Theoretical Physics II B – Quantum Mechanics

Lecture 14

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28.2.2012

Solutions to previous control questions

13.1 (a) Commutators:

$$\left[\underline{\hat{J}}^2,\, \hat{J}_k\right] = \sum_{i=1}^{3}\left(\hat{J}_i^2\hat{J}_k - \hat{J}_k\hat{J}_i^2\right) = \sum_{i=1,\, i\neq k}^{3}\left(\hat{J}_i^2\hat{J}_k - \hat{J}_k\hat{J}_i^2\right)$$

$$= \sum_{i=1,\, i\neq k}^{3}\left\{\hat{J}_i\left[\hat{J}_i,\, \hat{J}_k\right] + \hat{J}_i\hat{J}_k\hat{J}_i - \hat{J}_k\hat{J}_i\hat{J}_i\right\}$$

$$= \sum_{i=1,\, i\neq k}^{3}\left\{\hat{J}_i\left[\hat{J}_i,\, \hat{J}_k\right] + \left[\hat{J}_i,\, \hat{J}_k\right]\hat{J}_i\right\}$$

$$= \sum_{i,j=1,\, i,j\neq k, i\neq j}^{3} i\hbar\epsilon_{ikj}\left\{\hat{J}_i\hat{J}_j + \hat{J}_j\hat{J}_i\right\} = 0$$

because the Levi-Civita symbol is anti-symmetric under the direct exchange of i and j:

$$\epsilon_{ikj} = -\epsilon_{jki}\,.$$

$$\left[\hat{J}_+,\, \hat{J}_-\right] = \left[\hat{J}_x + i\hat{J}_y,\, \hat{J}_x - i\hat{J}_y\right] = -i\left[\hat{J}_x,\, \hat{J}_y\right] + i\left[\hat{J}_y,\, \hat{J}_x\right] = 2\hbar\hat{J}_z\,.$$

$$\left[\hat{J}_\pm,\, \hat{J}_z\right] = \left[\hat{J}_x \pm i\hat{J}_y,\, \hat{J}_z\right] = -i\hbar\hat{J}_y \mp \hbar\hat{J}_x = \mp\hbar\left(\hat{J}_x \pm \hat{J}_y\right) = \mp\hbar\hat{J}_\pm$$

$$\left[\hat{J}_\pm,\, \underline{\hat{J}}^2\right] = \left[\hat{J}_x,\, \underline{\hat{J}}^2\right] \pm i\left[\hat{J}_y,\, \underline{\hat{J}}^2\right] = 0\,.$$

(b) The solution follows from rearranging the result of

$$\hat{J}_+\hat{J}_- = \hat{J}_x^2 + \hat{J}_y^2 + i\left(\hat{J}_y\hat{J}_x - \hat{J}_x\hat{J}_y\right) = \underline{\hat{J}}^2 - \hat{J}_z^2 + \hbar\hat{J}_z\,.$$

Using that $\hat{J}_- \left|j,\, m\right\rangle = c_{-,jm} \left|j,\, m-1\right\rangle$ we find

$$
\begin{aligned}
\left|c_{-,jm}\right|^2 \langle j,\, m-1|j,\, m-1\rangle &= \left\langle j,\, m-1 \left| \left(\hat{J}_-^\dagger \hat{J}_-\right) \right| j,\, m \right\rangle \\
&= \left\langle j,\, m-1 \left| \left(\hat{J}_+ \hat{J}_-\right) \right| j,\, m \right\rangle = \left\langle j,\, m-1 \left| \left(\underline{\hat{J}}^2 - \hat{J}_z^2 + \hbar \hat{J}_z\right) \right| j,\, m \right\rangle \\
&= \hbar^2 \left[j(j+1) - m(m-1)\right] \langle j,\, m-1|j,\, m-1\rangle
\end{aligned}
$$

and therefore

$$
\left|c_{-,jm}\right|^2 = \hbar^2 \left[j(j+1) - m(m-1)\right] = \hbar^2 (j-m+1)(j+m)\,.
$$

13.2 Express $\hat{L}_{x,y}$ through $\hat{L}_\pm$:

$$\hat{L}_x = \frac{1}{2}\left(\hat{L}_+ + \hat{L}_-\right) \quad \text{and} \quad \hat{L}_y = \frac{1}{2i}\left(\hat{L}_+ - \hat{L}_-\right) .$$

Use the matrix elements of the ladder operators

$$\left\langle l'm' \left| \hat{L}_\pm \right| lm \right\rangle = \hbar\sqrt{(l \mp m)(l \pm m + 1)}\,\delta_{l'l}\delta_{m'\,m\pm 1}$$

to realise that their expectation value vanishes, since in this case we want to have $\left\langle lm \left| \hat{L_\pm} \right| lm \right\rangle$ and thus $m' = m \neq m \pm 1$.

