Quantum Mechanics M.T. 2002

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Problems

These problems cover all the material we will be studying in the lectures this term. The **Synopsis** tells you which problems are associated with which lectures.

Some of the problems have a double dagger ††; they are a bit more challenging but if you can do them you're really on top of the subject. Some of the problems have a single dagger †. They are straightforward extensions and applications of things we will do in the lectures; first time round they will take you some time and may raise difficulties that you'll need to discuss with your tutor but in a couple of years time they'll seem really easy! Finally there are problems with no daggers; these are either really easy or pretty much the same as problems we've done in the lectures. If you're paying attention you should be able to do them.

There are quite a lot of these problems, more than most of you will manage to do by the end of term, and your tutor may well tell you to do just a subset of them to start with. Still I hope that in the end you will try most of them, perhaps over the vac.

1 Orders of Magnitude

1. **Quanta of radiation**

   A beam of ultraviolet light of wavelength $\lambda = 124$ nm and intensity 1.6×10^{-12} W m^{-2} is suddenly turned on and falls on a metal surface, ejecting electrons through the photo-electric effect. The beam has a cross-sectional area of 10^{-4}m^2 and the work function of the metal is 5 eV. Estimate the time delay before the first photoelectron appears by the following approaches:

   (a) A crude estimate using classical physics is to calculate the time needed for the work function energy to be accumulated over the area of one atom (radius $\approx 10^{-10}$ m).

   (b) Lord Rayleigh showed that this is a bit pessimistic and that a better estimate of the effective area (or *scattering cross section*) that the atom presents is λ^2. Use this to revise your estimate of the time delay.

   (c) In the quantum approach, emission can occur as soon as the first photon arrives (why?). To obtain a time delay that can be compared to these classical estimates, calculate the average time interval between arrival of successive photons.

2. **Matter waves**

   The single-slit diffraction pattern for a monochromatic wave of wavelength λ incident normally on a narrow slit of width a is described (in the "Fraunhofer region") by the intensity

$$I(\theta) = I(0)\frac{\sin^2[(\pi a/\lambda)\sin\theta]}{[(\pi a/\lambda)\sin\theta]^2} \tag{1}$$

where θ is the deflection angle perpendicular to the incident wavefront. (We'll see how to derive this later in Question 5.4.)

(i) What is the value of $I(\theta)$ as $\theta \to 0$?

(ii) Sketch the form of $I(\theta)$ versus θ for the particular case $\lambda = a/2$. How does the sketch change as λ decreases? Show that the intensity peak centred on $\theta = 0$ falls to half its central intensity at

$$\theta = \sin^{-1}(0.443\lambda/a). \tag{2}$$

(iii) Nuclear reactors provide high fluxes of neutrons with energies $\sim 10^{-2}$ or $10^{-3} eV$. For neutrons with an energy of 4.18 x 10^{-3} eV, what is (a) their speed, (b) their wavelength?

(iv) In an experiment (C. G. Schull, Physical Review 179 (1969) 752-754) neutrons of energy 4.18 x 10^{-3} eV were incident on a slit of width 5.6 μm. It was found that the full width at half maximum of the central intensity peak (measured downstream from the slit) was 15.4 arc seconds. Is this consistent with the above diffraction formula $I(\theta)$?

3. **The importance of $\hbar$**

   Planck's constant $\hbar$ is equal to 1.0×10^{-34} Js, to two significant figures. A system (e.g. a mechanical watch) has moving parts of size d and mass m, and the movement occurs on a characteristic timescale τ.

   (i) Construct a quantity, call it S, having the same dimensions as $\hbar$ from d, m and τ (such quantities are said to have the dimensions of *action*). The rule of thumb is that if S has numerical value much bigger than $\hbar$ then quantum effects are negligible.

   (ii) Evaluate your S and compare it to $\hbar$ for
   a) The final stage of a turbofan engine (the thing that makes an aircraft fly; typically the final stage turbine rotates at an incredible 30,000 rpm!).
   b) The motion of a mechanical wristwatch.
   c) A bacteria "swimming".

   (iii) Now take d to be a typical atomic size, and m to be the electron mass. Find τ such that your action quantity is equal to $\hbar$ in this case. Defining an average velocity by $v = d/\tau$, calculate the corresponding kinetic energy of the electron, in eV.

4. Microscopes using waves with wavelength λ can resolve objects roughly as small as λ but no smaller. Determine the kinetic energy of electrons in an electron microscope needed to resolve

(i) a DNA molecule (10^{-8}m)

(ii) a proton (10^{-15}m).

[Use the de Broglie relation $\lambda = h/p$; in each case consider whether you should use the non-relativistic expression $T = p^2/2m$ for the kinetic energy T, or the relativistic one $T + mc^2 = [m^2c^4 + c^2p^2]^{1/2}$.

2 Time Dependent Schrödinger Equation

The 1-D TDSE is

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t). \tag{3}$$

1. **Einstein - de Broglie - Schrödinger waves**

   A plane wave solution of the time-dependent Schrödinger equation in one dimension is given by

   $$\psi(x,t) = Ae^{ikx-i\omega t}. \tag{4}$$

   (i) By substituting this solution into the TDSE for the case that $V(x) = 0$ find the relation between ω and k for such waves.

   (ii) The "phase velocity" v_p is defined to be ω/k and the "group velocity" v_g is defined to be $d\omega/dk$. Find expressions for v_p and v_g in terms of the "particle velocity" defined by $v = p/m$. Are the results what you expect, and why?

