Quantum Mechanics M.T. 2000

I. J. R. Aitchison

Problem Set No. 5

Separation of r, θ, ϕ for spherically symmetric V; angular momentum operators

1. The 3-D time-independent Schrödinger equation for a particle of mass m in a spherically symmetric potential (i.e. one that only depends on r, not on θ and ϕ) is

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\psi(\mathbf{r}) = E\psi(\mathbf{r}).$$

(i) By writing ∇^2 in terms of r, θ, ϕ show that this can be written as

$$-\frac{\hbar^2}{2m}\,\frac{1}{r^2}\,\frac{\partial}{\partial r}\,r^2\frac{\partial\psi}{\partial r} \;+\; \frac{\hat{\mathbf{L}}^2}{2mr^2}\;\psi + V\psi = E\psi \tag{1}$$

where

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

(ii) The *angular momentum operators* $\hat{L}_x, \hat{L}_y$ and $\hat{L}_z$ are defined in q.m. by $\hat{\mathbf{L}} = \mathbf{r}\times\hat{\mathbf{p}}$ where $\hat{\mathbf{p}} = -i\hbar\nabla$ (would it make any difference if we defined $\hat{\mathbf{L}} = -\hat{\mathbf{p}}\times\mathbf{r}$?). So, for example

$$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right).$$

Using the relations

$$\begin{aligned}x &= r\sin\theta\cos\phi\\ y &= r\sin\theta\sin\phi\\ z &= r\cos\theta\end{aligned}$$

show that

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$$

[hint: it is easier to show that this expression is equal to the previous one, rather than the other way round; use the chain rule

$$\frac{\partial f}{\partial \phi} = \frac{\partial x}{\partial \phi}\frac{\partial f}{\partial x} + \frac{\partial y}{\partial \phi}\frac{\partial f}{\partial y} + \frac{\partial z}{\partial \phi}\frac{\partial f}{\partial z}$$

for any f.]

Expressions for $\hat{L}_x$ and $\hat{L}_y$ can also be worked out. Amazingly, when $\hat{\mathbf{L}}^2$ is calculated it is exactly the operator (in terms of $\frac{\partial}{\partial\theta}$'s and $\frac{\partial}{\partial\phi}$'s) given in (i)! See any book on q.m., and part (iv) below. *Is this *really* amazing or should we expect it?

(iii) Writing $\psi(\mathbf{r}) = R(r)Y(\theta,\phi)$ show that Y must satisfy $\hat{\mathbf{L}}^2 Y = cY$ where c is a constant, and where

$$-\frac{\hbar^2}{2mr^2}\frac{d}{dr}r^2\frac{dR}{dr} + \left(V + \frac{c}{2mr^2}\right)R = ER$$

(here is another use of "separation variables"). Writing $R = f(r)/r$, show that $f(r)$ satisfies the equation

$$-\frac{\hbar^2}{2m}\frac{d^2 f}{dr^2} + \left(V + \frac{c}{2mr^2}\right)f = Ef.$$

This is of exactly the same form as a 1-D time independent Schrödinger equation, with V replaced by $V + c/2mr^2$. [*Harder*: So, can we conclude that the spectrum in the original 3D problem is the same as for this 1D problem?]

(iv) In classical mechanics, the kinetic energy T is given by

$$T = \frac{1}{2}m\dot{\mathbf{r}}^2$$

Show that

$$\frac{dr}{dt} = \mathbf{r}.\dot{\mathbf{r}}/r$$

(write $r = (x^2+y^2+z^2)^{\frac{1}{2}}$ and evaluate $\frac{d}{dt}$ of it) and

$$(\mathbf{r}\times\dot{\mathbf{r}})^2 = \mathbf{r}^2\dot{\mathbf{r}}^2 - (\mathbf{r}.\dot{\mathbf{r}})^2$$

(Hint: write $(\mathbf{r}\times\dot{\mathbf{r}})^2 = (\mathbf{r}\times\dot{\mathbf{r}}).(\mathbf{r}\times\dot{\mathbf{r}})$.).