On the other hand,

$$\hat{L}_x^2 = \frac{1}{4}\left(\hat{L}_+^2 + \hat{L}_-^2 + \hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+\right) = \frac{1}{4}\left(\hat{L}_+^2 + \hat{L}_-^2 + 2\hat{\underline{L}}^2 - 2\hat{L}_z^2\right)$$

and similarly

$$\hat{L}_y^2 = -\frac{1}{4}\left(\hat{L}_+^2 + \hat{L}_-^2 - \hat{L}_+\hat{L}_- - \hat{L}_-\hat{L}_+\right) = -\frac{1}{4}\left(\hat{L}_+^2 + \hat{L}_-^2 - 2\hat{\underline{L}}^2 + 2\hat{L}_z^2\right)$$

yields

$$\left\langle lm \left| \hat{L^2_{x,y}} \right| lm \right\rangle = \frac{1}{2}\left\langle lm \left| \left(\hat{\underline{L}}^2 - \hat{L}_z^2\right) \right| lm \right\rangle = \hbar^2 \frac{l(l+1) - m^2}{2} \, .$$

Reminder: Commutation relations etc.

- Remember the commutation relations

$$\left[\hat{J}_i,\, \hat{J}_j\right] = i\hbar\epsilon_{ijk}\hat{J}_k \;, \quad \left[\underline{\hat{J}}^2,\, \hat{J}_k\right] = 0$$

and the ladder operators $\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$ with

$$\left[\hat{J}_+,\, \hat{J}_-\right] = 2\hbar\hat{J}_z \;, \quad \left[\hat{J}_z,\, \hat{J}_\pm\right] = \pm\hbar\hat{J}_\pm \quad \text{and} \quad \left[\underline{\hat{J}}^2,\, \hat{J}_\pm\right] = 0\,.$$

- Eigenvalues and eigenkets read

$$\underline{\hat{J}}^2 \left|jm\right\rangle = j(j+1)\hbar^2 \left|jm\right\rangle \quad \text{and} \quad \hat{J}_z \left|jm\right\rangle = m\hbar \left|jm\right\rangle \;.$$

- j and m are non-negative are integers or half-integers, and

$$m \in \{-j,\, -j+1,\, -j+2,\, \ldots,\, j-1,\, j\}\,.$$

Matrix elements of angular momentum operators

- The eigenkets $|jm\rangle$ form an orthonormal base: $\langle j'm'|jm\rangle = \delta_{jj'}\delta_{mm'}$
- Operator sandwiches:

$$\left\langle j'm'\left|\hat{\underline{J}}^2\right|jm\right\rangle = j(j+1)\hbar^2\delta_{jj'}\delta_{mm'} \quad \text{and} \quad \left\langle j'm'\left|\hat{\underline{J}}^2\right|jm\right\rangle = m\hbar\delta_{jj'}\delta_{mm'}$$

- Action of ladder operators:

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

Angular momentum operators for spin-$\frac{1}{2}$

- Eigenvalue j also called the **spin**.
- Angular momentum operators for $j = \frac{1}{2}$ proportional to Pauli's:

$$\hat{J}_i \quad \stackrel{j=\frac{1}{2}}{\longrightarrow} \quad \frac{\hbar}{2}\hat{\sigma}_i\,,$$

with

$$\hat{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\,, \quad \hat{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\,, \quad \hat{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\,.$$

- Easy to check: $\hat{S}_i$ have same algebra as $\hat{J}_i$.
- Additional identities for $\hat{\sigma}_i$:

$$\begin{aligned} [\hat{\sigma}_i,\,\hat{\sigma}_j] &= 2i\epsilon_{ijk}\hat{\sigma}_k\,, \quad \{\hat{\sigma}_i,\,\hat{\sigma}_j\} = 2\delta_{ij}\hat{\mathbf{1}}\,, \quad \hat{\sigma}_i^\dagger = \hat{\sigma}_i\,, \\ \sigma_i^2 &= \hat{\mathbf{1}}\,, \quad \det(\hat{\sigma}_i) = -1\,, \quad \mathrm{Tr}(\hat{\sigma}_i) = 0\,. \end{aligned}$$