2. **Probability interpretation of the wavefunction**

   In Max Born's original paper (Zeitschrift für Physik 37 863-67 (1926)) the sentences proposing the probability interpretation of the wavefunction read as follows (quoting from the English translation, printed in "Quantum Theory and Measurement", Edited by J A Wheeler and W H Zurek, Princeton University Press, 1983, pages 52-55):

   "If one translates this result into terms of particles, only one interpretation is possible. $\Phi_{\eta\tau m}(\alpha,\beta,\gamma)$ [the wavefunction for the particular problem he is considering] gives the probability *for the electron, arriving from the z-direction, to be thrown out into the direction designated by the angles α,β,γ ... .

   * Addition in proof: More careful considerations show that the probability is proportional to the square of the quantity $\Phi_{\eta\tau m}$. "

   Give as many "considerations" as you can why a general wavefunction ψ does **not** have suitable properties to be interpreted as a probability density, but the square modulus $|\psi|^2$ does.

3. **Continuous probability distributions**

   For a certain continuous variable x, the probability that it has a value lying between x and $x + dx$ is $\rho(x)dx$. The possible values of x range from a to b.

(i) What conditions must $\rho(x)$ satisfy?

(ii) Define the average value $\langle f(x) \rangle$ of a function of x, $f(x)$.

(iii) The *variance* of the distribution is σ^2, defined by $\sigma^2 = \langle (x - \langle x \rangle)^2 \rangle$. Show that $\sigma^2 = \langle x^2 \rangle - (\langle x \rangle)^2$. (A customary measure of the "spread" of a distribution is σ, which by the above result is equal to $[\langle x^2 \rangle - (\langle x \rangle)^2]^{1/2}$. Frequently this may be written as Δx.)

4. **Solutions of the TDSE separated in x and t**

   Consider solutions in which the x- and t- dependence is *separated* ie we write $\psi(x, t) = \phi(x) \times T(t)$.

   (i) Show that

$$\frac{1}{T(t)} i\hbar \frac{dT(t)}{dt} = \frac{1}{\phi(x)} \left(-\frac{\hbar^2}{2m} \frac{d^2\phi(x)}{dx^2} \right) + V(x) \tag{5}$$

   and explain why each side of this equation must equal the same constant "A".

   (ii) Solve the T-equation for $T(t)$ given that $T(0) = 1$. Show that if A is real, $| \psi(x, t) |^2$ is independent of t. What is the frequency ω of the wave in terms of A? Assuming the Einstein relation $E = \hbar\omega$, find E in terms of A, and obtain an expression for the average value of x. Such solutions are called *stationary state solutions*: why? Do all wavefunctions have to satisfy the TISE?

   (iii) Suppose V depends on t as well as on x: $V(x, t)$. Will such a separation of the x and t variables be possible, in general? Can you invent a $V(x, t)$ for which it would be mathematically possible (even if not physically sensible)?

   (iv) Returning to the case $V(x)$, suppose A is in fact complex, $A = E - i\Gamma/2$. Show that the total (integrated over x) probability decays exponentially with a half-life of $(\hbar \ln 2)/\Gamma$. Suggest a physical problem in which such a solution might be useful.

3 Particle in a Box

1. **Necessary integrals**

   You will need certain integrals repeatedly over the next few weeks. They are given here; make sure that you can do them and then keep this piece of paper handy.

$$\int_0^a \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) = \begin{cases} \frac{a}{2}, & \text{if } n = m; \\ 0, & \text{otherwise.} \end{cases} \tag{6}$$

$$\int_0^a \sin\left(\frac{n\pi x}{a}\right) \cos\left(\frac{m\pi x}{a}\right) = \begin{cases} \frac{2an}{\pi(n^2 - m^2)}, & \text{if } n + m \text{ is odd;} \\ 0, & \text{otherwise.} \end{cases} \tag{7}$$

2. **Particle in a box: average values**

   Consider the particle in the infinitely deep square well potential ($V = 0$ for $0 < x < a$, $V = \infty$ for $x \leq 0, x \geq a$).

(i) Show that the allowed energy values are $E_n = \hbar^2 n^2 \pi^2 / 2ma^2$ for $n = 1, 2, \ldots$ and that the associated normalised eigenfunctions are

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \tag{8}$$

Why is there no state with $E = 0$? What does it mean to say that the ϕ_n are orthogonal?

(ii) Show qualitatively by means of a sketch that the eigenfunctions $\phi_1(x)$ and $\phi_2(x)$ are orthogonal.

(iii) For a particle with energy E_1, calculate the quantum-mechanical expectation value of x, denoted by $\langle x \rangle$.

(iv) Without working out any integrals, show that $\langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - a^2/4$. Hence find $\langle (x - \langle x \rangle)^2 \rangle$ using the result

$$\int_0^a x^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{a^3}{6} - \frac{a^3}{4n^2\pi^2}. \tag{9}$$

(v) A classical analogue of this problem is that of a particle bouncing back and forth between two perfectly elastic walls, with uniform velocity between bounces. Calculate the classical averages values $\langle x \rangle_c$ and $\langle (x - \langle x \rangle_c)^2 \rangle_c$, and show that for high values of n the quantum and classical results tend to each other.

