B7.3 Further quantum theory lecture 6

Now we are ready to take a look at the structures associated with rotational symmetry in quantum systems. On the basis of our discussion in lecture 5, expect a unitary (projective) representation of the rotation group $SO(3)$ on our Hilbert space.

First let's look at wave-functions, $\mathcal{H} \cong L^2(\mathbb{R}^3)$. We have $SO(3): \mathbb{R}^3 \longrightarrow \mathbb{R}^3$, $\underline{x} \longmapsto R\underline{x}$

R: 3×3 orthogonal matrix.

This induces an action on wave functions: $U: \mathcal{H} \times SO(3) \longrightarrow \mathcal{H}$, $(\Psi, R) \longmapsto \tilde{\Psi}(\underline{x}) = \Psi(R\underline{x})$

This is a unitary operator b/c orthogonal change of variables preserves d^3x measure on $\mathbb{R}^3$. On general grounds, rotation about a given axis should be inf. generated by a self-adjoint operator. Let's find it for the coordinate axes.

$$R_1(\delta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\delta & \sin\delta \\ 0 & -\sin\delta & \cos\delta \end{pmatrix} \qquad R_2(\delta) = \begin{pmatrix} \cos\delta & 0 & -\sin\delta \\ 0 & 1 & 0 \\ \sin\delta & 0 & \cos\delta \end{pmatrix} \qquad R_3(\delta) = \begin{pmatrix} \cos\delta & \sin\delta & 0 \\ -\sin\delta & \cos\delta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\approx \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \delta \\ 0 & -\delta & 0 \end{pmatrix} \qquad \approx \begin{pmatrix} 1 & 0 & -\delta \\ 0 & 1 & 0 \\ \delta & 0 & 1 \end{pmatrix} \qquad \approx \begin{pmatrix} 1 & \delta & 0 \\ -\delta & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

So
$$\left(\mathcal{U}(\underline{e}_1,\delta)\Psi\right)(\underline{x}) = \Psi\left(R_1(\epsilon)\,\underline{x}\right) = \Psi\left(x_1, \cos(\delta)x_2 + \sin(\delta)x_3, -\sin(\delta)x_2 + \cos(\delta)x_3\right)$$
$$\approx \Psi(x_1, x_2 + \delta x_3, x_3 - \delta x_2) \approx \Psi(\underline{x}) + \delta\left(x_3\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_3}\right)\Psi(\underline{x})$$
$$= \Psi(\underline{x}) - \frac{iL_1\epsilon}{\hbar}\Psi(\underline{x}) \quad \text{where } L_1 = i\hbar\left(x_3\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_3}\right) = X_2P_3 - X_3P_2$$

Similarly $L_2 = X_3P_1 - X_1P_3$ and $L_3 = X_1P_2 - X_2P_1$, or $L_i = \sum_{j,k=1}^{3} \epsilon_{ijk} X_j P_k$

or $\underline{L} = \underline{X} \wedge \underline{P}$

These are the "orbital angular momentum" operators from part A. They obey the commutation relations

completely antisymmetric tensor on $\mathbb{R}^3$.

$$[L_i, L_j] = i\hbar \sum_k \epsilon_{ijk} L_k$$

Can compute this directly, but it follows from the structure of the group $SO(3)$! Indeed, writing $R_i(\theta) = \mathbb{1} + \theta\omega_i + O(\theta^2)$, we have

$$(*) \quad [\omega_i, \omega_j] = \sum_k \epsilon_{ijk}\,\omega_k$$

So L_i's obey commutators of $(i\hbar\omega_i)$'s. The algebra $(*)$ is the Lie algebra $so(3)$ associated to the Lie group $SO(3)$.

Def: A representation of angular momentum on $\mathcal{H}$ is a triplet of Hermitian operators $\{J_{1,2,3}\}$ satisfying the "angular momentum commutation relations"

$$[J_i, J_j] = i\hbar \sum_{k=1}^{3} \epsilon_{ijk} J_k$$

So for *any* quantum system with an action of 3d rotations, we should get a representation of angular momentum on $\mathcal{H}$. We are making a standard move from studying Lie group reps to those of the associated Lie algebra.

