PAPER CODE NO.
MATH325

THE UNIVERSITY
of LIVERPOOL

JANUARY 2001 ANSWERS

QUANTUM MECHANICS

TIME ALLOWED : Two Hours and a Half

These are brief answers, just to allow you to check your own results. You should show much more working, and write more explanation, than you see here!

In this paper, bold-face quantities such as $\mathbf{r}$ represent three-dimensional vectors.

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1. *The normalised eigenfunctions of the Hamiltonian of a particle of mass m confined to the region of the x-axis between $x = 0$ and $x = L$ are*

$$\phi_n(x) = \begin{cases} A \sin \frac{n\pi x}{L} & : \quad 0 \le x \le L \\ 0 & : \quad x < 0 \quad or \quad x > L \end{cases}$$

where A is a real, positive normalisation constant and the corresponding energy eigenvalues are

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \qquad (n = 1, 2, 3 \ldots).$$

Find the value of A.

The particle is initially in the ground state *of this potential well of width L. Suddenly the well expands to twice its original size, the right wall moving from $x = L$ to $x = 2L$, leaving the wavefunction momentarily undisturbed. A measurement of the energy is now made.*

(a) Write down the wavefunction ψ of the particle in the modified potential (indicating its value for all *x).*

(b) By expressing ψ in terms of eigenfunctions of the modified system, find the probabilities for each possible result of the energy measurement. What is the most likely result?

(c) By using the result that

$$\sum_{n=1,3,5\ldots} \frac{1}{(n^2 - 4)^2} = \frac{\pi^2}{64},$$

verify that the probabilities evaluated in (b) do indeed add to 1.

(d) If the result of the energy measurement was in fact E_1', where

$$E_n' = \frac{\hbar^2 \pi^2 n^2}{8mL^2} \qquad (n = 1, 2, 3 \ldots),$$

what is the probability that a subsequent energy measurement will give E_2'?

[*For part (b), you may find it helpful to use the result:* $2 \sin A \sin B = \cos(A - B) - \cos(A + B)$].

To find A, require

$$\int_0^L |\phi_n(x)^2|\, dx = 1 \quad \Rightarrow \quad |A^2|\, \frac{L}{2} = 1 \quad \Rightarrow \quad A = \sqrt{\frac{2}{L}}.$$

(a) Initial wave-function is the ground state ($n = 1$) of the box of length L,

$$\psi(x) = \begin{cases} \sqrt{\frac{2}{L}}\, \sin\frac{\pi x}{L} & : \quad 0 \le x \le L \\ 0 & : \quad x < 0 \quad \text{or} \quad x > L \end{cases}$$

(b) We get the eigenfunctions in the new box by changing L to $2L$ in the formula for ϕ_n.

$$\phi_n'(x) = \begin{cases} \frac{1}{\sqrt{L}}\, \sin\frac{n\pi x}{2L} & : \quad 0 \le x \le 2L \\ 0 & : \quad x < 0 \quad \text{or} \quad x > 2L \end{cases}$$

Writing $\psi(x) = \sum_n c_n \phi_n'(x)$ we find the c_n from the scalar product (or overlap integral)

$$c_n = \langle \phi_n' | \psi \rangle = \int_0^{2L} \phi_n'^*(x)\psi(x)\, dx = \frac{\sqrt{2}}{L} \int_0^L \sin\frac{n\pi x}{2L} \sin\frac{\pi x}{L}\, dx + \int_L^{2L} 0\, dx$$

Using the hint gives

$$c_n = \begin{cases} \dfrac{4\sqrt{2}\, \sin\frac{n\pi}{2}}{\pi(4 - n^2)} & n \ne 2 \\ \\ \dfrac{1}{\sqrt{2}} & n = 2 \end{cases}$$

The probabilities are

$$P(n) = |c_n|^2 = \begin{cases} \dfrac{32}{\pi^2(n^2 - 4)^2} & \text{n odd} \\ \frac{1}{2} & \text{n} = 2 \\ 0 & \text{otherwise} \end{cases}$$

The most likely result is that $n = 2$.

(c)

$$\sum_n |c_n|^2 = \frac{1}{2} + \frac{32}{\pi^2} \sum_{n=1,3,5\ldots} \frac{1}{(n^2-4)^2} = \frac{1}{2} + \frac{32}{\pi^2}\frac{\pi^2}{64} = 1$$

(d) The probability is zero: the only possible outcome of subsequent measurements is E_1'.

Reason: Immediately after a measurement that gives E_1' the wave-function is $\psi = \phi_1'$. If we evolve this in time we get

$$\psi(x,t) = \phi_1'(x) e^{-i\omega_1' t} \qquad \text{where} \;\; \hbar\omega_1' = E_1'.$$

ψ is proportional to ϕ_1', so measurements are 100% sure to give E_1' , all other results are impossible.