Deduce that

$$\begin{aligned} T &= \frac{1}{2}m\left(\frac{dr}{dt}\right)^2 + \frac{1}{2}\,m\,\frac{(\mathbf{r}\times\dot{\mathbf{r}})^2}{\mathbf{r}^2} \\ &= \frac{1}{2}m\left(\frac{dr}{dt}\right)^2 + \mathbf{L}^2/2mr^2 \end{aligned}$$

where $\mathbf{L} = (\mathbf{r} \times m\dot{\mathbf{r}})$, classically. So the first two terms of (1) in part (i) can be interpreted as the quantum mechanical expressions for the K.E. associated with purely radial oscillations and for the K.E. associated with rotation, respectively; the third term is the (original) potential energy. Notice that $\hat{\mathbf{L}}^2/2mr^2$ can be added to V to make the "effective potential" $\hat{V}_{eff} = \hat{\mathbf{L}}^2/2mr^2 + V$, and this (from (iii)) actually has the form $c/2mr^2 + V$ where c is a constant - which is the eigenvalue of $\hat{\mathbf{L}}^2$, namely $\ell(\ell+1)\hbar^2$ where ℓ is zero or a positive integer.

(v) Suppose $V(r)$ is the attractive Coulomb potential $-z_1 z_2 e^2/4\pi\epsilon_0 r$. Sketch the form of the "effective potential" for $\ell = 0$ and for $\ell = 1$. Taking m to be the electron mass, at what value of r is this effective potential zero, for $\ell = 1$ and $z_1 = z_2 = 1$?

2. Write down expressions for $\hat{L}_x, \hat{L}_y$ and $\hat{L}_z$ in terms of x, y, z and $\frac{\partial}{\partial x}, \frac{\partial}{\partial y}$ and $\frac{\partial}{\partial z}$. Show that, for any differentiable function $f(x, y, z)$,

$$(\hat{L}_x \hat{L}_y - \hat{L}_y \hat{L}_x) f(x, y, z) = i\hbar \hat{L}_z f(x, y, z).$$

Since the above relation is true for any f, it is usually written as an operator equation

$$[\hat{L}_x, \hat{L}_y] = \hat{L}_x \hat{L}_y - \hat{L}_y \hat{L}_x = i\hbar \hat{L}_z.$$

By cyclic interchange we can also infer that

$$[\hat{L}_y, \hat{L}_z] = \hat{L}_y \hat{L}_z - \hat{L}_z \hat{L}_y = i\hbar \hat{L}_x$$

and

$$[\hat{L}_z, \hat{L}_x] = \hat{L}_z \hat{L}_x - \hat{L}_x \hat{L}_z = i\hbar \hat{L}_y.$$

Using the result $[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$, *deduce* (without going back to the differential operators) that if $\hat{\mathbf{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ then

$$[\hat{L}_x, \hat{\mathbf{L}}^2] = [\hat{L}_y, \hat{\mathbf{L}}^2] = [\hat{L}_z, \hat{\mathbf{L}}^2] = 0.$$

Explain why it is *not* possible, in general, to have states for which more than one component of $\hat{\mathbf{L}}$ has a definite value (the special case $\psi(x, y, z) = \psi(r)$ obviously has $\hat{L}_x = \hat{L}_y = \hat{L}_z = 0$); also, explain why it *is* possible to have states with simultaneously definite values of $\hat{\mathbf{L}}^2$ and of one component of $\hat{\mathbf{L}}$. (Often the component chosen by convention is $\hat{L}_z$.)

3. (i) Verify by brute force that the three functions $\cos\theta, \sin\theta e^{i\phi}, \sin\theta e^{-i\phi}$ are all eigenfunctions of $\hat{\mathbf{L}}^2$ and of $\hat{L}_z$ and find the corresponding eigenvalues.

(ii) Find normalisation constants N such that $\int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} N^2 \mid \psi(\theta, \phi) \mid^2 \sin\theta d\theta d\phi =$ 1 for each of the three above functions. (This means that they are normalised over the full 4π solid angle subtended at the centre of the unit sphere).

