§ 3.5. Dirac Notation and Representations

14. QM Probability Amplitude and Interference Effect.

Let $|\psi_1\rangle$ and $|\psi_2\rangle$ be two orthogonal normalized states:

$$\langle\psi_1|\psi_2\rangle = 0, \quad \langle\psi_1|\psi_1\rangle = \langle\psi_2|\psi_2\rangle = 1.$$

For a given observable $\hat{A}$, $\{|u_n\rangle\}$ are complete orthonormal eigenstates corresponding to the eigenvalues $\{a_n\}$: $\hat{A}|u_n\rangle = a_n|u_n\rangle$, $\langle u_m|u_n\rangle = \delta_{mn}$.

* If the system is in the state $|\psi_1\rangle$, the probability $P_1(a_n)$ of finding a_n when $\hat{A}$ is measured on the system is given by

$$P_1(a_n) = |\langle u_n|\psi_1\rangle|^2.$$

* If the system is in the state $|\psi_2\rangle$, the probability $P_2(a_n)$ of finding a_n when $\hat{A}$ is measured on the system is given by

$$P_2(a_n) = |\langle u_n|\psi_2\rangle|^2.$$

* Now consider a normalized state $|\psi\rangle$ which is a linear superposition of $|\psi_1\rangle$ and $|\psi_2\rangle$: $\quad |\psi\rangle = \lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle$

$$|\lambda_1|^2 + |\lambda_2|^2 = 1.$$

The probability $P(a_n)$ of finding the eigenvalue a_n when the observable $\hat{A}$ is measured on the system in the state $|\psi\rangle$ is

$$P(a_n) = |\langle u_n|\psi\rangle|^2.$$

Substituting $|\psi\rangle$ expression into $P(a_n)$ and further deriving it:

$$\begin{aligned} P(a_n) &= |\langle u_n|\psi\rangle|^2 = |\lambda_1\langle u_n|\psi_1\rangle + \lambda_2\langle u_n|\psi_2\rangle|^2 \\ &= (\lambda_1 \langle u_n|\psi_1\rangle + \lambda_2\langle u_n|\psi_2\rangle)(\lambda_1^*\langle u_n|\psi_1\rangle^* + \lambda_2^*\langle u_n|\psi_2\rangle^*) \\ &= |\lambda_1|^2|\langle u_n|\psi_1\rangle|^2 + |\lambda_2|^2|\langle u_n|\psi_2\rangle|^2 \\ &\quad + \lambda_1\lambda_2^*\langle u_n|\psi_1\rangle\langle u_n|\psi_2\rangle^* + \lambda_1^*\lambda_2\langle u_n|\psi_1\rangle^*\langle u_n|\psi_2\rangle \\ &= |\lambda_1|^2 P_1(a_n) + |\lambda_2|^2 P_2(a_n) + 2\mathrm{Re}(\lambda_1\lambda_2^*\langle u_n|\psi_1\rangle\langle u_n|\psi_2\rangle) \end{aligned}$$

Thus, the cross term shows the interference effect.

Since $P(a_n)$, $P_1(a_n)$ and $P_2(a_n)$ are the probabilities, $\langle u_n|\psi\rangle$, $\langle u_n|\psi_1\rangle$, and $\langle u_n|\psi_2\rangle$ are called the probability amplitudes. The interference effect is explained by the superposition of the probality amplitudes,

$$\langle u_n|\psi\rangle = \lambda_1\langle u_n|\psi_1\rangle + \lambda_2\langle u_n|\psi_2\rangle.$$

15. Representations:

Above descriptions of QM concepts and principles have been using the abstract state vectors and the abstract linear operators in the abstract state space. They are perfect for expressing the exact meaning of QM principle of superposition of states, principle of uncertainty, principle of motion, and principle of measurements. They also give clear presentation of some derivations like projector operator, mean value, etc.

However, when facing practical problems, we need to project these abstract vectors and operators to a concrete representation in order to do some actual computation. Choosing a representation means choosing an orthonormal basis, either discrete or continuous, in the state space. We then project the state vector and linear operator onto the basis so that the state vector and linear operator are represented by numbers or functions in the actual representation. The choice of a representation is, in theory, arbitrary. In practice, it obviously depends on the particular problem being studied: in each case, one chooses the representation which leads to the simplest calculation.

