Quantum Mechanics by Cohen

Self-learning Notes

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Don't try to teach yourself quantum mechanics.

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Chapter 1
Basic Mathematical tools of Quantum Mechanics

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1.1 Wave Function and Wave Function Space $\mathscr{F}$

1.1.1 Wave Function

As people uncovered that, in the study of atomic emission and absorption spectra, these spectra are composed of **narrow lines**. In other words, **the energy of the atom is quantized**. Later in 1923, de Broglie came up with the hypothesis:

Postulate 1.1 (de Broglie hypothesis)

Material particles just like photons, can have a wavelike aspect, with wavelength λ *given by de Broglie relation:*

$$\lambda = \frac{2\pi}{|\boldsymbol{k}|} = \frac{h}{|\boldsymbol{p}|}$$

♡

So instead of using classical concepts like position and momentum, since the possible particle positions form a **continuum**, which was verified by the Electron diffraction experiments, we use a time-varying **state** to describe a particle, which is characterized by a **wave function** $\psi(\boldsymbol{r}, t)$.

Definition 1.1 (Wave Function)

We use a time-varying function $\psi(\boldsymbol{r}, t)$ *to describe the state of a particle, which contains all the information it is possible to obtain about the particle. And it is interpreted as a* ***probability amplitude of the particle's presence****:* $\mathrm{d}\mathscr{P}(\boldsymbol{r}, t)$ *is the probability of particle in volume* $\mathrm{d}^3 r$ *situated at* $\boldsymbol{r}$ *at time* t*, and* $|\psi(\boldsymbol{r}, t)|$ *is the corresponding* ***probability density****:*

$$\mathrm{d}P(\boldsymbol{r}, t) = C|\psi(\boldsymbol{r}, t)|^2 \mathrm{d}^3 r$$

♣

Postulate 1.2 (Spectra Decomposition)

The result of any measurement of an arbitrary physical quantity must belong to a set of eigen results $\{a\}$*, with each eigenvalue* a *associated an eigenstate, characterized by* $\psi_a(\boldsymbol{r})$*. And the* *probability to get a at time t_0 can be obtained by decomposition:*

$$\psi(\boldsymbol{r}, t_0) = \sum_a c_a \psi_a(\boldsymbol{r})$$

then

$$P_a = \frac{|c_a|^2}{\sum_a |c_a|^2}$$

And after measurement, the wave function immediately is $\psi'(\boldsymbol{r}, t_0) = \psi_a(\boldsymbol{r})$. ♡

And since the wave function is dependent with time, its evolution rule is provided by **Schrödinger Equation**:

Theorem 1.1 (Schrödinger Equation)

Suppose the particle of mass m in a potential $V(\boldsymbol{r}, t)$, its wave function evolutes like

$$\mathrm{i}\hbar \frac{\partial}{\partial t}\psi(\boldsymbol{r}, t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{r}, t) + V(\boldsymbol{r}, t)\psi(\boldsymbol{r}, t)$$

♡

So it is important to figure out the structure of the set of wave function, which is the **wave function space**, and we would find its properties similar to what we learned an inner product vector space.

1.1.2 Wave Function Space $\mathscr{F}$

According to the hypothesis before, since the probability should be normalized, that is

$$\int \mathrm{d}^3 r \, |\psi(\boldsymbol{r}, t)|^2 = 1$$

which means that the wave function is absolutely square integrable, and in math it is called L^2, but in physics we want more constrains on it to obtain physical and practical results:

Definition 1.2 (Wave Function Space)

We call the set of function in L^2 and also everywhere defined, continuous, infinitely differentiable, have a bounded domain (which makes it can be found within a finite region, like inside the lab), etc. a ***wave function space****, denote as $\mathscr{F}$.* ♣

Proposition 1.1 ($\mathscr{F}$ is a vector space)

In field $\mathbb{C}$, $\forall \psi_1, \psi_2 \in \mathscr{F}$, then

$$\psi = \lambda_1\psi_1 + \lambda_2\psi_2 \in \mathscr{F}$$

where $\lambda_1, \lambda_2 \in \mathbb{C}$. ♠

Proof We only need to show that ψ is also absolutely square integrable:

$$\begin{aligned}|\psi(\boldsymbol{r})|^2 &= (\lambda_1\psi_1(\boldsymbol{r}) + \lambda_2\psi_2(\boldsymbol{r}))(\lambda_1\psi_1(\boldsymbol{r}) + \lambda_2\psi_2(\boldsymbol{r}))^* \\ &= |\lambda_1|^2|\psi_1(\boldsymbol{r})|^2 + |\lambda_2|^2|\psi_2(\boldsymbol{r})|^2 + \lambda_1\lambda_2^*\psi_1(\boldsymbol{r})\psi_2^*(\boldsymbol{r}) + \lambda_1^*\lambda_2\psi_1^*(\boldsymbol{r})\psi_2(\boldsymbol{r}) \\ &\le |\lambda_1|^2|\psi_1(\boldsymbol{r})|^2 + |\lambda_2|^2|\psi_2(\boldsymbol{r})|^2 + 2|\lambda_1||\lambda_2||\psi_1(\boldsymbol{r})||\psi_2(\boldsymbol{r})| \\ &\le |\lambda_1|^2|\psi_1(\boldsymbol{r})|^2 + |\lambda_2|^2|\psi_2(\boldsymbol{r})|^2 + |\lambda_1||\lambda_2|\left(\psi_1^2(\boldsymbol{r}) + \psi_2^2(\boldsymbol{r})\right)\end{aligned}$$

□

And we define the inner product in $\mathscr{F}$:

Definition 1.3 (Inner Product)

Inner product $()$: $\mathscr{F} \times \mathscr{F} \to \mathbb{C}$ *takes a pair* (φ, ψ) *in* $\mathscr{F}$ *to a complex number, which is defined*

$$(\varphi, \psi) = \int \mathrm{d}^3 r\, \varphi^*(\boldsymbol{r})\psi(\boldsymbol{r})$$

♣

It is similar to the inner product in math, just change the complex conjugate to another place. The properties like **Schwarz inequality** it also holds.

In $\mathscr{F}$ we also has operators to act on wave function, and we prefer the **linear operators**, just like in linear algebra.

1.1.3 Basis in $\mathscr{F}$

To truly study a vector space, we must study its bases, which gives us way to represents its element. In the following we would learn that bases in Quantum Mechanics is just a "**representation**".

Definition 1.4 (Discrete Orthonormal Bases)

A countable set $\{u_i\}$ *of orthonormal functions in* $\mathscr{F}$*, labeled by discrete index* i*, that any function in* $\mathscr{F}$ *can be expanded uniquely by the linear combination (needn't to be finite) of it.*

♣

Proposition 1.2 (Closure Relation)

Any discrete orthonormal basis $\{u_i\}$ *for* $\mathscr{F}$ *satisfies the* ***closure relation****:*

$$\sum_i u_i(\boldsymbol{r})u_i^*(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}')$$

♠

Proof Since u_i is orthonormal, any $\psi \in \mathscr{F}$ can be written as

$$\begin{aligned}\psi(\boldsymbol{r}) &= \sum_i (u_i, \psi)u_i(\boldsymbol{r}) \\ &= \sum_i \left[\int \mathrm{d}^3 r'\, u_i^*(\boldsymbol{r}')\psi(\boldsymbol{r}')\right] u_i(\boldsymbol{r}) \\ &= \int \mathrm{d}^3 r'\, \psi(\boldsymbol{r}')\left[\sum_i u_i(\boldsymbol{r})u_i^*(\boldsymbol{r}')\right]\end{aligned}$$

since it satisfies for any ψ, and thus it acts like a delta function, which is the closure relation. □

Similarly we can define the continuous orthonormal basis (labeled by continuous index α) and get its closure relation:

$$\psi(\boldsymbol{r}) = \int \mathrm{d}\alpha\, c(\alpha) w_\alpha(\boldsymbol{r})$$

$$\int \mathrm{d}\alpha\, w_\alpha(\boldsymbol{r}) w_\alpha^*(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}')$$

1.1.4 Basis not in $\mathscr{F}$

Although we introduce $\mathscr{F}$ to make the wave function more "good", we can introduce basis that not in $\mathscr{F}$ but it would gives us great convenience. The first example is the **plane wave basis**. Recall that by fourier transformation, we can obtain a function by doing transformation:

$$f(x) = \int_{-\infty}^{\infty} F(\omega) \mathrm{e}^{\mathrm{i}\omega x}\, \mathrm{d}\omega$$

thus we introduce function $v_{\boldsymbol{p}}(\boldsymbol{r})$:

Definition 1.5 (Plane Wave Basis)

Plane wave basis $\{v_{\boldsymbol{p}}(\boldsymbol{r})\}$ is defined as

$$v_{\boldsymbol{p}}(\boldsymbol{r}) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}$$

with continuous index $\boldsymbol{p}$. Then all function ψ in $\mathscr{F}$ can be expanded as:

$$\psi(\boldsymbol{r}) = \int \mathrm{d}^3 p\, \overline{\psi}(\boldsymbol{p}) v_{\boldsymbol{p}}(\boldsymbol{r})$$

where $\overline{\psi}(\boldsymbol{p})$ is the fourier transformation of $\psi(\boldsymbol{r})$:

$$\overline{\psi}(\boldsymbol{p}) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int \mathrm{d}^3 r\, \psi(\boldsymbol{r}) \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}} = \int \mathrm{d}^3 r\, v_{\boldsymbol{p}}^*(\boldsymbol{r}) \psi(\boldsymbol{r}) = (v_{\boldsymbol{p}}, \psi)$$

♣

Hence we see it is much similar to the basis we familiar with. Moreover, it it "orthonormal" and also we can get its closure relation.

