Theoretical Physics II B – Quantum Mechanics

Lecture 16

Frank Krauss

7.3.2012

Solutions to previous control questions

15.1 To see how this works, consider first the commutation relations

$$\left[\hat{L}_k,\, \hat{x}_l\right] = \left[\sum_{ij} \epsilon_{ijk}\hat{x}_i\hat{p}_j,\, \hat{x}_l\right] = \sum_{ij} \epsilon_{ijk}\left[\hat{x}_i\hat{p}_j,\, \hat{x}_l\right]$$
$$= \sum_{ij} \epsilon_{ijk}\left(\hat{x}_i\left[\hat{p}_j,\, \hat{x}_l\right] + \left[\hat{x}_i,\, \hat{x}_l\right]\hat{p}_j\right) = -i\hbar\sum_{ij}\epsilon_{ijk}\delta_{jl}\hat{x}_i = i\hbar\sum_i \epsilon_{ikl}\hat{x}_i\,.$$

(a) This implies that

$$\begin{aligned}
\left[\hat{L}_3,\, \hat{x}_3\right] &= 0 \\
\left[\hat{L}_3,\, \hat{x}_{1,2}\right] &= \pm i\hbar\hat{x}_{2,1} \quad\longrightarrow\quad \left[\hat{L}_3,\, \mp\frac{1}{\sqrt{2}}\left(\hat{x}_1 \pm i\hat{x}_2\right)\right] = \frac{\hbar}{2}\left(\hat{x}_1 \pm i\hat{x}_2\right) \\
\left[\hat{L}_{1,2},\, \hat{x}_3\right] &= \mp i\hbar\hat{x}_{2,1} \quad\longrightarrow\quad \left[\hat{L}_1 \pm i\hat{L}_2,\, \hat{x}_3\right] = \mp\hbar\left(\hat{x}_1 \pm i\hat{x}_2\right)\,,
\end{aligned}$$

as demanded, identifying $\hat{R}_{\pm 1} = \frac{1}{\sqrt{2}}\left(\hat{x}_1 \pm i\hat{x}_2\right)$ and $\hat{L}_\pm = \hat{L}_1 \pm i\hat{L}_2$.

Solutions to previous control questions

(b) Use the results above to write

$$\left[\hat{L}_j,\, \hat{\underline{R}}^2\right] = \left[\hat{L}_j,\, \sum_k \hat{x}_k\hat{x}_k\right] = \sum_k \left[\hat{L}_j,\, \hat{x}_k\hat{x}_k\right]$$

$$= \sum_k \left(\hat{x}_k \left[\hat{L}_j,\, \hat{x}_k\right] + \left[\hat{L}_j,\, \hat{x}_k\right]\hat{x}_k\right) = i\hbar \sum_{k,i} \epsilon_{ijk} \left(\hat{x}_k\hat{x}_i + \hat{x}_i\hat{x}_k\right) = 0\,,$$

because we multiply the antisymmetric Levi-Civita tensor ϵ_{ijk} with the symmetric operator product $(\hat{x}_k\hat{x}_i + \hat{x}_i\hat{x}_k)$.

Note: Similar equations can be shown to hold true for corresponding commutators with the components of the momentum operator, i.e.

$$\left[\hat{L}_i,\, \hat{p}_j\right] = i\hbar \sum_k \epsilon_{ijk}\hat{p}_k \quad \text{and} \quad \left[\hat{L}_i,\, \hat{\underline{p}}^2\right] = 0\,.$$

This renders the position and the momentum operators components of a *vector operator*, i.e. of an operator that transforms like an "ordinary vector" under rotations. Clearly, we would have suspected that anyway, but this was the proof.