2. *A beam of particles of mass m and energy E is incident in the positive x direction on a potential well whose potential V is given by*

$$V(x) = \begin{cases} 0 & : \quad x < 0 \qquad \textit{(region I)} \\ -V_0 & : \quad 0 \le x \le a \quad \textit{(region II)} \\ 0 & : \quad x > a \qquad \textit{(region III)} \end{cases}$$

where $E > 0$ and $V_0 > 0$.

(a) Show that the particle wave function in the x regions defined above can be written

$$\begin{aligned} \psi_{\mathrm{I}} &= Ae^{iKx} + Be^{-iKx} \\ \psi_{\mathrm{II}} &= Ce^{iqx} + De^{-iqx} \\ \psi_{\mathrm{III}} &= Fe^{iKx} \end{aligned}$$

where you should find expressions for K and q.

(b) State the conditions on the particle wave function ψ and its derivative ψ' which must be satisfied at the boundaries between regions I, II and III and use these to show that

$$\frac{A}{F} = \frac{(K+q)^2 e^{i(K-q)a} - (K-q)^2 e^{i(K+q)a}}{4Kq} .$$

(c) The incident particle current density for the above scattering problem is defined by

$$j_I = \frac{\hbar K}{m} |A|^2 .$$

Give the corresponding expressions for the reflected and transmitted particle current densities j_R and j_T. Hence define the reflection and transmission coefficients R and T.

(d) Use the result of part (b) to evaluate the transmission coefficient T in the case when $qa = n\pi$ (where n is some integer). Without explicitly evaluating it, state what the value of R will be, giving reasons.

2.(a) The Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

and its eigenvalue equation is $\hat{H}\psi = E\psi$.

In region I or region III the potential is 0 and the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x)$$

which has the solutions

$$\psi(x) = e^{\pm iKx} \quad \text{where } K^2 = \frac{2mE}{\hbar^2} \text{ if } \; E \geq 0.$$

In region I both solutions will be present, so we write

$$\psi_{\text{I}}(x) = Ae^{iKx} + Be^{-iKx}$$

which is the general solution of the Schrödinger equation. In region III there will be no e^{-iKx} term present because there is no source of incoming particles from large x (we are told in the question that the incoming beam is travelling in the positive x direction).

$$\psi_{\text{III}}(x) = Fe^{iKx}.$$

In region II the potential is $-V_0$ and the Schrödinger equation is

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V_0\right)\psi(x) = E\psi(x) \quad \Rightarrow \quad -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = (E+V_0)\psi(x)$$

which has the solutions

$$\psi(x) = e^{\pm iqx} \quad \text{where } q^2 = \frac{2m(E+V_0)}{\hbar^2} \text{ if } \; E+V_0 \geq 0.$$

The general solution in region II is

$$\psi_{\text{II}}(x) = Ce^{iqx} + De^{-iqx}.$$

(b) Both ψ and ψ' must be continuous at $x = 0$ and $x = a$.

There are only 3 unknowns at the $x = a$ boundary, but 4 at $x = 0$, so it is probably easiest to start at $x = a$. There we have to solve the simultaneous equations

$$\begin{aligned} \psi_{\text{II}}(a) = \psi_{\text{III}}(a) \quad &\Rightarrow \quad Ce^{iqa} + De^{-iqa} = Fe^{iKa} \\ \psi'_{\text{II}}(a) = \psi'_{\text{III}}(a) \quad &\Rightarrow \quad q(Ce^{iqa} - De^{-iqa}) = KFe^{iKa} \end{aligned}$$

which has the solutions

$$\begin{aligned} Ce^{iqa} &= \frac{q+K}{2q}Fe^{iKa} \\ De^{-iqa} &= \frac{q-K}{2q}Fe^{iKa}\,. \end{aligned}$$

The continuity equations at $x = 0$ read

$$\begin{aligned}
\psi_{\mathrm{I}}(0) = \psi_{\mathrm{II}}(0) \quad &\Rightarrow \quad A + B = C + D \\
\psi'_{\mathrm{I}}(0) = \psi'_{\mathrm{II}}(0) \quad &\Rightarrow \quad K(A - B) = q(C - D)
\end{aligned}$$

Solving these equations for A gives

$$2KA = (K+q)C + (K-q)D = \frac{(K+q)^2}{2q} e^{i(K-q)a} F - \frac{(K-q)^2}{2q} e^{i(K+q)a} F$$

$$\Rightarrow \frac{A}{F} = \frac{(K+q)^2 \, e^{i(K-q)a} - (K-q)^2 \, e^{i(K+q)a}}{4Kq}$$

as required.

(c)

$$\begin{aligned}
j_R &= \frac{\hbar K}{m} |B|^2 \\
j_T &= \frac{\hbar K}{m} |F|^2 \\
R &= \frac{j_R}{j_I} = \frac{|B|^2}{|A|^2} \\
T &= \frac{j_T}{j_I} = \frac{|F|^2}{|A|^2}
\end{aligned}$$

(d) If $qa = n\pi$ the result from (b) becomes

$$\frac{A}{F} = e^{i(Ka - n\pi)} \, \frac{(K+q)^2 - (K-q)^2 \, e^{i2n\pi}}{4Kq} = e^{i(Ka - n\pi)}$$

because $e^{i2n\pi} = 1$. This gives

$$T = \left| \frac{F}{A} \right|^2 = 1.$$

If $T = 1$ we expect $R = 0$ by conservation of probability flux j.