3. †**Superposition of eigenfunctions**

Suppose the state is described at time $t = 0$ by the wavefunction

$$\psi(x, t = 0) = \frac{1}{\sqrt{2}} \left(\phi_1(x) + \phi_2(x)\right) \tag{10}$$

i) Show that ψ is correctly normalized.

ii) Show that this is not an energy eigenfunction. What are the possible results of a measurement of the energy of the particle, what are the corresponding amplitudes, and what are the corresponding probabilities? What do you expect the expectation value of the energy to be?

iii) Repeat (ii) but with the wavefunction

$$\psi'(x, t = 0) = \frac{1}{\sqrt{2}} \left(\phi_1(x) + e^{i\theta} \phi_2(x)\right) \tag{11}$$

iv) Reverting to ψ, explain why at subsequent times the wavefunction is given by

$$\psi(x, t) = \frac{1}{\sqrt{2}} \left(\phi_1(x) e^{-iE_1 t/\hbar} + \phi_2(x) e^{-iE_2 t/\hbar}\right) \tag{12}$$

Does the outcome of a measurement of the energy of the particle depend on when the measurement is made?

v) Show that

$$|\psi(x,t)|^2 = \frac{1}{a}\left\{\sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + 2\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\cos\omega t\right\} \tag{13}$$

where $\omega = (E_2 - E_1)/\hbar = 3E_1/\hbar$. Make rough sketches of $|\psi|^2$ for $t = 0$, $t = h/12E_1$, $t = h/6E_1$, $t = h/4E_1$. Does the outcome of a measurement of the position of the particle depend on when the measurement is made?

vi) Given that

$$\int_0^a x\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)dx = -\frac{8a^2}{9\pi^2}, \tag{14}$$

show that a particle with this wavefunction has $\langle x\rangle = a/2$ - $(16a/9\pi^2)\cos\omega t$. Discuss the connection between this result and the sketches of $|\psi|^2$.

vii) What is the value of ω for an electron confined to a distance comparable to the size of an atom (say 10^{-10} m)? What is the wavelength of radiation having this (circular) frequency?

4 Operators, Expectation Values, Conservation Laws

1. **Hermitian Operators**

Why are dynamical quantities (energy, momentum ...) represented by Hermitian operators in quantum mechanics?

The Hermitian conjugate $A^\dagger$ of a differential operator A is defined via its matrix elements between arbitrary wavefunctions ϕ_1 and ϕ_2,

$$\int_{-\infty}^{\infty}\phi_1^*(x)A^\dagger\phi_2(x)dx \stackrel{def}{=} \int_{-\infty}^{\infty}\left(A\phi_1(x)\right)^*\phi_2(x)dx \tag{15}$$

provided ϕ_1 and ϕ_2 vanish at $x = \pm\ \infty$. Show that

$$\left(\frac{\partial}{\partial x}\right)^\dagger = -\frac{\partial}{\partial x} \tag{16}$$

(you will need to do an integration by parts - see Rae p67,68) and

$$\left(\frac{\partial^2}{\partial x^2}\right)^\dagger = \frac{\partial^2}{\partial x^2} \tag{17}$$

Deduce from (16) that the momentum operator $-i\hbar(\partial/\partial x)$ is Hermitian and from (17) that the kinetic energy operator is Hermitian.

2. **Eigenfunctions**

   (i) Is $e^{ipx/\hbar} + e^{-ipx/\hbar}$ an eigenfunction of momentum? Is it an eigenfunction of kinetic energy?

   (ii) Is $\mathrm{e}^{-|x|/a}$ an eigenfunction of momentum? (Careful: a sketch and some thought is the best approach).

3. **Probability current density and the 1-D barrier**

   Derive the continuity equation relating the rate of change of probability density $\psi^*\psi$ to the gradient of a probability current density j, and find the expression for j. Find j for the plane wave solution $\psi(x,t) = A\ e^{ikx-i\omega t}$ and express your answer in terms of the particle velocity p/m. [Note: A is in general complex].

   Particles of mass m and energy E are incident from the region $x < 0$ on the "finite step" potential $V(x) = 0$ for $x \leq 0$, $V(x) = V_0$ for $x > 0$, with $V_0 > E$.

   (i) Explain why the solution of the time independent Schrodinger equation in the region $x \leq 0$ may be taken to have the form $\phi_1(x) = e^{ikx} + re^{-ikx}$ where $k = (2mE/\hbar^2)^{\frac{1}{2}}$, and why the solution in the region $x > 0$ has the form $\phi_2(x) = ae^{-Kx}$ where $K = [2m(V_0 - E)/\hbar^2]^{\frac{1}{2}}$.

   (ii) By imposing suitable boundary conditions at $x = 0$ show that

   $$r = \frac{k - iK}{k + iK}, \quad a = \frac{2k}{k + iK}. \tag{18}$$

   (iii) Is your solution for the wavefunction an energy eigenstate? Is it a momentum eigenstate?

   (iv) Compute the probability current density in the two regions. Discuss your result.

   (v) Show that r can be written as $e^{-2i\alpha}$ where $\alpha = \tan^{-1}(K/k)$, and hence show that

   $$|\phi_1(x)|^2 = 4\cos^2(kx + \alpha). \tag{19}$$

   Make two separate sketches, for the special cases $E = V_0/2$ and $E = V_0$, of $|\phi_1|^2$, and of $|\phi_2|^2$, showing how they match at $x = 0$.

   (vi) Estimate the penetration distance into the region $x > 0$ for an electron with $V_0 - E = 1eV$.

4. †**Equations of motion for expectation values**

   Prove that

   $$\frac{d}{dt}\langle\psi|A|\psi\rangle = \frac{i}{\hbar}\langle\psi|[H, A]|\psi\rangle \tag{20}$$

   where A is any operator (not explicitly depending on t) representing an observable dynamical quantity. You can do this either by writing out $\langle\psi|A|\psi\rangle$

as an integral, and differentiating with respect to time or directly in the Dirac notation by using

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}|\psi\rangle &= H|\psi\rangle \\
-i\hbar\frac{\partial}{\partial t}\langle\psi| &= \langle\psi|H
\end{aligned}
\tag{21}
$$

What is the corresponding result if the operator A does depend explicitly on t?

