Quantum Physics Exercise Class III

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Requirement: A symmetry transformation does not change possible results of any observation or experiment.

Ray: Normalized kets in Hilbert space $|\Psi\rangle$ and $\xi|\Psi\rangle$ with $|\xi| = 1$ represent the same state of the system. Ray is a collection of all the states $\{\xi|\Psi\rangle\} \equiv \mathcal{R}_\Psi \subset \mathcal{H}$.

The results of an observation experiment are given by states in orthogonal rays $\mathcal{R}_1, \mathcal{R}_2, \cdots$.

Two experiments observing a same thing have two sets $\{\mathcal{R}_n\}$ and $\{\mathcal{R}'_n\}$, but the symmetry requires

$$\mathbb{P}(\mathcal{R} \to \mathcal{R}_n) = \mathbb{P}(\mathcal{R}' \to \mathcal{R}'_n) \tag{1}$$

Wigner shows:

- Such a transformation $\mathcal{R} \to \mathcal{R}'$ can be expressed as an operator $\hat{U}$ in Hilbert space, such that $|\Psi\rangle \in \mathcal{R}$ and $\hat{U}|\Psi\rangle \in \mathcal{R}'$. The operator $\hat{U}$ can be unitary and linear, i.e.,

$$\langle \hat{U}\Phi|\hat{U}\Psi\rangle = \langle \Phi|\Psi\rangle \quad \text{and} \quad \hat{U}(a|\Psi\rangle + b|\Phi\rangle) = a\hat{U}|\Psi\rangle + b\hat{U}|\Phi\rangle \tag{2}$$

or anti–unitary and anti–linear,

$$\langle \hat{U}\Phi|\hat{U}\Psi\rangle = \langle \Phi|\Psi\rangle^* \quad \text{and} \quad \hat{U}(a|\Psi\rangle + b|\Phi\rangle) = a^*\hat{U}|\Psi\rangle + b^*\hat{U}|\Phi\rangle \tag{3}$$

Classification of symmetries:

- Discrete symmetry: Space reflection ($\boldsymbol{r} \to -\boldsymbol{r}$), time reversal ($t \to -t$), point group symmetry (lattice structure), particle exchange, etc.

- Continuous symmetry (expressed by several continuous parameters): Space translation ($\boldsymbol{r} \to \boldsymbol{r} + \boldsymbol{r}_0$), space rotation $\boldsymbol{r} \to \mathrm{R}\boldsymbol{r}$, Lorentz transformation, gauge symmetry, etc.

A type of symmetries form a group. The multiplication of two symmetry operators is still a symmetry operator.

In quantum mechanics, most of the symmetries correspond to unitary linear operators except for the time reversal symmetry. For continuous symmetries, the unitary operators can be expressed with several parameters ε and satisfy

$$\hat{U} = 1 + i\varepsilon t, \tag{4}$$

when ε are small enough.

Displacement operator

- Infinitesimal definition:

$$\hat{D}(\boldsymbol{a}) \equiv 1 - \frac{i}{\hbar}\hat{\boldsymbol{p}} \cdot \boldsymbol{a} + \mathcal{O}(\boldsymbol{a}^2) \tag{5}$$

  with commutation relations $[\hat{p}_i, \hat{p}_j] = 0$.

- Requirement:

$$\hat{D}^\dagger(\boldsymbol{a})\hat{\boldsymbol{x}}\hat{D}(\boldsymbol{a}) = \hat{\boldsymbol{x}} + \boldsymbol{a} \tag{6}$$

  or

$$\hat{D}(\boldsymbol{a})|\boldsymbol{x}\rangle = |\boldsymbol{x} + \boldsymbol{a}\rangle \tag{7}$$

  These lead to $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$.