15.2 Check the first two identities by writing the orbital angular momentum operators as, e.g., $\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$. To apply them, use identities such as

$$\hat{y}\hat{p}_z \left| \begin{pmatrix} x \\ y \\ z \end{pmatrix} \right\rangle = \hat{p}_z\hat{y} \left| \begin{pmatrix} x \\ y \\ z \end{pmatrix} \right\rangle = -iy\hbar\frac{\partial}{\partial z} \left| \begin{pmatrix} x \\ y \\ z \end{pmatrix} \right\rangle = -iy\hbar \left| \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\rangle$$

and, after that, rewrite the components of the position kets in spherical coordinates.

$$\begin{aligned}
\left[\hat{\mathbf{1}} - \frac{i\delta\phi}{\hbar}\hat{L}_x\right] \left| \begin{pmatrix} r\sin\theta\cos\phi \\ r\sin\theta\sin\phi \\ r\cos\theta \end{pmatrix} \right\rangle &= \left| \begin{pmatrix} r\sin\theta\cos\phi \\ r(\sin\theta\sin\phi - \cos\theta\delta\phi) \\ r(\cos\theta + \sin\theta\sin\phi\delta\phi) \end{pmatrix} \right\rangle \\
\longrightarrow \quad \hat{L}_x \left|\underline{x}\right\rangle &= i\hbar \left| \begin{pmatrix} 0 \\ -r\cos\theta \\ r\sin\theta\sin\phi \end{pmatrix} \right\rangle \\
&= \quad i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)\left|\underline{x}\right\rangle
\end{aligned}$$

yielding the desired result.

Repeating the same exercise for $\hat{L}_y$ yields

$$\left[\hat{\mathbf{1}} - \frac{i\delta\phi}{\hbar}\hat{L}_y\right]\left|\begin{pmatrix} r\sin\theta\cos\phi \\ r\sin\theta\sin\phi \\ r\cos\theta \end{pmatrix}\right\rangle = \left|\begin{pmatrix} r(\sin\theta\cos\phi + \cos\theta\delta\phi) \\ r\sin\theta\sin\phi \\ r(\cos\theta - \sin\theta\cos\phi\delta\phi) \end{pmatrix}\right\rangle$$

$$\begin{aligned} \longrightarrow \quad & \hat{L}_x\left|\underline{x}\right\rangle = i\hbar\left|\begin{pmatrix} r\cos\theta \\ 0 \\ -r\sin\theta\cos\phi \end{pmatrix}\right\rangle \\ = \quad & i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)\left|\underline{x}\right\rangle \end{aligned}$$

This also proves the form of $\hat{L}_\pm$, given by

$$\left\langle\underline{x}\left|\hat{L_\pm}\right|\psi\right\rangle = -i\hbar e^{\pm i\phi}\left(\pm i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right)\left\langle\underline{x}|\psi\right\rangle \;.$$

Using that $\underline{\hat{L}}^2 = \hat{L}_z^2 + \frac{1}{2}\left(\hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+\right)$ leaves us to calculate

$$
\begin{aligned}
\hat{L}_z^2 &= -\hbar^2\frac{\partial^2}{\partial\phi^2} \\
\frac{\hat{L}_+\hat{L}_-}{2} &= -\frac{\hbar^2}{2}\left[e^{i\phi}\left(i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right)\right]\left[e^{-i\phi}\left(-i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right)\right] \\
&= -\frac{\hbar^2}{2}\left[\frac{\partial^2}{\partial\theta^2} + \frac{i}{\sin^2\theta}\frac{\partial^2}{\partial\theta\partial\phi} - \cot\theta\left(i - \frac{\partial}{\partial\phi}\right)\left(i\frac{\partial}{\partial\theta} + \cot\theta\frac{\partial}{\partial\phi}\right)\right. \\
\frac{\hat{L}_-\hat{L}_+}{2} &= -\frac{\hbar^2}{2}\left[e^{-i\phi}\left(-i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right)\right]\left[e^{i\phi}\left(i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right)\right] \\
&= -\frac{\hbar^2}{2}\left[\frac{\partial^2}{\partial\theta^2} - \frac{i}{\sin^2\theta}\frac{\partial^2}{\partial\theta\partial\phi} - \cot\theta\left(i + \frac{\partial}{\partial\phi}\right)\left(i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right)\right.
\end{aligned}
$$