Proposition 1.3 (Plane Wave Basis is Orthonormal)

As we defined above, plane wave basis is orthonormal, means that

$$(v_{\boldsymbol{p}}(\boldsymbol{r}), v_{\boldsymbol{p}'}(\boldsymbol{r})) = \delta(\boldsymbol{p} - \boldsymbol{p}')$$

♠

Proof

$$\begin{aligned}(v_{\boldsymbol{p}}(\boldsymbol{r}), v_{\boldsymbol{p}'}(\boldsymbol{r})) &= \frac{1}{(2\pi\hbar)^3} \int \mathrm{d}^3 r\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\boldsymbol{p}-\boldsymbol{p}')\cdot\boldsymbol{r}} \\ &= \delta(\boldsymbol{p} - \boldsymbol{p}')\end{aligned}$$

□

Proposition 1.4 (Closure Relation for Plane Wave Basis)

$$\int \mathrm{d}^3 p\, v_{\boldsymbol{p}}(\boldsymbol{r}) v_{\boldsymbol{p}}^*(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}')$$

♠

Proof

$$\int \mathrm{d}^3 p\, v_{\boldsymbol{p}}(\boldsymbol{r}) v_{\boldsymbol{p}}^*(\boldsymbol{r}') = \frac{1}{(2\pi\hbar)^3} \int \mathrm{d}^3 p\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}')}$$
$$= \delta(\boldsymbol{r}-\boldsymbol{r}')$$

□

Another example is the ”δ function”:

Definition 1.6 (Delta Function Basis)

We introduce set $\{\xi_{\boldsymbol{r}_0}(\boldsymbol{r})\}$ with continuous index $*r_0$:

$$\xi_{\boldsymbol{r}_0}(\boldsymbol{r}) = \delta(\boldsymbol{r}-\boldsymbol{r}_0)$$

Then $\forall \psi \in \mathscr{F}$:

$$\psi(\boldsymbol{r}) = \int \mathrm{d}^3 r_0\, \psi(\boldsymbol{r}_0)\xi_{\boldsymbol{r}_0}(\boldsymbol{r})$$

♣

Similarly we get the ”orthonormal” property and the closure relation.

$$(\xi_{\boldsymbol{r}_0}(\boldsymbol{r}), \xi_{\boldsymbol{r}_0'}(\boldsymbol{r})) = \delta(\boldsymbol{r}_0 - \boldsymbol{r}_0')$$
$$\int \mathrm{d}^3 r_0\, \xi_{\boldsymbol{r}_0}(\boldsymbol{r})\xi_{\boldsymbol{r}_0}^*(\boldsymbol{r}') = \delta(\boldsymbol{r}-\boldsymbol{r}')$$

Now we have introduce bases in wave function space $\mathscr{F}$, in future we would see that bases is a powerful tool in representations of states.

1.2 State Space

As we are in senior high school, we have learned the analytic geometry to represent curves in Cartesian coordinate system, like the circle equation is $x^2 + y^2 = r^2$. But do not forget that we have all learned the geometry in junior high school, which is independent of the functions, coordinates etc., just like Euclid’s Elements.

Similarly, what we have learned above is like the analytic geometry, we use a function $\psi(\boldsymbol{r}, t)$ to represent a state of a particle. But in different coordinates, different bases, we would get different representations of it, and thus it seems a little miscellaneous. In this section, we would introduce the **state space**, which is like the pure geometry, we study the **state vector** itself instead of its representation in wave function.

Definition 1.7 (State Space)

*Like a wave function, we use a **state vector** to characterize a quantum state of a particle, belonging to an abstract space $\mathscr{E}_{\boldsymbol{r}}$ is the **state space** of the particle. The fact that $\mathscr{F}$ is a subspace of L^2 means that $\mathscr{E}_{\boldsymbol{r}}$ is a subspace of a Hilbert space. Generally, we consider $\mathscr{E}$ be the state space is the set of all state vectors.*

♣

So in this section we would study the calculation in $\mathscr{E}$. And for convenience, we introduce the

Dirac notations, which is quite natural and simple for Quantum Mechanics.

1.2.1 Dirac Notation

Definition 1.8 (Ket)

We use a ket vector $|\psi\rangle \in \mathscr{E}_{\boldsymbol{r}}$ *to represent the state vector, associated with the wave function* $\psi(\boldsymbol{r}) \in \mathscr{F}$. *Here we ignore the index* $\boldsymbol{r}$ *and just emphasize the vector* ψ *itself.* ♣

Similar to linear algebra, we have the concept of **linear functional**, and dual space, while in Dirac notation we call it **bra**, belongs to the dual space $\mathscr{E}^*$.

Definition 1.9 (Bra)

For each state vector $|\psi\rangle \in \mathscr{E}$, *the vector in* $\mathscr{E}^*$, *called the linear functional, denote as* χ *that maps the state space to a complex number:* $\chi : \mathscr{E} \to \mathbb{C}$. *And we use* ***bra*** $\langle\chi|$ *to represent a linear functional:*

$$\chi(|\psi\rangle) = \langle\chi|\psi\rangle$$

♣

Moreover, since we have defined the inner product for wave functions, for pair $|\psi\rangle, |\varphi\rangle \in \mathscr{E}$, we can find the linear functional corresponding to $|\varphi\rangle$, that the result of it of $|\psi\rangle$ is the inner product. That is $\exists \langle\varphi| \in \mathscr{E}^*$ s.t.

$$\langle\varphi|\psi\rangle = (|\varphi\rangle, |\psi\rangle)$$

Thus every ket corresponds a bra.

Note *Since the inner product is* ***antilinear*** *in the first position, thus the link between ket and bra is also antilinear, that is*

$$\langle\lambda\psi| = \lambda^* \langle\psi|$$

and consequently we have relation

$$\langle\psi|\varphi\rangle = \langle\varphi|\psi\rangle^*$$

But conversely, does any bra corresponds to a ket? As in the last section we learn two bases that not in $\mathscr{F}$: $\{v_{\boldsymbol{p}}(\boldsymbol{r})\}, \{\xi_{\boldsymbol{r}_0}(\boldsymbol{r})\}$, thus then do not have the corresponding ket, but there exist bra that act correctly with these two bases. So this means that $\mathscr{E}$ and $\mathscr{E}^*$ is not isomorphic, which is different to what we learned that any finite-dimensional vector space is isomorphic to its dual space. But we still use a notation dagger: $\cdot^\dagger$ to represent the link between ket and bra (if exists): $|\psi\rangle^\dagger = \langle\psi|, \langle\psi|^\dagger = |\psi\rangle$.

1.2.2 Linear Operators

Like in linear algebra, we can define **linear operators** that acts on state vectors.

Definition 1.10 (Linear Operators)

A linear operator $\hat{A}$ is a linear map that maps a state vector $|\psi\rangle$ to another ket $|\psi'\rangle$ both in $\mathscr{E}$. We use the hat to distinguish operators and vectors. ♣

Notice that in order to distinguish operators and quantities, we add a "hat" $\hat{\cdot}$ on the operators.

Definition 1.11 (Matrix Element)

We call the matrix element of an operator $\hat{A}$ between $|\psi\rangle$ and $|\varphi\rangle$ be the inner product: $(|\varphi\rangle, \hat{A}|\psi\rangle) := \langle\varphi|\hat{A}|\psi\rangle$. ♣

Notice that here we do not distinguish the operator $\hat{A}$ belongs to $|\psi\rangle$, because for operator acting on bra, we define it as:

$$\langle\varphi|\hat{A} = \langle\varphi'| \text{ s.t. } \langle\varphi'|\psi\rangle = \left\langle\varphi\middle|\hat{A}\psi\right\rangle, \forall\psi \in \mathscr{E}$$

We also have the **Hermitian conjugate** of an operator, as the adjoint of operator in linear algebra.

