Part IB — Quantum Mechanics Example Sheet 3

Supervised by Dr Warnick
Examples worked through by Christopher Turnbull

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QUESTION 1

Time independent Schrödinger Equation is

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\left(\frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z}\right) = E$$

Can split this into 3 equations, eg.

$$-\frac{\hbar^2}{2m}\frac{X''}{X} = E_1$$

$$X'' + k^2 X = 0 \qquad \text{where } E_1 = \frac{\hbar^2 k^2}{2m}$$

Note we take $E_i > 0$, as boundary conditions mean $E_i < 0$ has no eigenstate solutions.

$X(0) = X(a) = 0 \Rightarrow k = n_1\pi/a$ Repeat for Y and Z.

$$\begin{aligned} E &= E_1 + E_2 + E_3 \\ &= \frac{\hbar^2\pi^2}{2m}\left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2}\right) \end{aligned}$$

With $a = b = c$, ground state is $E = \frac{3\hbar^2\pi^2}{2ma^2}$ where $n_1 = n_2 = n_3 = 1$, and next when $\sum_i n_i = 4$ (which happens in 3 different ways) we have $E = \frac{2\hbar^2\pi^2}{ma^2}$, so first excited state has degeneracy 3.

QUESTION 2

Time independent Schrödinger Equation is

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \frac{1}{2}m\omega^2(x_1^2 + x_2^2 + x_3^2)\psi = E\psi$$

The Hamiltonian splits into $H = H_1 + H_2 + H_3$
Seek solutions of the form $\psi = X(x_1)Y(x_2)Z(x_3)$. Separating variables shows

$$-\frac{\hbar^2}{2m}\left(\frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z}\right) + \frac{1}{2}m\omega^2(x_1^2 + x_2^2 + x_3^2) = E$$

As X cannot vary for fixed Y, Z, we have

$$-\frac{\hbar^2}{2m}\frac{X''}{X} + \frac{1}{2}m\omega^2 x_1^2 = E_1$$

This is the one dimensional harmonic oscillator equation; with eigenstates and eigenvalues

$$X_{n_1}(x_1) = h_{n_1}(y_1)\exp\left(-y_1^2/2\right), \qquad E_1 = \hbar\omega(n_1 + \frac{1}{2})$$

$$y_1 = \left(\left(\frac{m\omega}{\hbar}\right)^{1/2} x_1\right)$$

for $n_1 = 0, 1, 2, \cdots$
Similarly, recover that $E_i = \hbar\omega(n_i + \frac{1}{2})$

$$\begin{aligned} E &= E_1 + E_2 + E_3 \\ &= \hbar\omega\left(n_1 + n_2 + n_3 + \frac{3}{2}\right) \end{aligned}$$

where $n_i = 0, 1, 2, \cdots$

To count the number of linearly independent eigenstates corresponding to energy $E = (N + \frac{3}{2})\hbar\omega$, need $n_1 + n_2 + n_3 = N$. With $n_1 = 0$, need $n_2 + n_3 = N$, which can happen in $N + 1$ ways. Then $n_1 = 1$, have N more states. So the total number of states is given by

$$\begin{aligned} \text{Degeneracy } &= (N+1) + N + \cdots + 2 + 1 \\ &= (N+2)(N+1)/2 \end{aligned}$$

Now have

$$\psi(\mathbf{x}) = h_{n_1}(y_1)h_{n_2}(y_2)h_{n_3}(y_3)\exp\left(-(y_1^2 + y_2^2 + y_3^2)/2\right)$$

Note $\exp\left(-(y_1^2 + y_2^2 + y_3^2)/2\right) = \exp(-\alpha r^2)$ for some constant α, ie. this term is spherically symmetrical. We just need to look at the hermite polynomials.

For $N := n_1 = n_2 = n_3 = 0$ (ground state), $h_0(y_i) =$ constant , so this is spherically symmetric. For a solution with $N = 2$, consider

$$
\begin{aligned}
\psi(\mathbf{x}) &= \psi_0(x_1)\psi_0(x_2)\psi_0(x_3) \\
&= A(1 - 2y_3^2)e^{-r^2/2}
\end{aligned}
$$

Now adding similar solutions gives

$$
\begin{aligned}
\psi(\mathbf{x}) &= A(1 - 2y_1^2 - 2y_2^2 - 2y_3^2)e^{-r^2/2} \\
&= A(1 - 2r^2)e^{-r^2/2}
\end{aligned}
$$

QUESTION 3

QUESTION 4

QUESTION 5

Laplacian for a spherically symmetric potential is

$$\begin{aligned}\nabla^2\psi &= \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}\psi}{\mathrm{d}r}\right)\\ &= \psi'' + \frac{2}{r}\psi'\end{aligned}$$