Def: an irreducible representation (irrep) of the angular momentum operators is a Hilbert space $\mathcal{H}$ w/ self-adjoint $\{J_i\}$ obeying A.M. commutators and such that $\mathcal{H} \neq \mathcal{H}_1 \oplus \mathcal{H}_2$ with $\mathcal{H}_1 \perp \mathcal{H}_2$ and $J_i : \mathcal{H}_{1,2} \to \mathcal{H}_{1,2}$ for $i = 1,2,3$.

(there is no proper subrepresentation).

Most of the time in quantum mechanics, the relevant Hilbert space $\mathcal{H}$ doesn't furnish an irreducible representation of the $\{J_i\}$. However, one can relatively easily show that due to self-adjointness of the L_i, any representation is completely decomposable, i.e.,

$$\mathcal{H} = \bigoplus_{i \in I} \mathcal{H}_i \quad \text{, each } \mathcal{H}_i \text{ irreducible}$$

The structure of possible irreps of the angular momentum operators were considered in part A. Let's refresh how this works:

- Define $J^2 = \underline{J} \cdot \underline{J} = J_1^2 + J_2^2 + J_3^2$. We have $[J_i, J^2] = 0$ so can diagonalize, say, J^2 & J_3. In an irrep, J^2 will act by a constant.
- Define ladder operators $J_\pm = J_1 \pm i J_2$ $\left(J_+ = J_-^*\right)$. These obey $[J_3, J_\pm] = \pm\hbar J_\pm$. Thus, if $J_3|m\rangle = m\hbar|m\rangle$, we have

$$\begin{aligned} J_3 \left(J_\pm|m\rangle\right) &= \left([J_3, J_\pm] + J_\pm J_3\right)|m\rangle \\ &= \pm\hbar J_\pm|m\rangle + m\hbar J_\pm|m\rangle \\ &= (m \pm 1)\hbar J_\pm|m\rangle \end{aligned}$$

  so ladder operators raise & lower J_3 eigenvalue by one (leaving J^2 fixed).
- From positivity of norm, show that in a given irrep w/ $J^2 = \hbar^2 j(j+1)$, the range of J_3 eigenvalues runs from $-j, -j+1, \ldots, j-1, j$ with $j \in \frac{1}{2}\mathbb{Z}_{\geq 0}$. (Exercise!)

One more subtlety: could there be degeneracy at some value of m?

We can compute $J_+J_- = J_1^2 + J_2^2 - i[J_1, J_2] = J^2 - J_3^2 + \hbar J_3$

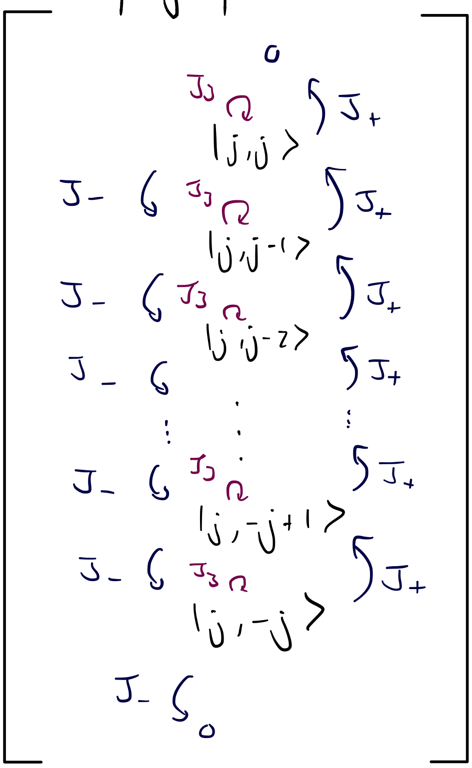
$$J_-J_+ = J_1^2 + J_2^2 + i[J_1, J_2] = J^2 - J_3^2 - \hbar J_3$$

So if Ψ, Φ are orthogonal w/ $J_3|\Psi\rangle = m\hbar|\Psi\rangle$, $J_3|\Phi\rangle = m\hbar|\Phi\rangle$, then acting with $J_\pm$:

$\langle J_\pm \Psi | J_\pm \Phi \rangle = \langle \Psi | J_\mp J_\pm | \Phi \rangle = \hbar^2 (j(j+1) - m(m\pm 1)) \langle \Psi | \Phi \rangle = 0$ and so on.