3.(i) *The Hamiltonian of a particle undergoing simple harmonic motion in one dimension is given by*

$$\hat{H} = \frac{\hat{p}^2}{2m} + \tfrac{1}{2}m\omega^2\hat{x}^2$$

and ϕ_0 *is the normalised ground state wave function such that* $a\phi_0 = 0$ *where*

$$a = \frac{\alpha}{\sqrt{2}}\left(\frac{1}{m\omega}\hat{p} - i\hat{x}\right), \qquad \alpha^2 = \frac{m\omega}{\hbar}.$$

(a) Given that $[\hat{x}, \hat{p}] = i\hbar$, *show that* $[a, a^\dagger] = 1$.

(b) Show that one may write the Hamiltonian in the form

$$\hat{H} = \hbar\omega(a^\dagger a + \tfrac{1}{2})$$

and hence find the eigenvalue corresponding to the groundstate wave function ϕ_0.

(c) Show that $\phi_1 = Aa^\dagger\phi_0$ *is also an eigenfunction of* $\hat{H}$ *and find the associated eigenvalue. [Here,* A *is a normalisation constant.]*

(d) Given that the properly normalised ground state wave function is

$$\phi_0 = \sqrt{\frac{\alpha}{\sqrt{\pi}}}e^{-\frac{1}{2}\alpha^2x^2},$$

obtain the properly normalised eigenfunction $\phi_1(x)$.

(ii) Establish, giving reasons, which of the following operators could represent quantum mechanical observables:

$$\hat{A} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{B} = \begin{pmatrix} 0 & i \\ -i & 2 \end{pmatrix}, \quad \hat{C} = x\frac{d}{dx}, \quad \hat{D} = i(x\frac{d}{dx} + \tfrac{1}{2})$$

where the space of wave functions $\psi(x)$ *acted upon by* $\hat{C}$ *and* $\hat{D}$ *is such that* $a \leq x \leq b$ *and* $\psi(a) = \psi(b) = 0$.

3.(i)

$$a = \frac{\alpha}{\sqrt{2}}(\frac{1}{m\omega}\hat{p} - i\hat{x}) \quad \Rightarrow \quad a^\dagger = \frac{\alpha}{\sqrt{2}}(\frac{1}{m\omega}\hat{p}^\dagger + i\hat{x}^\dagger) = \frac{\alpha}{\sqrt{2}}(\frac{1}{m\omega}\hat{p} + i\hat{x})$$

because $\hat{p}$ and $\hat{x}$ are both Hermitian.

$$\begin{aligned}[a, a^\dagger] = aa^\dagger - a^\dagger a &= \frac{\alpha^2}{2}\left\{\left(\frac{\hat{p}}{m\omega}\right)^2 + \frac{\hat{p}}{m\omega}i\hat{x} - i\hat{x}\frac{\hat{p}}{m\omega} + \hat{x}^2 - \left(\frac{\hat{p}}{m\omega}\right)^2 - i\hat{x}\frac{\hat{p}}{m\omega} + \frac{\hat{p}}{m\omega}i\hat{x} - \hat{x}^2\right\} \\ &= -i\frac{\alpha^2}{m\omega}[\hat{x}, \hat{p}] = 1\end{aligned}$$

(b)

$$\begin{aligned}a^\dagger a &= \frac{\alpha^2}{2}\left\{\left(\frac{\hat{p}}{m\omega}\right)^2 - \frac{\hat{p}}{m\omega}i\hat{x} + i\hat{x}\frac{\hat{p}}{m\omega} + \hat{x}^2\right\} = \frac{\hat{p}^2}{2m\hbar\omega} + \frac{i[\hat{x}, \hat{p}]}{2\hbar} + \frac{m\omega}{2\hbar}\hat{x}^2 = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2} \\ \Rightarrow \hat{H} &= \hbar\omega(a^\dagger a + \tfrac{1}{2}). \\ \hat{H}\phi_0 &= \hbar\omega a^\dagger a\phi_0 + \tfrac{1}{2}\hbar\omega\phi_0 = 0 + \tfrac{1}{2}\hbar\omega\phi_0\end{aligned}$$

so the eigenvalue is $E_0 = \frac{1}{2}\hbar\omega$.

(c)

$$\hat{H}Aa^\dagger\phi_0 = A\hbar\omega(a^\dagger aa^\dagger + \tfrac{1}{2}a^\dagger)\phi_0 = A\hbar\omega a^\dagger(aa^\dagger + \tfrac{1}{2})\phi_0 = A\hbar\omega a^\dagger(a^\dagger a + \tfrac{3}{2})\phi_0 = \tfrac{3}{2}\hbar\omega Aa^\dagger\phi_0$$

so $\phi_1 = Aa^\dagger\phi_0$ is an eigenfunction of $\hat{H}$ with eigenvalue $E_1 = \frac{3}{2}\hbar\omega$.

