# Part IB — Quantum Mechanics Example Sheet 3

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# QUESTION 1

When the particle is inside the box, the time independent Schrödinger Equation is

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

The Hamiltonian then splits into

$$H = H_1 + H_2 + H_3$$

where

$$H_i = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i^2}$$

The SE then gives (upon division by $\psi = \chi_1\chi_2\chi_3$)

$$\sum_{i=1}^{3} -\frac{\hbar^2}{2m}\frac{\chi_i''}{\chi_i} = E$$

Since each term is independent of the other two, we have

$$H_i\chi_i = E_i\chi_i$$

with

$$E_1 + E_2 + E_3 = E$$

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

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

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 $\alpha$, 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

$$\begin{aligned}
i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle Q\rangle_\Psi &= i\hbar\frac{\mathrm{d}}{\mathrm{d}t}(\Psi, Q\Psi) \\
&= i\hbar(\dot{\Psi}, Q\psi) + (\Psi, Q\dot{\psi}) \\
&= (-i\hbar\dot{\Psi}, Q\psi) + (\Psi, Qi\hbar\dot{\Psi}) \\
&= (-H\Psi, Q\Psi) + (\Psi, QH\Psi) \\
&= (\Psi, -HQ\Psi) + (\Psi, QH\Psi) \\
&= (\Psi, (QH - HQ)\Psi) \\
&= \langle [Q, H]\rangle_\Psi
\end{aligned}$$

In one dimension, Ehrenfest's Theorem showed that

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{x}\rangle_\Psi &= \frac{1}{m}\langle\hat{p}\rangle_\Psi \\
\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{p}\rangle_\Psi &= -\langle V'(\hat{x})\rangle_\Psi
\end{aligned}$$

Similarly, using the above result,

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\mathbf{x}}\rangle_\Psi = \langle[\hat{\mathbf{x}}, H]\rangle_\Psi$$

$$\begin{aligned}
[\hat{x}_i, H_i] &= -\frac{1}{2m}[\hat{x}_i, \hat{p}_i^2] + \underbrace{[\hat{x}_i, V(\hat{x}_i)]}_{=0} \\
&= -\frac{1}{2m}\left([\hat{x}_i, \hat{p}_i]\hat{p}_i + \hat{p}_i[\hat{x}_i, \hat{p}_i^2]\right) \\
&= -\frac{1}{2m}(-2i\hbar\hat{p}_i) \\
&= \frac{i\hbar}{m}\hat{p}_i
\end{aligned}$$

Thus

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\mathbf{x}}\rangle_\Psi = \frac{1}{m}\langle\hat{\mathbf{p}}\rangle_\Psi$$

Next,

$$\begin{aligned}
[\hat{p}_i, H_i]\Psi &= -\frac{1}{2m}\underbrace{[\hat{p}_i, \hat{p}_i^2]}_{=0}\Psi + [\hat{p}_i, V(\hat{x}_i)]\Psi \\
&= -i\hbar\frac{\partial}{\partial x_i}(V(\hat{x}_i)\Psi) - V(\hat{x}_i)(-i\hbar\frac{\partial\Psi}{\partial x}) \\
&= -i\hbar V'(\hat{x}_i)\Psi
\end{aligned}$$

Thus

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\mathbf{p}}\rangle_\Psi = -\langle V'(\hat{\mathbf{x}})\rangle_\Psi$$

# QUESTION 4

Suppose $A, B$ Hermitian. Then

$$\begin{aligned}
(\psi, i[A,B]\psi) &= (\psi, i(AB-BA)\psi) \\
&= (\psi, iAB\psi) - (\psi, iBA\psi) \\
&= (-iBA\psi, \psi) + (iAB\psi, \psi) \\
&= (i(AB-BA)\psi, \psi) \\
&= (i[A,B]\psi, \psi)
\end{aligned}$$

Hence $i[A,B]$ Hermitian.
Consider $||(A+i\lambda B)\psi||^2 \geq 0$.

$$\begin{aligned}
||(A+i\lambda B)\psi||^2 &= ((A+i\lambda B)\psi, (A+i\lambda B)\psi) \\
&= (A\psi, A\psi) + (A\psi, i\lambda B\psi) + (i\lambda B, A\psi) + (i\lambda B, i\lambda B) \\
&= (\psi, A^2\psi) + \lambda(\psi, iAB\psi) - \lambda(\psi, iBA\psi) + \lambda^2(\psi, B^2\psi) \\
&= \langle A^2\rangle_\psi + \lambda\langle i[A,B]\rangle_\psi + \lambda^2\langle B^2\rangle_\psi
\end{aligned}$$

Quadratic in $\lambda$, and is $\geq 0$, so discriminant must be negative, ie

$$|\langle i[A,B]\rangle_\psi|^2 \leq 4\left|\langle A^2\rangle_\psi\right|\left|\langle B^2\rangle_\psi\right|$$

showing the required result.
Have that $(\Delta A)^2_\psi = \langle A^2\rangle_\psi - \langle A\rangle^2_\psi$,

# 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 $\psi(r) = Ce^{-r/a}$, time indep SE becomes something easy, and you should get (use the fine structure const.)

Should get $a$ is the Bohr radius, $E$ is the ground energy state.

And $C = \left(\frac{1}{\pi a}\right)^{1/2}$, expected value

$$\frac{1}{4}\left(\frac{a}{\pi}\right)^{1/2}$$

can check this is more than the Bohr radius as $\alpha \approx 1/137$

# 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 $\frac{\partial\phi}{\partial x_i} = \frac{\phi'(r)}{r}x_i$.
Also $L_2\phi = L_1\phi = 0$
Now,

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

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 $\pm i\hbar$.

# QUESTION 7

SE

$$H = -\frac{\hbar}{2\mu}\nabla^2 + V(r)$$

# QUESTION 8

By the Leibnitz property

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

for $i = 1, 2, 3$, and we get 0 since we are contracting the antisymmetric tensor $\varepsilon_{ijk}$ with the symmetric tensor $L_kL_j + L_jL_k$.

# QUESTION 9

Calculation shows

$$[S_1, S_2] = i\hbar S_3$$
$$[S_2, S_3] = i\hbar S_1$$
$$[S_3, S_1] = i\hbar S_2$$

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

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