Finite rotations for spin-$\frac{1}{2}$

- Consider now a two-component ket $|\alpha\rangle$ to be rotated by rotation $\mathcal{R}$ (around z-axis by ϕ), of course generated by $\hat{S}_z$:

$$|\alpha\rangle \quad \xrightarrow{\mathcal{R}} \quad |\alpha'\rangle = \hat{R}_z^{(\frac{1}{2})}(\phi)\,|\alpha\rangle = \exp\left(-\frac{i\hat{S}_z\phi}{\hbar}\right)|\alpha\rangle$$

- Check for rotation: Calculate $\langle\hat{S}_x\rangle_{|\alpha\rangle}$ before and after rotation.

$$\begin{aligned}\left\langle\alpha'\left|\hat{S}_x\right|\alpha'\right\rangle &= \left\langle\alpha\left|\exp\left(\frac{i\hat{S}_z\phi}{\hbar}\right)\hat{S}_x\exp\left(-\frac{i\hat{S}_z\phi}{\hbar}\right)\right|\alpha\right\rangle\\ &= \left\langle\alpha\left|\hat{S}_x\right|\alpha\right\rangle\cos\phi - \left\langle\alpha\left|\hat{S}_y\right|\alpha\right\rangle\sin\phi\,.\end{aligned}$$

(To see this use the identity for $\exp(\hat{L})\hat{M}\exp(-\hat{L})$ from lecture 4.)

Rotating the kets in spin-$\frac{1}{2}$ representation

- When applied on expectation values, the rotations generated by the angular momentum matrices deliver the correct behaviour.
- Now let's see what happens when acting on a ket alone. Decompose $|\alpha\rangle$ into the two eigenkets of $\hat{S}_z$, $|\uparrow\rangle$ and $|\downarrow\rangle$:

$$|\alpha\rangle = \alpha_\uparrow |\uparrow\rangle + \alpha_\downarrow |\downarrow\rangle\ .$$

- Be ready for a surprise! Rotate by 2π:

$$\begin{aligned} |\alpha'\rangle &= \exp\left(-\frac{2i\pi\hat{S}_z}{\hbar}\right)|\alpha\rangle = \exp\left(-i\pi\hat{\sigma}_z\right)|\alpha\rangle \\ &= \exp(-i\pi)\alpha_\uparrow|\uparrow\rangle + \exp(i\pi)\alpha_\downarrow|\downarrow\rangle = -\alpha_\uparrow|\uparrow\rangle - \alpha_\downarrow|\downarrow\rangle = -|\alpha\rangle\ . \end{aligned}$$

- A rotation by 2π is just half the way around - for a full rotation of a ket one needs to rotate by 4π.

General rotations for spin-$\frac{1}{2}$

- In general, rotations can be characterised by a rotation axis $\underline{n}$ ($\underline{n}^2 = 1$) and an angle ϕ.
  Therefore the rotation operator in the spin-$\frac{1}{2}$ representation reads

$$\hat{R}^{(\frac{1}{2})}(\underline{n},\,\phi) \equiv \hat{R}^{(\frac{1}{2})}(\underline{\phi}) = \exp\left(-\frac{i\underline{\hat{\sigma}}\cdot\underline{n}\phi}{2}\right)$$

- In general,

$$\underline{\hat{\sigma}}\cdot\underline{a} = \left(\begin{array}{cc} a_3 & a_1 - ia_2 \\ a_1 + ia_2 & -a_3 \end{array}\right) \quad \text{and} \quad (\underline{\hat{\sigma}}\cdot\underline{a})^2 = |\underline{a}|^2$$

- Therefore

$$\exp\left(-\frac{i\underline{\hat{\sigma}}\cdot\underline{n}\phi}{2}\right) = \hat{\mathbf{1}}\cos\left(\frac{\phi}{2}\right) - i\underline{\hat{\sigma}}\cdot\underline{n}\sin\left(\frac{\phi}{2}\right)\,.$$

Euler rotations

- From classical meachnics: General rotations of a rigid body can be accomplished in three steps, a.k.a. **Euler rotations**.
  They are characterised by three angles α, β, and γ around three axes (z, y, and z-axis):

$$\begin{array}{rcccl} & \mathcal{R}(\underline{n},\,\phi) & = \mathcal{R}(\alpha,\,\beta,\,\gamma) & = & \mathcal{R}_z(\alpha)\mathcal{R}_y(\beta)\mathcal{R}_z(\gamma) \\ \longrightarrow & \hat{R}(\mathcal{R}) & = \hat{R}(\alpha,\,\beta,\,\gamma) & = & \hat{R}_z(\alpha)\hat{R}_y(\beta)\hat{R}_z(\gamma) \end{array}$$