(d) First find A

$$\langle\phi_1|\phi_1\rangle = |A|^2\langle\phi_0|aa^\dagger\phi_0\rangle = |A|^2\langle\phi_0|(a^\dagger a + 1)\phi_0\rangle = |A|^2\langle\phi_0|\phi_0\rangle \quad \Rightarrow |A| = 1.$$

$$\phi_1 = a^\dagger\phi_0 = \frac{\alpha}{\sqrt{2}}\left(-i\frac{\hbar}{m\omega}\frac{d}{dx} + ix\right)\phi_0 = i\left(\frac{4\alpha^6}{\pi}\right)^{\frac{1}{4}} xe^{-\frac{1}{2}\alpha^2x^2}.$$

3.(ii) The matrices $\hat{A}$ and $\hat{B}$ are both Hermitian, so they could represent observables.

Integrating by parts

$$\langle\hat{C}\psi|\phi\rangle = -\langle\psi|\phi\rangle - \langle\psi|\hat{C}\phi\rangle \neq \langle\psi|\hat{C}\phi\rangle$$

so $\hat{C}$ is *not* Hermitian, so it could *not* represent an observable.

For $\hat{D}$, integrating by parts gives $\langle\hat{D}\psi|\phi\rangle = \langle\psi|\hat{D}\phi\rangle$ so $\hat{D}$ *is* Hermitian, and it can represent an observable.

4. *Given that the angular momentum operators* L_i $(i = 1, 2, 3)$ *satisfy the commutation relations* $[L_1, L_2] = i\hbar L_3$ *(and cyclic permutations), show that*

$$[\mathbf{L}^2, L_1] = [\mathbf{L}^2, L_2] = [\mathbf{L}^2, L_3] = 0\,,$$

where $\mathbf{L}^2 = L_1^2 + L_2^2 + L_3^2$.

*From the above commutation relations it is possible to deduce the following results (*which you may assume*). There exist normalised eigenfunctions* $|l, m\rangle$ *such that*

$$L_3|l, m\rangle = \hbar m|l, m\rangle, \qquad \mathbf{L}^2|l, m\rangle = \hbar^2 l(l + 1)|l, m\rangle,$$

where $2l$ *is a positive integer and the possible values of* m *are* $-l, -l + 1, \ldots l - 1, l$. *Moreover,*

$$L_+|l, m\rangle = M_{l,m}|l, m + 1\rangle \quad \textit{and} \quad L_-|l, m\rangle = N_{l,m}|l, m - 1\rangle,$$

where $L_+ = L_1 + iL_2$ *and* $L_- = L_1 - iL_2$*, and* $M_{l,m}$ *and* $N_{l,m}$ *are real, positive constants.*

(a) Show that

$$L_-L_+ = \mathbf{L}^2 - L_3^2 - \hbar L_3$$

and, by considering the norm of $L_+|l, m\rangle$*, show that*

$$M_{l,m} = \hbar\sqrt{l(l + 1) - m(m + 1)}\,.$$

(b) A particle is in the normalised angular momentum state

$$|\psi\rangle = A(|1, -1\rangle + |1, 1\rangle - 2|1, 0\rangle)$$

where A *is a real normalisation constant which you should find. By expressing* L_1 *in terms of* L_+ *and* L_-*, find the expectation values* $\langle L_1\rangle$ *and* $\langle L_1^2\rangle$ *for this state. Hence find the standard deviation* ΔL_1 *for this state.* $((\Delta A)^2 \equiv \langle (A - \langle A\rangle)^2\rangle$ *.)*

[*You may assume that*

$$N_{l,m} = \hbar\sqrt{l(l + 1) - m(m - 1)} \quad \textit{and} \quad L_+L_- = \mathbf{L}^2 - L_3^2 + \hbar L_3\,.]$$

4. Doing this case by case:

$$[\mathbf{L}^2, L_1] = [L_1^2, L_1] + [L_2^2, L_1] + [L_3^2, L_1] = 0 + [L_2^2, L_1] + [L_3^2, L_1].$$

There are many ways to check that this is zero, here is one (don't worry if your method was a bit different).

Look first at the $[L_2^2, L_1]$ term, and "push" the L_1 operator through to the back:

$$\begin{aligned}
[L_2^2, L_1] &= L_2^2 L_1 - L_1 L_2^2 \\
&= L_2^2 L_1 - L_2 L_1 L_2 - [L_1, L_2] L_2 \\
&= L_2^2 L_1 - L_2^2 L_1 - L_2 [L_1, L_2] - [L_1, L_2] L_2 \\
&= -i\hbar L_2 L_3 - i\hbar L_3 L_2
\end{aligned}$$

Similarly

$$\begin{aligned}
& [L_3^2, L_1] = \cdots = +i\hbar L_3 L_2 + i\hbar L_2 L_3 \\
\Rightarrow \quad & [L_2^2, L_1] + [L_3^2, L_1] = 0 \\
\Rightarrow \quad & [\mathbf{L}^2, L_1] = 0.
\end{aligned}$$

Repeat for $[\mathbf{L}^2, L_2]$ and $[\mathbf{L}^2, L_3]$ (or say that they are clearly also 0 by symmetry).