5. †**Commutators and Consequences**

   i) Verify that if the momentum operator p is represented by $-i\hbar(\partial/\partial x)$ (in one dimension) acting on wavefunctions, then

$$
[p, x]\phi(x) = -i\hbar\phi(x) \tag{22}
$$

   for any differentiable wavefunction $\phi(x)$, where $[A, B]$ means $AB - BA$.

   ii) Find $[p, V(x)]$.

   iii) For any operators A, B, verify that

$$
[A, B^2] = [A, B]B + B[A, B] \tag{23}
$$

   For $H = \frac{p^2}{2m} + V(x)$ use (23) together with your results for i) and ii) to show that

$$
\begin{aligned}
[H, x] &= -i\hbar\frac{p}{m} \\
[H, p] &= i\hbar\frac{dV}{dx}
\end{aligned}
\tag{24}
$$

   iiiA) Alternatively, if you're not happy with iii) use the differential operator representation $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$ to calculate the commutators (24) directly.

   iv) Use the commutators (24) and the equation of motion (20) to show that

$$
\begin{aligned}
\frac{d}{dt}\langle x\rangle &= \langle\frac{p}{m}\rangle \\
\frac{d}{dt}\langle p\rangle &= -\langle\frac{dV}{dx}\rangle.
\end{aligned}
\tag{25}
$$

   v) Let $V(x) = \frac{1}{2}m\omega^2x^2$ (ie the S.H.O. potential). Plug this into (25), solve the resulting differential equations and show that $\langle x\rangle$ has the same time dependent behaviour as x does classically.

6. ††Discuss the relationship between the results (25) and the classical equations of motion. In classical physics the equations of motion are second order in time dervatives and we need to specify both the position and the velocity at $t = 0$. But the Schrodinger equation is first order in time. Can you resolve these two facts?

7. ††**Two Particles**

   The Hamiltonian for two particles of mass m moving in one dimension interacting via their mutual potential energy $V(x_1 - x_2)$ is given by

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2} + V(x_1 - x_2) \tag{26}$$

   where x_1 and x_2 are the coordinates of the two particles. Show that the total momentum of the two particles is conserved. [Hint: the total momentum operator P is $P = p_1 + p_2$ where $p_1 = -i\hbar\frac{\partial}{\partial x_1}$ and similarly for p_2.]

8. ††**Eigenvalues and Eigenfunctions of Hermitian Operators**

   In Dirac's notation if Q is a Hermitian operator then $|v\rangle = Q|u\rangle$ implies $\langle v| = \langle u|Q$. Eigenstates of Q are labelled by their eigenvalues $q_1, \ldots$ and satisfy $Q|q_n\rangle = q_n|q_n\rangle$.

   Show that $\langle u|Q|v\rangle = (\langle v|Q|u\rangle)^*$ and hence that the eigenvalues of Q must be real.

   Show that when $q_n \neq q_m$ then $\langle q_n|q_m\rangle = 0$.

   Suppose that $|a\rangle$ and $|b\rangle$ are eigenstates of Q with the *same* eigenvalue; then the previous proof of orthogonality fails. However it is always possible to construct linear combinations of $|a\rangle$ and $|b\rangle$, let's call them $|\tilde{a}\rangle$ and $|\tilde{b}\rangle$, which *are* orthogonal. Do it.

5 Measurement

1. **Change of state following a measurement**

   A particle in the infinite-sided box has the wavefunction (10) at $t = 0$. At that time its energy is measured and found to have the value $h^2/2ma^2$. What is the probability of finding the particle in the region $0 \leq x \leq a/2$ (i) before the energy measurement? (ii) after it? Explain the answers qualitatively, with the aid of a sketch.

2. **Compatibility**

   Explain why it is possible to have quantum states for a particle in which the momentum and the kinetic energy both have well-defined values, but that this is possible for the momentum and the total energy only if the potential energy is a constant.

   Find a wavefunction (not normalised) such that $p_x = -i\hbar\frac{\partial}{dx}, p_y = -i\hbar\frac{\partial}{\partial y}$ and $p_z = -i\hbar\frac{\partial}{\partial z}$ all have well-defined values, say $\hbar k_x, \hbar k_y$, and $\hbar k_z$ (i.e. you are looking for a wavefunction for a particle with definite momentum (vector) $\hbar\mathbf{k}$). Why can all three components of momentum have well-defined values?

   Two operators A and B do not commute. Is it true that

$$[A, B]|\psi\rangle \neq 0 \tag{27}$$

for any state ψ?

3. **Uncertainty relations**

   As a simple example of a time-independent wavepacket, consider the function

$$\phi(x) = \frac{1}{2\Delta k}\int_{k_0-\Delta k}^{k_0+\Delta k} e^{ikx}dk \tag{28}$$

   which may be regarded as a superposition of (complex) waves e^{ikx} with different k's, lying within Δk on either side of a central value k_0. Evaluate this integral and show that

$$|\phi(x)|^2 = \frac{\sin^2(\Delta k.x)}{(\Delta k.x)^2}. \tag{29}$$

   Sketch $|\phi(x)|^2$ versus x (recall that Δk is the spread in the wavenumbers of the packet). $|\phi(x)|^2$ is mostly concentrated in the region bounded by its first zeros on either side of the origin; if the size of this region is denoted by "Δx", show that "Δx" $\Delta k = 2\pi$. Relate this to the uncertainty relation $\Delta x \Delta p \geq \frac{1}{2}\hbar$.

