbar}{2\mu c}\vec{\sigma}\cdot\vec{B} + \frac{(\vec{p}+e\vec{A}/c)^2}{2\mu} \\ &= \frac{e}{\mu c}\vec{S}\cdot\vec{B} + \frac{(\vec{p}+e\vec{A}/c)^2}{2\mu} \\ &= -\vec{\mu}_s\cdot\vec{B} + \frac{(\vec{p}+e\vec{A}/c)^2}{2\mu}\ , \end{aligned} \tag{S.2.9}$$

where $-\vec{\mu}_s = [e\hbar/(2\mu c)]\vec{\sigma} = [e/(\mu c)]\vec{S}$ is the magnetic moment due to the electron spin, which is an intrinsic property.

In summary, we have:

$$\frac{\mu_l}{l} = \frac{e}{2\mu c} = g_l\frac{e}{2\mu c}\ , \tag{S.2.10}$$

$$\frac{\mu_s}{S} = \frac{e}{\mu c} = g_s\frac{e}{2\mu c}\ , \tag{S.2.11}$$

where $g_l = 1$ and $g_s = 2$ are called g-factor, which is an important factor in quantum electrodynamics.

S.3 Total Angular Momentum

We now obtain the Hamiltonian including the spin and angular momentum:

$$\begin{aligned} H &= \frac{1}{2\mu}\left(\vec{p}+\frac{e\vec{A}}{c}\right)^2 - \vec{\mu}_s\cdot\vec{B} \\ &= \frac{1}{2\mu}\left(\vec{p}^2+\frac{e^2\vec{A}^2}{c^2}\right) - \vec{\mu}_l\cdot\vec{B} - \vec{\mu}_s\cdot\vec{B}\ . \end{aligned} \tag{S.3.1}$$

However, this is not the complete Hamiltonian. There is another interaction called *Thomas coupling*, which considers the interaction between the spin and the angular momentum and is a relativistic phenomenon. The coupling Hamiltonian is expressed as:

$$H_{\text{coupling}} = \frac{1}{2\mu^2c^2}\frac{1}{r}\frac{\mathrm{d}\,V}{\mathrm{d}\,r}\vec{S}\cdot\vec{l} \equiv \xi(r)\vec{S}\cdot\vec{l}\ . \tag{S.3.2}$$

This coupling Hamiltonian can affect the spin and angular momentum states, in other words, the angular momentum and the spin can affect each other through this coupling. Therefore, the coupling Hamiltonian does not commute with $\vec{S}$ and $\vec{l}$:

$$[\vec{S},\vec{S}\cdot\vec{l}] \neq 0\ , \quad [\vec{l},\vec{S}\cdot\vec{l}] \neq 0\ . \tag{S.3.3}$$

Now, since the spin and the angular momentum can affect each other, we combine them together and define it as

$$\vec{j} \equiv \vec{S}+\vec{l}\ , \tag{S.3.4}$$

which is called *total angular momentum*. It is easy to check that the total angular momentum follows the same algebra as the spin and the angular momentum:

$$[j_\alpha, j_\beta] = \mathrm{i} \sum_\gamma \epsilon_{\alpha\beta\gamma} j_\gamma \ , \quad [j^2, j_\alpha] = 0 \ . \tag{S.3.5}$$

In addition, the commutator of the total angular momentum and the coupling term is:

$$\begin{aligned} [j_\alpha, \vec{S} \cdot \vec{l}] &= [S_\alpha + l_\alpha, \vec{S} \cdot \vec{l}] \\ &= \sum_\beta \left([S_\alpha, S_\beta l_\beta] + [l_\alpha, S_\beta l_\beta] \right) \\ &= \sum_\beta \left([S_\alpha, S_\beta] l_\beta + [l_\alpha, l_\beta] S_\beta \right) \\ &= \sum_\beta \sum_\gamma \mathrm{i}\, \epsilon_{\alpha\beta\gamma} \left(S_\gamma l_\beta + l_\gamma S_\beta \right) \\ &= \sum_\beta \sum_\gamma \mathrm{i}\, \epsilon_{\alpha\beta\gamma} \left(S_\gamma l_\beta + l_\gamma S_\beta \right) = 0 \ . \end{aligned} \tag{S.3.6}$$

The zero comes from the opposite sign of permutation. Alternatively, we can write it in the vector form:

$$[\vec{j}, \vec{S} \cdot \vec{l}] = 0 \ . \tag{S.3.7}$$

By a similar trick, we can obtain:

$$[j^2, \vec{S} \cdot \vec{l}] = 0 \ . \tag{S.3.8}$$

Therefore, the complete set of commuting observables is:

$$\{ \ H, \ l^2, \ j^2, \ j_z \ \} \ . \tag{S.3.9}$$

S.4 Spin-Orbit Coupling

S.5 Applications