The quickest method, if you are confident with the ε_{ijk} symbol, is to do everything in one go by considering $[L_i^2, L_j]$.

(a) $$\begin{aligned}
L_- L_+ = (L_1 - iL_2)(L_1 + iL_2) &= L_1^2 + iL_1 L_2 - iL_2 L_1 + L_2^2 \\
&= L_1^2 + L_2^2 + i[L_1, L_2] \\
&= \mathbf{L}^2 - L_3^2 - \hbar L_3
\end{aligned}$$

The norm of $L_+|l,m\rangle$ is $\langle l,m|L_+^\dagger L_+|l,m\rangle = \langle l,m|L_- L_+|l,m\rangle$.

$$\langle l,m|L_- L_+|l,m\rangle = \langle l,m|(\mathbf{L}^2 - L_3^2 - \hbar L_3)|l,m\rangle = \hbar^2 \left\{ l(l+1) - m^2 - m \right\}.$$

Because $L_+|l,m\rangle$ can also be written $M_{l,m}|l,m+1\rangle$,

$$M_{l,m}^2 = \hbar^2 \{ l(l+1) - m(m+1) \}.$$

(b) $$\langle\psi|\psi\rangle = |A|^2 \left(1^2 + 1^2 + (-2)^2\right) \quad \Rightarrow \quad A = \frac{1}{\sqrt{6}}.$$

From the definitions of L_+ and L_- we find $L_1 = \frac{1}{2}(L_+ + L_-)$.

$$\begin{aligned}
L_1|\psi\rangle &= \tfrac{1}{2}(L_+ + L_-)|\psi\rangle \\
&= \frac{A}{2}\Big(L_+|1,-1\rangle + L_+|1,1\rangle - 2L_+|1,0\rangle + L_-|1,-1\rangle + L_-|1,1\rangle - 2L_-|1,0\rangle\Big) \\
&= \frac{A}{2}\Big(M_{1,-1}|1,0\rangle + M_{1,1}|1,2\rangle - 2M_{1,0}|1,1\rangle + N_{1,-1}|1,-2\rangle + N_{1,1}|1,0\rangle - 2N_{1,0}|1,-1\rangle\Big) \\
&= \frac{A}{2}\hbar\sqrt{2}\Big(|1,0\rangle + 0 - 2|1,1\rangle + 0 + |1,0\rangle - 2|1,-1\rangle\Big) \\
&= \frac{\hbar}{\sqrt{3}}\Big(- |1,-1\rangle + |1,0\rangle - |1,1\rangle\Big)
\end{aligned}$$

We can now work out the expectation values,

$$
\begin{aligned}
\langle L_1 \rangle &= \langle \psi | L_1 | \psi \rangle \\
&= \frac{1}{\sqrt{6}} \frac{\hbar}{\sqrt{3}} \Big(\langle 1,-1| - 2\langle 1,0| + \langle 1,1| \Big) \cdot \Big(-|1,-1\rangle + |1,0\rangle - |1,1\rangle \Big) \\
&= -\hbar \, \frac{\sqrt{8}}{3}. \\
\langle L_1^2 \rangle &= \langle \psi | L_1 L_1 | \psi \rangle \\
&= \frac{\hbar^2}{3} \Big(-\langle 1,-1| + \langle 1,0| - \langle 1,1| \Big) \cdot \Big(-|1,-1\rangle + |1,0\rangle - |1,1\rangle \Big) \\
&= \hbar^2 \, . \\
\Delta L_1 &= \sqrt{\langle L_1^2 \rangle - \langle L_1 \rangle^2} = \frac{\hbar}{3} \, .
\end{aligned}
$$

5. *The Hamiltonian for a stationary electron of mass m and charge e in a constant magnetic field B along the z-axis is given by*

$$\hat{H} = \hbar\omega\sigma_3$$

where

$$\omega = \frac{eB}{2m} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

(a) By solving Schrödinger's equation, show that at time t the state of the electron is given by

$$\psi(t) = \begin{pmatrix} ae^{-i\omega t} \\ \\ be^{i\omega t} \end{pmatrix},$$

where a, b are constants.

(b) An observable $\hat{O}$ is represented by

$$\hat{O} = \gamma \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

where γ is a real constant. Compute the eigenvalues and normalised eigenvectors of $\hat{O}$ and deduce the possible results of a measurement of $\hat{O}$.

(c) At $t = 0$, the electron is in the state

$$\psi(0) = \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix} .$$

By writing $\psi(t)$ as a linear combination of the eigenvectors of $\hat{O}$, find the probabilities of each possible result of a measurement of $\hat{O}$ at time t.

What is the effect on the system of such a measurement?