Two important examples of representations and observables are the coordinate (position) $\{|\vec{r}\rangle\}$ and momentum $\{|\vec{p}\rangle\}$ representations and observables ($\hat{\vec{r}}$ and $\hat{\vec{p}}$). We will use these two as examples to show how to project state and operator to a representation, how to do actual calculation, and how to change from representation to another.

(1) State vector versus wave function in $\{|\vec{r}\rangle\}$ and $\{|\vec{p}\rangle\}$ rep:
Recall the principle of superposition of states, for the complete orthonormal states $\{|\vec{r}\rangle\}$, we have $\langle \vec{r}'|\vec{r}\rangle = \delta(\vec{r}-\vec{r}')$.
Similarly, for orthonormal $\{|\vec{p}\rangle\}$, we have $\langle \vec{p}'|\vec{p}\rangle = \delta(\vec{p}-\vec{p}')$.

* Any arbitrary state vector $|\psi\rangle$ can be expanded in terms of $\{|\vec{r}\rangle\}$ as: $|\psi\rangle = \int c(\vec{r}')|\vec{r}'\rangle d^3r'$, where $c(\vec{r}')$ is the probability amplitude of the system being in the state of $|\vec{r}'\rangle$, i.e., $|c(\vec{r}')|^2$ is the probability of finding the system at position $\vec{r}'$. As explained earlier,

$$\langle \vec{r}|\psi\rangle = \int c(\vec{r}')\langle \vec{r}|\vec{r}'\rangle d^3r' = \int c(\vec{r}')\delta(\vec{r}-\vec{r}')d^3r' = c(\vec{r})$$

Thus, we repeat the expression for $c(\vec{r})$ [i.e., $c(\alpha)$].
We can write $c(\vec{r}) = \langle \vec{r}|\psi\rangle \equiv \psi(\vec{r})$,
which is called the wave function in the $\{|\vec{r}\rangle\}$ representation.

* Similary, $|\psi\rangle$ can be projected onto $\{|\vec{p}\rangle\}$ representation:

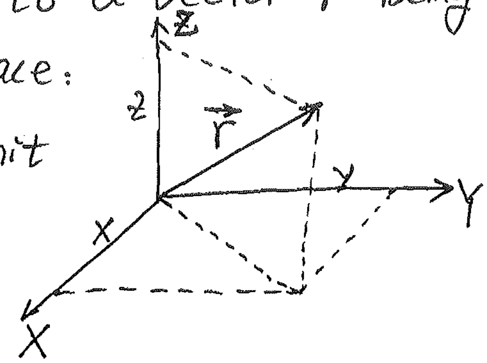
$$|\psi\rangle = \int c(\vec{p}')|\vec{p}'\rangle d^3p' \Rightarrow$$

$$c(\vec{p}) = \langle \vec{p}|\psi\rangle \equiv \psi(\vec{p}),$$

which is the wave function in the $\{|\vec{p}\rangle\}$ representation.

* Wave function $\psi(\vec{r}) = \langle \vec{r}|\psi\rangle$ has the following meaning: it is the probability amplitude of finding a particle at position $\vec{r}$.
In other words, $|\psi(\vec{r})|^2 = |\langle \vec{r}|\psi\rangle|^2$ is the probability of the particle appearing at position $\vec{r}$. Similarly, $|\psi(\vec{p})|^2 = |\langle \vec{p}|\psi\rangle|^2$ is the probability of finding the particle with momentum $\vec{p}$.

* Wave function $\psi(\vec{r})$ is the projection of the state vector $|\psi\rangle$ onto the $\{|\vec{r}\rangle\}$ representation, analogy to a vector $\vec{r}$ being projected onto a (X, Y, Z) coordinate space:



$\vec{r} = x\vec{i} + y\vec{j} + z\vec{k}$ ($\vec{i}, \vec{j}, \vec{k}$ are unit vectors along x, y, z axes)

$\therefore \vec{r} \Rightarrow (x, y, z)$.

Analogy: $|\psi\rangle = \int \psi(\vec{r})\,|\vec{r}\rangle\, d^3r$

$\therefore |\psi\rangle \Rightarrow \{\psi(\vec{r})\}$

* In 1-dimension case, $\vec{r} \rightarrow x$, so $|\psi\rangle \Rightarrow \{\psi(x)\}$. The conjugate of $|\psi\rangle$, i.e., $\langle\psi| \Rightarrow \{\psi^*(x)\}$. These are the wave functions used in HW #2, problem #2.

