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Quantum Mechanics

Lecture 6

AM matrices: spin 1/2 example;
Reduction of the two-body problem;
Angular momentum revisited;
Commutation relations;
Simultaneous eigenstates.

A quick recap

Angular momentum eigenstates satisfy:

$$J^2 |j, m\rangle = j(j+1)\hbar^2 |j, m\rangle \qquad J_z |j, m\rangle = m\hbar |j, m\rangle$$

The eigenvalues are constrained:

Allowed values for j are: $j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$

$2j$+1 total states: $m = j, j-1, j-2, \ldots, -j$

The matrix elements of the raising and lowering operators are:

$$\langle j, m' | J_\pm | j, m\rangle = \sqrt{j(j+1) - m(m \pm 1)}\,\hbar\delta_{m', m\pm1}$$

Example: spin 1/2

Let's derive the spin operators for a spin-1/2 system using these formulas.

Recall: $\langle j, m' | J_\pm | j, m \rangle = \sqrt{j(j+1) - m(m \pm 1)}\hbar \delta_{m', m\pm 1}$

Set $j = 1/2$.

$$\left\langle \frac{1}{2}, m' \middle| J_\pm \middle| \frac{1}{2}, m \right\rangle = \sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right) - m(m \pm 1)}\hbar \delta_{m', m\pm 1} = \sqrt{\frac{3}{4} - m(m \pm 1)}\hbar \delta_{m', m\pm 1}$$

Now m = +1/2 or -1/2 only.

$$J_\pm = \begin{bmatrix} \left\langle \frac{1}{2}, \frac{1}{2} \middle| J_\pm \middle| \frac{1}{2}, \frac{1}{2} \right\rangle & \left\langle \frac{1}{2}, \frac{1}{2} \middle| J_\pm \middle| \frac{1}{2}, -\frac{1}{2} \right\rangle \\ \left\langle \frac{1}{2}, -\frac{1}{2} \middle| J_\pm \middle| \frac{1}{2}, \frac{1}{2} \right\rangle & \left\langle \frac{1}{2}, -\frac{1}{2} \middle| J_\pm \middle| \frac{1}{2}, -\frac{1}{2} \right\rangle \end{bmatrix} = \begin{bmatrix} 0 & \left\langle \frac{1}{2}, \frac{1}{2} \middle| J_\pm \middle| \frac{1}{2}, -\frac{1}{2} \right\rangle \\ \left\langle \frac{1}{2}, -\frac{1}{2} \middle| J_\pm \middle| \frac{1}{2}, \frac{1}{2} \right\rangle & 0 \end{bmatrix}$$

Example: spin 1/2

Let's derive the spin operators for a spin-1/2 system using these formulas.

Recall: $\left\langle \frac{1}{2}, m' \middle| J_\pm \middle| \frac{1}{2}, m \right\rangle = \sqrt{\frac{3}{4} - m(m \pm 1)}\,\hbar\,\delta_{m',m\pm1}$

We also have: $J_+\left|\frac{1}{2},\frac{1}{2}\right\rangle = 0$ and $J_-\left|\frac{1}{2},-\frac{1}{2}\right\rangle = 0$ therefore:

$$J_+ = \begin{bmatrix} 0 & \left\langle \frac{1}{2},\frac{1}{2} \middle| J_+ \middle| \frac{1}{2},-\frac{1}{2} \right\rangle \\ 0 & 0 \end{bmatrix}$$

$$\left\langle \frac{1}{2},\frac{1}{2} \middle| J_+ \middle| \frac{1}{2},-\frac{1}{2} \right\rangle = \sqrt{\frac{3}{4} - \left(-\frac{1}{2}\right)\left(-\frac{1}{2}+1\right)}\,\hbar = \hbar$$

therefore: $J_+ = \hbar \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$ and $J_- = J_+^\dagger = \hbar \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$

Example: spin 1/2

Let's derive the spin operators for a spin-1/2 system using these formulas.

Recall: $J_\pm = J_x \pm iJ_y$

$$\frac{1}{2}(J_+ + J_-) = J_x \qquad \frac{1}{2}(J_+ - J_-) = iJ_y$$

$$J_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad iJ_y = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \Rightarrow J_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad J_z = \frac{1}{i\hbar}[J_x, J_y] = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

These formulas exactly recover the Pauli spin matrices in the z-basis!

$$\left|\frac{1}{2},\frac{1}{2}\right\rangle = |\uparrow\rangle = |\mathbf{z}_+\rangle \quad \text{and} \quad \left|\frac{1}{2},-\frac{1}{2}\right\rangle = |\downarrow\rangle = |\mathbf{z}_-\rangle$$

Also notice that total AM is:

$$|J| = \sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right)}\hbar = \frac{\sqrt{3}}{2}\hbar$$

Two-body Hamiltonian with interaction

Consider a Hamiltonian with two interacting particles that are otherwise free:

$$H = \frac{\hat{\mathbf{p}}_1^2}{2m_1} + \frac{\hat{\mathbf{p}}_2^2}{2m_2} + V(|\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2|)$$

Position ket in 3D: $|\mathbf{r}\rangle = |x, y, z\rangle$

Total state space: $|\mathbf{r}_1, \mathbf{r}_2\rangle = |\mathbf{r}_1\rangle \otimes |\mathbf{r}_2\rangle$

Total linear momentum: $\hat{\mathbf{p}}_1^2 = \hat{p}_{1x}^2 + \hat{p}_{1y}^2 + \hat{p}_{1z}^2$

The potential energy depends only on the **distance** between the particles.