Summing them yields

$$\begin{aligned}\hat{\underline{L}}^2 &= -\hbar^2\left[\left(1-\cot^2\theta\right)\frac{\partial^2}{\partial\phi^2}+\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}\right]\\ &= -\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]\,.\end{aligned}$$

Definition of spherical harmonics

- The Hamiltonian of a spin-less particle in a spherically symmetric potential reads

$$\hat{H} = \frac{\hat{\underline{p}}^2}{2m} + \hat{V}(r)$$

and the energy eigenfunctions are labelled by the energy levels n and the angular quantum numbers l and m, $|nlm\rangle$. In position space they can be decomposed as (with $\underline{x}$ given by the distance r and the angles θ and ϕ)

$$\langle \underline{x} | lm \rangle = R_n(r)\, Y_{lm}(\theta,\, \phi)$$

In other words, with the unit vector $\check{\underline{x}}$ in the direction of $\underline{x}$:

$$Y_{lm}(\theta,\, \phi) \equiv \langle \check{\underline{x}} | lm \rangle$$

Properties: Normalisation

- The orthonormality of the $|lm\rangle$ translates to

$$\langle lm|l'm'\rangle = \delta_{ll'}\delta_{mm'} = \int\limits_{-1}^{1} \mathrm{d}\cos\theta \int\limits_{0}^{2\pi} \mathrm{d}\phi\, Y^*_{lm}(\theta,\phi)Y_{l'm'}(\theta\phi)$$

using the completeness relation

$$1 = \int\limits_{0}^{4\pi} \mathrm{d}\Omega\, |\underline{\check{x}}\rangle\langle\underline{\check{x}}| = \int\limits_{-1}^{1} \mathrm{d}\cos\theta \int\limits_{0}^{2\pi} \mathrm{d}\phi\, |\underline{\check{x}}\rangle\langle\underline{\check{x}}| \,.$$

Further properties

- From last lectures we know that

$$\begin{aligned}\hat{L}_z\,|lm\rangle &= \hbar m\,|lm\rangle\\ \hat{\underline{L}}^2\,|lm\rangle &= \hbar^2 l(l+1)\,|lm\rangle\ .\end{aligned}$$

- When sandwiched with a position-bra the first operator becomes

$$\left\langle \underline{x}\left|\hat{L}_z\right|\psi\right\rangle = -i\hbar\frac{\partial}{\partial\phi}\langle\underline{x}|\psi\rangle$$

which leads to the differential equation

$$-i\hbar\frac{\partial}{\partial\phi}Y_{lm}(\theta,\,\phi) = m\hbar Y_{lm}(\theta,\,\phi) \quad\longrightarrow\quad Y_{lm}(\theta,\,\phi)\propto e^{im\phi}\,.$$

- In addition, for the $\underline{\hat{L}}^2$-identity we find

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

Constructing the spherical harmonics

- To find the form of the $Y_{lm}(\theta,\,\phi)$, start with $\hat{L}_+$ acting on $|ll\rangle$:

$$\hat{L}_+\,|ll\rangle = 0 \quad\longrightarrow\quad -i\hbar e^{i\phi}\left[i\frac{\mathrm{d}}{\mathrm{d}\theta} - \cot\theta\frac{\mathrm{d}}{\mathrm{d}\phi}\right]\,Y_{ll}(\theta,\,\phi) = 0\,.$$

- Since the ϕ-dependence of Y_{ll} is $e^{il\phi}$, this leads

$$Y_{ll}(\theta,\,\phi) = c_l e^{il\phi}\sin^l\theta\,.$$

- Applying, successively, $\hat{L}_-$ will yield the other Y_{lm}, i.e.:

$$\begin{aligned} Y_{l(m-1)} &= \frac{\left\langle \check{\underline{x}} \middle| \hat{L_-} \middle| lm \right\rangle}{\hbar\sqrt{(l+m)(l-m+1)}} \\ &= \frac{e^{-i\phi}}{\hbar\sqrt{(l+m)(l-m+1)}}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)\,Y_{lm}(\theta,\,\phi)\,. \end{aligned}$$