* Note $|\langle\vec{r}|\psi\rangle|^2 \equiv \langle\vec{r}|\psi\rangle^* \langle\vec{r}|\psi\rangle$

$$|\psi(\vec{r})|^2 \equiv \psi^*(\vec{r})\,\psi(\vec{r}).$$

* In principle, different representations are equivalent, since they represent the same state vector $|\psi\rangle$ and same operator $\hat{A}$.

(2) Operator in $\{|\vec{r}\rangle\}$ and $\{|\vec{p}\rangle\}$ representations.

In $\{|\vec{r}\rangle\}$ representation, the coordinate $\hat{\vec{r}}$ and momentum $\vec{p}$ operators are:

$$\hat{x} \to x, \qquad \hat{\vec{r}} \to \vec{r}$$

$$\hat{p}_x \to -i\hbar\frac{\partial}{\partial x}, \qquad \hat{\vec{p}} \to -i\hbar\vec{\nabla}, \qquad \vec{\nabla} = \vec{e}_x\frac{\partial}{\partial x} + \vec{e}_y\frac{\partial}{\partial y} + \vec{e}_z\frac{\partial}{\partial z}.$$

In $\{|\vec{p}\rangle\}$ representation, $\hat{\vec{r}}$ and $\hat{\vec{p}}$ operators are

$$\hat{p}_x \to p_x, \qquad \hat{\vec{p}} \to \vec{p}$$

$$\hat{x} \to i\hbar\frac{\partial}{\partial p_x}, \qquad \hat{\vec{r}} \to i\hbar\vec{\nabla}_p, \qquad \vec{\nabla}_p = \vec{e}_{p_x}\frac{\partial}{\partial p_x} + \vec{e}_{p_y}\frac{\partial}{\partial p_y} + \vec{e}_{p_z}\frac{\partial}{\partial p_z}$$

Because $\psi(\vec{r})$ and $\psi(\vec{p})$ are the Fourier transform of each other, we have $\hat{\vec{p}} = -i\hbar\vec{\nabla}$ in $\{|\vec{r}\rangle\}$ representation, while $\hat{\vec{r}} = i\hbar\vec{\nabla}_p$ in $\{|\vec{p}\rangle\}$ representation.

* $\{|\vec{r}\rangle\}$ is the most common and widely used representation, also called the Schrödinger representation, in which Schrödinger developed the Schrödinger equation. Let us write down a few other operators in the $\{|\vec{r}\rangle\}$ representation.

① Kinetic energy operator: the classical kinetic energy is given by $E_k = \frac{\vec{p}^2}{2m}$. To quantize it to derive its operator, replace $\vec{p}$ with its corresponding operator $\hat{\vec{p}}$:

$$\hat{E}_k = \frac{\hat{\vec{p}}^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) = -\frac{\hbar^2}{2m}\nabla^2.$$

② Hamiltonian operator $\hat{H}(t)$: the classical $H = \frac{\vec{p}^2}{2m} + V$

Then in QM, $\hat{H}(t) = \frac{\hat{\vec{p}}^2}{2m} + \hat{V}$. If $\hat{V} = V(\hat{\vec{r}})$, then $\hat{V} = V(\vec{r})$

Since $\hat{\vec{r}} = \vec{r}$ in $\{|\vec{r}\rangle\}$, $\hat{H}(t) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(\vec{r})$.

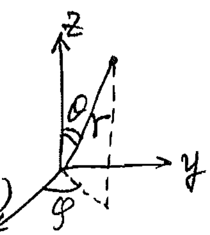
③ Angular momentum operator: the classical angular momentum is $\vec{l} = \vec{r} \times \vec{p}$, where $\vec{r}$ is position vector, $\vec{p}$ is momentum vector.