- Finite form:

$$\hat{D}(\boldsymbol{a}) = e^{-i\hat{\boldsymbol{p}}\cdot\boldsymbol{a}/\hbar} \tag{8}$$

- For the wave function, it recovers the conventional Taylor expansion,

$$\psi(\boldsymbol{x} - \boldsymbol{a}) = e^{-\nabla\cdot\boldsymbol{a}}\psi(\boldsymbol{x}) = \left(1 - \boldsymbol{a}\cdot\nabla + \frac{1}{2}\sum_{ij} a_i a_j \partial_i \partial_j + \cdots\right)\psi(\boldsymbol{x}) \tag{9}$$

Rotation

- Infinitesimal definition:

$$\hat{\mathcal{D}}(\hat{\mathbf{n}}, \theta) \equiv 1 - \frac{i}{\hbar}\theta\hat{\mathbf{n}} \cdot \hat{\boldsymbol{J}} + \mathcal{O}(\theta^2) \tag{10}$$

where $\hat{\mathbf{n}}$ is the rotation axis and θ is the rotation angle. Here, the generators, $\hat{\boldsymbol{J}}$, are the angular momentum operators, satisfying

$$[\hat{J}_i, \hat{J}_j] = i\hbar\epsilon_{ijk}\hat{J}_k \tag{11}$$

- One can simultaneously diagonalize $\hat{J}^2$ and $\hat{J}_z$ as

$$\hat{J}^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle \quad \text{and} \quad \hat{J}_z|j,m\rangle = \hbar m|j,m\rangle \tag{12}$$

with $j = 0, \frac{1}{2}, 1, \cdots$ and $m = -j, -j+1, \cdots, j$. The orthogonal and complete relations are

$$\langle j,m|j',m'\rangle = \delta_{jj'}\delta_{mm'} \quad \text{and} \quad \sum_{j,m}|j,m\rangle\langle j,m| = 1 \tag{13}$$

- Define $\hat{J}_\pm \equiv \hat{J}_x \pm i\hat{J}_y$, and we have

$$\hat{J}_\pm|j,m\rangle = \hbar\sqrt{(j \mp m)(j \pm m + 1)}|j, m \pm 1\rangle \tag{14}$$

- Definition:

$$\hat{\boldsymbol{L}} \equiv \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}} \tag{15}$$

- Commutation relations:

$$[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k \tag{16}$$

- Eigenstates: $|l, m\rangle$ with $l = 0, 1, 2, \cdots$.
- Spherical harmonics: $Y_{l,m}(\theta, \phi) \equiv \langle\theta, \phi|l, m\rangle$, satisfying

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + l(l+1)\right]Y_{l,m}(\theta, \phi) = 0 \tag{17}$$

Relation to classical rotation

- Classical rotation:

$$\boldsymbol{x}' = \mathsf{R}\boldsymbol{x} \tag{18}$$

with R being an orthogonal matrix satisfying $\mathsf{R}^T\mathsf{R} = \mathsf{R}\mathsf{R}^T = \mathsf{I}$ and $\det \mathsf{R} = 1$.

- Parametrize it as

$$\mathsf{R}(\hat{\mathbf{n}}, \theta) = e^{\theta \hat{\mathbf{n}} \cdot \vec{\mathsf{J}}} \tag{19}$$

with

$$(\mathsf{J}_i)_{jk} = -\epsilon_{ijk} \tag{20}$$

- In quantum mechanics,

$$\hat{\mathcal{D}}^\dagger(\hat{\mathbf{n}}, \theta)\hat{\boldsymbol{x}}\hat{\mathcal{D}}(\hat{\mathbf{n}}, \theta) = \mathsf{R}\hat{\boldsymbol{x}} \tag{21}$$

Generalize it: If $\hat{\boldsymbol{V}}$ is a vector operator, it satisfies

$$\hat{\mathcal{D}}^\dagger(\hat{\mathbf{n}}, \theta)\hat{\boldsymbol{V}}\hat{\mathcal{D}}(\hat{\mathbf{n}}, \theta) = \mathsf{R}\hat{\boldsymbol{V}} \tag{22}$$

or equivalently, $[\hat{V}_i, \hat{J}_j] = i\hbar\epsilon_{ijk}\hat{V}_k$. If $\hat{K}$ is a scalar, it satisfies

$$\hat{\mathcal{D}}^\dagger(\hat{\mathbf{n}}, \theta)\hat{K}\hat{\mathcal{D}}(\hat{\mathbf{n}}, \theta) = \hat{K} \tag{23}$$

