Quantum PS1

Richard Fern

1 1.1) Kinetic Energies

Find the kinetic energy in eV (electron volts) of a neutron, an electron and an electromagnetic wave, each of wavelength 0.1 nm. (For the electron and the neutron, first try a non-relativistic formula for the kinetic energy, and then justify afterwards why it was reasonable to do that.) [2]

We know that $p = \frac{h}{\lambda}$ but we should derive this from quantum mechanics. Thus, consider

$$\hat{\boldsymbol{p}}\psi = \boldsymbol{p}\psi$$

where ψ is our eigenstate of momentum and $\hat{\boldsymbol{p}} = -i\hbar\nabla$ is the corresponding operator. We can solve this to find

$$\psi = \exp\left(\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{x}\right).$$

Therefore, one wavelength, λ, satisfies the equation

$$\frac{p\lambda}{\hbar} = 2\pi \qquad \implies \qquad p = \frac{h}{\lambda}.$$

As such, the momentum is

$$p = \frac{h}{\lambda} = 6.6 \times 10^{-24} \text{ kg m s}^{-2}$$

in all three cases. For the neutron and electron we assume that the energy is simply the classical $E = \frac{p^2}{2m}$. Thus,

$$E_{\text{neutron}} = 81.8 \text{ meV},$$

$$E_{\text{neutron}} = 150 \text{ eV}.$$

We will analyse the validity of this classical approximation in the next question. As for the photon, the formula is simple,

$$E_{\text{photon}} = pc = 12.4 \text{ keV}.$$

2 1.2) Relativistic Waves

For the electron and the neutron in the previous problem, estimate in each case the approximate wavelength below which the non-relativistic formula would fail to give a good answer (and make a reasonable choice for what 'good' means here). [2]

We know the classical formula holds well for speeds much smaller than the speed of light. So we require

$$\frac{p}{m} \ll c \qquad \Longrightarrow \qquad \frac{h}{mc} \ll \lambda.$$

We can calculate the left hand side here for the neutron and electron,

$$\frac{h}{m_{\text{neutron}} c} = 1.32 \times 10^{-15} \text{ m},$$

$$\frac{h}{m_{\text{electron}} c} = 2.42 \times 10^{-12} \text{ m}.$$

Therefore, λ must be a factor of about 10 larger than this.

The above method is a rather quick and dirty way of finding our cutoff. We can also just expand the formula for the relativistic kinetic energy and find the size of the sub-leading term.

$$\begin{aligned} E_K &= \sqrt{(mc^2)^2 + (pc)^2} - mc^2 \\ &= mc^2 \left(\sqrt{1 + \frac{p^2}{m^2c^2}} - 1 \right) \\ &= mc^2 \left(\frac{p^2}{2m^2c^2} - \frac{p^4}{8m^4c^4} + \dots \right) \\ &= \frac{p^2}{2m} \left(1 - \frac{p^2}{4m^2c^2} \right). \end{aligned}$$

This is effectively the same condition. We require

$$\frac{p^2}{m^2c^2} \ll 1 \qquad \Longrightarrow \qquad \frac{p}{m} \ll c.$$

3 1.3) Neutron Beams

A beam of neutrons with energy E runs horizontally into a crystal. The crystal transmits half the neutrons and deflects the other half vertically upwards. After climbing to height H these neutrons are deflected through $90°$ onto a horizontal path parallel to the originally transmitted beam. The two horizontal beams now move a distance L down the laboratory, one distance H above the other. After going distance L, the lower beam is deflected vertically upwards and is finally deflected into the path of the upper beam such that the two beams are co-spatial as they enter the detector. Given that particles in both the lower and upper beams are in states of well-defined momentum, show that the wavenumbers k, k' of the lower and upper beams are related by

$$k' \simeq k\left(1 - \frac{m_\mathrm{n} g H}{2E}\right)$$

where m_n is the neutron mass and g the acceleration due to gravity. In an actual experiment (R. Colella *et al.*, *Phys. Rev. Lett.*, **34**, 1472, 1975) $E = 0.042$ eV and $LH \sim 10^{-3}$ m^2 (the actual geometry was slightly different). Determine the phase difference between the two beams at the detector. Sketch the intensity in the detector as a function of H. [5]

We assume the energy of the beams is conserved and so

$$E = \frac{p^2}{2m_\mathrm{n}} = \frac{p'^2}{2m_\mathrm{n}} + m_\mathrm{n} g H$$

$$\implies \qquad p^2\left(1 - \frac{m_\mathrm{n} g H}{E}\right) = p'^2.$$

We know that $p = \hbar k$ and so we use this, taking a square root to find

$$k' \simeq k\left(1 - \frac{m_\mathrm{n} g H}{2E}\right),$$

assuming that $m_\mathrm{n} g H \ll E$.