Definition 1.12 (Hermitian Conjugate)

The Hermitian conjugate of an operator $\hat{A}$ is denote as $\hat{A}^\dagger$, defined by

$$\left(\hat{A}|\psi\rangle\right)^\dagger = \langle\psi|\hat{A}^\dagger$$

♣

Notice that we use the same notation $\cdot^\dagger$ to represent the Hermitian conjugate and the link between ket and bra, in fact it is natural, since it acts just like transpose $\cdot^\top$:$\left(\hat{A}|\psi\rangle\right)^\dagger = (|\psi\rangle)^\dagger\hat{A}^\dagger$ and $(Ax)^\top = x^\top A^\top$

Use the definition we immediately obtain:

$$\langle\psi|\hat{A}^\dagger|\varphi\rangle = \langle\varphi|\hat{A}|\psi\rangle^*$$

1.2.3 Basis in State Space

Firstly we define basis in state space.

Definition 1.13 (Basis in State Space)

We call a discrete set $\{|u_i\rangle\}$ or a continuous set $\{|w_\alpha\rangle\}$ is a basis iff. any $|\psi\rangle \in \mathscr{E}$ can be uniquely expanded by it:

$$|\psi\rangle = \sum_i c_i |u_i\rangle$$

$$|\psi\rangle = \int \mathrm{d}\alpha\, c(\alpha)\, |w_\alpha\rangle$$

♣

Moreover if the basis is orthonormal, then we can get the **closure relation**:

Proposition 1.5 (Closure Relation for State Space)

If $\{|u_i\rangle\}$ and $\{|w_\alpha\rangle\}$ are orthonormal basis for $\mathscr{E}$, then

$$\sum_i |u_i\rangle\langle u_i| = \mathbb{1}$$

$$\int \mathrm{d}\alpha\, |w_\alpha\rangle\langle w_\alpha| = \mathbb{1}$$

here $\mathbb{1}$ is the ***identity operator*** *in $\mathscr{E}$.*

Proof Since $\{|u_i\rangle\}$ and $\{|w_\alpha\rangle\}$ are orthonormal, we can write as

$$|\psi\rangle = \sum_i |u_i\rangle \langle u_i|\psi\rangle = \left(\sum_i |u_i\rangle\langle u_i|\right) |\psi\rangle$$

$$|\psi\rangle = \int \mathrm{d}\alpha\, |w_\alpha\rangle \langle w_\alpha|\psi\rangle = \left(\int \mathrm{d}\alpha\, |w_\alpha\rangle\langle w_\alpha|\right) |\psi\rangle$$

for $\forall\, |\psi\rangle \in \mathscr{E}$. □

1.2.4 Representations in State Space

As in linear algebra, a vector has its **coordinate representation** and a linear transformation has its **matrix representation** with a basis for the vector space, in Quantum Mechanics, the **representation** is just those numbers that represent the state vectors and operators in a specific basis.

Definition 1.14 (Representations of ket, bra and linear operator)

Similar to linear algebra, we can use a ***column vector***, ***row vector*** *and a* ***matrix*** *to represent a ket, bra and linear operator respectively w.r.t. a basis. That is:*

$$\begin{aligned} c_i &= \langle u_i|\psi\rangle \\ c_j^\dagger &= \langle \psi|u_i\rangle \\ A_{ij} &= \langle u_i|\hat{A}|u_j\rangle \\ A_{ij}^\dagger &= \langle u_i|\hat{A}^\dagger|u_j\rangle = A_{ji}^* \end{aligned}$$

And we also have the transformation matrix just like the change coordinate matrix.

Definition 1.15 (Transformation Matrix)

Let $\{|u_i\rangle\}, \{|t_k\rangle\}$ be orthonormal bases for $\mathscr{E}$, then set

$$S_{ik} = \langle u_i|t_k\rangle$$

then S is the matrix to transform representations, its Hermitian conjugate is

$$\left(S^\dagger\right)_{ki} = (S_{ik})^* = \langle t_k|u_i\rangle$$

Just remember the closure relation of basis, we can quickly obtain the relation between representations of different bases:

$$\begin{aligned}
\langle t_k|\psi\rangle &= \langle t_k|\mathbb{1}|\psi\rangle \\
&= \langle t_k|\left(\sum_i |u_i\rangle\langle u_i|\right)|\psi\rangle \\
&= \sum_i \langle t_k|u_i\rangle \langle u_i|\psi\rangle \\
&= S^\dagger_{ki} \langle u_i|\psi\rangle
\end{aligned}$$

and conversely:

$$\langle u_i|\psi\rangle = S_{ik} \langle t_k|\psi\rangle$$

For bra just take the Hermitian conjugate:

$$\langle\psi|t_k\rangle = \langle\psi|u_i\rangle S_{ik}$$
$$\langle\psi|u_i\rangle = \langle\psi|t_k\rangle S^\dagger_{ki}$$

For operators:

$$\begin{aligned}
\langle t_k|\hat{A}|t_l\rangle &= \langle t_k|\mathbb{1}\hat{A}\mathbb{1}|t_l\rangle \\
&= \sum_{k,l} \langle t_k|u_i\rangle \langle u_i|\hat{A}|u_j\rangle \langle u_j|t_l\rangle \\
&= \sum_{k,l} S^\dagger_{ki} \langle u_i|\hat{A}|u_j\rangle S_{jl}
\end{aligned}$$

and

$$\langle u_i|\hat{A}|u_j\rangle = \sum_{k,l} S_{ik} \langle t_k|\hat{A}|t_l\rangle S^\dagger_{lj}$$

1.3 Observables

In this section, we would focus on operators which are corresponding to the measurement in real world, called **observables**. We would introduce the properties of it, and in the next chapter we would see its physical interpretations.

In linear algebra, we see that for a Hermitian (or self-adjoint) operator, we can use its eigenvectors to build an orthonormal basis for a finite dimensional vector space. But in $\mathscr{E}$, it do not guaranteed. And hence we introduce the **observables**.

1.3.1 Fundamental Knowledge

Definition 1.16 (Observables)

We call a Hermitian operator $\hat{A}$ a observable if we can find a basis for $\mathscr{E}$ that consists of its eigenvectors. ♣

Definition 1.17 (Spectrum)

We call the set of the eigenvalues the spectrum.

Similar to what we have learned in linear algebra, an observable has the following properties.

Proposition 1.6 (Properties of Observables)

Consider an observable $\hat{A}$, then:

(a) *All eigenvalues of $\hat{A}$ is real.*

(b) *eigenvectors corresponding to distinct eigenvalues are orthogonal.*

(c) *We can always build an orthonormal basis of eigenvectors of $\hat{A}$.*

Since the properties above are just trivial (if you have learned linear algebra), we ignore the proof. And we give an example of observable: the projector.

Definition 1.18 (Projector)

Consider a space which is spanned by a set of orthonormal vectors:

$$\mathscr{E}_q = \mathrm{span}\{|\psi_i\rangle\}_{i=1}^q$$

Then the projector onto $\mathscr{E}_q$ is defined as

$$\hat{P}_q = \sum_i^q |\psi_i\rangle\langle\psi_i|$$

Note *Since in definition we let those vectors $|\psi_i\rangle$ are orthonormal, so here the projector is actually an "orthogonal projection".*

Proposition 1.7

$\hat{P}_q^2 = \hat{P}_q = \hat{P}_q^\dagger$

Proof

$$\begin{aligned}\hat{P}_q^2 &= \left[\sum_{i=1}^q |\psi_i\rangle\langle\psi_i|\right]\left[\sum_{j=1}^q |\psi_j\rangle\langle\psi_j|\right] = \sum_{i,j=1}^q |\psi_i\rangle \langle\psi_i|\psi_j\rangle \langle\psi_j| \\ &= \sum_{i,j=1}^q |\psi_i\rangle\langle\psi_j|\, \delta_{ij} = \sum_i^q |\psi_i\rangle\langle\psi_i| = \hat{P}_q\end{aligned}$$

For the second equality, just notice that $(|u\rangle\langle v|)^\dagger = |v\rangle\langle u|$, thus

$$\hat{P}_q^\dagger = \left(\sum_{i=1}^q |\psi_i\rangle\langle\psi_i|\right)^\dagger = \sum_{i=1}^q |\psi_i\rangle\langle\psi_i| = \hat{P}_q$$

□

Proposition 1.8

Any projector is an observable.