   [The reason we used quotes in "Δx" is that it is not quite the same as the mathematically precise definition $\Delta x = [\langle (x - \langle x \rangle)^2 \rangle]^{\frac{1}{2}}$].

4. †**Interference**

   Consider the two slit interference set-up

   Let the amplitude for a particle from the source S to reach slit 1 be $\langle 1|S\rangle$, to get from slit 1 to point x on the screen $\langle x|1\rangle$ etc. Assume that each slit is infinitely narrow but that if a particle hits the slit it goes through with amplitude 1.

   i) Write down expressions for the amplitude for a particle to leave S and reach the point x via slit 1, via slit 2, and via both slits. Explain why the result of measuring the number of particles arriving at the screen is qualitatively different when both slits are open compared to when only one slit is open.

   ii) Assume that the source is infinitely far away, and that the amplitude for a particle starting at $\mathbf{x}_1$ to end at $\mathbf{x}_2$ is

$$\langle \mathbf{x}_2|\mathbf{x}_1\rangle = |\mathbf{x}_2 - \mathbf{x}_1|^{-1} e^{i\mathbf{k}.(\mathbf{x}_2-\mathbf{x}_1)}. \tag{30}$$

   Compute *exactly* the probability distribution $P(x)$ for particles arriving at the screen.

   iii) Now simplify $P(x)$ in the regime $L \gg d$ and $L \gg x$. It is interesting to look at how the pattern behaves when these simplifying assumptions are not valid. There is a Maple worksheet at http://www-thphys.physics.ox.ac.uk/users/JohnWheater to help you do this.

   iv) Use similar methods find the single slit diffraction pattern (1).

5. †The eigenstates of two commuting operators A and B are denoted $|a,b\rangle$ and satisfy the eigenvalue equations $A|a,b\rangle = a|a,b\rangle$ and $B|a,b\rangle = b|a,b\rangle$. A system is set up in the state

$$|\psi\rangle = N\left(|1,2\rangle + |2,2\rangle + |1,3\rangle\right) \tag{31}$$

What is the value of the normalization constant N?

A measurement of the value of A yields the result 1. What is the probability of this happening? What is the new state $|\psi'\rangle$ of the system?

Then a measurement of the value of B yields the result 2. What is the probability of this happening? What is the new state $|\psi''\rangle$ of the system?

Given that the system starts in the state $|\psi\rangle$ and then A is measured and then B is measured what is the probability that it ends up in the state $|\psi''\rangle$?

Repeat the above but measure B first and then A. Comment on your results.

6. ††The operators A and B do not commute. The eigenstates of A are $|0\rangle$ and $|1\rangle$ and satisfy $A|a\rangle = a|a\rangle$. The eigenstates of B are

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle) \tag{32}$$

with eigenvalues ± 1 respectively.

A system starts in the state $|0\rangle$. A measurement of B yields the value $+1$. What is the probability of this and what is now the state of the system?

Now a measurement of A is made. What are the possible outcomes and what state will the system be in afterwards?

Suppose the measurements of A and B are made in the opposite order. Discuss what happens.

Suppose alternating measurements of A and B are made *ad infinitum*. Discuss what happens.

6 The Simple Harmonic Oscillator

1. **Eigenfunctions, eigenvalues**

The eigenvalue equation for the SHO is

$$\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right)\phi = E\phi \tag{33}$$

where ω is the classical frequency of the oscillator.

i) Show that by making the change of variables $x = y\sqrt{\frac{\hbar}{m\omega}}$ (33) becomes

$$\frac{\hbar\omega}{2}\left(-\frac{\partial^2}{\partial y^2} + y^2\right)\phi = E\phi \tag{34}$$

ii) Show that $\phi(y) = e^{-\frac{y^2}{2}}$ satisfies the eigenvalue equation for the SHO and find E. In fact this is the ground state. Show that the correctly normalized wavefunction is

$$\phi_0(x) = \left(\frac{1}{\pi a^2}\right)^{\frac{1}{4}} \exp(-x^2/2a^2) \quad \text{where} \quad a^2 = \hbar/m\omega. \tag{35}$$

iii) Find the expectation values of x, x^2, p and p^2 for a particle in the ground state. [Hint: for $\langle p^2 \rangle$ use $p^2/2m + \frac{1}{2}m\omega^2 x^2 = E$].

iv) Defining $\Delta x = [\langle (x - \langle x \rangle)^2 \rangle]^{\frac{1}{2}}$, $\Delta p = [\langle (p - \langle p \rangle)^2 \rangle]^{1/2}$ show that in this case $\Delta x \Delta p = \frac{1}{2}\hbar$. Comment on this result.

You will need the integrals

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}; \qquad \int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx = \frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}. \tag{36}$$

2. **Pictures**

On the same diagram, plot carefully (paying particular attention to the points of intersection of the various curves)

i) $\phi_0(x)$ from (35) versus x, indicating where $\frac{d^2\phi_0}{dx^2} = 0$

ii) the potential energy $\frac{1}{2}m\omega^2 x^2$ versus x

iii) the total energy $E = \frac{1}{2}\hbar\omega$ versus x

iv) the region in x to which the particle would be confined according to classical mechanics.

Why do the x-values such that $\frac{d^2\phi_0}{dx^2} = 0$ lie at the limits of the classically allowed region?