Corresponding QM operator is:

$$\hat{\vec{l}} = \hat{\vec{r}} \times \hat{\vec{p}} = -i\hbar\, \vec{r} \times \vec{\nabla}.$$

Angular momentum operator components are

$$\begin{cases} \hat{l}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right) \\ \hat{l}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) = i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right) \\ \hat{l}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial\varphi} \end{cases}$$



The last equality is in spherical coordinates:

$$r = \sqrt{x^2+y^2+z^2}, \quad \theta = \arctan\left(\sqrt{x^2+y^2}/z\right), \quad \varphi = \arctan(y/x)$$

④ The square of angular momentum:

$$\hat{\vec{l}}^2 \equiv \hat{l}_x^2 + \hat{l}_y^2 + \hat{l}_z^2$$

$$= -\hbar^2\left[\frac{1}{\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right].$$

(3) Mean values in the $\{|\vec{r}\rangle\}$ and $\{|\vec{p}\rangle\}$ representations.

In the abstract state space, as we proved above, the mean value of an observable $\hat{A}$ in the state $|\psi\rangle$ of a system is given by

$$\bar{A} \equiv \langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle.$$

Now project state vector and operator to $\{|\vec{r}\rangle\}$ representation,

recall $\int |\vec{r}\rangle\langle\vec{r}| d^3r = 1$, we have

$$\begin{aligned}\bar{A} &= \langle \psi | \hat{A} | \psi \rangle \\ &= \langle \psi | \left(\int |\vec{r}\rangle\langle\vec{r}| d^3r\right) \hat{A} | \psi \rangle \\ &= \int d^3r \langle \psi | \vec{r}\rangle \langle \vec{r} | \hat{A} | \psi \rangle.\end{aligned}$$

Recall $\langle \psi | \vec{r}\rangle = \psi^*(\vec{r})$.

If $\hat{A}$ is a function of $\hat{\vec{r}}$, i.e., $\hat{A} = A(\hat{\vec{r}})$, then since $|\vec{r}\rangle$ is an eigenstate of $\hat{\vec{r}}$, it is also an eigenstate of $A(\hat{\vec{r}})$, i.e., $A(\hat{\vec{r}})|\vec{r}\rangle = A(\vec{r})|\vec{r}\rangle$.

Thus, $\langle \vec{r} | \hat{A} | \psi \rangle = \langle \vec{r} | A(\hat{\vec{r}}) | \psi \rangle = A(\vec{r}) \langle \vec{r} | \psi \rangle = A(\vec{r})\psi(\vec{r})$,

$$\therefore \bar{A} = \int d^3r\, \psi^*(\vec{r}) A(\vec{r}) \psi(\vec{r}).$$

<u>Example</u>: In HW #2, Problem #7 (1), 1-D case, $\hat{X}^2$ is a function of $\hat{X}$, i.e., $\widehat{X^2} = (\hat{X})^2$. $\because \hat{X}|x\rangle = x|x\rangle$, $\therefore \hat{X}^2|x\rangle = x^2|x\rangle$.

$$\therefore \overline{X^2} = \int dx\, \psi^*(x) X^2 \psi^*(x).$$

Furthermore, since x^2 is just a polynomial term of x, it can exchange order with $\psi^*(x)$ or $\psi(x)$, so

$$\overline{X^2} = \int x^2 |\psi(x)|^2 dx.$$

For the momentum operator $\hat{\vec{p}} = -i\hbar\vec{\nabla}$ in $\{|\vec{r}\rangle\}$ representation, which is NOT a simple function of $\vec{r}$, but involves derivatives.

$$\bar{p} \equiv \langle\hat{\vec{P}}\rangle = \langle\psi|\hat{\vec{P}}|\psi\rangle$$
$$= \langle\psi|\left(\int|\vec{r}\rangle\langle\vec{r}|d^3r\right)(-i\hbar\vec{\nabla})|\psi\rangle$$
$$= \int d^3r\,\langle\psi|\vec{r}\rangle(-i\hbar)\langle\vec{r}|\vec{\nabla}|\psi\rangle.$$

It can be proven that $\langle\vec{r}|\vec{\nabla}|\psi\rangle = \vec{\nabla}\langle\vec{r}|\psi\rangle = \vec{\nabla}\psi(\vec{r})$

$$\therefore\ \bar{p} = \int d^3r\,\psi^*(\vec{r})(-i\hbar\vec{\nabla})\psi(\vec{r}).$$

If an operator is a function of $\hat{\vec{P}}$, e.g., $\hat{B} = B(\hat{\vec{P}})$,

then $\hat{B}|\vec{r}\rangle = B(-i\hbar\vec{\nabla})|\vec{r}\rangle$

$$\therefore\ \bar{B} = \int d^3r\,\psi^*(\vec{r})B(-i\hbar\vec{\nabla})\psi(\vec{r})$$