- Because $\left[\hat{\underline{J}},\,\hat{J}_i\right] = 0$

$$\hat{\underline{J}}^2\,\hat{R}(\mathcal{R})\,|jm\rangle \;=\; \hat{R}\,\hat{\underline{J}}^2(\mathcal{R})\,|jm\rangle \;=\; j(j+1)\hbar^2\,\hat{R}(\mathcal{R})\,|jm\rangle\;.$$

  This means that **under rotations the j values are constant**.
- Thus: Only need j-representations of the $\hat{J}_i$.

Matrix elements of rotation operators

- This implies that it makes sense to characterise the rotation operators through matrix elements $\hat{R}^{(j)}_{m'm}(\mathcal{R})$:

$$\hat{R}^{(j)}_{m'm}(\mathcal{R}) = \left\langle jm' \left| \exp\left(-\frac{i\underline{\hat{J}}\cdot\underline{n}\phi}{\hbar}\right) \right| jm \right\rangle$$

In other words the rotation matrix is given by the individual amplitudes for a rotated state to be in state $|jm'\rangle$ when the original state was $|jm\rangle$:

$$\hat{R}(\mathcal{R})\,|jm\rangle = \sum_{m'} |jm'\rangle \left\langle jm' \left| \hat{R} \right| jm \right\rangle \,.$$

Properties

- Composition and inverse:

$$\begin{aligned}
\sum_{m'} \hat{R}^{(j)}_{m'm}(\mathcal{R}_1)\hat{R}^{(j)}_{m'm''}(\mathcal{R}_2) &= \hat{R}^{(j)}_{mm''}(\mathcal{R}_1 \times \mathcal{R}_2) \\
\hat{R}^{(j)}_{m'm}(\mathcal{R}^{-1}) &= \hat{R}^{(j)*}_{mm'}(\mathcal{R})\,.
\end{aligned}$$

  The $\hat{R}$ operators are unitary, since the $\hat{J}_i$ are Hermitian.

- Realize that the $|jm\rangle$ are eigenstates of $\hat{J}_z$:

$$\begin{aligned}
&\hat{R}^{(j)}_{m'm}(\alpha,\,\beta,\,\gamma) \\
&= \left\langle jm' \left| \exp\left(-\frac{i\hat{J}_z\alpha}{\hbar}\right) \exp\left(-\frac{i\hat{J}_y\beta}{\hbar}\right) \exp\left(-\frac{i\hat{J}_z\gamma}{\hbar}\right) \right| jm \right\rangle \\
&= \exp\left[-i(m'\alpha + m\gamma)\right] \left\langle jm' \left| \exp\left(-\frac{i\hat{J}_y\beta}{\hbar}\right) \right| jm \right\rangle
\end{aligned}$$

Euler rotations for spin-$\frac{1}{2}$ systems

- For spin-$\frac{1}{2}$ systems therefore

$$
\begin{aligned}
\hat{R}^{(\frac{1}{2})}(\alpha,\,\beta,\,\gamma) &= \exp\left(-\frac{i\hat{\sigma}_3\alpha}{2}\right)\exp\left(-\frac{i\hat{\sigma}_2\beta}{2}\right)\exp\left(-\frac{i\hat{\sigma}_3\gamma}{2}\right)\\
&= \begin{pmatrix} \exp\left[-\frac{i(\alpha+\gamma)}{2}\right]\cos\frac{\beta}{2} & -\exp\left[-\frac{i(\alpha-\gamma)}{2}\right]\sin\frac{\beta}{2} \\ \exp\left[\frac{i(\alpha-\gamma)}{2}\right]\sin\frac{\beta}{2} & \exp\left[\frac{i(\alpha+\gamma)}{2}\right]\cos\frac{\beta}{2} \end{pmatrix}
\end{aligned}
$$

- This is a unimodular unitary operator (more in homework question).
- The reduced matrix elements read:

$$
\left\langle \frac{1}{2} m' \left| \exp\left(-\frac{i\hat{J}_y\beta}{\hbar}\right) \right| \frac{1}{2} m \right\rangle = \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}
$$