One may worry that we are just using a classical result here. However, it is simple to prove. The Hamiltonian describing a system in a linear potential should look like

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m_\mathrm{n}} + m_n g \hat{z}$$

where we take the z-direction to be vertically upwards. We then send in states along the x direction. These states, by their construction, have the form

$$\psi_{p,h}(x) = \exp\left(\frac{i}{\hbar} p x\right) |h\rangle$$

where this state $|z\rangle$ is just defined such that $\hat{z}\,|h\rangle = h\,|h\rangle$. These wavefunctions are then eigenstates of the Hamiltonian with energies

$$E_{p,h} = \frac{p^2}{2m_\mathrm{n}} + m_\mathrm{n} g h.$$

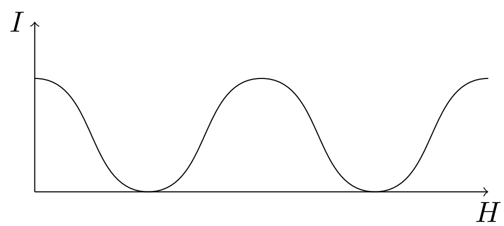
The phase difference at the detector will simply be the phase accrued over the distance L. So

$$\begin{aligned}\Delta\phi = (k - k')L &\simeq k\frac{m_\mathrm{n} g H}{2E} L \\ &= \frac{\sqrt{2m_\mathrm{n}E}}{\hbar}\frac{m_\mathrm{n} g}{2E} LH \\ &= 55.2 = (8.8 \times 2\pi)\,\text{radians}.\end{aligned}$$

At the detector, the total phases of the two waves add and we get the intensity

$$\begin{aligned}I &= \left|\frac{1}{2}e^{i\phi_0} + \frac{1}{2}e^{i(\phi_0+\Delta\phi)}\right|^2 \\ &= \frac{1}{4}\left|1 + e^{i\Delta\phi}\right|^2 \\ &= \cos^2\left(\frac{\Delta\phi}{2}\right).\end{aligned}$$

Sketching this, we find the following graph.



4 1.4) Cliff Scattering

Particles move in the potential

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x > 0 \end{cases}.$$

Particles of mass m and energy $E > V_0$ are incident from $x = -\infty$. Show that the probability that a particle is reflected is

$$\left(\frac{k-K}{k+K}\right)^2,$$

where $k = \frac{\sqrt{2mE}}{\hbar}$ and $K = \frac{\sqrt{2m(E-V_0)}}{\hbar}$. Show directly from the time-independent Schrödinger equation that the probability of transmission is

$$\frac{4kK}{(k+K)^2}$$

and check that the flux of particles moving away from the origin is equal to the incident particle flux. [5]

Consider first what the wavefunctions are for particles travelling in one dimension along a flat plane of height V,

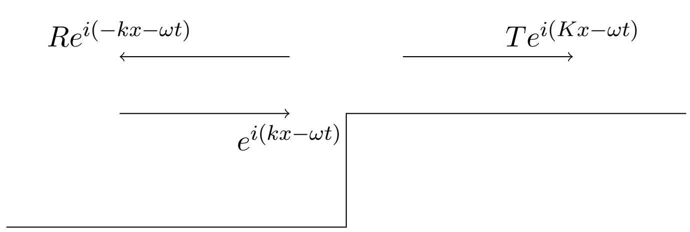
$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\psi = E\psi$$

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{2m(E-V)}{\hbar^2}\psi = -k'^2\psi \tag{4.1}$$

where we have define $k'(V) = \sqrt{2m(E-V)}/\hbar$. Thus,

$$\psi(x) = Ae^{ik'x} + Be^{-ik'x}$$

where $k'(0) = k$ and $k'(V_0) = K$. We can then consider that the $e^{ik'x}$ solution has positive momentum eigenvalue and so travels right whilst the negative solution must travel left. Therefore, we can consider the system as in the diagram. The incident wave has amplitude 1 and the reflected and transmitted waves have amplitude R and T respectively.