3. **†Spectrum**

The form (34) strongly suggests that we should try factorizing the differential operator. So define

$$\begin{aligned} D^\dagger &= \frac{1}{\sqrt{2}}\left(-\frac{d}{dy} + y\right) \\ D &= \frac{1}{\sqrt{2}}\left(\frac{d}{dy} + y\right) \end{aligned} \tag{37}$$

i) Show that

$$\begin{aligned} D^\dagger D f &= \frac{1}{2}\left(-\frac{d^2 f}{dy} + y^2 f - f\right) \\ D\, D^\dagger f &= \frac{1}{2}\left(-\frac{d^2 f}{dy} + y^2 f + f\right) \end{aligned} \tag{38}$$

and hence that (34) may be written

$$\hbar\omega\left(D^\dagger D+\frac{1}{2}\right)\phi=E\phi \tag{39}$$

and that

$$D^\dagger D-D\,D^\dagger=-1 \tag{40}$$

ii) Now *assume* that ϕ satisfies (39). Show that $\phi'=D\,\phi$ also satisfies (39) but with E replaced by $E'=E-\hbar\omega$. (Most easily done by acting on (39) with D and then using the commutator to reverse the order of D and $D^\dagger$.)

iii) Explain why there must be a ϕ_0 satisfying $D\,\phi_0=0$. Writing this condition out explicitly gives a first order differential equation for ϕ_0; solve it. To what value of E does ϕ_0 correspond?

iv) Now show that if ϕ satisfies (39) then $\phi'=D^\dagger\phi$ also satisfies (39) but with E replaced by $E'=E+\hbar\omega$.

v) Now assemble everything to give the spectrum E_n and a recipe for generating the eigenfunctions ϕ_n. Write out the first three eigenfunctions explicitly and plot them on a graph.

vi) Is the ground state wavefunction an even or odd function of x? How do the excited states behave under $x\to -x$? (This property is called the *parity* of the state.)

4. ††**A slicker way**

Of course what we did in the previous question didn't really depend on a differential equation; just on the properties of some operators. So actually it can be done at a more abstract level without reference to differential operators at all. So let

$$\begin{aligned} H &= \frac{p^2}{2m}+\frac{m\omega^2x^2}{2} \\ A &= \sqrt{\frac{m\omega}{2}}x+i\frac{p}{\sqrt{2m\omega}} \\ A^\dagger &= \sqrt{\frac{m\omega}{2}}x-i\frac{p}{\sqrt{2m\omega}} \end{aligned} \tag{41}$$

i) Show that $[A,A^\dagger]=\hbar$ and $H=\omega A^\dagger A+\hbar\omega/2$.

ii) Show that $[H,A]=-\hbar\omega A$ and $[H,A^\dagger]=\hbar\omega A^\dagger$

iii) Assume that $H|\psi\rangle=E|\psi\rangle$; show that $|\psi'\rangle=A|\psi\rangle$ satisfies $H|\psi'\rangle=(E-\hbar\omega)|\psi'\rangle$. Deduce that there must be a state $|0\rangle$ satisfying $A|0\rangle=0$ and give its energy.

iv) Show that $|\psi'\rangle=A^\dagger|\psi\rangle$ satisfies $H|\psi'\rangle=(E+\hbar\omega)|\psi'\rangle$. Now you can deduce the spectrum E_n and how the corresponding states $|n\rangle$ are related to $|0\rangle$.

v) It's easy to compute the correct normalization too. Being careful we have

$$|n+1\rangle = C_n A^\dagger |n\rangle \tag{42}$$

where the states are all normalised and C_n is a constant. Show that

$$1 = \langle n+1|n+1\rangle = |C_n|^2 \hbar (n+1). \tag{43}$$

This tells you C_n; find the constant N_n such that

$$|n\rangle = N_n (A^\dagger)^n |0\rangle \tag{44}$$

is correctly normalized.

7 Barriers and Wavepackets

1. †**Momentum probability distribution I**

   Consider the following two normalised wavefunctions

   $$\phi_1(x) = \frac{1}{\sqrt{a}} \exp(-|x|/a), \quad \phi_2(x) = e^{ikx} \frac{1}{\sqrt{a}} \exp(-|x|/a). \tag{45}$$

   Calculate $\langle x\rangle$ and $\langle p\rangle$ for both of these wavefunctions.

   Sketch $|\phi_1|^2$ and $|\phi_2|^2$ versus x for fixed a.

   The momentum probability amplitude corresponding to a position probability amplitude $\phi(x)$ is (see Question 7.2)

   $$\tilde{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \phi(x) dx \tag{46}$$

   Evaluate $\tilde{\phi}_1(p)$ and $\tilde{\phi}_2(p)$ and sketch both as a function of p, for fixed a. Give an informal (qualitative) definition of the "spreads" of $|\phi_1(x)|^2$ in x and of $|\tilde{\phi}_1(p)|^2$ in p. Show that their product is of order $\hbar$.

2. ††**Momentum probability distribution II**

   A particle is in the state $|\psi\rangle$. Describe in words what information the amplitude $\langle x|\psi\rangle$ contains; what do we usually call this amplitude?

   Let $|p\rangle$ be an eigenstate of the *momentum* operator $\hat{p}$ (contrary to our usual practice we need a hat on the operator here to avoid getting confused) so that $\hat{p}|p\rangle = p|p\rangle$. Describe in words what information the amplitude $\langle x|p\rangle$ contains. Explain why $\langle x|p\rangle \propto \exp(ipx/\hbar)$.

   Describe in words what information the amplitude $\langle p|x\rangle$ contains and give its form as a function of p and x.

