Theoretical Physics II B – Quantum Mechanics

Lecture 15

Frank Krauss

5.3.2013

Solutions to previous control questions

14.1 Proving three identities:

$$\begin{aligned}(\underline{\hat{\sigma}}\cdot\underline{a})(\underline{\hat{\sigma}}\cdot\underline{b}) &= \sum_{i,j} a_i b_j\,(\hat{\sigma}_i\hat{\sigma}_j) = \sum_{i,j} a_i b_j \left(\frac{1}{2}\,[\hat{\sigma}_i,\,\hat{\sigma}_j] + \frac{1}{2}\,\{\hat{\sigma}_i,\,\hat{\sigma}_j\}\right)\\ &= \sum_{i,j} a_i b_j\,(i\epsilon_{ijk}\hat{\sigma}_k + \delta_{ij}) = i\left(\underline{a}\times\underline{j}\right)\cdot\underline{\hat{\sigma}} + \underline{a}\cdot\underline{b}\hat{\mathbf{1}}\,.\end{aligned}$$

With $\underline{a} = \underline{b}$ this becomes $|\underline{a}|^2\cdot\hat{\mathbf{1}}$.

Using this result and $|\underline{n}|^2 = 1$ yields

$$\begin{aligned}
&\exp\left(-\frac{i\underline{\hat{\sigma}}\cdot\underline{n}\,\phi}{2}\right)\\
&= \hat{\mathbf{1}} + \frac{1}{1!}\left(-\frac{i\underline{\hat{\sigma}}\cdot\underline{n}\,\phi}{2}\right) + \frac{1}{2!}\left(-\frac{i\underline{\hat{\sigma}}\cdot\underline{n}\,\phi}{2}\right)^2 + \frac{1}{3!}\left(-\frac{i\underline{\hat{\sigma}}\cdot\underline{n}\,\phi}{2}\right)^3 + \ldots\\
&= \hat{\mathbf{1}} - i\underline{\hat{\sigma}}\cdot\underline{n}\left(\frac{\phi}{2}\right) + \frac{1}{2!}\hat{\mathbf{1}}\left(-\frac{\phi}{2}\right)^2 + i\underline{\hat{\sigma}}\cdot\underline{n}\frac{1}{3!}\left(\frac{\phi}{2}\right)^3 + \ldots\\
&= \hat{\mathbf{1}}\cos\frac{\phi}{2} - i\underline{\hat{\sigma}}\cdot\underline{n}\sin\frac{\phi}{2}\,.
\end{aligned}$$

(c) Explicit calculations yields:

$$\hat{U} = [a_0 + i\underline{\hat{\sigma}} \cdot \underline{a}]\,[a_0 - i\underline{\hat{\sigma}} \cdot \underline{a}]^{-1}$$
$$= \frac{1}{a_0^2 + a_1^2 + a_2^2 + a_3^2} \begin{pmatrix} a_0 + ia_3 & ia_1 + a_2 \\ ia_1 - a_2 & a_0 - ia_3 \end{pmatrix} \begin{pmatrix} a_0 + ia_3 & ia_1 + a_2 \\ ia_1 - a_2 & a_0 - ia_3 \end{pmatrix}$$
$$= \begin{pmatrix} \frac{a_0^2 - a_3^2 - a_1^2 - a_2^2 + 2ia_0a_3}{a_0^2+a_1^2+a_2^2+a_3^2} & \frac{2a_0[ia_1+a_2]}{a_0^2+a_1^2+a_2^2+a_3^2} \\ \frac{2a_0[ia_1-a_2]}{a_0^2+a_1^2+a_2^2+a_3^2} & \frac{a_0^2 - a_1^2 - a_2^2 - a_3^2 - 2ia_0a_3}{a_0^2+a_1^2+a_2^2+a_3^2} \end{pmatrix} = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} .$$

Reading of a and b and squaring indeed results in

$$|a|^2 + |b|^2 = \frac{(a_0^2 - a_1^2 - a_2^2 - a_3^2)^2 + 4a_0^2(a_1^2 + a_2^2 + a_3^2)}{(a_0^2 + a_1^2 + a_2^2 + a_3^2)^2} = 1\,,$$

and hence the operator $\hat{U}$ is unimodular.