So this rep^n is reducible; states obtained from $|\Psi\rangle$ all $\perp$ to states obtained from $|\Phi\rangle$.
Thus, general irrep has orthonormal basis $|j, m\rangle$ $m = -j, -j+1, \ldots, j-1, j$.

"spin-j representation"



$$|j, m\pm 1\rangle = \frac{J_\pm |j, m\rangle}{\hbar\sqrt{j(j+1) - m(m\pm 1)}}$$

When we realize these in terms of wave functions in $\mathbb{R}^3$ (or really on S^2), the eigenstates are given by the spherical harmonics

- $L_\pm = i\hbar e^{\pm i\phi}(\cot\theta\, \partial_\phi \pm i\, \partial_\theta)$
- $L_3 = -i\hbar\, \partial_\phi$
- L^2 = spherical Laplacian

$L^2(S^2)$ is infinitely reducible as an A.M. rep^n: $L^2(S^2) \cong \bigoplus_{\ell=0}^{\infty} \mathcal{H}_{\text{spin-}\ell}$, $|\ell, m\rangle \leftrightarrow Y_{\ell,m}(\phi, \theta)$

$$Y_{\ell,m}(\phi,\theta) \sim \underbrace{P_\ell^m}_{\text{Legendre polynomial}}(\cos(\theta))\, \exp(im\phi)$$

$m \in \mathbb{Z}$ for single-valued wave-function.

Spin-1/2: the smallest non-trivial rep. is the $j = 1/2$ "spin-$\frac{1}{2}$" representation. Here $\mathcal{H}_{j=\frac{1}{2}} \cong \mathbb{C}^2$ and we can take

$$J_1 = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_1$$
$$J_2 = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_2$$
$$J_3 = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}\sigma_3$$

$$\left.\begin{matrix} \\ \end{matrix}\right\} \quad J_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad J_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Some observations

- these σ_i (and identity matrix) span 2×2 Hermitian matrices, so these ang. mom. operators are ubiquitous; arise any time there is a 2-state system (qubit).
- can express general rotation in $SO(3)$ as rotation about an axis ($\underline{n}$) by an angle $\theta \in [0, 2\pi)$. Can work out the corresponding action on $\mathbb{C}^2$:

$$U(R(\underline{n},\theta)) = \exp\left(\frac{-i}{\hbar}(\underline{J}\cdot\underline{n})\theta\right) = \exp\left(\frac{-i\theta}{2}\underline{\sigma}\cdot\underline{n}\right)$$
$$= \cos\left(\frac{\theta}{2}\right) \times \mathbb{1}_{2\times 2} + i\sin\left(\frac{\theta}{2}\right)\underline{\sigma}\cdot\underline{n}$$

This is actually the most general matrix in $SU(2)$ $\left(2\times 2 \text{ unitaries w/ } \det = 1\right)$. However, we see a subtlety: as $\theta \to 2\pi$, our matrix approaches minus the identity!

$$U(R(\underline{n}, 2\pi)) = -\mathbb{1}_{2\times 2}$$

Rather, the map is 4π-periodic. What's going on? We have

$$U(R(\underline{n},\pi))\,U(R(\underline{n},\pi)) = -U(R(\underline{n},2\pi))$$
$$= -U(R(\underline{n},0))$$

This is only a projective unitary rep$^{\underline{n}}$ of $SO(3)$. Physicists just say "under rotations, state comes back to itself up to a phase" (really a sign). There's some beautiful mathematics behind this: $SU(2)$ is the "universal cover" of $SO(3)$, a double cover. A thm. of Bargmann (1954) says that projective unitary reps of G are unitary reps of the universal cover of G.

Now we see why half-integer spins can't show up in wave functions. By construction, wave functions are acted upon by the honest rotation group $SO(3)$.

Next week we'll start w/ addition of angular momentum; how to combine multiple ingredients that are acted upon by the same rotation group.