5.(a)

Write the wave-function as a two-component vector $\psi(t) = \begin{pmatrix} \psi_1(t) \\ \psi_2(t) \end{pmatrix}$

The Schrödinger equation is

$$i\hbar\frac{d}{dt}\psi(t) = H\psi(t) \quad \Rightarrow i\hbar\frac{d}{dt}\begin{pmatrix} \psi_1(t) \\ \psi_2(t) \end{pmatrix} = \hbar\omega\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \psi_1(t) \\ \psi_2(t) \end{pmatrix}$$

This splits into two independent equations

$$i\frac{d}{dt}\psi_1(t) = +\omega\psi_1(t) \quad \text{and} \quad i\frac{d}{dt}\psi_2(t) = -\omega\psi_2(t)$$

The general solutions are $\psi_1(t) = ae^{-i\omega t}$ and $\psi_2(t) = be^{i\omega t}$, where a and b are complex constants. Therefore the general solution of Schrödinger's equation is

$$\psi(t) = \begin{pmatrix} ae^{-i\omega t} \\ \\ be^{i\omega t} \end{pmatrix},$$

(b) Finding the eigenvalues of a 2×2 matrix should be easy by now, the results are

$$\begin{aligned} \lambda_1 = 3\gamma \qquad & \text{with eigenvector} \quad \phi_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ \text{and} \quad \lambda_2 = \gamma \qquad & \text{with eigenvector} \quad \phi_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \end{aligned}$$

The possible outcomes of a measurement are the operator's eigenvalues, (3γ or γ).
(c) At $t = 0$

$$\psi(0) = \frac{1}{\sqrt{2}}\begin{pmatrix} i \\ 1 \end{pmatrix}.$$

so $a = i/\sqrt{2}$ and $b = 1/\sqrt{2}$.

$$\psi(t) = \frac{1}{\sqrt{2}}\begin{pmatrix} i\, e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix}$$

We want to express $\psi(t)$ as a combination of eigenvectors of $\hat{O}$, $\psi(t) = c_1\phi_1 + c_2\phi_2$. The coefficients are given by

$$\begin{aligned} c_1 &= \langle\phi_1|\psi(t)\rangle = \phi_1^\dagger \cdot \psi(t) = \frac{1}{2}\begin{pmatrix} 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} i\, e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix} = \frac{1}{2}\left(i\, e^{-i\omega t} + e^{i\omega t}\right), \\ c_2 &= \langle\phi_2|\psi(t)\rangle = \phi_2^\dagger \cdot \psi(t) = \frac{1}{2}\begin{pmatrix} 1 & -1 \end{pmatrix} \cdot \begin{pmatrix} i\, e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix} = \frac{1}{2}\left(i\, e^{-i\omega t} - e^{i\omega t}\right). \end{aligned}$$

The probability of getting result λ_i is $|c_i|^2$.

$$\begin{aligned} P(3\gamma) &= |c_1|^2 = c_1^* c_1 = \tfrac{1}{4}\left(-i\, e^{i\omega t} + e^{-i\omega t}\right)\left(i\, e^{-i\omega t} + e^{i\omega t}\right) = \tfrac{1}{2}(1 + \sin 2\omega t) \\ P(\gamma) &= |c_2|^2 = c_2^* c_2 = \tfrac{1}{4}\left(-i\, e^{i\omega t} - e^{-i\omega t}\right)\left(i\, e^{-i\omega t} - e^{i\omega t}\right) = \tfrac{1}{2}(1 - \sin 2\omega t) \end{aligned}$$

After a measurement the wave-function "collapses" to the corresponding eigenvector (ϕ_i if the outcome is λ_i.)

6(i) *Use integration by parts to show that for* $n \geq 2$

$$I_{n-2} = \frac{2\beta^2}{n-1} I_n\,, \qquad \textit{where} \quad I_n \equiv \int_0^\infty r^n e^{-\beta^2 r^2}\, dr\,.$$

Given that

$$I_0 = \frac{\sqrt{\pi}}{2\beta}\,,$$

find I_2*. Evaluate* I_1 *and deduce the value of* I_3*.*

[6 marks]

(ii) The Hamiltonian for a particle of mass m *moving in three dimensions under the influence of a three-dimensional harmonic oscillator potential is*

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \tfrac{1}{2}m\omega^2 r^2\,,$$

where $r = |\mathbf{r}| = \sqrt{x^2+y^2+z^2}$ *and the radial part of the Laplacian operator is*

$$\nabla^2_{\text{rad}} = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}.$$

(a) Given that the normalised ground state wave function is

$$\psi_0(\mathbf{r}) = Ae^{-\frac{1}{2}\beta^2 r^2}$$

where A *is real, determine* β *and the ground state energy* E_0*.*

(b) Calculate the normalisation constant A*.*

(c) The potential is perturbed by the addition of a term λH_1 *where*

$$H_1(r) = r^3\Big(\frac{m\omega}{\hbar}\Big)^{\frac{3}{2}} \qquad \textit{and } \lambda \textit{ is small.}$$