   Describe in words what information the amplitude $\langle p|\psi\rangle$ contains and explain why

   $$\langle p|\psi\rangle \propto \int_{-\infty}^{\infty} dx\, \langle p|x\rangle\langle x|\psi\rangle, \tag{47}$$

which, up to a constant factor, is (46). Confirm that the factor $1/\sqrt{2\pi\hbar}$ ensures that

$$\int_{-\infty}^{\infty} |\tilde{\phi}(p)|^2 dp = 1 \tag{48}$$

if $\phi(x)$ is normalised. (You'll need to use the Dirac delta function covered in the Mathematical Physics lectures.)

3. †**The 1-D finite well**

   Remember that there is a Maple worksheet to do most of the algebra of this question. You can download it from
   http://www-thphys.physics.ox.ac.uk/users/JohnWheater .

   A particle of mass m is in a "finite well" potential

$$\begin{aligned} V(x) &= V_0 \quad \text{for} \quad |x| > a \\ &= 0 \quad \text{for} \quad |x| \leq a \end{aligned} \tag{49}$$

   where V_0 is positive. It may be shown that for such a potential, which satisfies the condition $V(-x) = V(x)$, each energy eigenfunction has a definite parity, which can be either *even* ($\psi(-x) = \psi(x)$) or *odd* ($\psi(-x) = -\psi(x)$). (We'll meet parity again next term.)

   (i) Assuming that the well parameters V_0 and a are such that these bound states are possible, sketch the form of the wavefunctions for the first two bound states ($E < V_0$) of even parity, and for the first two bound states of odd parity (*not* exact wavefunctions; just the right number of wiggles, the right parity, and the right behaviour at the edge of the well and as $x \to \pm\infty$).

   (ii) The bound state wavefunction for even parity states has the form

$$\psi(x) = A\cos kx \quad \text{for} \quad 0 \leq x \leq a \tag{50}$$

$$\quad\;\; = Be^{-Kx} \quad \text{for} \quad x \geq a, \tag{51}$$

   where $k = \left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}}$ and $K = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$. Write down $\psi(x)$ for $-a \leq x \leq 0$ and for $x \leq -a$. By applying the boundary condition at $x = a$, show that the allowed k (i.e. E) values are determined by the roots of the equation

$$(v^2 - s^2)^{\frac{1}{2}} = s\tan s \tag{52}$$

   where $v = [2mV_0a^2/\hbar^2]^{\frac{1}{2}}$ and $s = ka$. Check that v and s are dimensionless. Why is it not necessary to consider the boundary condition at $x = -a$ as well? This equation (52) can be solved for s, given v, by a graphical method. For positive s, sketch the function $s\tan s$ versus s, and the function $(v^2 - s^2)^{\frac{1}{2}}$ versus s. Where these curves meet, you have a solution for s. Show (a) that there is always *one* solution, whatever the value of v; (b) that a second "even" bound state is possible as soon as v becomes greater than π.

   (iii) Write down a similar form of the wavefunction for odd-parity states, and show that the energy eigenvalue condition is

$$(v^2 - s^2)^{\frac{1}{2}} = -s\cot s \tag{53}$$

Sketch both sides of (53) as a function of s, and show that there is no odd-parity bound state if $v < \pi/2$.

(iv) Explain why the number of bound states (even + odd) is given by the next integer greater than the value of $2v/\pi$ (which is called the "well parameter").

(v) The roots of (52) and (53) can be found by using the fsolve command on Maple - or by trial and error. Take m = electron mass, $a = 0.5$ nm and $V_0 =$ 20 eV. How many bound states are there?

Verify that the two lowest roots for s are $s = 1.44438$ and $s = 2.88685$ and find the corresponding eigenvalues in eV.

(vi) Use Maple to produce accurate plots of the ground and first excited states.

4. †**Barrier penetration and transmission**

Remember that there is a Maple worksheet to do most of the algebra of this question. You can download it from
http://www-thphys.physics.ox.ac.uk/users/JohnWheater

A particle of mass m is incident with energy $E < V_0$ from the region $x < 0$ on the finite potential barrier

$$\begin{aligned} V(x) &= 0 \quad \text{for} \quad x < 0, x > a \\ &= V_0 \quad \text{for} \quad 0 \leq x \leq a. \end{aligned} \tag{54}$$

Take the wavefunction in $x < 0$ to be

$$\psi_1 = e^{ikx} + Re^{-ikx}, \tag{55}$$

in $0 \leq x \leq a$ to be

$$\psi_2 = Ae^{Kx} + Be^{-Kx} \tag{56}$$

and in $x > a$ to be

$$\psi_3 = Ce^{ikx} \tag{57}$$

where $K^2 = \frac{2m}{\hbar^2}(V_0 - E), k^2 = 2mE/\hbar^2$.
i) Is the wavefunction an energy eigenstate?
ii) Is the wavefunction a momentum eigenstate?
iii) From the boundary conditions at $x = 0$ deduce that

$$2 = A(1 - \frac{iK}{k}) + B(1 + \frac{iK}{k}) \tag{58}$$

and from the boundary conditions at $x = a$ deduce that

$$A = \frac{1}{2}e^{-Ka}(1 + \frac{ik}{K})e^{ika}C \tag{59}$$

and

$$B = \frac{1}{2}e^{Ka}(1 - \frac{ik}{K})e^{ika}C. \tag{60}$$

Substitute these expressions for A and B into the previous equation to show that

$$C = \frac{2e^{-ika}}{\left[2\cosh Ka - i\left(\frac{k}{K} - \frac{K}{k}\right)\sinh Ka\right]} \tag{61}$$