Transform to center-of-mass and relative coordinates:

$$\hat{\mathbf{P}} := \hat{\mathbf{p}}_1 + \hat{\mathbf{p}}_2$$

Total linear momentum.

$$M := m_1 + m_2$$

Total mass.

$$\hat{\mathbf{R}} := \frac{m_1}{M}\hat{\mathbf{r}}_1 + \frac{m_2}{M}\hat{\mathbf{r}}_2$$

Center-of-mass position

$$\hat{\mathbf{p}} := \frac{m_2}{M}\hat{\mathbf{p}}_1 - \frac{m_1}{M}\hat{\mathbf{p}}_2$$

Relative linear momentum.

$$\mu := \frac{m_1 m_2}{m_1 + m_2}$$

Reduced mass.

$$\hat{\mathbf{r}} := \hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2$$

Relative position.

Reduced Hamiltonian

Rewrite the Hamiltonian in the new coordinates:

$$H = \frac{\hat{\mathbf{P}}^2}{2M} + \frac{\hat{\mathbf{p}}^2}{2\mu} + V(|\hat{\mathbf{r}}|)$$

Energy eigenstates can be labeled by total momentum P:

$$[\hat{\mathbf{P}}, \hat{\mathbf{r}}] = [\hat{\mathbf{p}}_1 + \hat{\mathbf{p}}_2, \hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2] = 0$$

We can always choose a co-moving frame so that:

$$P = 0 \quad \Rightarrow \quad H = \frac{\hat{\mathbf{p}}^2}{2\mu} + V(|\hat{\mathbf{r}}|)$$

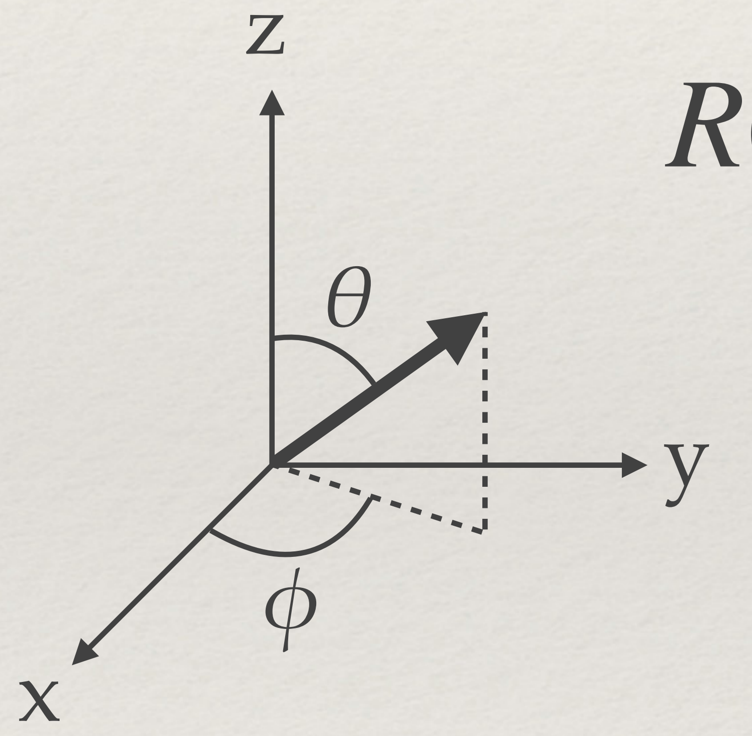
We have reduced the problem to a single-particle problem.

Angular momentum operator revisited

The new Hamiltonian is radially symmetric, so we expect AM conservation.

$$H = \frac{\hat{\mathbf{p}}^2}{2\mu} + V(|\hat{\mathbf{r}}|)$$

To show this, consider an AM operator L_z and it's associated rotation operator:



Spherical coordinates

$$\begin{aligned} R(\mathrm{d}\phi\mathbf{e_z})\,|\,x, y, z\rangle &= |\,x - y\,\mathrm{d}\phi, y + x\,\mathrm{d}\phi, z\rangle \\ &= \left(1 - \frac{i}{\hbar}\hat{p}_x(-y\mathrm{d}\phi)\right)\left(1 - \frac{i}{\hbar}\hat{p}_y(x\mathrm{d}\phi)\right)|\,x, y, z\rangle \\ &= \left(1 - \frac{i}{\hbar}(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x)\mathrm{d}\phi\right)|\,x, y, z\rangle \end{aligned}$$

To first order in $\mathrm{d}\phi$.

$$R(\mathrm{d}\phi\mathbf{e_z}) = 1 - \frac{i}{\hbar}L_z\mathrm{d}\phi = 1 - \frac{i}{\hbar}(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x)\mathrm{d}\phi \quad \Rightarrow \quad L_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

Obtain L_x and L_y by cyclic symmetry.