Proof For any vector $|\psi\rangle$, we can rewrite it as

$$|\psi\rangle = \hat{P}_q |\psi\rangle + \left(\mathbb{1} - \hat{P}_q\right) |\psi\rangle$$

then $\hat{P}_q |\psi\rangle$ and $\left(\mathbb{1} - \hat{P}_q\right)$ are all eigenvectors of $\hat{P}_q$, since

$$\hat{P}_q\left(\hat{P}_q |\psi\rangle\right) = \hat{P}_q^2 |\psi\rangle = \hat{P}_q |\psi\rangle$$

and

$$\hat{P}_q\left[\left(\mathbb{1} - \hat{P}_q\right) |\psi\rangle\right] = \hat{P}_q |\psi\rangle - \hat{P}_q^2 |\psi\rangle = 0$$

means that 0 and 1 are two eigenvalues of $\hat{P}_q$. Thus any vector can be expanded by the eigenvectors of $\hat{P}_q$, hence $\hat{P}_q$ is an observable. □

Since for observables we can use eigenvectors of it to express any vector, we can also use projectors onto its eigenspaces to express the observables:

Theorem 1.2 (Spectral Theorem)

Suppose $\hat{A}$ is an observable and let $\hat{P}_n$ is the projector onto $\mathscr{E}_n$, which is the eigenspace of $\hat{A}$:

$$\hat{P}_n = \sum_{i=1}^{g_n} |\psi_n^i\rangle\langle\psi_n^i|$$

where g_n is the degeneracy. Then $\hat{A}$ can be factored as

$$\hat{A} = \sum_n a_n \hat{P}_n$$

where a_n is the corresponding eigenvalue. ♡

Proof Just act the right side to any vector $|\psi\rangle$, and use the definition. □

Use the projector onto the eigenspace, we can get another property:

Proposition 1.9 (The Resolution of the Identity Operator)

Let $\hat{A}$ be an observable and $\hat{P}_n$ is the projector onto $\mathscr{E}_n$ which is the eigenspace of $\hat{A}$ corresponding to the eigenvalue a_n, then

$$\sum_n \hat{P}_n = \mathbb{1}$$

♠

Proof This comes from that the eigenvectors of $\hat{A}$ can form an orthonormal basis for $\mathscr{E}$. □

1.3.2 Sets of Commuting Observables

In linear algebra we learned that if two self-adjoint operators T, U commutes, then are simultaneous diagonalizable, means that we can find orthonormal basis of vectors that are eigenvectors of both T and U. In Quantum Mechanics, we want to find a set of commuting observables that all are simultaneous diagonalizable. Firstly we introduce the notation: commutator.

Definition 1.19 (Commutator)

The commutator of two operators $\hat{A}, \hat{B}$ is

$$\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

To reach our goal, we first see a lemma.

Lemma 1.1

If two operators $\hat{A}, \hat{B}$ commute, and $|\psi\rangle$ is an eigenvector of $\hat{A}$, then $\hat{B}|\psi\rangle$ is also an eigenvector of $\hat{A}$ with same eigenvalue, and hence the eigenspace of $\hat{A}$ is invariant under $\hat{B}$.

Proof Suppose $\hat{A}|\psi\rangle = a|\psi\rangle$, then

$$\hat{A}\left(\hat{B}|\psi\rangle\right) = \hat{B}\left(\hat{A}|\psi\rangle\right) = \hat{B}(a|\psi\rangle) = a\left(\hat{B}|\psi\rangle\right)$$

Thus $\forall\, |\psi\rangle \in \mathscr{E}_a$, $\hat{B}|\psi\rangle \in \mathscr{E}_a$, so eigenspace of $\hat{A}$ is invariant under $\hat{B}$. □

Theorem 1.3 (Fundamental)

If two observables $\hat{A}, \hat{B}$ commute, then we can construct an orthonormal basis of the state space with eigenvectors common to $\hat{A}, \hat{B}$.

Proof Since $\hat{A}$ is observable, there exists orthonormal basis of eigenvectors of $\hat{A}$, denote by $|u_n^i\rangle$:

$$\hat{A}\left|u_n^i\right\rangle = a_n\left|u_n^i\right\rangle$$

where $i = 1, 2, \cdots, g_n$ is the **degree of degeneracy** of eigenvalue of a_n (in math we call it geometry multiplicity), and each n label the n-th eigenspace $\mathscr{E}_n$. And they are orthonormal:

$$\left\langle u_n^i \middle| u_{n'}^{i'} \right\rangle = \delta_{nn'}\delta_{ii'}$$

By lemma 1, $\mathscr{E}_n$ is $\hat{B}$-invariant, $\forall n$, then we restrict $\hat{B}$ to $\hat{B}_{\mathscr{E}_n} : \mathscr{E}_n \to \mathscr{E}_n$, since $\hat{B}$ is an observable, thus $\hat{B}_{\mathscr{E}_n}$ is Hermitian, so we can find basis consisting eigenvectors of $\hat{B}_{\mathscr{E}_n}$, so does $\hat{B}$, to form an orthonormal basis, denote β_n, for $\mathscr{E}_n$, and then are also eigenvectors of $\hat{A}$ since they are in eigenspace of $\hat{A}$. Thus for each n we can always do so, obtained $\beta_n, n = 1, 2, \cdots$, and $\beta = \bigcup\limits_{n=1}^{\infty} \beta_n$ is the orthonormal basis consisting eigenvectors of both $\hat{A}$ and $\hat{B}$. □

Note *We use notation $\left|u_{n,p}^i\right\rangle$ to label the eigenvector that corresponds to eigenvalue a_n of $\hat{A}$ and b_p of $\hat{B}$, the superscript i is used to distinguish different vectors that both in eigenspace $\mathscr{E}_{\hat{A},n}$ and $\mathscr{E}_{\hat{B},p}$. And it is easy to prove the inverse of Theorem 1.3, since*

$$\hat{B}\hat{A}\left|u_{n,p}^i\right\rangle = \hat{B}a_n\left|u_{n,p}^i\right\rangle = a_n b_p\left|u_{n,p}^i\right\rangle$$
$$\hat{A}\hat{B}\left|u_{n,p}^i\right\rangle = \hat{A}b_p\left|u_{n,p}^i\right\rangle = a_n b_p\left|u_{n,p}^i\right\rangle$$

hence we get

$$\left[\hat{A}, \hat{B}\right]\left|u_{n,p}^i\right\rangle = 0$$

since $\{\left|u_{n,p}^i\right\rangle\}$ forms a basis, thus $\left[\hat{A}, \hat{B}\right] = 0$.

In Theorem 1.3 we see that, for observables $\hat{A}$ and $\hat{B}$, even though eigenvalues of $\hat{A}$ can be degenerate, we can introduce $\hat{B}$ to "shrink" the degree of degeneracy, since each index i of $|u_n^i\rangle$ of

$\hat{A}$ would split into index i of $|u^i_{n,p}\rangle$ of $\hat{A}$ and $\hat{B}$. And we want to construct what called a **complete sets of commuting observables** or **C.S.C.O.**:

Definition 1.20 (C.S.C.O.)

We call a set of observables: $\{\hat{A}, \hat{B}, \hat{C}, \cdots\}$ is a C.S.C.O. if we can find a basis for state space and, each ket is an eigenvector of all the observables in it, and, moreover, every list of eigenvalues $(a_n, b_p, c_r, \cdots)$ corresponds to only **one** *vector (to within phase factor). And hence we use notation $|a_n, b_p, c_r, \cdots\rangle$ to label the basis.*

♣

1.4 Two Important Examples of Representations and Observables

In this section, we would return to the $\mathscr{F}$-space, or more exactly, the $\mathscr{E}_{\boldsymbol{r}}$ space: For each wave function $\psi(\boldsymbol{r})$, we correspond it to a ket $|\psi\rangle \in \mathscr{E}_{\boldsymbol{r}}$. Thus $\mathscr{E}_{\boldsymbol{r}}$ is a state space of a (spinless) particle.

1.4.1 The $|r\rangle$-representation and $|p\rangle$-representation

Recall the "basis" not belong to $\mathscr{F}$ (Delta function basis: 1.6 and plane wave basis: 1.5):

$$\xi_{\boldsymbol{r}_0}(\boldsymbol{r}) = \delta(\boldsymbol{r} - \boldsymbol{r}_0)$$

$$v_{\boldsymbol{p}_0}(\boldsymbol{r}) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\boldsymbol{p}_0 \cdot \boldsymbol{r}}$$

And their corresponding ket is denoted as $|\boldsymbol{r}_0\rangle$ and $|\boldsymbol{p}_0\rangle$.

For convenience we ignore the subscript 0, and it is easy to verify that they satisfy the following fundamental relations:

Proposition 1.10 (Fundamental Relation for $|r_0\rangle$ and $|p_0\rangle$)

$$\langle \boldsymbol{r}, \boldsymbol{r}' \rangle = \delta(\boldsymbol{r} - \boldsymbol{r}')$$

$$\langle \boldsymbol{p}, \boldsymbol{p}' \rangle = \delta(\boldsymbol{p} - \boldsymbol{p}')$$

$$\int \mathrm{d}^3 r \, |\boldsymbol{r}\rangle\langle\boldsymbol{r}| = \mathbb{1}$$

$$\int \mathrm{d}^3 p \, |\boldsymbol{p}\rangle\langle\boldsymbol{p}| = \mathbb{1}$$

♠

Furthermore, if we calculate the components of a ket:

Proposition 1.11 (Components of a ket)

$$\langle \boldsymbol{r}, \psi \rangle = \int \mathrm{d}^3 r' \, \delta(\boldsymbol{r} - \boldsymbol{r}')\psi(\boldsymbol{r}') = \psi(\boldsymbol{r})$$

$$\langle \boldsymbol{p}, \psi \rangle = \int \mathrm{d}^3 r' \, \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}'} \psi(\boldsymbol{r}') = \overline{\psi}(\boldsymbol{p})$$

♠

This means that **the value $\psi(\boldsymbol{r})$ of the wave function at point $\boldsymbol{r}$ is the component of ket $|\psi\rangle$ on basis $|\boldsymbol{r}\rangle$ of the $|\boldsymbol{r}\rangle$-representation**, and $\overline{\psi}(\boldsymbol{p})$ is analogously.

