Problem sheet - MT vacation

Main questions

Q1. Probability current density and a 1D 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

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

(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

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

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 $V_0 - E = 1eV$.

[JMR QM Q4.3]

Q2. Momentum distributions

Consider the following two normalised wavefunctions

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

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

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

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 $\hbar$.

[JMR QM Q7.1]

Q3. Bound states of a 1D finite well

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

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

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

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

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

$$(v^2 - s^2)^{\frac{1}{2}} = s\tan s \tag{61}$$

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 (61) 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

$$(v^2 - s^2)^{\frac{1}{2}} = -s\cot s \tag{62}$$

Sketch both sides of (62) 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 (61) and (62) 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. 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.

[JMR QM Q7.3]

Q4. Transmission through a 1D finite barrier

Obtain the probability of passing through the square barrier

$$V = \begin{cases} V_0 & \text{for } |x| < a \\ 0 & \text{otherwise,} \end{cases}$$

in the case $E > V_0 > 0$. Verify that the probability you obtain joins at $E = V_0$ to the transition probability for $E < V_0$, which is

$$P(E) = \frac{1}{\cosh^2 2Ka + \frac{1}{4}(k/K - K/k)^2 \sinh 2Ka} \quad \text{with} \quad K^2 \equiv \frac{2m(V_0 - E)}{\hbar^2}.$$

[JB QM Q3.7]

Q5. Barrier penetration and transmission

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

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

Take the wavefunction in $x < 0$ to be

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

in $0 \leq x \leq a$ 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

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

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

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

which can also be written as

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

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

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

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).

[JMR QM Q7.4]

Q6. Transmission resonances [JMR QM Q7.5]

In Question 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

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

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

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 $0 \leq x \leq a$ look like at these values of E?