Lecture 5: Orbital angular momentum, spin and rotation

1 Orbital angular momentum operator

According to the classic expression of orbital angular momentum $\vec{L} = \vec{r} \times \vec{p}$, we define the quantum operator

$$L_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y, L_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z, L_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x. \tag{1}$$

(From now on, we may omit the hat on the operators.) We can check that the three components of operators of $\vec{L}$ are Hermitian, and satisfy the commutation relation

$$[L_i, L_j] = i\varepsilon_{ijk}\hbar L_k. \tag{2}$$

The non-commutativity of $L_i (i = x, y, z)$ is absent in the classic physics, which is a quantum effect. We can normalize L_i by dividing l, roughly speaking the magnitude of orbital angular momentum, we have

$$[\frac{L_i}{l}, \frac{L_j}{l}] = \frac{1}{l} i\varepsilon_{ijk} \frac{L_k}{l}. \tag{3}$$

As we can see, that in the limit of $l \to \infty$, the non-commutativity approaches zero and thus the classic physics is recovered.

2 Rotation operator

Let us define the rotation operator. Consider a single particle state $|\Psi\rangle$, and after a rotation operation $g(\hat{n}, \theta)$ where $\hat{n}$ is the rotation axis and θ is the rotation angle, we arrive at $|\Psi^g\rangle$. The operation of g on three-vectors, such as $\vec{r}$, $\vec{p}$, and $\vec{S}$, is described by a 3×3 special orthogonal matrix, i.e., SO(3), $g_{\alpha\beta}$ as

$$(g\vec{r})_\alpha = g_{\alpha\beta} r_\beta; \quad (g\vec{p})_\alpha = g_{\alpha\beta} p_\beta; \quad (g\vec{S})_\alpha = g_{\alpha\beta} S_\beta. \tag{4}$$

For example, for $\hat{n} = \hat{z}$, we have

$$g(\hat{z}, \theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{5}$$

For infinitesimal rotation angle θ,

$$g(\hat{z}, \theta) \approx 1 + \theta \frac{\partial}{\partial_\theta} g(\hat{z}, \theta)|_{\theta=0} = 1 + \theta \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{6}$$

Exercise 1: Please find the explicit matrices for $g(\hat{x},\theta)$ and $g(\hat{y},\theta)$, and find their infinitesimal rotation generators $\frac{\partial}{\partial_\theta} g(\hat{x},\theta)|_{\theta=0}$ and $\frac{\partial}{\partial_\theta} g(\hat{y},\theta)|_{\theta=0}$.

By the physical meaning of rotation, we should have

$$\langle \Psi^g | \Psi^g \rangle = \langle \Psi | \Psi \rangle, \quad \langle \Psi^g | \vec{p} | \Psi^g \rangle = \langle \Psi | g\vec{p} | \Psi \rangle, \quad \langle \Psi^g | \vec{S} | \Psi^g \rangle = \langle \Psi | g\vec{S} | \Psi \rangle. \tag{7}$$

We denote that $|\Psi^g\rangle = D(g)|\Psi\rangle$, and assume that $D(g)$ is a linear unitary operator. We should have

$$\begin{aligned} D(g(\vec{n},0)) &= 1, \\ D^\dagger(g)D(g) &= D(g)D^\dagger(g) = 1, \\ D^\dagger(g)\vec{r}D(g) &= g\vec{r}, \\ D^\dagger(g)\vec{p}D(g) &= g\vec{p} \\ D^\dagger(g)\vec{S}D(g) &= g\vec{S}. \end{aligned} \tag{8}$$

For two successive rotations g_1 and g_2, their net effect is another rotation g whose matrix is defined as $g = g_1 g_2$. Their corresponding rotation operators satisfy the similar relation of product as

$$D(g_1 g_2) = D(g_1)D(g_2). \tag{9}$$

Using the group theory language, $D(g)$'s form a unitary representation for the SO(3) (3D special orthogonal) rotation group.

Next we discuss the relation between the rotation operator and total angular momentum. In the limit of small rotation angle $\theta \to 0$,

$$D(g(\hat{n},\delta\theta))|\Psi(t)\rangle = |\Psi(t)\rangle + \delta\theta \frac{\partial D(\hat{n},\theta)}{\partial\theta}|_{\theta=0}|\Psi(t)\rangle + ..., \tag{10}$$

thus

$$\langle \Psi(t)|D(g)|\Psi(t)\rangle - \langle \Psi(t)|\Psi(t)\rangle = \delta\theta \langle \Psi(t)| \frac{\partial D(\hat{n},\theta)}{\partial\theta}|_{\theta=0}|\Psi(t)\rangle + ... \tag{11}$$