1.4.2 The $\hat{r}$ and $\hat{p}$ operators

Definition 1.21 (The $\hat{r}$ operator)

For $\forall\,|\psi\rangle \in \mathscr{E}_{\boldsymbol{r}}$, we define the operator $\hat{x}$ as:

$$|\psi'\rangle = \hat{x}\,|\psi\rangle$$

where $|\psi'\rangle$ is the ket that its corresponding wave function is:

$$\psi'(\boldsymbol{r}) = \langle \boldsymbol{r}|\psi'\rangle = x\psi(\boldsymbol{r}) = x\,\langle \boldsymbol{r}|\psi\rangle$$

Similarly we can define the $\hat{y}$ and $\hat{z}$ operators, and finally the $\hat{\boldsymbol{r}}$ operator, with the components are $\hat{x}, \hat{y}, \hat{z}$. We condense it as:

$$\langle \boldsymbol{r}|\hat{\boldsymbol{r}}|\psi\rangle = \boldsymbol{r}\,\langle \boldsymbol{r}|\psi\rangle$$

♣

Similarly we can define the $\hat{\boldsymbol{p}}$ operator:

Definition 1.22 (The $\hat{p}$ operator)

$$\langle \boldsymbol{p}|\hat{\boldsymbol{p}}|\psi\rangle = \boldsymbol{p}\,\langle \boldsymbol{p}|\psi\rangle$$

♣

Let us ascertain how the $\hat{\boldsymbol{p}}$ operator acts in the $\hat{\boldsymbol{r}}$-representation:

Proposition 1.12

The $\hat{\boldsymbol{p}}$ operator in $\hat{\boldsymbol{r}}$-representation:

$$\langle \boldsymbol{r}|\hat{\boldsymbol{p}}|\psi\rangle = -\mathrm{i}\hbar\boldsymbol{\nabla}\,\langle \boldsymbol{r}|\psi\rangle$$

♠

Proof For $\forall\psi \in \mathscr{E}_{\boldsymbol{r}}$, consider

$$\begin{aligned}
\langle \boldsymbol{r}|\hat{\boldsymbol{p}}|\psi\rangle &= \langle \boldsymbol{r}|\left[\int \mathrm{d}^3p\,|\boldsymbol{p}\rangle\langle \boldsymbol{p}|\right]\hat{\boldsymbol{p}}|\psi\rangle \\
&= \int \mathrm{d}^3p\left(\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}\right)\boldsymbol{p}\overline{\psi}(\boldsymbol{p}) \\
&= \int \mathrm{d}^3p\,(-\mathrm{i}\hbar\boldsymbol{\nabla})\left(\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}\right)\overline{\psi}(\boldsymbol{p}) \\
&= -\mathrm{i}\hbar\boldsymbol{\nabla}\psi(\boldsymbol{r})
\end{aligned}$$

□

Proposition 1.13 (Canonical Commutation Relations)

$$[\hat{r}_i, \hat{r}_j] = 0$$
$$[\hat{p}_i, \hat{p}_j] = 0$$
$$[\hat{r}_i, \hat{p}_j] = \mathrm{i}\hbar\delta_{ij}$$

♠

Proof

$$\begin{aligned}\langle \boldsymbol{r}|[\hat{r}_i, \hat{r}_j]|\psi\rangle &= \langle \boldsymbol{r}|\hat{r}_i\hat{r}_j|\psi\rangle - \langle \boldsymbol{r}|\hat{r}_j\hat{r}_i|\psi\rangle \\ &= r_i r_j \langle \boldsymbol{r}|\psi\rangle - r_j r_i \langle \boldsymbol{r}|\psi\rangle \\ &= 0\end{aligned}$$

Similarly

$$\langle \boldsymbol{p}|[\hat{p}_i, \hat{p}_j]|\psi\rangle = 0$$

And the final one:

$$\begin{aligned}\langle \boldsymbol{r}|[\hat{r}_i, \hat{p}_j]|\psi\rangle &= r_i \langle \boldsymbol{r}|\hat{p}_j|\psi\rangle - \left(-\mathrm{i}\hbar\frac{\partial}{\partial r_j}\right)\langle \boldsymbol{r}|\hat{r}_i|\psi\rangle \\ &= \mathrm{i}\hbar\frac{\partial}{\partial r_j}[r_i\psi(\boldsymbol{r})] - \mathrm{i}\hbar r_i\frac{\partial}{\partial r_j}\psi(\boldsymbol{r}) \\ &= \mathrm{i}\hbar\frac{\partial r_i}{\partial r_j}\langle \boldsymbol{r}|\psi\rangle \\ &= \mathrm{i}\hbar\delta_{ij}\langle \boldsymbol{r}|\psi\rangle\end{aligned}$$

□

Since $\boldsymbol{r}, \boldsymbol{p}$ are both real, it is not difficult to find that:

Proposition 1.14

$\hat{\boldsymbol{r}}$ and $\hat{\mathbf{p}}$ are both Hermitian operator.

Another important proposition is about the eigenvectors of them.

Proposition 1.15

Eigenvectors of $\hat{\boldsymbol{r}}$ and $\hat{\mathbf{p}}$ are $\boldsymbol{r}$ and $\boldsymbol{p}$ respectively. Or:

$$\begin{aligned}\hat{\boldsymbol{r}}\,|\boldsymbol{r}\rangle &= \boldsymbol{r}\,|\boldsymbol{r}\rangle \\ \hat{\mathbf{p}}\,|\boldsymbol{p}\rangle &= \boldsymbol{p}\,|\boldsymbol{p}\rangle\end{aligned}$$

Proof Consider

$$\begin{aligned}\langle \boldsymbol{r}|\hat{\boldsymbol{r}}|\boldsymbol{r}_0\rangle &= \boldsymbol{r}\langle \boldsymbol{r}|\boldsymbol{r}_0\rangle \\ &= \boldsymbol{r}\delta(\boldsymbol{r}-\boldsymbol{r}_0) \\ &= \boldsymbol{r}_0\delta(\boldsymbol{r}-\boldsymbol{r}_0) \\ &= \boldsymbol{r}_0\langle \boldsymbol{r}|\boldsymbol{r}_0\rangle\end{aligned}$$

thus we have

$$\hat{\boldsymbol{r}}\,|\boldsymbol{r}_0\rangle = \boldsymbol{r}_0\,|\boldsymbol{r}_0\rangle$$

Similarly for $\hat{\boldsymbol{p}}$. □

Proposition 1.16

$\hat{\boldsymbol{r}}$ and $\hat{\mathbf{p}}$ are both observables. And we can build C.S.C.O. by these operators.

Note *Since we introduce $\hat{\boldsymbol{r}}$ and $\hat{\mathrm{p}}$ by the two "basis", then obviously they are observables. Meanwhile, for three given eigenvalues of $\hat{x}, \hat{y}, \hat{z}$: x_0, y_0, z_0, we can uniquely determine an eigenvector $|\mathrm{r}_0\rangle$, hence*

$\{\hat{x}, \hat{y}, \hat{z}\}$ *constitutes a C.S.C.O. in* $\mathscr{E}_{\mathbf{r}}$*, the same as* $\{\hat{p_x}, \hat{p_y}, \hat{p_z}\}$*. Also notice the canonical commutation relations:* $[\hat{r_i}, \hat{p_j}] = \mathrm{i}\hbar\delta_{ij}$*, then* $\{\hat{x}, \hat{p_y}, \hat{p_z}\}$ *can also be a C.S.C.O..*

Chapter 3
The Postulates of Quantum Mechanics

3.1 Introduction

In classical mechanics, we use **generalized coordinates** $q_i(t)$ and **generalized velocities** $\dot{q}_i(t)$ to describe a system. By Lagrange Mechanics, they are characterized by the **Lagrange Equation**:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \frac{\partial L}{\partial q_i}$$

or we can introduce the **conjugate momentum** p_i of each of the generalized coordinates q_i:

$$p_i = \frac{\partial L}{\partial \dot{q}_i}$$

and use the **Hamilton-Jacobi Canonic Equations**:

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = \frac{\partial H}{\partial p_i}$$
$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = -\frac{\partial H}{\partial q_i}$$

And by the knowledge of PDE, we know that once the initial state of the system is given, there is only one solution to this system. In summary, the classical description of a physical system is the following points:

(i) The state of the system at a fixed time t_0 is defined by the those $q_i(t_0)$ and $p_i(t_0)$.