Now, consider what boundary conditions we have. We can integrate our Schrödinger equation, (4.1), from $-\epsilon$ to ϵ around the origin,

$$\left.\frac{\partial\psi}{\partial x}\right|_{\epsilon} - \left.\frac{\partial\psi}{\partial x}\right|_{-\epsilon} = -\int_{-\epsilon}^{\epsilon} \mathrm{d}x \left(k'^2\psi\right). \tag{4.2}$$

As the limit of this integral approach 0 the integral vanishes. Therefore, the derivative must be constant across the boundary and, by extension, the wavefunction itself. Let's apply these conditions,

$$1 + R = T,$$

$$k - kR = KT.$$

We then rearrange to get rid of T,

$$\frac{1-R}{1+R} = \frac{K}{k}$$

$$\implies R = \frac{k-K}{k+K}.$$

Similarly we find that

$$T = \frac{2k}{k+K}.$$

Finding the reflection and transmission probabilities is then not as simple as one might immediately expect. We are tempted to just take the mod squared of the wavefunction for each part but this will overestimate the probability for transmission. The physical reason is that the particles move slower there and so the density of that beam is higher. We must instead consider the probability flux,

$$\boldsymbol{J} = \frac{i\hbar}{2m}\left(\psi \nabla \psi^* - \psi^* \nabla \psi\right).$$

The probability of reflection must then be the modulus of the reflected flux divided by the modulus of the incident flux. For the incident, reflected and transmitted parts of the wave then the fluxes are

$$J_I = \frac{\hbar k}{m},$$

$$J_R = -\frac{\hbar k}{m}|R|^2,$$

$$J_T = \frac{\hbar K}{m}|T|^2.$$

Thus,

$$P_{\text{reflected}} = |R|^2 = \left(\frac{k-K}{k+K}\right)^2,$$

$$P_{\text{transmitted}} = \frac{K}{k}|T|^2 = \frac{4kK}{(k+K)^2}.$$

These do indeed add to one, so the flux out is the flux in.

To recall where this probability flux come from consider some time dependent probability distribution $P(x,t) = |\psi(x,t)|^2$. This must be conserved and so satisfies a continuity equation,

$$\frac{\partial P(x,t)}{\partial t} + \nabla \cdot \boldsymbol{J} = 0$$

$$\frac{\partial \psi}{\partial t}\psi^* + \psi\frac{\partial \psi^*}{\partial t} + \nabla \cdot \boldsymbol{J} = 0.$$

Here we make use of the time-dependent Schrödinger equation,

$$H\psi = i\hbar\frac{\partial \psi}{\partial t}$$

to find

$$\frac{i}{\hbar}\left(\psi(H\psi^*) - (H\psi)\psi^*\right) + \nabla \cdot \boldsymbol{J} = 0.$$

If we use a simple Hamiltonian, $H = p^2/2m + V(x)$, then we simply find

$$-\frac{i\hbar}{2m}\left(\psi(\nabla^2\psi^*) - (\nabla^2\psi)\psi^*\right) + \nabla \cdot \boldsymbol{J} = 0.$$

This can be solved by taking

$$\boldsymbol{J} = \frac{i\hbar}{2m}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right)$$

as we have seen.

5 1.5) Finite Well

Show that the energies of bound, odd-parity stationary states of the square potential well

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

are governed by

$$\cot(ka) = -\sqrt{\frac{W^2}{(ka)^2} - 1}\,,$$

$$\text{where} \qquad W = \sqrt{\frac{2mV_0a^2}{\hbar^2}} \qquad \text{and} \qquad k^2 = \frac{2mE}{\hbar^2}.$$

Show that for a bound odd-parity state to exist, we require $W > \frac{\pi}{2}$. [7]

We are searching for odd-parity solution, $\psi(-x) = -\psi(x)$. Therefore, consider the general solution to

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi$$

where V is some constant. In this 1D case,

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

where k' could well be imaginary if $E < V$. The solutions here are

$$\psi(x) = Ae^{ik'x} + Be^{-ik'x}. \tag{5.1}$$

However, we have odd parity symmetry which instantly tells us that $B = -A$,

$$\psi(x) = A\left(e^{ik'x} - e^{-ik'x}\right).$$

We can make this simplification because the parity operator, $\mathcal{P}$, commutes with our Hamiltonian. This is quite obvious because $H(x) = H(-x)$ quite obviously. Why this allows us to consider eigenstates which are also eigenvalues of this operator is less clear. So consider some $\psi(x)$ which is an eigenvalue of H,

$$H\psi(x) = E\psi(x).$$

Then consider creating some state $\mathcal{P}\psi(x)$. Is this also an eigenvalue? Because of the commutation relation, yes.

$$H\left(\mathcal{P}\psi(x)\right) = \mathcal{P}H\psi(x) = E\left(\mathcal{P}\psi(x)\right).$$

Therefore, we simplify proceedings by working in a basis of eigenstates of $\mathcal{P}$.