14.2 (a) Represent $\hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-)$ and realise that

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

(b) Use the explicit form of $\hat{J}_y$ from (a):

$$\begin{aligned}
\hat{J}_y{}^2 &= \frac{\hbar^2}{2}\begin{pmatrix} -1 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & -1 \end{pmatrix} \\
\hat{J}_y{}^3 &= i\frac{\hbar^3}{2\sqrt{2}}\begin{pmatrix} 0 & -2 & 0 \\ -2 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix} = -\hbar^2\hat{J}_y\,.
\end{aligned}$$

Therefore, with the superscript $^{(j=1)}$ understood,

$$\begin{aligned}
\exp\left(-\frac{i\hat{J}_y\beta}{\hbar}\right)
&= \hat{\mathbf{1}} - \hat{J}_y\sum_{n=0}^{\infty}\frac{\hbar^{2n}}{(2n+1)!}\left(\frac{i\beta}{\hbar}\right)^{2n+1} + \hat{J}_y^2\sum_{n=0}^{\infty}\frac{\hbar^{2n}}{(2n+2)!}\left(\frac{i\beta}{\hbar}\right)^{2n+2}\\
&= \hat{\mathbf{1}} - \frac{i\hat{J}_y}{\hbar}\sin\beta + \frac{\hat{J}_y^2}{\hbar^2}(1-\cos\beta)\,,
\end{aligned}$$

as demanded.

(c) Using this, we find

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

as demanded.

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

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

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

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

Orbital angular momentum operators

- Ignoring the spin of a particle, its angular momentum equals its orbital angular momentum, in analogy to classical mechanics it is

$$\underline{\hat{L}} = \underline{\hat{x}} \times \underline{\hat{p}}\,.$$

- Direct caclulation shows that $\underline{\hat{L}}$ enjoys the same commutation relations as $\underline{\hat{J}}$:

$$\begin{aligned}\left[\hat{L}_x,\,\hat{L}_y\right] &= [\hat{y}\hat{p}_z - \hat{z}\hat{p}_y,\,\hat{z}\hat{p}_x - \hat{x}\hat{p}_z] \\ &= [\hat{y}\hat{p}_z,\,\hat{z}\hat{p}_x] - \underbrace{[\hat{y}\hat{p}_z,\,\hat{x}\hat{p}_z]}_{=0} - \underbrace{[\hat{z}\hat{p}_y,\,\hat{z}\hat{p}_x]}_{=0} + [\hat{z}\hat{p}_y,\,\hat{x}\hat{p}_z] \\ &= \hat{y}\hat{p}_x\underbrace{[\hat{p}_z,\,\hat{z}]}_{-i\hbar} + \hat{p}_y\hat{x}\underbrace{[\hat{z},\,\hat{p}_z]}_{i\hbar} = i\hbar\left(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x\right) = i\hbar\hat{L}_z\end{aligned}$$

and similar for the other combinations such that $\left[\hat{L}_i,\,\hat{L}_j\right] = i\hbar\epsilon_{ijk}\hat{L}_k$.

Orbital angular momentum operators and spatial rotations

- Try to identify the $\hat{L}_i$ with generators of spatial rotations.
- Write the generator of an infinitesimal rotation around the z-axis as

$$\hat{\mathbf{1}} - \frac{i\delta\phi}{\hbar}\hat{L}_z = \hat{\mathbf{1}} - \frac{i\delta\phi}{\hbar}\left(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x\right)$$

and let this operator act on a position eigenket $|\underline{x}\rangle = |x,\, y,\, z\rangle$:

$$\left[\hat{\mathbf{1}} - \frac{i\delta\phi}{\hbar}\left(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x\right)\right]|x,\, y,\, z\rangle = |x - y\delta\phi,\, y + x\delta\phi,\, z\rangle$$

and on an arbitrary state ket $|\psi\rangle$:

$$\left\langle x,\, y,\, z\left|\left[\hat{\mathbf{1}} - \frac{i\delta\phi}{\hbar}\left(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x\right)\right]\right|\psi\right\rangle = \langle x + y\delta\phi,\, y - x\delta\phi,\, z|\psi\rangle$$

Differential forms of the operators

- The action on a position eigenket can also be written as

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

- Therefore, rewriting the cartesian as polar coordinates results in

$$
\begin{aligned}
\left\langle r,\,\theta,\,\phi\left|\left[\hat{\mathbf{1}}-\frac{i\delta\phi}{\hbar}\hat{L}_z\right]\right|\psi\right\rangle &= \langle r,\,\theta,\,\phi-\delta\phi|\psi\rangle\\
&= \langle r,\,\theta,\,\phi|\psi\rangle-\delta\phi\frac{\partial}{\partial\phi}\langle r,\,\theta,\,\phi|\psi\rangle\ .
\end{aligned}
$$

- Repeating the same exercise for rotations around the x and y axis by expressing the position eigenket in spherical coordinates results in

$$\begin{aligned}
\left\langle \underline{x} \middle| \hat{L}_x \middle| \psi \right\rangle &= -i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)\langle \underline{x}|\psi\rangle \\
\left\langle \underline{x} \middle| \hat{L}_y \middle| \psi \right\rangle &= -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)\langle \underline{x}|\psi\rangle \\
\left\langle \underline{x} \middle| \hat{L}_z \middle| \psi \right\rangle &= -i\hbar\left(\frac{\partial}{\partial\phi}\right)\langle \underline{x}|\psi\rangle\ .
\end{aligned}$$