(ii) Once know the state of the system at some time, all value of physical quantities is completely determined, and we can predict with certainty the result of any measurement performed at this time.

(iii) The time evolution of the state of the system is given by the Hamilton-Jacobi Equations, and the state is known for all time if its initial state is known.

In QM, the description of physical system is based on the postulates we shall study in this chapter, and this postulates will provide us with answers to this questions:

(i) How is the state of a quantum system at a given time described mathematically?

(ii) Given this state, how can we predict the results of the measurement of various physical quantities?

(iii) How can the state of the system at an arbitrary time t be found when the state at t_0 time is known?

3.2 Statement of the Postulates

Postulate 3.1 (Description of the State of a System)

At a fixed time t_0, the state of an isolated physical system is defined by specifying a ket $|\psi(t_0)\rangle$ belonging to the state space $\mathscr{E}$. ♡

Since $\mathscr{E}$ is a vector space, this first postulate implies a superposition principle: a linear combination of a state vector is still a state vector.

Postulate 3.2 (Description of Physical Quantities)

Every measurable physical quantity A is described by an operator $\hat{A}$ acting in $\mathscr{E}$, which is an observable. ♡

Postulate 3.3 (Possible Results of the Measurememt of Physical Quantites)

The only possible result of the measurement of a physical quantity A is one of the eigenvalues of the corresponding observable $\hat{A}$. ♡

Since $\hat{A}$ is an observable, then all eigenvalues of $\hat{A}$ is real. Also if the spectrum of $\hat{A}$ is discrete, then the results are consequently quantized. But remember this is not a obvious thing. Only after we solve those eigenvalue equations can we find that the results are discrete, which can be measured experimentally. We stress the fact that these results will be obtained using the same fundamental interaction law used in classical mechanics in the macroscopic domain.

Postulate 3.4 (Principle of Specturm Decomposition (Discrete))

When the physical quantity A is measured on a system in the ***normalized*** *state $|\psi\rangle$, the probability $P(a_n)$ of obtaining the eigenvalue a_n of the corresponding observable $\hat{A}$ is*

$$P(a_n) = \sum_{i=1}^{g_n} \left|\langle u_n^i|\psi\rangle\right|^2$$

where g_n is the degree of degeneracy of a_n and $\{|u_n^i\rangle\}$ $(i = 1, 2, \cdots, g_n)$ is an orthonormal basis for the eigenspace $\mathscr{E}_n$ associated with the eigenvalue a_n of $\hat{A}$. ♡

For this postulate to make sense, the probability should be independent of the choice of the basis. Actually, from the view of geometry, the probability is just the square norm of the projection of the ket onto the eigenspace, or use the language of projector: Let

$$\hat{P}_n = \sum_{i=1}^{g_n} |u_n^i\rangle\langle u_n^i|$$

be the projector onto the eigenspace $\mathscr{E}_n$, let $|\psi_n\rangle$ be the projection of $|\psi\rangle$ onto $\mathscr{E}_n$:

$$|\psi_n\rangle = \hat{P}_n |\psi\rangle = \sum_{i=1}^{g_n} \langle u_n^i|\psi\rangle\, |u_n^i\rangle$$

thus the probability is

$$P(a_n) = \langle\psi_n|\psi_n\rangle = \langle\psi|\hat{P}_n^\dagger \hat{P}_n|\psi\rangle = \langle\psi|\hat{P}_n|\psi\rangle$$

which is independent of $\{|u_n^i\rangle\}$.

Similarly we can obtain postulate for continuous case. For convenience we only consider the non-degenerate case:

$$\rho(\alpha) = \frac{\mathrm{d}P(\alpha)}{\mathrm{d}\alpha} = |\langle v_\alpha|\psi\rangle|^2$$

where $\rho(\alpha)$ is the probability density and $|v_\alpha\rangle$ is a basis.

Note *Based on the postulate above, we know that a global phase factor does not affect the physical predictions, but the relative phases of the coefficients of an expansion are significant:*

$$\mathrm{e}^{\mathrm{i}\theta}|\psi\rangle \leftrightarrow |\psi\rangle$$

$$\lambda_1 \mathrm{e}^{\mathrm{i}\theta_1}|\psi_1\rangle + \lambda_2 \mathrm{e}^{\mathrm{i}\theta_2}|\psi_2\rangle \not\leftrightarrow \lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle$$

Also, recall that we also gives the spectra decomposition 1.2 use the language of wave function, indeed postulate 3.4 is consistent with the previous postulate, just observe that the wave function is the components of the state vector in $\{|\hat{\boldsymbol{r}}\rangle\}$-representation: $\psi(\boldsymbol{r},t) = \langle \boldsymbol{r}|\psi(t)\rangle$.

Postulate 3.5 (Reduction of the Wave Packet)

If the measurement of the physical quantity A on the system in the state $|\psi\rangle$ gives the result a_n, then state of the system immediately after the measurement is the normalized projection: $\dfrac{\hat{P}_n|\psi\rangle}{\sqrt{\langle\psi|\hat{P}_n|\psi\rangle}}$, of $|\psi\rangle$ onto the eigenspace associated with a_n.

We stress that the state of the system after the measurement is always an eigenvector of $\hat{A}$ with eigenvalue a_n, but this vector is not an arbitrary ket of the eigenspace $\mathscr{E}_n$, but the part of the $|\psi\rangle$ that belongs to $\mathscr{E}_n$ (suitably normalized, for convenience).

Postulate 3.6 (Time Evolution of Systems)

The time evolution of the state vector $|\psi(t)\rangle$ is governed by the Schrödinger equation:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$$

where $\hat{H}(t)$ is the observable associated with the total energy of the system, called the ***Hamiltonian operator****, obtained from the classical Hamiltonian.*

Finally, we introduce the rules to construct a operator for a physical quantity A:

Postulate 3.7 (Quantization Rules)

With the position $\boldsymbol{r}(x,y,z)$ of the particle is associated the observable $\hat{\boldsymbol{r}}(\hat{x},\hat{y},\hat{z})$. With the momentum $\boldsymbol{p}(p_x,p_y,p_z)$ of the particle is associated the observable $\hat{\boldsymbol{p}}(\hat{p}_x,\hat{p}_y,\hat{p}_z)$. Since any physical quantity A can be expressed in terms of the fundamental dynamical variables $\boldsymbol{r}$ and $\boldsymbol{p}$: $A(\boldsymbol{r},\boldsymbol{p},t)$. To obtain the corresponding observable $\hat{A}$, just replace $\boldsymbol{r}$ and $\boldsymbol{p}$ in suitable ***symmetrized*** *expression by $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{p}}$ respectively.*

Note *Here the momentum is the* ***canonic momentum****, not the mechanical momentum. For example,* *in electromagnetic field, the classical Hamiltonian is*

$$H(\boldsymbol{r},\boldsymbol{p}) = \frac{1}{2m}[\boldsymbol{p} - q\boldsymbol{A}(\boldsymbol{r},t)]^2 + qU(\boldsymbol{r},t)$$

where $U(\boldsymbol{r},t)$ and $\boldsymbol{A}(\boldsymbol{r},t)$ is the scalar and vector potentials which describe the electromagnetic field, while $\boldsymbol{p}$ is given by

$$\boldsymbol{p} = m\boldsymbol{v} + q\boldsymbol{A}(\boldsymbol{r},t)$$

where $\boldsymbol{v}$ is the velocity of the particle. Hence after quantized the Hamilton operator becomes

$$\hat{H}(t) = \frac{1}{2m}[\hat{\boldsymbol{p}} - q\boldsymbol{A}(\hat{\boldsymbol{r}},t)]^2 + qU(\hat{\boldsymbol{r}},t)$$

and the Schrödinger equation is written:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle = \left\{\frac{1}{2m}[\hat{\boldsymbol{p}} - q\boldsymbol{A}(\hat{\boldsymbol{r}},t)]^2 + qU(\hat{\boldsymbol{r}},t)\right\}\left|\psi(t)\right\rangle$$

3.3 The Physical Interpretation of the Postulates Concerning Observables and Their Measurement

3.3.1 Mean Value and Heisenberg Relations

Proposition 3.1 (Mean Value of an Observable in a Given State)

We define the mean value of an observable $\hat{A}$ in a give state $|\psi\rangle$, denoted as $\langle\hat{A}\rangle_\psi$, or just $\langle\hat{A}\rangle$, is given by the formula:

$$\langle\hat{A}\rangle_\psi = \langle\psi|\hat{A}|\psi\rangle$$

♠

Proof When the times of measurement N is large: $N \to \infty$, the mean value of $\hat{A}$ is

$$\begin{aligned}\langle\hat{A}\rangle &= \sum_n a_n P(a_n) \\ &= \sum_n a_n \langle\psi|\hat{P}_n|\psi\rangle\end{aligned}$$

since $\hat{P}_n|\psi\rangle$ is an eigenvector of $\hat{A}$, hence $\hat{A}\hat{P}_n|\psi\rangle = a_n\hat{P}_n|\psi\rangle$, thus

$$\begin{aligned}\langle\hat{A}\rangle &= \sum_n \langle\psi|a_n\hat{P}_n|\psi\rangle \\ &= \sum_n \langle\psi|\hat{A}\hat{P}_n|\psi\rangle \\ &= \langle\psi|\hat{A}\left[\sum_n \hat{P}_n\right]|\psi\rangle \\ &= \langle\psi|\hat{A}|\psi\rangle\end{aligned}$$

the last equality comes from the resolution of the identity operator 1.9.