For $\psi(r) = Ce^{-r/a}$,

$$\begin{aligned}\nabla^2\psi &= \frac{1}{r^2}\left(\frac{r^2}{a^2} - \frac{1}{a}\right)\psi + \frac{2}{r}\left(\frac{-r}{a}\psi\right)\\ &= \left(\frac{1}{a^2} - \frac{2}{a}\right)\psi - \frac{1}{r^2a}\psi\\ &=\end{aligned}$$

QUESTION 6

For any any spherically symmetric wavefunction $\phi(r)$, we have that $L_3\phi = 0$.

$$\begin{aligned}
L_3\phi(r) &= -i\hbar\left(x_1\frac{\partial\phi(r)}{\partial x_2} - x_2\frac{\partial\phi(r)}{\partial x_1}\right)\\
&= -i\hbar\left(x_1\frac{\partial r}{\partial x_2}\phi'(r) - x_2\frac{\partial r}{\partial x_1}\phi'(r)\right)\\
&= -i\hbar\left(x_1\frac{x_2}{r}\phi'(r) - x_2\frac{x_1}{r}\phi'(r)\right)\\
&= 0
\end{aligned}$$

Note that $\frac{\partial\phi}{\partial x_i} = \frac{\phi'(r)}{r}x_i$.
Now,

$$\begin{aligned}
L_3[x_1\phi(r)] &= -i\hbar\left(x_1\frac{\partial[x_1\phi(r)]}{\partial x_2} - x_2\frac{\partial[x_1\phi(r)]}{\partial x_1}\right)\\
&= -i\hbar\left(x_1^2 x_2\frac{\phi'(r)}{r} - x_2\phi(r) - x_1^2 x_2\frac{\phi'(r)}{r}\right)\\
&= i\hbar x_2\phi(r)
\end{aligned}$$

Similarly,

$$L_3[x_2\phi(r)] = -i\hbar x_1\phi(r), \qquad L_3[x_3\phi(r)] = 0$$

We can use these results we calculate L_3^2

$$\begin{aligned}
L_3^2[x_1\phi(r)] &= i\hbar L[x_2\phi(r)]\\
&= i\hbar(-i\hbar x_1\phi(r))\\
&= \hbar^2 x_1\phi(r)
\end{aligned}$$

Similarly,

$$L_3^2[x_2\phi(r)] = \hbar^2 x_2\phi(r), \qquad L_3^2[x_3\phi(r)] = 0$$

The total angular momentum operator is

$$L^2 = L_1^2 + L_2^2 + L_3^2$$

We can use symmetry to deduce that

$$L_i^2[x_j\phi(r)] = \begin{cases}\hbar^2 x_j\phi(r) & \text{if } i \neq j\\ 0 & \text{if } i = j\end{cases}$$

Thus

$$L^2[x_j\phi(r)] = 2\hbar^2 x_j\phi(r)$$

ie. $\psi_i(\mathbf{x}) = x_j\phi(r)$ is an eigenfunction of L^2 with eigenvalue $2\hbar^2$.

Also, letting $\psi_{\pm}(\mathbf{x}) = x_1\phi(r) \pm x_2\phi(r)$

$$\begin{aligned} L_3[x_1\phi(r) \pm x_2\phi(r)] &= i\hbar[x_2\phi(r)] \mp i\hbar[x_1\phi(r)] \\ &= \pm i\hbar\psi_{\pm}(\mathbf{x}) \end{aligned}$$

ie. $\psi_{\pm}(\mathbf{x})$ are eigenvalues of L_3 with eigenvalues ± 1.

QUESTION 7

QUESTION 8

By the Leibniz property

$$\begin{aligned}[L_i, \mathbf{L}] &= [L_i, L_{jj}] \\ &= [L_i, L_j]L_j + L_j[L_i, L_j] \\ &= i\hbar\varepsilon_{ijk}(L_k L_j + L_j L_k) \\ &= 0\end{aligned}$$

for $i = 1, 2, 3$, and we get 0 since we are contracting the antisymmetric tensor ε_{ijk} with the symmetric tensor $L_k L_j + L_j L_k$.

QUESTION 9

Calculation shows

$$\begin{aligned}
[S_1, S_2] &= i\hbar S_3 \\
[S_2, S_3] &= i\hbar S_1 \\
[S_3, S_1] &= i\hbar S_2
\end{aligned}$$

ie. $[S_i, S_j] = \varepsilon_{ijk} i\hbar S_k$
Also find that

$$\begin{aligned}
S^2 &= S_1^2 + S_2^2 + S_3^2 \\
&= \frac{3\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\end{aligned}$$