Show that, to first order in λ*, the perturbed ground state energy can be written in the form*

$$\tfrac{3}{2}\hbar\omega + \lambda K$$

where K *is a numerical constant which you should find.*

[14 marks]

[*Standard results from perturbation theory may be assumed without proof.*]

5.(i) Proof:

$$I_{n-2} = \int_0^\infty r^{n-2} e^{-\beta^2 r^2}\, dr = \left[\frac{r^{n-1}}{n-1} e^{-\beta^2 r^2}\right]_0^\infty - \int_0^\infty \frac{r^{n-1}}{n-1}(-2\beta^2 r) e^{-\beta^2 r^2}\, dr = \frac{2\beta^2}{n-1} I_n$$

To find I_1, make the substitution $r^2 = u$

$$I_1 = \int_0^\infty r e^{-\beta^2 r^2}\, dr = \frac{1}{2}\int_0^\infty e^{-\beta^2 u}\, du = -\frac{1}{2\beta^2}\left[e^{-\beta^2 u}\right]_0^\infty = \frac{1}{2\beta^2}$$

From the recursion formula

$$I_2 = \frac{1}{2\beta^2} I_0 = \frac{\sqrt{\pi}}{4\beta^3}, \quad I_3 = \frac{2}{2\beta^2}\, I_1 = \frac{1}{2\beta^4}$$

(ii)(a) To find β and E_0 we plug the wave-function into Schrödinger's equation.

$$\begin{aligned}
& \hat{H}\psi_0(\mathbf{r}) = E_0\psi_0(\mathbf{r}) \\
\Rightarrow \quad & -\frac{\hbar^2}{2m}\nabla^2\psi_0(\mathbf{r}) + \frac{1}{2}m\omega^2 r^2 \psi_0(\mathbf{r}) = E_0\psi_0(\mathbf{r}) \\
\Rightarrow \quad & -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) A e^{-\frac{1}{2}\beta^2 r^2} + \frac{1}{2}m\omega^2 r^2 A e^{-\frac{1}{2}\beta^2 r^2} = E_0 A e^{-\frac{1}{2}\beta^2 r^2} \\
\Rightarrow \quad & \frac{\hbar^2}{2m}3\beta^2 e^{-\frac{1}{2}\beta^2 r^2} - \frac{\hbar^2}{2m}\beta^4 r^2 e^{-\frac{1}{2}\beta^2 r^2} + \frac{1}{2}m\omega^2 r^2 e^{-\frac{1}{2}\beta^2 r^2} = E_0 e^{-\frac{1}{2}\beta^2 r^2} \\
\Rightarrow \quad & \frac{\hbar^2}{2m}3\beta^2 - \frac{\hbar^2}{2m}\beta^4 r^2 + \frac{1}{2}m\omega^2 r^2 = E_0
\end{aligned}$$

Equating coefficients (to make this equation true for all r) gives

$$\beta^4 = \frac{m^2\omega^2}{\hbar^2} \quad \Rightarrow \quad \beta = \sqrt{\frac{m\omega}{\hbar}}$$

and

$$E_0 = \frac{3}{2}\frac{\hbar^2}{m}\beta^2 = \frac{3}{2}\hbar\omega.$$

(b) We now know β and E_0. To find A we impose

$$\int_0^\infty 4\pi r^2 |\psi_0|^2\, dr = 1 \quad \Rightarrow \quad 4\pi |A|^2 \int_0^\infty r^2 e^{-\beta^2 r^2}\, dr = 1 \quad \Rightarrow \quad 4\pi|A|^2 I_2 = 1.$$

From the recursion relation

$$I_2 = \frac{1}{2\beta^2} I_0 = \frac{\sqrt{\pi}}{4\beta^3}$$

so

$$|A|^2 \frac{\pi^{\frac{3}{2}}}{\beta^3} = 1 \qquad \Rightarrow A = \frac{\beta^{\frac{3}{2}}}{\pi^{\frac{3}{4}}} = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{3}{4}}$$

(c) The oscillator is perturbed by adding a term

$$\lambda H_1 = \lambda r^3 \left(\frac{m\omega}{\hbar}\right)^{\frac{3}{2}} = \lambda\beta^3 r^3.$$

We remember the first-order perturbation formula

$$\mathcal{E}_n = E_n + \langle\psi_n|\lambda H_1 \psi_n\rangle + O(\lambda^2)$$

Applying this to the ground state

$$\begin{aligned}
\langle\psi_0|\lambda H_1\psi_0\rangle &= \lambda\beta^3|A|^2 \int_0^\infty dr\; 4\pi r^2 e^{-\beta^2 r^2} r^3 = \lambda\beta^3|A|^2 4\pi\, I_5 = \lambda\frac{4}{\sqrt{\pi}} \\
\Rightarrow \mathcal{E}_0 &= \frac{3}{2}\hbar\omega + \lambda\frac{4}{\sqrt{\pi}} + O(\lambda^2) \qquad \Rightarrow \quad K = \frac{4}{\sqrt{\pi}}.
\end{aligned}$$

7. *An arbitrary, normalised wave function* ψ *is expanded in terms of orthogonal, normalised eigenfunctions* ϕ_n *of the Hamiltonian* $\hat{H}$*:*

$$\psi = \sum_n c_n \phi_n \qquad \hat{H}\phi_n = E_n \phi_n$$

and the eigenfunctions are ordered so that $E_0 \leq E_1 \leq E_2 \ldots$.