For continuous case, just substitute the $\sum_n$ to $\int \mathrm{d}\alpha$. □

Definition 3.1 (The (Root) Mean Square Deviation)

For an observable $\hat{A}$, the mean square deviation, denoted $(\Delta\hat{A})^2$ is

$$(\Delta\hat{A})^2 = \langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$$

and the root mean square deviation is $\Delta\hat{A}$ by setting

$$\Delta\hat{A} = \sqrt{\langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle}$$

♣

Use these definitions, we can obtain the Heisenberg relations, with precise lower limit. First we introduce a useful lemma.

Lemma 3.1

The mean value of Hermitian operator is purely real, of anti-Hermitian operator is purely imaginary.

♡

Proof By 3.1, since

$$\langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle$$

hence

$$\Big(\langle\hat{A}\rangle\Big)^\dagger = \Big(\langle\psi|\hat{A}|\psi\rangle\Big)^\dagger = \pm\langle\psi|\hat{A}|\psi\rangle = \pm\langle\hat{A}\rangle$$

□

Theorem 3.1 (Heisenberg Relations)

Apply definition 3.1 to the observables $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$, using the commutation relations, for any state $|\psi\rangle$, we have

$$\begin{cases} \Delta\hat{x}\Delta\hat{p}_x \geq \dfrac{\hbar}{2} \\ \Delta\hat{y}\Delta\hat{p}_y \geq \dfrac{\hbar}{2} \\ \Delta\hat{z}\Delta\hat{p}_z \geq \dfrac{\hbar}{2} \end{cases}$$

♡

Proof Consider any two **incompatible** observables $\hat{A}, \hat{B}$, means that $[\hat{A}, \hat{B}] \neq 0$, then we can deduce the uncertainty relation for $\Delta\hat{A}\Delta\hat{B}$. For any state $|\psi\rangle$, consider the following two kets:

$$|\alpha\rangle = \hat{A}'|\psi\rangle$$
$$|\beta\rangle = \hat{B}'|\psi\rangle$$

where

$$\hat{A}' = \hat{A} - \langle\hat{A}\rangle$$
$$\hat{B}' = \hat{B} - \langle\hat{B}\rangle$$

then use the Schwarz inequality:

$$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$$

since $\hat{A}', \hat{B}'$ is Hermitian, hence we get

$$\langle\hat{A}'^2\rangle\langle\hat{B}'^2\rangle \geq \Big|\langle\hat{A}'\hat{B}'\rangle\Big|^2$$

while by definition, $\langle \hat{A}'^2 \rangle = (\Delta \hat{A})^2$, $\langle \hat{B}'^2 \rangle = (\Delta \hat{B})^2$, and the right side we can rewrite as

$$\hat{A}'\hat{B}' = \frac{1}{2}[\hat{A}', \hat{B}'] + \frac{1}{2}\{\hat{A}', \hat{B}'\}$$

where $\{\hat{A}', \hat{B}'\} = \hat{A}'\hat{B}' + \hat{B}'\hat{A}'$ is the anticommutator. Thus we have

$$\Delta\hat{A}\Delta\hat{B} \geq \frac{1}{2}\Big| \langle [\hat{A}', \hat{B}'] + \{\hat{A}', \hat{B}'\} \rangle \Big|$$

by lemma 3.1, since the commutator is anti-Hermitian and the anticommutator is Hermitian, we get

$$\begin{aligned}
\Delta\hat{A}\Delta\hat{B} &\geq \frac{1}{2}\Big| \langle [\hat{A}', \hat{B}'] \rangle \Big| \\
&= \frac{1}{2}\Big| \langle (\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle) - (\hat{B} - \langle \hat{B} \rangle)(\hat{A} - \langle \hat{A} \rangle) \rangle \Big| \\
&= \frac{1}{2}\Big| \langle [\hat{A}, \hat{B}] \rangle \Big|
\end{aligned}$$

Then for $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{p}}$, since $[\hat{r}_i, \hat{p}_i] = \mathrm{i}\hbar$, we have $\Delta\hat{r}_i\Delta\hat{p}_i \geq \dfrac{\hbar}{2}$ and that is the Heisenberg relations. □

3.3.2 Compatibility of Observables

In this part, we want to dig properties of compatibile or incompatible observables, first we give the definition of compatibility.

Definition 3.2 (Compatibility)

Consider two observables $\hat{A}$ and $\hat{B}$, if they commute: $[\hat{A}, \hat{B}] = 0$, we say they are compatibile, if they are not commut, they are incompatible. ♣

As in theorem 1.3 shows, if two observables $\hat{A}$, $\hat{B}$ commute, or compatibile, we can construct an orthonormal basis of the state space with eigenvectors common to $\hat{A}$ and $\hat{B}$: $\{|a_n, b_p, i\rangle\}$ with

$$\hat{A}\,|a_n, b_p, i\rangle = a_n\,|a_n, b_p, i\rangle$$
$$\hat{B}\,|a_n, b_p, i\rangle = b_p\,|a_n, b_p, i\rangle$$

where i allow us to distinguish different vectors corresponding to the same pair of eigenvalues (if necessary). On the other hand, if two observables are incompatible, we can not construct such basis.

Then, consider the measurement of these two compatibile observables on a system, with arbitrary initial state $|\psi\rangle$. It can be written:

$$|\psi\rangle = \sum_{n,p,i} c_{n,p,i}\,|a_n, b_p, i\rangle$$

Assume we first measure A and immediately afterwards, B, let's caculate the probability $P(a_n, b_p)$ of obtaining a_n in first measurememt and b_p in second one. First measurememt:

$$P(a_n) = \sum_{p,i} |c_{n,p,i}|^2$$

With state becomes

$$|\psi_n\rangle = \frac{1}{\sqrt{\sum_{p,i} |c_{n,p,i}|^2}} \sum_{p,i} c_{n,p,i}\,|a_n, b_p, i\rangle$$

then the second measurememt:

$$P(b_p \mid a_n) = \frac{1}{\sqrt{\sum_{p,i} |c_{n,p,i}|^2}} \sum_i |c_{n,p,i}|^2$$

with state becomes:

$$|\psi_{n,p}\rangle = \frac{1}{\sqrt{\sum_i |c_{n,p,i}|^2}} \sum_i c_{n,p,i} |a_n, b_p, i\rangle$$

hence the total probability is

$$P(a_n, b_p) = P(a_n)P(b_p \mid a_n) = \sum_i |c_{n,p,i}|^2$$

Conversely, if we first measure B and then A:

$$P(b_p) = \sum_{n,i} |c_{n,p,i}|^2$$

with state

$$|\psi_p\rangle = \frac{1}{\sqrt{\sum_{n,i} |c_{n,p,i}|^2}} \sum_{n,i} c_{n,p,i} |a_n, b_p, i\rangle$$

the second:

$$P(a_n \mid b_p) = \frac{1}{\sqrt{\sum_{n,i} |c_{n,p,i}|^2}} \sum_i |c_{n,p,i}|^2$$

with state

$$|\psi_{p,n}\rangle = \frac{1}{\sqrt{\sum_i |c_{n,p,i}|^2}} \sum_i c_{n,p,i} |a_n, b_p, i\rangle$$

hence the total probability is

$$P(b_p, a_n) = P(b_p)P(a_n \mid b_p) = \sum_i |c_{n,p,i}|^2$$

From the previous computation we find that:

$$P(a_n, b_p) = P(b_p, a_n)$$
$$|\psi_{n,p}\rangle = |\psi_{p,n}\rangle$$

hence we see that if two observables are compatibile, the measurememt of B does not cause any loss of information previously obtained from a measurement of A (and vice versa). Also, the order of measuring two observables are not important, furthermore, this enables us to envisage the **simultaneous measurement** of A and B, and generalized the result in postulate 3.4 and 3.5. Conversely, if two observables are incompatible, we cannot obtain the relation above, means that

$$P(a_n, b_p) \neq P(b_p, a_n)$$
$$|\psi_{n,p}\rangle \neq |\psi_{p,n}\rangle$$

and hence we cannot simultaneous measure two incompatible observables. This is consistent with the discussion of uncertainty relations: $\Delta\hat{A}\Delta\hat{B} \geq \frac{1}{2}\left| \langle[\hat{A}, \hat{B}]\rangle \right|$.