Hence show that the transmission coefficient (defined as the transmitted flux divided by the incident flux) is

$$|C|^2 = \left(1 + \frac{(K^2+k^2)^2}{4K^2k^2}\sinh^2 Ka\right)^{-1}, \tag{62}$$

which can also be written as

$$|C|^2 = \left(1 + \frac{\sinh^2[v^2(1-E/V_0)]^{\frac{1}{2}}}{4(E/V_0)(1-E/V_0)}\right)^{-1} \tag{63}$$

where v is as defined in Q 1, $v = (2mV_0a^2/\hbar^2)^{\frac{1}{2}}$.

iv) Compute the probability flux *inside* the barrier, ie from ψ_2. [Hint: caution - A and B are complex!] Compare your result with part iii).

v) Show that if $E/V_0 \ll 1$ and $v \gg 1, |C|^2$ is given approximately by

$$|C|^2 \approx \frac{16E}{V_0}e^{-2v}. \tag{64}$$

This shows the characteristic *exponential tunnelling probability*: the amplitude for waves with $E < V_0$ is exponentially attenuated by the barrier (though of course classical particles wouldn't get through at all); it is analogous to the evanescent waves in optics (e.g. in total internal reflection).

Suppose $E = 1eV, V_0 = 6eV$ and $a = 1$nm. By what factor will $|C|^2$ change if a increases to 1.1 nm?

The "Scanning Tunnelling Microscope" is just one application of quantum tunnelling - see G. Binnig and H. Rohrer Reviews of Modern Physics **59** (1987) 615 (their Nobel lecture).

5. ††**Transmission resonances**

In Question 4 above, imagine the energy gradually increasing until it becomes equal to V_0. What is $|C|^2$ when $E = V_0$? Now suppose E becomes greater than V_0. Then K^2 becomes negative, $K \to i|K|$ (or maybe $-i|K|$?) and $\sinh^2 Ka \to (i\sin|K|a)^2$, so

$$|C|^2 \to \left(1 + \frac{\sin^2[v^2(E/V_0-1)]^{\frac{1}{2}}}{4(E/V_0)(E/V_0-1)}\right)^{-1} \tag{65}$$

(if you don't like this, you can of course repeat the whole calculation from scratch . . . ; there is a worksheet at http://www-thphys.physics.ox.ac.uk/users/JohnWheater to do this too).

Show that this new $|C|^2$ is equal to unity when $\left[\frac{2m}{\hbar^2}(E-V_0)\right]^{\frac{1}{2}} = n\pi/a$. What does the wave in the region $0 \le x \le a$ look like at these values of E?

6. ††**Time dependent packets; dispersion**

A simple example of a time-dependent wave packet is provided by a superposition of waves for which the *frequency is proportional to the wavenumber*: $\omega = ck$. Light, of course, is such a wave. Consider the packet

$$\phi(x,t) = \frac{1}{2\Delta k}\int_{k_0-\Delta k}^{k_o+\Delta k} e^{ik(x-ct)}dk \tag{66}$$

(Note that $\phi(x,0)$ is the packet in Question 5.3).

(i) Evaluate the integral and show that

$$|\phi(x,t)|^2 = \frac{\sin^2[\Delta k(x-ct)]}{[\Delta k(x-ct)]^2} \tag{67}$$

(as in Q5.3). For fixed t, at what x is $|\phi(x,t)|^2$ a maximum, and at what values of x do the first zeros of $|\phi(x,t)|^2$ away from the maximum occur? Sketch $|\phi(x,t)|^2$ for fixed t versus x.

Describe how the packet moves along in x as t varies. Does the *shape* of the function $|\phi(x,t)|^2$ change?

Consider now the packet for fixed x, as t varies. Where is the maximum as a function of t for fixed x, and where do the first minima on either side of it occur? If the spread in the packet in time, "Δt", is defined as the distance between the first minima on either side of the central maximum, show that $\Delta\omega$ "Δt" $= 2\pi$, where $\Delta\omega = c\Delta k$. Relate this to the uncertainty relation $\Delta E\ \Delta t\ \ge \frac{1}{2}\hbar$.

(ii) A time-dependent free-particle (plane wave) solution of the 1-D Schrödinger equation is $\psi(x,t) = N\exp(ikx - iEt/\hbar)$ where N is a normalization constant and $E = p^2/2m = \hbar^2k^2/2m = \hbar\omega$. It follows that for these waves the frequency ω is *not* proportional to k but to k^2: $\omega = \hbar k^2/2m$. This makes a dramatic difference to the way a packet of these waves evolves with time: the packet does *not* maintain its shape, but "flattens out", a phenomenon called *dispersion* (of the packet). Consider the packet

$$\psi(x,t) = \frac{1}{2\Delta k}\int_{k_0-\Delta k}^{k_0+\Delta k} e^{ikx - i\hbar k^2 t/2m}dk \tag{68}$$

(note that $\psi(x,0)$ is again the packet from Q5.3). This time the integral can *not* be done in terms of elementary functions. However, if $k_0 \gg \Delta k$ and the t-term in the exponent is "not too big" we can expand "k^2" about the point

$k = k_0$ by a Taylor series: $k^2 = k_0^2 + (k - k_0).2k_0$, and we are back to only a *linear* term in the exponent, which can be integrated exactly. Show that in this approximation

$$|\psi(x,t)|^2 = \frac{\sin^2[\Delta k(x - vt)]}{[\Delta k(x - vt)]^2} \tag{69}$$

where $v = \hbar k_0/m$, and describe how this packet moves as t varies.