Euler rotations for spin-1 systems

- Missing ingredient: spin-1 representation of $\hat{J}_y$.
- From the identity $\hat{J}_y = \frac{\hat{J}_+ - \hat{J}_-}{2i}$ and the form of the ladder operators:

$$\left(\hat{J}_y^{(j=1)}\right)_{m'm} = \frac{i\hbar}{\sqrt{2}}\left[\delta_{m'(m-1)} - \delta_{m'(m+1)}\right] = \frac{i\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

Therefore,

$$\left\langle 1m' \middle| \exp\left(-\frac{i\hat{J}_y\beta}{\hbar}\right) \middle| 1m \right\rangle = \begin{pmatrix} \frac{1}{2}(1+\cos\beta) & -\frac{1}{\sqrt{2}}\sin\beta & \frac{1}{2}(1-\cos\beta) \\ \frac{1}{\sqrt{2}}\sin\beta & \cos\beta & -\frac{1}{\sqrt{2}}\sin\beta \\ \frac{1}{2}(1-\cos\beta) & \frac{1}{\sqrt{2}}\sin\beta & \frac{1}{2}(1+\cos\beta) \end{pmatrix}$$

Learning outcomes

- Finite rotations and Euler angles
- Matrix representation of finite rotations through angular momentum operators: unitary matrices.
- Rotations do not change spin j.
- Effective form for evaluating them:

$$\hat{R}^{(j)}_{m'm}(\alpha,\,\beta,\,\gamma) = \exp\left[-i(m'\alpha + m\gamma)\right]\left\langle jm'\left|\exp\left(-\frac{i\hat{J}_y\beta}{\hbar}\right)\right|jm\right\rangle$$

- How to construct representations for spin $\frac{1}{2}$ and spin 1.

Control questions

14.1 Some algebra.

(a) Check that the following relations hold true:

$$
\begin{aligned}
(\hat{\underline{\sigma}} \cdot \underline{a})(\hat{\underline{\sigma}} \cdot \underline{b}) &= \underline{a} \cdot \underline{b}\,\hat{\mathbf{1}} + i\hat{\underline{\sigma}} \cdot (\underline{a} \times \underline{b}) \\
(\hat{\underline{\sigma}} \cdot \underline{a})^2 &= |\underline{a}|^2\,\hat{\mathbf{1}} \\
\exp\left(-\frac{i\hat{\underline{\sigma}} \cdot \underline{n}\phi}{2}\right) &= \hat{\mathbf{1}}\cos\left(\frac{\phi}{2}\right) - i\hat{\underline{\sigma}} \cdot \underline{n}\sin\left(\frac{\phi}{2}\right) \quad \text{for} \;\; |\underline{n}|^2 = 1\,.
\end{aligned}
$$

(b) A 2×2 matrix is called unimodular, if it can be written as

$$
\begin{pmatrix} a & b \\ -b^* & a* \end{pmatrix} \quad \text{with} \;\; |a|^2 + |b|^2 = 1\,.
$$

Show that

$$
\hat{U} = [a_0 + i\hat{\underline{\sigma}} \cdot \underline{a}]\,[a_0 - i\hat{\underline{\sigma}} \cdot \underline{a}]^{-1}
$$

with real numbers a_0 and $\underline{a} = (a_1,\, a_2,\, a_3)$ forms an unitary unimodular matrix.

14.2 $j = 1$ representations.

(a) Explicitly write the 3×3 matrix for $\left\langle (j=1)m' \left| \hat{J}_y \right| (j=1)m \right\rangle$.

(b) By explicitly calculating powers of $\hat{J}_y^{(j=1)}$, show that

$$\exp\left(-\frac{i\hat{J}_y^{(j=1)}\beta}{\hbar}\right) = \hat{\mathbf{1}} - i\frac{\hat{J}_y^{(j=1)}}{\hbar}\sin\beta - \left(\frac{\hat{J}_y^{(j=1)}}{\hbar}\right)^2 (1-\cos\beta)\,.$$

(c) Use the findings of (a) and (b) to prove that

$$\left\langle 1m' \left| \exp\left(-\frac{i\hat{J}_y\beta}{\hbar}\right) \right| 1m \right\rangle = \begin{pmatrix} \frac{1}{2}(1+\cos\beta) & -\frac{1}{\sqrt{2}}\sin\beta & \frac{1}{2}(1-\cos\beta) \\ \frac{1}{\sqrt{2}}\sin\beta & \cos\beta & -\frac{1}{\sqrt{2}}\sin\beta \\ \frac{1}{2}(1-\cos\beta) & \frac{1}{\sqrt{2}}\sin\beta & \frac{1}{2}(1+\cos\beta) \end{pmatrix}$$