Therefore, within the well

$$\psi(x) = A'\sin(kx) \qquad\qquad k^2 = \frac{2mE}{\hbar^2}.$$

Outside the well the situation is a little less immediately obvious. We can return to the general solution, (5.1), with an imaginary k' and consider boundary conditions. The wavefunction must integrate to something finite by conservation of probability and so it must go to zero at infinity. This means that our solution outside looks like

$$\psi(x) = \begin{cases} B'e^{-Kx} & \text{for } x > a \\ -B'e^{Kx} & \text{for } x < a \end{cases} \qquad\qquad K^2 = \frac{2m(V_0 - E)}{\hbar^2}.$$

Note that $K^2 = \left(\frac{W}{a}\right)^2 - k^2$ for W as defined in the question.

Now we must satisfy boundary conditions. We need only do this at one boundary as parity will automatically take care of the other for us. So equating the wavefunction and the derivative at $x = a$,

$$A' \sin(ka) = B'e^{-Ka},$$

$$kA' \cos(ka) = -KB'e^{-Ka}.$$

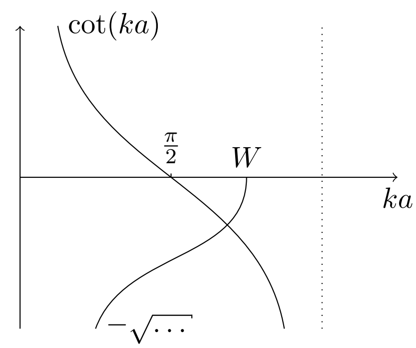
Dividing the two equations we find

$$\cot(ka) = -\frac{K}{k}.$$

Finally, we note our earlier observation about K and so find the form given,

$$\cot(ka) = -\sqrt{\frac{W^2/a^2 - k^2}{k^2}} = -\sqrt{\frac{W^2}{(ka)^2} - 1}\,.$$

Finally, we look for the case in which this has no solutions. What do these two graphs look like?



Thus, from the graph it is clear we require $W > \frac{\pi}{2}$. Furthermore, in the large-W limit we can imagine pulling W along to the right, giving a series of solutions at $k = \frac{n\pi}{a}$. This makes sense with the infinite-well problem.

6 1.8) Current

Given that the wavefunction is $\psi = Ae^{i(kz-\omega t)} + Be^{-i(kz+\omega t)}$, where A and B are constants, show that the probability current density is

$$\boldsymbol{J} = v\left(|A|^2 - |B|^2\right)\hat{\boldsymbol{z}},$$

where $v = \frac{\hbar k}{m}$. Interpret the result physically. [3]

We simply need to apply the formula we saw earlier for this,

$$\begin{aligned}
\boldsymbol{J} &= \frac{i\hbar}{2m}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right) \\
&= \frac{i\hbar}{2m}\left(\left(Ae^{i} + Be^{-i}\right)\left(-ikA^*e^{-i} + ikB^*e^{i}\right)\hat{\boldsymbol{z}} - \left(A^*e^{-i} + B^*e^{i}\right)\left(ikAe^{i} - ikBe^{-i}\right)\hat{\boldsymbol{z}}\right) \\
&= \frac{i\hbar}{2m}\left(-2ik|A|^2 + 2ik|B|^2\right)\hat{\boldsymbol{z}} \\
&= \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right)\hat{\boldsymbol{z}}
\end{aligned}$$

as required.

Physically, this wavefunction describes particles moving upwards (with amplitude A) and downwards (amplitude B). Therefore, the total flux along $\hat{\boldsymbol{z}}$ (upwards) is expected to be proportional to $|A|^2 - |B|^2$, the probability a particle is moving up minus the probability it moves down. The flux is then also proportional to the speed. We can see this is the expected speed of the particles with wavevector k because the momentum is $p = \hbar k$ and so $p = mv$ as expected.