If the space is isotropic around the axis $\hat{n}$, and if $|\Psi(t)\rangle$ is a state vector, then $D(g)|\Psi(t)\rangle$ is also a valid time-dependent state vector, thus the left-hand-side is independent of time. Then $\langle \Psi(t)| \frac{\partial D(\hat{n},\theta)}{\partial\theta}|_{\theta=0}|\Psi(t)\rangle$ is a conserved quantity associated with rotation around the axis $\vec{n}$. It is also easy to show that $\frac{\partial D(\hat{n},\theta)}{\partial\theta}|_{\theta=0}$ is an anti-Hermitian operator. It should be the angular momentum projection to the axis $\vec{n}$ up to a constant α as

$$\frac{\partial D(\hat{n},\theta)}{\partial\theta}|_{\theta=0} = -\frac{i}{\alpha}\hat{n}\cdot\vec{J}. \tag{12}$$

$\vec{J}$ should be the total angular momentum $\vec{J} = \vec{L} + \vec{S}$. Next we need to determine the constant

α. From $D^\dagger(g)\vec{r}D(g) = g\vec{r}$, we have

$$i\alpha[\hat{n}\cdot\vec{J}, r_i] = \frac{\partial g(\hat{n},\theta)}{\partial\theta}|_{\theta=0,ij} r_j \tag{13}$$

By taking $\vec{n}$ along the z-axis and $r_i = r_x$, we can obtain that $\alpha = \hbar$, and thus

$$D(g(\hat{n},\theta)) = e^{-i\frac{\theta}{\hbar}\hat{n}\cdot\vec{J}} \tag{14}$$

From the Eq. 8 relation $D^\dagger(g)S_iD(g) = g_{ij}S_j$, and take the infinitesimal rotation, we arrive the commutation relation between spin operators

$$[S_i, S_j] = i\varepsilon_{ijk}\hbar S_k. \tag{15}$$

Exercise 2

1. Prove that above statement that $\alpha = \hbar$.
2. Prove Eq. 15.
3. From $D^\dagger(g)L_iD(g) = g_{ij}L_j$, please derive that $[L_i, L_j] = i\varepsilon_{ijk}\hbar L_k$, which is consistent with the direct calculation using the canonical quantization condition.
4. From $D^\dagger(g)p_iD(g) = g_{ij}p_j$, please derive that $[L_i, p_j] = i\varepsilon_{ijk}\hbar p_j$.

3 Pauli matrices for spin-$\frac{1}{2}$ particles

For spin-$\frac{1}{2}$, we can explicitly construct its operators due to its simplicity. The projection of spin along any direction can only take values of $\pm\frac{\hbar}{2}$, thus

$$S_x^2 = S_y^2 = S_z^2 = \frac{1}{4}\hbar^2, \quad S_x^2 + S_y^2 + S_z^2 = \frac{3}{4}\hbar^2. \tag{16}$$

Set $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$, such that $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$ which are all Hermitian matrices. The satisfy the commutation relation

$$\sigma_x\sigma_y - \sigma_y\sigma_x = 2i\sigma_z, \quad \sigma_y\sigma_z - \sigma_z\sigma_y = 2i\sigma_x, \quad \sigma_z\sigma_x - \sigma_x\sigma_z = 2i\sigma_y. \tag{17}$$

A convenient choice of representations of Pauli matrices is

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{18}$$

Pauli matrices have a special properties that other spin matrices do not have, they anti-commute with each other, i.e.,

$$\sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}, \tag{19}$$

and consequently

$$\sigma_i\sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k. \tag{20}$$

Pauli matrices are actually the lowest order Clifford algebra. They are also isomorphic to quaternions (the Hamilton number) following the correspondce of

$$i \leftrightarrow -i\sigma_x \quad j \leftrightarrow -i\sigma_y \quad k \leftrightarrow -i\sigma_z. \tag{21}$$

Exercise 3 1) Prove the anti-commutation relation $\sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}$ which is independent of the concrete representation.

2) Prove that for the rotation operator from the spin part $D_s(n,\theta) = \exp\{-\frac{i}{2}\theta\vec{\sigma}\cdot\vec{n}\}$, it equals to $\cos\frac{\theta}{2} - i(\vec{\sigma}\cdot\vec{n})\sin\frac{\theta}{2}$.

