Quantum Mechanics M.T. 2000

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Problem Set No. 4

1. The 1-D finite well

A particle of mass m is in a "finite well" potential $V(x) = V_0$ for $\mid x \mid> a$, $V(x) = 0$ for $\mid x \mid\leq a$.
It may be shown (see Q 13 and Q 14 on Set No. 3) 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* ($\psi(-x) = -\psi(x)$).

(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

$$\begin{aligned} \psi(x) &= A \cos kx \quad \text{for} \quad 0 \leq x \leq a \\ &= Be^{-Kx} \quad \text{for} \quad x \geq a, \end{aligned}$$

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

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

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 **??** 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

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

Sketch both sides of **??** 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 **??** and **??** can be found by (for example) using the Find Root command on Mathematica - or by trial and error. Take m = electron mass, $a = 0.5$ nm and $V_0 = 20$ eV (these are the default parameters in the Finite Square Well programme in McMurry's disk). 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. Compare with McMurry (her "L" is our "2a").

(vi) Suppose you are running a programme (such as McMurry's) that plots $\psi(x)$ (for given V_0 and a) for a guessed-at value of E, the eigenvalue. If you are near an eigenvalue, you will find the following behaviour: for the guessed E just less than the true eigenvalues $\psi(x)$ will diverge "upwards" to $+\infty$ for $x > a$ (i.e. without crossing the axis), whereas if your guessed E is just larger than the true eigenvalue $\psi(x)$ will diverge "downwards" to $-\infty$ for $x > a$ (i.e. it will cross the x-axis) - this is assuming that $\psi(x) > 0$ at $x = a$, by convention. Can you explain this behaviour? [Hint: consider $\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V(x) - E)\psi$.]

2. <u>Barrier penetration and transmission</u>

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

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

Take the wavefunction in $x < 0$ to be

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

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

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

and in $x > a$ to be

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

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

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

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

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

and

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

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

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

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

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

which can also be written as

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

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 $v \gg 1$, $\mid C \mid^2$ is given approximately by

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

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 $\mid C \mid^2$ change if a increases to 1.1 nm?

The programme "Transmission: plane wave, barrier" in McMurry's disk can be run to see the effect of changing parameters.

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).

3. <u>The 1-D S.H.O.</u>

   Q 9 (i) Set 2 and Q 11 Set 3 show that the ground state wavefunction, with energy $E = \frac{1}{2}\hbar\omega$, is

$$\psi_0(x) = \left(\frac{1}{\pi a^2}\right)^{\frac{1}{4}} \exp(-x^2/2a^2) \quad \text{where} \quad a^2 = \hbar/m\omega.$$

   On the same diagram, plot carefully (paying particular attention to the points of intersection of the various curves)
   (a) $\psi_0(x)$ versus x, indicating where $\frac{d^2\psi_0}{dx^2} = 0$

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

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

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

   Why do the x-values such that $\frac{d^2\psi_0}{dx^2} = 0$ lie at the limits of the classically allowed region?

4. Show that any even-parity solution is orthogonal to any odd-parity solution. In terms of the dimensionless variable $y = x\left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}$ introduced in Q 9 (i) Set 2, the wavefunctions (unnormalised) for the three lowest energy eigenstates have the forms $\phi_0 = e^{-y^2/2}, \phi_1 = ye^{-y^2/2}, \phi_2 = (a + by^2)e^{-y^2/2}$. Calculate the ratio a/b from the condition that ϕ_0 is orthogonal to ϕ_2. Sketch ϕ_0, ϕ_1 and ϕ_2 versus y.

   [McMurry's disk has a programme for solving and plotting the 1D S.H.O.].

5. <u>2-D S.H.O.</u>

   Consider a particle moving in the $x-y$ plane in the potential $V(x,y) = \frac{1}{2}m\omega^2(x^2 + y^2)$. Write down the stationary state Schrödinger equation, with energy eigenvalue E. By writing the wavefunction in the form

$$\psi(x,y) = X(x)Y(y)$$

and applying the method of *separation of variables* (i.e. in x and y), show - *assuming* any necessary results for the 1-D oscillator - that the energy eigenvalues have the form $E = (n_x + n_y + 1)\hbar\omega$ where n_x and n_y are integers or zero.

So these states are described by *two* quantum numbers. Write down $\psi(x, y)$ for the states with $E = \hbar\omega$ and $2\hbar\omega$ (caution: there are *two different* wavefunctions in the second case; this is called "degeneracy"). What is the degeneracy of the state with $E = 3\hbar\omega$?

What would happen to the degeneracy of the levels if the potential had different frequencies for x and for y? (e.g. $\frac{1}{2}m\omega_x^2 x^2 + \frac{1}{2}m\omega_y^2 y^2$).

6. Cubical box

Show that the energy eigenvalues of a particle confined inside a cubical box of side a (i.e. the potential is infinite at the walls) are given by

$$E(n_x, n_y, n_z) = \frac{\hbar^2\pi^2}{2ma^2}(n_x^2 + n_y^2 + n_z^2)$$

where n_x, n_y and n_z are positive integers. Why can't they be negative, or zero?

Consider an electron in a room of size 4m x 4m x 4m. What is the rough value of $n_x^2 + n_y^2 + n_z^2$ if the energy of the electron is 5 eV? What is the approximate energy difference $E(2, 1, 1) - E(1, 1, 1)$ for an electron in an ordinary room? Repeat the last calculation for an electron in a small room of side 10^{-10}m.

[Extra problem]

7. In Q2 above, imagine the energy gradually increasing until it becomes equal to V_0. What is $\mid C \mid^2$ when $E = V_0$? Now suppose E becomes greater than V_0. Then K^2 becomes negative, $K \to i \mid K \mid$ (or maybe $-i \mid K \mid$?) and $\sinh^2 Ka \to (i \sin \mid K \mid a)^2$, so

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

(if you don't like this, you can of course repeat the whole calculation from scratch ...).

Show that this new $\mid C \mid^2$ 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 $0 \leq x \leq a$ look like at these values of E?

McMurry's programme can be run to show these "transmission resonances" for $E > V_0$.