- The normalisation follows from

$$1 = \int\limits_{-1}^{1} \mathrm{d}\cos\theta \int\limits_{0}^{2\pi} \mathrm{d}\phi\, Y_{ll}^*(\theta,\,\phi)\,Y_{ll}(\theta,\,\phi)$$

$$= \quad 2\pi|c_l|^2 \int\limits_{-1}^{1} \mathrm{d}\cos\theta \sin^{2l}\theta = 2\pi|c_l|^2 \int\limits_{-1}^{1} \mathrm{d}x(1-x^2)^l\,.$$

leading to

$$c_l = \frac{(-1)^l}{2^l\, l!}\sqrt{\frac{(2l+1)(2l)!}{4\pi}}\,,$$

where we used the freedom in the phase of c_l to fix it to be $(-1)^l$.

(This guarantees to find Y_{l0} with the same sign as the Legendre polynomial $P_l(\cos\theta)$, see later.)

General form of spherical harmonics

- In general thus

$$Y_{lm}(\theta,\,\phi) = \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)}{4\pi}\,\frac{(l+m)!}{(l-m)!}}\,\frac{e^{im\phi}}{\sin^m\theta}\,\frac{\mathrm{d}^{l-m}\sin^{2l}\theta}{\mathrm{d}(\cos\theta)^{l-m}}\,,$$

  and, by definition

$$Y_{l(-m)}(\theta,\,\phi) = (-1)^m\left[Y_{lm}(\theta,\,\phi)\right]^*\,.$$

- For $m = 0$, the spherical harmonics are given by the Legendre polynomials

$$Y_{l0}(\theta,\,\phi) = \sqrt{\frac{2l+1}{4\pi}}\,P_l(\cos\theta)\,,$$

  defined in the maths lecture.

Explicit expressions

- For up to $l = 2$ the spherical harmonics are given by

$$\begin{aligned}
Y_{00}(\theta,\,\phi) &= \frac{1}{\sqrt{4\pi}}\\
Y_{10}(\theta,\,\phi) &= \sqrt{\frac{3}{4\pi}}\,\cos\theta\\
Y_{1\pm1}(\theta,\,\phi) &= \mp\sqrt{\frac{3}{8\pi}}\,\sin\theta\,e^{\pm i\phi}\\
Y_{20}(\theta,\,\phi) &= \sqrt{\frac{5}{16\pi}}\,(3\cos^2\theta-1)\\
Y_{2\pm1}(\theta,\,\phi) &= \mp\sqrt{\frac{15}{8\pi}}\,\sin\theta\cos\theta\,e^{\pm i\phi}\\
Y_{2\pm2}(\theta,\,\phi) &= \sqrt{\frac{15}{32\pi}}\,\sin^2\theta\,e^{\pm 2i\phi}
\end{aligned}$$

No half-integer spherical harmonics

- For half-integer l (and therefore for half-integer m), the wave function is not single-valued in position space, since $e^{im(2\pi)} = -1$. In other words, a rotation by 2π, which in position space brings you back to where you started will not yield the same wave-function. To see this consider a 2π rotation around the z-axis, generated by $\underline{\hat{L}}$. Using $\underline{\hat{L}} = \underline{\hat{x}} \times \underline{\hat{p}}$

$$\left\langle \underline{x} \left| \exp\left(-\frac{i\hat{L}_z 2\pi}{\hbar}\right) \right| \psi \right\rangle = \left\langle \left(\begin{array}{c} x\cos(2\pi)+y\sin(2\pi) \\ y\cos(2\pi)-x\sin(2\pi) \\ z \end{array} \right) \middle| \psi \right\rangle = \left\langle \underline{x} \middle| \psi \right\rangle$$