- With $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$ and $e^{\pm i\phi} = \cos\phi \pm i\sin\phi$ this leads to

$$\begin{aligned}\left\langle \underline{x} \middle| \hat{L_\pm} \middle| \psi \right\rangle = \left\langle \underline{x} \middle| \left[\hat{L}_x \pm i\hat{L}_y\right] \middle| \psi \right\rangle \\ &= -i\hbar\left[(-\sin\phi \pm i\cos\phi)\frac{\partial}{\partial\theta} - \cot\theta\,(\cos\phi \pm i\sin\phi)\frac{\partial}{\partial\phi}\right]\langle \underline{x}|\psi\rangle \\ &= -i\hbar e^{\pm i\phi}\left(\pm i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right)\langle \underline{x}|\psi\rangle\ .\end{aligned}$$

- Using $\hat{\underline{L}}^2 = \hat{L}_z^2 + \frac{1}{2}(\hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+)$ yields

(Don't forget to let the differential operators act on everything to the right!)

$$\begin{aligned}\left\langle \underline{x} \left| \hat{\underline{L}}^2 \right| \psi \right\rangle &= \left\langle \underline{x} \left| \left[\hat{L}_z^2 + \frac{1}{2}(\hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+) \right] \right| \psi \right\rangle \\ &= -\hbar^2 \left[\frac{\partial^2}{\partial\phi^2} + \frac{1}{2}\left(\frac{2\partial^2}{\partial\theta^2} + \cot\theta \frac{2\partial}{\partial\theta} + \cot^2\theta \frac{2\partial^2}{\partial\phi^2} \right) \right] \langle \underline{x} | \psi \rangle \\ &= -\hbar^2 \left[\frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) \right] \langle \underline{x} | \psi \rangle \ ,\end{aligned}$$

where $\cot\theta = \cos\theta / \sin\theta$ has been used.

- Note that up to a factor of $1/r^2$ this last expression is nothing but the angular-dependent part of the Laplacian expressed in polar coordinates.

$\hat{\underline{L}}^2$ and the Laplacian operator

- First realise that

$$\hat{\underline{L}}^2 = \hat{\underline{x}}^2\hat{\underline{p}}^2 - \left(\hat{\underline{x}}\cdot\hat{\underline{p}}\right)^2 + i\hbar\left(\hat{\underline{x}}\cdot\hat{\underline{p}}\right) .$$

- Proof:

$$\begin{aligned}
\hat{\underline{L}}^2 = \left(\hat{\underline{x}}\times\hat{\underline{p}}\right)^2 &= \sum_{ijkl}\epsilon_{aij}\epsilon_{akl}\hat{x}_i\hat{p}_j\hat{x}_k\hat{p}_l = \sum_{ijkl}\left(\delta_{ik}\delta_{jl}-\delta_{il}\delta_{jk}\right)\hat{x}_i\hat{p}_j\hat{x}_k\hat{p}_l\\
&= \sum_{ijkl}\left[\delta_{ik}\delta_{jl}\hat{x}_i\left(\hat{x}_k\hat{p}_j - i\hbar\delta_{kj}\right)\hat{p}_l - \delta_{il}\delta_{jk}\hat{x}_i\hat{p}_j\left(\hat{p}_l\hat{x}_k + i\hbar\delta_{kl}\right)\right]\\
&= \hat{\underline{x}}^2\hat{\underline{p}}^2 - i\hbar\left(\hat{\underline{x}}\cdot\hat{\underline{p}}\right) - \sum_{ijkl}\delta_{il}\delta_{jk}\left[i\hbar\delta_{kl}\hat{x}_i\hat{p}_j + \hat{x}_i\hat{p}_l\left(\hat{x}_k\hat{p}_j + i\hbar\delta_{kj}\right)\right]\\
&= \hat{\underline{x}}^2\hat{\underline{p}}^2 - 2i\hbar\left(\hat{\underline{x}}\cdot\hat{\underline{p}}\right) - \left(\hat{\underline{x}}\cdot\hat{\underline{p}}\right)^2 + \underbrace{\delta_{kk}}_{=3} i\hbar\left(\hat{\underline{x}}\cdot\hat{\underline{p}}\right)
\end{aligned}$$