Spin

- Spin as an internal degree of freedom of particles also satisfies the algebra of angular momentum.
- For spin–$\frac{1}{2}$, $j = \frac{1}{2}$ and we denote

$$\hat{S}_z|\pm\rangle = \pm\frac{\hbar}{2}|\pm\rangle, \quad \hat{S}^2|\pm\rangle = \frac{3}{4}\hbar^2|\pm\rangle \tag{24}$$

- Pauli matrices:

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{25}$$

  with $\hat{S}_i = \frac{\hbar}{2}\hat{\sigma}_i$.
- Properties:

$$[\hat{\sigma}_i, \hat{\sigma}_j] = 2i\epsilon_{ijk}\hat{\sigma}_k, \quad \{\hat{\sigma}_i, \hat{\sigma}_j\} = 2\delta_{ij}, \quad \hat{\sigma}_i\hat{\sigma}_j = \delta_{ij} + i\epsilon_{ijk}\hat{\sigma}_k \tag{26}$$

- The rotation transformation operator can be evaluated as

$$\hat{\mathcal{D}}(\hat{\mathbf{n}}, \theta) = e^{-i\theta\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}/2} = \cos\frac{\theta}{2} - i\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}\sin\frac{\theta}{2} \tag{27}$$

- Pauli matrices together with unit matrix form a basis of 2×2 matrix space, i.e.,

$$\mathbf{A} = a_0\mathbf{I} + \sum_{j=1}^{3} a_j\hat{\sigma}_j, \quad a_0 = \frac{1}{2}\mathrm{Tr}\mathbf{A}, \quad a_j = \frac{1}{2}\mathrm{Tr}(\hat{\sigma}_j\mathbf{A}) \tag{28}$$

- Consider two angular momenta, $\hat{\boldsymbol{J}}_1$ and $\hat{\boldsymbol{J}}_2$. Define their addition as

$$\hat{\boldsymbol{J}} \equiv \hat{\boldsymbol{J}}_1 \otimes 1 + 1 \otimes \hat{\boldsymbol{J}}_2 \tag{29}$$

- Total Hilbert space is expanded via

$$|j_1 j_2; m_1 m_2\rangle \equiv |j_1, m_1\rangle \otimes |j_2, m_2\rangle \tag{30}$$

- On the other hand, we can construct eigenbasis from

$$[\hat{J}^2, \hat{J}_z] = [\hat{J}^2, \hat{J}_1^2] = [\hat{J}^2, \hat{J}_2^2] = 0 \tag{31}$$

as $|j_1 j_2; jm\rangle$. For given j_1 and j_2, we have

$$|j_1 j_2; jm\rangle = \sum_{m_1, m_2} |j_1 j_2; m_1 m_2\rangle\langle j_1 j_2; m_1 m_2 | j_1 j_2; jm\rangle \tag{32}$$

Here $\langle j_1 j_2; m_1 m_2 | j_1 j_2; jm\rangle$ is called Clebsch–Gordan (CG) coefficient.

Addition of angular momenta

- From

$$(m - m_1 - m_2)\langle j_1 j_2; m_1 m_2 | j_1 j_2; jm\rangle = 0 \tag{33}$$

we know CG coefficients vanish unless $m = m_1 + m_2$.

- The maximum of j goes by

$$j_{\max} = m_{\max} = j_1 + j_2 \tag{34}$$

- From the identity

$$(2j_1 + 1)(2j_2 + 1) = \sum_{|j_1 - j_2|}^{j_1 + j_2} (2j + 1) \tag{35}$$

we know $j_{\min} = |j_1 - j_2|$.