- Another reason is provided by looking at some *hypothetical* spherical harmonics for half-integers, for example, following the for for a general $Y_{ll}(\theta,\,\phi) = c_l e^{il\phi}\sin^l\theta$:

$$Y_{\frac{1}{2}\frac{1}{2}}(\theta,\,\phi) = c_{\frac{1}{2}}\,e^{\frac{i\phi}{2}}\sqrt{\sin\theta}\,.$$

Using $\hat{L}_-$ to obtain $Y_{\frac{1}{2}-\frac{1}{2}}(\theta,\,\phi)$ would yield

$$\begin{aligned} Y_{\frac{1}{2}-\frac{1}{2}}(\theta,\,\phi) = \hat{L}_-\,Y_{\frac{1}{2}\frac{1}{2}}(\theta,\,\phi) &= e^{-i\phi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)Y_{\frac{1}{2}\frac{1}{2}}(\theta,\,\phi) \\ &= c_{\frac{1}{2}}\,e^{-\frac{i\phi}{2}}\cot\theta\sqrt{\sin\theta}\,, \end{aligned}$$

which is singular for $\theta = 0$ and $\theta = \pi$. Moreover, using

$$0 \equiv \left\langle \underline{\check{x}} \left| \hat{L_-} \right| \frac{1}{2}\,-\frac{1}{2} \right\rangle \quad\longrightarrow\quad Y_{\frac{1}{2}-\frac{1}{2}}(\theta,\,\phi) = c'_{\frac{1}{2}}\,e^{-\frac{i\phi}{2}}\sqrt{\sin\theta}$$

results in a striking inconsistency.

Learning outcomes

- Spherical harmonics defined as $Y_{lm}(\theta, phi) = \langle \underline{\check{x}} | lm \rangle$ and normalised to 1 after integration over solid angle (4π).
- Construction from differential from of orbital angular momentum operators. In particular,

$$\begin{aligned}
Y_{ll}(\theta, \phi) &= c_l e^{il\phi} \sin^l \theta \\
Y_{l0}(\theta, \phi) &= \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta) \\
Y_{lm}(\theta, \phi) &= \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)}{4\pi} \frac{(l+m)!}{(l-m)!}} \frac{e^{im\phi}}{\sin^m \theta} \frac{\mathrm{d}^{l-m} \sin^{2l}\theta}{\mathrm{d}(\cos\theta)^{l-m}} \\
Y_{l(-m)}(\theta, \phi) &= (-1)^m \left[Y_{lm}(\theta, \phi)\right]^* .
\end{aligned}$$

Control questions

16.1 A rotor - a system with θ and ϕ as the only two dynamical degrees of freedom - has a wave function given by

$$\psi(\theta,\,\phi) = N\left[\sqrt{3}\cos\theta + \sin\theta\cos\phi + \sin\theta\sin\phi\right]\,,$$

where N is a constant guaranteeing normalisation of the wave function:

$$\int\limits_{-1}^{1}\mathrm{d}\cos\theta\int\limits_{0}^{2\pi}\mathrm{d}\phi|\psi(\theta,\,\phi)|^2 = 1\,.$$

(a) Fix the normalisation constant N.
(b) What is the expectation value of the squared orbital angular momentum squared, $\underline{\mathcal{L}}^2$?
(c) What is the probability to measure the z-component of the orbital angular momentum, $\mathcal{L}_z$ to be zero?

16.2 Consider a particle of mass m constrained to move on a ring of radius a.

(a) By suitably orienting the ring, show that the Hamiltonian reads

$$\hat{H} = \frac{\hat{L}_z^2}{2I}\,, \quad \text{where } I = mr^2\,.$$

(b) Find the energy eigenkets of the system. What are the corresponding eigenfunctions of the system?

(c) Show that the expectation value of the orbital angular momentum in z-direction is a constant.

(d) Construct the time evolution operator and confirm by explicit calculation the finding in part (c).