<u>Example</u>. In HW #2, Problem #7, 1-D case, $\hat{P}_x = -i\hbar\frac{\partial}{\partial x}$,

so $(\hat{P}_x - P_0)^2 = (-i\hbar\frac{\partial}{\partial x} - P_0)^2 = -\hbar^2\frac{\partial^2}{\partial x^2} + 2i\hbar P_0\frac{\partial}{\partial x} + P_0^2$.

$$\therefore\ \overline{(\hat{P}_x - P_0)^2} = \int dx\,\psi^*(x)\left[-\hbar^2\frac{\partial^2}{\partial x^2} + 2i\hbar P_0\frac{\partial}{\partial x} + P_0^2\right]\psi(x).$$

Note, since $\frac{\partial^2}{\partial x^2}$, $\frac{\partial}{\partial x}$ are derivatives, not a polynomial of x, they <u>CANNOT</u> switch order with $\psi^*(x)$ or $\psi(x)$!!!

As $\psi(x) = Ae^{-ax^2/2}e^{+iP_0x/\hbar}$, $\psi^*(x) = Ae^{-ax^2/2}e^{-iP_0x/\hbar}$,

you cannot cancel out the imaginary part <u>BEFORE</u> taking derivatives!

(Of course, after taking derivatives, you only have x polynomial terms left, then you can swith these x terms with $\psi^*(x)$ or $\psi(x)$, and cancel out $e^{\pm iP_0x/\hbar}$ part!)

If you follow this procedure, Problem #2 (4) should reach a correct answer $\Delta p = \hbar\sqrt{\frac{a}{2}}$.

The same state and same operator can also be projected to different representations, e.g., $\{|\vec{p}\rangle\}$ presentation, and they are equivalent.

The momentum operator $\hat{\vec{p}} = \vec{p}$ in the $\{|\vec{p}\rangle\}$ representation,

$$\therefore \ \bar{p} \equiv \langle \hat{\vec{p}} \rangle = \langle \psi | \hat{\vec{p}} | \psi \rangle$$

$$= \langle \psi | \left(\int d^3p \, |\vec{p}\rangle\langle\vec{p}| \right) \vec{p} \, |\psi\rangle$$

$$= \int d^3p \, \langle \psi | \vec{p} \rangle \langle \vec{p} | \vec{p} | \psi \rangle$$

$$= \int d^3p \, \langle \psi | \vec{p} \rangle \, \vec{p} \, \langle \vec{p} | \psi \rangle$$

To distinguish $\langle \vec{p} | \psi \rangle$ from $\langle \vec{r} | \psi \rangle$, we write $\langle \vec{p} | \psi \rangle = C(\vec{p})$.

$$\therefore \ \bar{p} = \int d^3p . \, C^*(p) \, \vec{p} \, C(p)$$

Similarly, if $\hat{B} = B(\hat{\vec{p}})$, then

$$\bar{B} = \int d^3p . \, C^*(p) \, B(\vec{p}) \, C(p).$$

Example: In HW #2, Problem #7 (2), $C(P_x)$ is the Fourier transform of $\psi(x)$, and $\hat{P}_x = P_x$, $(\hat{P}_x - P_0)^2 = (P_x - P_0)^2$.

$$\therefore \ \overline{(\hat{P}_x - P_0)^2} = \int dP_x \, C^*(P_x) \, (P_x - P_0)^2 \, C(P_x) = \hbar \sqrt{\frac{a}{2}}$$

It gives the same result as problem #2(4). This indicates that the $\{|\vec{p}\rangle\}$ representation is equivalent to the $\{|\vec{r}\rangle\}$. With the same state $|\psi\rangle$ and same operator $\hat{p}$, you will get the same results (the root-mean-square) in the $\{|\vec{r}\rangle\}$ and $\{|\vec{p}\rangle\}$ representations. In other words, the results only depend on the state vector $|\psi\rangle$ and the observable operator $\hat{A}$, but independent of representations. But choosing different representations makes the calculation easier or complicated, just like $\hat{p}$ operator has more straightforward calculation in $\{|\vec{p}\rangle\}$.