- N.B. It pays to memorize these three functions, which all have $\ell = 1$, and $m = 0$, $m = 1$, $m = -1$ respectively.
- The normalised eigenfunctions of $\hat{\mathbf{L}}^2$ and $\hat{L}_z$ with eigenvalues $\ell(\ell+1)\hbar^2$ and $m\hbar$ respectively are called $Y_{\ell m}(\theta, \phi)$. So

$$Y_{10}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta, Y_{11}(\theta,\phi) = \sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi}, Y_{1-1}(\theta,\phi) = \sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\phi}.$$

- Using $x = r\sin\theta\cos\phi, y = r\sin\theta\sin\phi, z = r\cos\theta$, these can also be written as

$$Y_{10} = \sqrt{\frac{3}{4\pi}}\frac{z}{r}, Y_{11} = \sqrt{\frac{3}{8\pi}}(x+iy)/r, Y_{1-1} = \sqrt{\frac{3}{8\pi}}(x-iy)/r.$$

Sketch $\mid Y_{10} \mid^2, \mid Y_{11} \mid^2$ and $\mid Y_{1-1} \mid^2$ (a cross section in the x-z plane will do - why?)

*The programme "Orbital angular momentum" in McMurry's disk can be run to see plots of many more Y's. Try $\ell = 4, m = 4, 3, 2, 1, 0$.

4. A particle is in the state with wavefunction

$$\psi = \frac{1}{\sqrt{2}}(Y_{11}(\theta,\phi) + Y_{1-1}(\theta,\phi))$$

Express ψ in terms of x, y, z and r. What value is obtained if $\hat{\mathbf{L}}^2$ is measured? Does the particle have a definite value of $\hat{L}_z$? What are the probabilities of getting results $\hbar, -\hbar$ and 0 for $\hat{L}_z$? Are any other $\hat{L}_z$ results possible?

Calculate $\langle\psi \mid \hat{L}_z \mid \psi\rangle = \iint_{\text{unit sphere}} \psi^*(\theta,\phi)\hat{L}_z\psi(\theta,\phi)\sin\theta d\theta d\phi$ and explain the answer.

5. The energy operator (Hamiltonian) for a particle of charge q, mass m_0, in a constant magnetic field $\mathbf{B}$ is (approximately)

$$\hat{H} = -\frac{\hbar^2\nabla^2}{2m_0} - \frac{qB}{2m_0}\hat{L}_z$$

where $\mathbf{B} = (0, 0, B)$.

(i) The eigenvalues of which of the following are good quantum numbers: $\hat{\mathbf{L}}^2, \hat{L}_x, \hat{L}_y, \hat{L}_z$?

(ii) Show (using Q 5 (iii) set 3) that the expectation values of $\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_z$ in a general state with wavefunction ψ satisfy the equations

$$\frac{d}{dt}\langle\hat{L}_x\rangle = \frac{qB}{2m_0}\langle\hat{L}_y\rangle$$

$$\frac{d}{dt}\langle \hat{L}_y \rangle = -\frac{qB}{2m_0}\langle \hat{L}_x \rangle$$

$$\frac{d}{dt}\langle \hat{L}_z \rangle = 0.$$

The magnetic moment operator $\hat{\boldsymbol{\mu}}$ is defined by $\hat{\boldsymbol{\mu}} = \frac{q}{2m_0}\hat{\mathbf{L}}$. Deduce that

$$\frac{d}{dt}\langle \hat{\boldsymbol{\mu}} \rangle = \gamma \langle \hat{\boldsymbol{\mu}} \rangle \times \mathbf{B}$$

where $\gamma = q/2m_0$.

Show that (a) $(\langle \hat{\boldsymbol{\mu}} \rangle)^2$ is constant in time, and (b) $\langle \hat{\boldsymbol{\mu}} \rangle.\mathbf{B}$ is constant in time.

Show that $\langle \hat{\boldsymbol{\mu}} \rangle$ precesses around the direction of $\mathbf{B}$ with angular frequency $\omega = \gamma B$. Calculate ω for the electron in a field of 1 tesla.

6. A particle of mass m is described by the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 - \frac{e^2}{4\pi\epsilon_0 r} - e\mathcal{E}x.$$

(i) What is the physical origin of the last term in $\hat{H}$?
(ii) Calculate the commutators $[\hat{L}_x, x], [\hat{L}_y, x], [\hat{L}_z, x]$.
(iii) Which of the observables represented by the operators $\hat{\mathbf{L}}^2, \hat{L}_x, \hat{L}_y, \hat{L}_z$ are constants of the motion assuming (a) $\mathcal{E} = 0$ (b) $\mathcal{E} \neq 0$?