Show that

$$E_0 \leq \langle \psi | \hat{H} \psi \rangle$$

and use this result to explain the variational method for estimating an upper bound on the ground state energy of a system with Hamiltonian $\hat{H}$.

A particle of mass m *moves on the* x*-axis subject to a potential* $V(x) = \eta|x|$*, where* η *is a positive constant.*

(i) Normalise the trial wave function $\psi(x) = Ae^{-\frac{1}{2}\beta^2 x^2}$*, (i.e. find* A*) and show that*

$$\langle \psi | \hat{H} \psi \rangle = \frac{\hbar^2 \beta^2}{4m} + \frac{\eta}{\sqrt{\pi}\beta}.$$

(ii) Hence use the variational method to show that the ground state energy is at most

$$E_0^{\max} = \tfrac{3}{2}\left(\frac{\hbar^2 \eta^2}{2m\pi}\right)^{\frac{1}{3}}.$$

How might you improve on this estimate of the ground state energy and how would you know if you had succeeded?

You may use the results:

$$\int_{-\infty}^{\infty} e^{-\beta^2 x^2}\,dx = \frac{\sqrt{\pi}}{\beta}, \qquad \int_{-\infty}^{\infty} x^2 e^{-\beta^2 x^2}\,dx = \frac{\sqrt{\pi}}{2\beta^3}.$$

7. Write the wavefunction ψ as a sum over the eigenfunctions of $\hat{H}$,

$$\psi = \sum_n a_n \phi_n.$$

If ψ and ϕ_n are properly normalised $\sum_n |a_n|^2 = 1$. The expectation value of $\hat{H}$ is

$$\begin{aligned}
\langle \hat{H} \rangle = \langle \psi | \hat{H} \psi \rangle &= \sum_n |a_n|^2 E_n \\
&= E_0 \sum_n |a_n|^2 + \sum_n |a_n|^2 (E_n - E_0) \\
&= E_0 + \sum_n |a_n|^2 (E_n - E_0) \geq E_0
\end{aligned}$$

because $(E_n - E_0) \geq 0$ and $|a_n|^2 \geq 0$.

We can use this to get an upper estimate on E_0. Choose a trial wave function ψ with some free parameters, and minimise $\langle \psi | \hat{H} \psi \rangle$ w.r.t. the parameters. This minimum value of $\langle \hat{H} \rangle$ is an upper bound on the ground state energy, which is usually close to the true E_0.

(i) Find A:

$$\int_{-\infty}^{\infty} dx |\psi|^2 = 1 \qquad \Rightarrow \qquad A = \sqrt{\frac{\beta}{\sqrt{\pi}}}$$

Find $\langle \hat{H} \rangle$:

$$\begin{aligned}
\langle T \rangle &= \frac{1}{2m} \int_{-\infty}^{\infty} dx \ |\hat{p}\psi|^2 = \cdots = \frac{\hbar^2 \beta^2}{4m} \\
\langle V \rangle &= \int_{-\infty}^{\infty} dx \ |\psi|^2 \eta |x| = 2 \int_0^{\infty} dx \ |\psi|^2 \eta x = \cdots = \frac{\eta}{\beta\sqrt{\pi}} \\
\Rightarrow \langle \psi | \hat{H} \psi \rangle &= \frac{\hbar^2 \beta^2}{4m} + \frac{\eta}{\beta \sqrt{\pi}}.
\end{aligned}$$

(ii) Minimise $\langle \psi | \hat{H} \psi \rangle$ wrt β:

$$\frac{\hbar^2 \beta}{2m} - \frac{\eta}{\beta^2 \sqrt{\pi}} = 0 \qquad \Rightarrow \qquad \beta = \left(\frac{4\eta^2 m^2}{\hbar^4 \pi} \right)^{\frac{1}{6}}$$

So the minimum expectation value is

$$\langle \psi | \hat{H} \psi \rangle_{min} = \frac{3}{2} \left(\frac{\eta^2 \hbar^2}{2\pi m} \right)^{\frac{1}{3}} = 0.812889 \ \left(\frac{\eta^2 \hbar^2}{m} \right)^{\frac{1}{3}}.$$

To get a better estimate one could try a trial function with more free parameters. If it gives a lower number for the bound on E_0 we know that we have a better estimate.

Note: The true ground-state energy is

$$E_0 = 0.808617 \ \left(\frac{\eta^2 \hbar^2}{m} \right)^{\frac{1}{3}}$$

so this estimate is just $\frac{1}{2}$% off.