Commutation relations

Repeating the argument with cyclic symmetry, we conclude that:

$$\mathbf{L} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$$

This implies commutation relations with position and momentum:

$$\begin{aligned}[L_z, \hat{p}_x] &= [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{p}_x] \\ &= [\hat{x}\hat{p}_y, \hat{p}_x] \\ &= [\hat{x}, \hat{p}_x]\hat{p}_y \\ &= i\hbar\hat{p}_y\end{aligned}$$

$$\begin{aligned}[L_z, \hat{p}_y] &= [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{p}_y] \\ &= -[\hat{y}\hat{p}_x, \hat{p}_y] \\ &= -[\hat{y}, \hat{p}_y]\hat{p}_x \\ &= -i\hbar\hat{p}_x\end{aligned}$$

$$\begin{aligned}[L_z, \hat{p}_z] &= [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{p}_z] \\ &= 0\end{aligned}$$

$$\begin{aligned}[L_z, \hat{\mathbf{p}}^2] &= [L_z, \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2] \\ &= \hat{p}_x[L_z, \hat{p}_x] + [L_z, \hat{p}_x]\hat{p}_x + \hat{p}_y[L_z, \hat{p}_y] + [L_z, \hat{p}_y]\hat{p}_y + [L_z, \hat{p}_z^2] \\ &= 2i\hbar\hat{p}_x\hat{p}_y - 2i\hbar\hat{p}_x\hat{p}_y = 0\end{aligned}$$

Commutation relations

Repeating the argument with cyclic symmetry, we conclude that:

$$\mathbf{L} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$$

This implies commutation relations with position and momentum:

$$\begin{aligned}[L_z, \hat{x}] &= [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{x}] \\ &= -\hat{y}[\hat{p}_x, \hat{x}] \\ &= i\hbar\hat{y}\end{aligned}$$

$$\begin{aligned}[L_z, \hat{y}] &= [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{y}] \\ &= \hat{x}[\hat{p}_y, \hat{y}] \\ &= -i\hbar\hat{x}\end{aligned}$$

$$\begin{aligned}[L_z, \hat{z}] &= [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{z}] \\ &= 0\end{aligned}$$

$$\begin{aligned}[L_z, \hat{\mathbf{r}}^2] &= [L_z, \hat{x}^2 + \hat{y}^2 + \hat{z}^2] \\ &= \hat{x}[L_z, \hat{x}] + [L_z, \hat{x}]\hat{x} + \hat{y}[L_z, \hat{y}] + [L_z, \hat{y}]\hat{y} + [L_z, \hat{z}^2] \\ &= 2i\hbar\hat{x}\hat{y} - 2i\hbar\hat{x}\hat{y} = 0\end{aligned}$$

Note: $[\hat{\mathbf{r}}^2, |\hat{\mathbf{r}}|] = 0$

The Hamiltonian conserves AM

We have established that the Hamiltonian conserves angular momentum:

$$H = \frac{\hat{\mathbf{p}}^2}{2\mu} + V(|\hat{\mathbf{r}}|)$$

$$[L_z, \hat{\mathbf{p}}^2] = [L_z, \hat{\mathbf{r}}^2] = 0 \quad \Rightarrow \quad [L_z, H] = 0$$

$$[L^2, \hat{\mathbf{p}}^2] = [L_z, \hat{\mathbf{r}}^2] = 0 \quad \Rightarrow \quad [L^2, H] = 0$$

There is nothing special about the z direction… the same is true for x and y!
But L_z does not commute with L_x or L_y, so we can only choose one simultaneous symmetry.

Simultaneous eigenstates

The rotational symmetry establishes the following commutations relations:

$$H = \frac{\hat{\mathbf{p}}^2}{2\mu} + V(|\hat{\mathbf{r}}|) \qquad [L_z, H] = [L^2, H] = [L_z, L^2] = 0$$

Therefore, a simultaneous eigenbasis exists for all three of H, L^2, L_z:

$$H|E,l,m\rangle = E|E,l,m\rangle$$
$$L^2|E,l,m\rangle = l(l+1)\hbar^2|E,l,m\rangle$$
$$L_z|E,l,m\rangle = m\hbar|E,l,m\rangle$$

Next lecture, we will see how this allows us to decouple the angular and radial parts of the wave function and solve the Schrödinger equation separately for each part.