3.3.3 Preparation of a State

As in postulate 3.5, consider a physical system in the state $|\psi\rangle$ and measure the observable A, whose spectrum is discrete, let $\{|u_n\rangle\}$ be the orthonormal basis of eigenvectors of $\hat{A}$, and

$$|\psi\rangle = \sum_i c_i |u_i\rangle$$

then if the measurememt yields a_n, the state immediately becomes $\frac{c_n}{|c_n|}|u_n\rangle$, which represents the same physical satate as $|u_n\rangle$ it self. In this case (non-degenerate), we can determine unambiguously the state of the system after this measurement.

However, if the eigenvalue a_n is degenerate, then the state becomes:

$$|\psi_n\rangle = \frac{1}{\sqrt{\sum_i |c_n^i|^2}} \sum_{i=1}^{g_n} c_n^i |u_n^i\rangle$$

which is dependent on the initial state $|\psi\rangle$. But luckily, if we have two compatibile observables A and B, then we can simultaneous measure the two observables, to get a pair of eigenvalues. Moreover, if $\{\hat{A}, \hat{B}\}$ is a C.S.C.O., then the result state is still uniquely determined:

$$|\psi_{n,p}\rangle = |\psi_{p,n}\rangle = \frac{c_{n,p}}{|c_{n,p}|} |a_n, b_p\rangle$$

which represents the same as $|a_n, b_p\rangle$. And hence we return to the non-degenerate case, and this is why we say that C.S.C.O. can "reduce" the degeneracy, and with C.S.C.O. we can uniquely determine the result state, independent with the initial state.

3.4 The Physical Implications of the Schrödinger Equation

3.4.1 General Properties of the Schrödinger Equation

Proposition 3.2 (Determinism in the Evolution of Physical Systems)

Since the Schrödinger Equation is of first order in t, consequently, once given the initial stae $|\psi\rangle(t_0)$, the state $|\psi(t)\rangle$ at any subsequent time t is determined.

Proposition 3.3 (The Superposition Principle)

Since the Schrödinger Equation is linear and homogeneous, its solution are linearly superposable.

Proposition 3.4 (Conversation of Probability)

The norm of the state vector remains constant.

Proof Since $\hat{H}$ is Hermitian, we can get

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \frac{1}{\mathrm{i}\hbar}\hat{H}(t)|\psi(t)\rangle$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)| = -\frac{1}{\mathrm{i}\hbar}\hat{H}(t)\langle\psi(t)|$$

take the deravative of the norm of the state vector:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)|\psi(t)\rangle &= \left[\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)|\right]|\psi(t)\rangle + \langle\psi(t)|\left[\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle\right] \\ &= \left[-\frac{1}{\mathrm{i}\hbar}\hat{H}(t) + \frac{1}{\mathrm{i}\hbar}\hat{H}(t)\right]\langle\psi(t)|\psi(t)\rangle \\ &= 0\end{aligned}$$

□

This verifies the Interpretation of "the square modulus of wave function is the probability", since in $\{|\hat{\boldsymbol{r}}\rangle\}$-representation, the norm of state vector is

$$\langle\psi(t)|\psi(t)\rangle = \int \mathrm{d}^3r\,|\psi(\boldsymbol{r},t)|^2 = 1$$

which is a constant, meaning that the total probability of finding the particle in all space is equal to 1, which is a constance.

Recall that in electrodynamics we have the conversation of charge:

$$\frac{\partial}{\partial t}\rho(\boldsymbol{r},t) + \boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{r},t) = 0$$

where $\boldsymbol{J}(\boldsymbol{r},t)$ is the current, $\rho(\boldsymbol{r},t)$ is the density of charge. Similarly, if we let $\rho(\boldsymbol{r},t)$ denote the **density of probability** and let $\boldsymbol{J}(\boldsymbol{r},t)$ denote the **probability current**, we can analogously build the same formula.

Consider the simple case that the particle under a scalar potential $V(\boldsymbol{r},t)$, its Hermitonian is:

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + \hat{V}(\hat{\boldsymbol{r}},t)$$

in $\{\hat{\boldsymbol{r}}\}$-representation, the Schrödinger equation is:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{r},t) + V(\boldsymbol{r},t)\psi(\boldsymbol{r},t)$$

take the c.c. we get

$$-\mathrm{i}\hbar\frac{\partial}{\partial t}\psi^*(\boldsymbol{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi^*(\boldsymbol{r},t) + V(\boldsymbol{r},t)\psi^*(\boldsymbol{r},t)$$

since $V(\boldsymbol{r},t)$ must be real. Combine the two equations, since the density of probability is $\rho(\boldsymbol{r},t) = |\psi(\boldsymbol{r},t)|^2 = \psi^*(\boldsymbol{r},t)\psi(\boldsymbol{r},t)$, we obtain

$$\begin{aligned}\frac{\partial}{\partial t}\rho(\boldsymbol{r},t) &= \frac{\partial}{\partial t}[\psi^*(\boldsymbol{r},t)\psi(\boldsymbol{r},t)] \\ &= -\frac{\hbar}{2\mathrm{i}m}\left[\psi^*(\boldsymbol{r},t)\nabla^2\psi(\boldsymbol{r},t) - \psi(\boldsymbol{r},t)\nabla^2\psi^*(\boldsymbol{r},t)\right]\end{aligned}$$

hence if we let

$$\begin{aligned}\boldsymbol{J} &= \frac{\hbar}{2\mathrm{i}m}[\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*] \\ &= \frac{1}{m}\,\mathrm{Re}\left[\psi^*\left(\frac{\hbar}{\mathrm{i}}\boldsymbol{\nabla}\psi\right)\right]\end{aligned}$$

then we have

$$\frac{\partial}{\partial t}\rho(\boldsymbol{r},t) + \boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{r},t) = 0$$

Note *Since the current density is the charge density times the velocity: $\boldsymbol{J} = \rho\boldsymbol{v}$, and also notice that ρ*

is the mean value of operator $|\boldsymbol{r}\rangle\langle\boldsymbol{r}|$ *and* $\boldsymbol{v} = \dfrac{\boldsymbol{p}}{m}$*, then if we define an operator*

$$\hat{\boldsymbol{K}}(\boldsymbol{r}) = \frac{1}{2m}[|\boldsymbol{r}\rangle\langle\boldsymbol{r}|\,\hat{\boldsymbol{p}} + \hat{\boldsymbol{p}}\,|\boldsymbol{r}\rangle\langle\boldsymbol{r}|]$$

then the probability current is just the mean value of $\hat{K}$ *in state* $|\psi\rangle$*:*

$$\boldsymbol{J} = \langle\psi|\hat{\boldsymbol{K}}|\psi\rangle$$

Moreover if the particle is in an electromagnetic field described by the potentials $U(\boldsymbol{r}, t)$ and $\boldsymbol{A}(\boldsymbol{r}, t)$, then we can get

$$\boldsymbol{J}(\boldsymbol{r}, t) = \frac{1}{m}\,\mathrm{Re}\left\{\psi^*\left[\frac{\hbar}{\mathrm{i}}\boldsymbol{\nabla} - q\boldsymbol{A}\right]\psi\right\}$$

Theorem 3.2 (Ehrenfest)

For any observable $\hat{A}$*, the deravative of mean value of* $\hat{A}$ *w.r.t.* t *is*

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

♡

Proof Just use the Schrödinger equation. □

Note *Consider the simple case: a spinless particle in a scalar stationary potential* $V(\boldsymbol{r})$*, we have*

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

then we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\boldsymbol{r}}\rangle = \frac{1}{\mathrm{i}\hbar}\langle[\hat{\boldsymbol{r}}, \hat{H}]\rangle = \frac{\langle\hat{\boldsymbol{p}}\rangle}{m}$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\boldsymbol{p}}\rangle = \frac{1}{\mathrm{i}\hbar}\langle[\hat{\boldsymbol{p}}, \hat{H}]\rangle = -\langle\boldsymbol{\nabla}\hat{V}(\hat{\boldsymbol{r}})\rangle$$

which is similar to the classical case. Combine the two equation we get

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\hat{\boldsymbol{r}}\rangle = -\langle\boldsymbol{\nabla}\hat{V}(\hat{\boldsymbol{r}})\rangle$$

if the wave function $\psi(\boldsymbol{r}, t)$ *describing the state of the particle is a wave packet, then* $\langle\hat{\boldsymbol{r}}\rangle$ *represents the* ***center of the wave packet****. However, this equation does not means that the motion of the center of the wave packet obeys the laws of classical mechanics. Since the right side is the mean value of the force on the packet, but not the force at the center of the wave packet:*

$$\boldsymbol{F}_{cl} = -\boldsymbol{\nabla}V(\boldsymbol{r})\bigg|_{\boldsymbol{r}=\langle\hat{\boldsymbol{r}}\rangle} \neq -\langle\boldsymbol{\nabla}\hat{V}(\hat{\boldsymbol{r}})\rangle$$

3.4.2 The Case of Conservative Systems