- Now use

$$\begin{aligned}
\left\langle \underline{x} \left| \hat{\underline{x}} \cdot \hat{\underline{p}} \right| \psi \right\rangle &= \underline{x} \cdot \left\langle \underline{x} \left| \hat{\underline{p}} \right| \psi \right\rangle = -i\hbar\, \underline{x} \cdot \underline{\nabla} \left\langle \underline{x} | \psi \right\rangle = -i\hbar\, r \frac{\partial}{\partial r} \left\langle \underline{x} | \psi \right\rangle \\
\left\langle \underline{x} \left| \left(\hat{\underline{x}} \cdot \hat{\underline{p}} \right)^2 \right| \psi \right\rangle &= -\hbar^2 \left(r \frac{\partial}{\partial r} \right)^2 \left\langle \underline{x} | \psi \right\rangle = -\hbar^2 \left(r^2 \frac{\partial^2}{\partial r^2} + r \frac{\partial}{\partial r} \right) \left\langle \underline{x} | \psi \right\rangle \\
\left\langle \underline{x} \left| \left(\hat{\underline{x}}^2 \hat{\underline{p}}^2 \right) \right| \psi \right\rangle &= \underline{x}^2 \left\langle \underline{x} \left| \hat{\underline{p}}^2 \right| \psi \right\rangle = -\hbar^2 r^2 \nabla^2 \left\langle \underline{x} | \psi \right\rangle
\end{aligned}$$

- This then yields that

$$\left\langle \underline{x} \left| \hat{\underline{L}}^2 \right| \psi \right\rangle = r^2 \left\langle \underline{x} \left| \hat{\underline{p}}^2 \right| \psi \right\rangle + \hbar^2 \left(r^2 \frac{\partial^2}{\partial r^2} + 2r \frac{\partial}{\partial r} \right) \left\langle \underline{x} | \psi \right\rangle$$

and therefore the kinetic energy can be written as

$$\frac{1}{2m} \left\langle \underline{x} \left| \hat{\underline{p}}^2 \right| \psi \right\rangle = -\frac{\hbar^2}{2m} \left[\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) \left\langle \underline{x} | \psi \right\rangle - \frac{1}{\hbar^2 r^2} \left\langle \underline{x} \left| \hat{\underline{L}}^2 \right| \psi \right\rangle \right]$$

Learning outcomes

- Orbital angular momentum as relaisation of general angular momentum.
- Differential form of operators
- Rewriting the Laplacian and connection to angular part of Laplacian in spherical coordinates

Control questions

15.1 Use the fundamental commutation relation $[\hat{x}_i,\, \hat{p}_j] = i\hbar\hat{\mathbf{1}}\delta_{ij}$

(a) to show that the operators

$$\begin{aligned}\hat{R}^{(l=1)}_{m=\pm 1} &= \mp\frac{1}{\sqrt{2}}(\hat{x}_1 \pm i\hat{x}_2) = \sqrt{\frac{4\pi}{3}}\hat{R}Y_{1\pm 1}(\theta,\,\phi)\\ \hat{R}^{(l=1)}_{m=0} &= \hat{x}_3 = \sqrt{\frac{4\pi}{3}}\hat{R}Y_{10}(\theta,\,\phi)\end{aligned}$$

fulfil the following commutation relations with components of the oribatal angular momentum operator,

$$\begin{aligned}\left[\hat{L}_\pm,\, \hat{R}^{(1)}_q\right] &= \sqrt{(1\mp q)(2\pm q)}\,\hbar\,\hat{R}^{(1)}_{q\pm 1}\\ \left[\hat{L}_3,\, \hat{R}^{(1)}_q\right] &= q\hbar\hat{R}^{(1)}_q\,,\end{aligned}$$

where $q = 0,\, \pm 1$.

(Note that in the definitions of the $\hat{R}_q$ above the spherical harmonics are just added to make some contact with the material in lecture 16 - you do not need to use them for this problem.)

Control questions

(b) to show that $\hat{\underline{R}}^2 = \hat{x}_1^2 + \hat{x}_2^2 + \hat{x}_3^2$ is a rotationally invariant operator with repsect to orbital angular momentum, i.e. that

$$\left[\hat{L}_i,\, \hat{\underline{R}}^2\right] = 0\,.$$

15.2 Check that indeed

$$\begin{aligned}
\left\langle \underline{x} \left| \hat{L}_x \right| \psi \right\rangle &= -i\hbar \left(-\sin\phi \frac{\partial}{\partial\theta} - \cot\theta\cos\phi \frac{\partial}{\partial\phi} \right) \langle \underline{x} | \psi \rangle \\
\left\langle \underline{x} \left| \hat{L}_y \right| \psi \right\rangle &= -i\hbar \left(\cos\phi \frac{\partial}{\partial\theta} - \cot\theta\sin\phi \frac{\partial}{\partial\phi} \right) \langle \underline{x} | \psi \rangle \\
\left\langle \underline{x} \left| \hat{\underline{L}}^2 \right| \psi \right\rangle &= -\hbar^2 \left[\frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) \right] \langle \underline{x} | \psi \rangle \;,
\end{aligned}$$