- For a scalar operator $\hat{K}$, we have

$$\langle \gamma', j', m' | \hat{K} | \gamma, j, m\rangle \propto \delta_{jj'}\delta_{mm'} \tag{36}$$

- For a vector operator $\hat{\boldsymbol{V}}$,

$$\langle \gamma', j', m' | \hat{V}_q | \gamma, j, m\rangle \propto \langle j1; j'm' | j1; mq\rangle \tag{37}$$

- Hamiltonian:

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m_e} - \frac{Ze^2}{\hat{r}} \tag{38}$$

- Eigenvalues (for boundary states):

$$E_n = -\frac{Z^2}{n^2}\mathcal{R} \tag{39}$$

with $n = 1, 2, \cdots$, $\mathcal{R} = \frac{e^2}{2a_0}$, and $a_0 = \frac{\hbar^2}{m_e e^2}$.

- Eigenstates:

$$\langle \boldsymbol{r}|n, l, m\rangle = R_{n,l}(Zr/a_0)Y_{l,m}(\theta, \phi) \equiv \psi_{n,l,m}(\boldsymbol{r}) \tag{40}$$

with

$$\langle n, l, m|n', l', m'\rangle = \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \sin\theta \mathrm{d}\theta \int_0^{\infty} r^2 \mathrm{d}r\, \psi^*_{n,l,m}(\boldsymbol{r})\psi_{n',l',m'}(\boldsymbol{r}) = \delta_{nn'}\delta_{ll'}\delta_{mm'} \tag{41}$$

- Definition:

$$\hat{\boldsymbol{R}} \equiv -\frac{Ze^2\hat{\boldsymbol{r}}}{\hat{r}} + \frac{1}{2m_e}(\hat{\boldsymbol{p}} \times \hat{\boldsymbol{L}} - \hat{\boldsymbol{L}} \times \hat{\boldsymbol{p}}) \tag{42}$$

- Properties:

$$[\hat{H}, \hat{\boldsymbol{R}}] = 0 \quad \text{and} \quad \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{R}} = \hat{\boldsymbol{R}} \cdot \hat{\boldsymbol{L}} = 0 \tag{43}$$

and

$$\hat{R}^2 = Z^2 e^4 + \frac{2\hat{H}}{m_e}(\hat{L}^2 + \hbar^2) \tag{44}$$

$$[\hat{R}_i, \hat{R}_j] = -\frac{2i}{m_e}\hbar \sum_k \epsilon_{ijk} \hat{H} \hat{L}_k \tag{45}$$

- Define

$$\hat{\boldsymbol{A}}_\pm \equiv \frac{1}{2}\left(\hat{\boldsymbol{L}} \pm \sqrt{\frac{m_e}{-2E}}\hat{\boldsymbol{R}}\right) \tag{46}$$

in the subspace of $E < 0$ with

$$[\hat{A}_{\pm,i}, \hat{A}_{\pm,j}] = i\hbar\epsilon_{ijk}\hat{A}_{\pm,k} \quad \text{and} \quad [\hat{A}_{\pm,i}\hat{A}_{\mp,j}] = 0 \tag{47}$$

and

$$\hat{A}_\pm^2 = \frac{1}{4}\left[\hat{L}^2 + \left(\frac{m_e}{-2E}\right)\hat{R}^2\right] \tag{48}$$

- $\hat{A}_{\pm}^2$ have common eigenvalues, being

$$\hbar^2 a(a+1) \tag{49}$$

with a being any half integer.

- This leads to

$$\begin{aligned} \hbar^2 a(a+1) &= \frac{1}{4}\left[\hat{L}^2 + \left(\frac{m_e}{-2E}\right)\hat{R}^2\right] \\ &= \frac{1}{4}\left[\hat{L}^2 + \left(\frac{m_e}{-2E}\right)Z^2 e^4 - (\hat{L}^2 + \hbar^2)\right] \\ &= \left(\frac{m_e}{-8E}\right)Z^2 e^4 - \frac{\hbar^2}{4} \end{aligned} \tag{50}$$

Thus

$$E = -\frac{Z^2 e^4 m_e}{2\hbar^2(2a+1)^2} \tag{51}$$