4 Hamiltonian operator for charged particles in the E-M field and gauge invariance

The classic Lagrangian is

$$L(x,\dot{x},t) = \frac{1}{2}m\dot{\vec{r}}^2 + \frac{e}{c}\dot{\vec{r}}\cdot\dot{\vec{A}} - e\phi, \tag{22}$$

the canonical momentum is

$$\vec{P} = \frac{\partial L}{\partial \dot{\vec{q}}} = m\dot{\vec{r}} + \frac{e}{c}\vec{A}. \tag{23}$$

Thus

$$H_c(\vec{r},\vec{P}) = \vec{P}\cdot\dot{\vec{r}} - L = \frac{(\vec{P}-\frac{e}{c}\vec{A})^2}{2m} + e\phi. \tag{24}$$

Quantum mechanically, we replace the canonical momentum $\vec{P}$, rather than the mechanical momentum, with the operator $-i\hbar\frac{\partial}{\partial x}$. Again it is because of the correspondence principle: In classical mechanics, it is the canonical momentum $\vec{P}$ satisfy the Poisson bracket, not the mechanical momentum. Then for the quantum mechanical Hamiltonian, however, what enters the Hamiltonian is the mechanical momentum which is an physical observable. The canonical momentum is not gauge invariant, and thus is not a physical observable.

$$H = \frac{(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}(\vec{r}))^2}{2m} + e\phi(\vec{r}). \tag{25}$$

If we expand the above Hamiltonian, we have

$$H = \frac{-\hbar^2\nabla^2}{2m} - \frac{e}{2mc} i\hbar\vec{\nabla}\cdot(\vec{A} - \frac{e}{2mc}\vec{A}\cdot i\hbar\vec{\nabla} + \frac{e^2}{c^2}\frac{\vec{A}^2(\vec{r})}{2m}. \tag{26}$$

The meaning of the second term in the above equation is that for any wavefunction $\psi(\vec{r})$, its effect is $-\frac{i}{2m}\hbar\vec{\nabla}\cdot\{\vec{A}(\vec{r})\psi(\vec{r})\}$. We often use Column like gauge such that $\vec{\nabla}\cdot\vec{A} = 0$, in this case, Eq. 26 is reduced to

$$H = \frac{-\hbar^2\nabla^2}{2m} - \frac{i\hbar e}{mc}\vec{A}\cdot\vec{\nabla} + \frac{e^2\vec{A}^2(\vec{r})}{2mc^2}. \tag{27}$$

In classic EM, we know that $\vec{A}(\vec{r})$ has gauge redundancy, i.e., for

$$\vec{A}'(\vec{r}) = \vec{A}(\vec{r}) + \nabla f(\vec{r},t), \quad \phi'(\vec{r}) = \phi(\vec{r}) - \frac{1}{c}\frac{\partial}{\partial t} f(\vec{r},t) \tag{28}$$

where $f(\vec{r},t)$ is an arbitrary scale field, $(\vec{A}', \phi')$ and $(\vec{A}, \phi)$ represent the same physical electric and magnetic fields. In classic EM, it is not a problem because the equation of motion can be written by using $\vec{E}$ and $\vec{B}$,

$$\vec{F} = m\frac{d^2\vec{r}}{dt^2} = e\vec{E} + e\frac{\vec{v}}{c}\times\vec{B}. \tag{29}$$

The introduction of $\vec{A}$ and ϕ is just a convenience not essential.

However, in quantum mechanics, the concept of force is ill-defined. We have to either use Hamiltonian, or, Lagrangian, both of which can only be expressed by $\vec{A}$ and ϕ not by $\vec{E}$ and $\vec{B}$. The form of Hamiltonian by using $\vec{A}'$ and ϕ' is written as

$$H' = \frac{(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}'(\vec{r}))^2}{2m} + e\phi'(\vec{r}). \tag{30}$$

A natural question is: Should H' and H give rise to the same physics?

We can prove that for any solution to the equation

$$i\hbar\frac{\partial}{\partial t}\psi(r,t) = H\psi(r,t) \tag{31}$$

with H defined in Eq. 25, we define the a new wavefunction $\psi^{'}(\vec{r},t)$

$$\psi^{'}(\vec{r},t) = e^{\frac{ie}{\hbar c} f(\vec{r},t)} \psi(\vec{r},t) \tag{32}$$

such that it satisfies

$$i\hbar \frac{\partial}{\partial t} \psi^{'}(r,t) = H^{'} \psi^{'}(r,t). \tag{33}$$

Exercise 4 Prove the above statement in Eq. 32 and Eq. 33. Hint: you may need to first verify that

$$(i\hbar \frac{\partial}{\partial t} - e\phi^{'})\psi^{'} = e^{\frac{ie}{\hbar c} f(\vec{r},t)} (i\hbar \frac{\partial}{\partial t} - e\phi)\psi, \tag{34}$$

and you can also find a similar expression with respect to the spatial gradient.