1. From Prelims, January 12, 2007. Electron with effective mass. An electron is moving in one dimension in a potential $V(x) = 0$ for $x > 0$ and $V(x) = V_0 > 0$ for $x < 0$. The region $x > 0$ is empty space, where the electron mass is the usual bare mass m_0 , but in the region $x < 0$ it has a modified "effective mass" m_1 . When the mass of a non-relativistic particle depends on its position, the Hamiltonian should be written in the operator-ordered form

$$H = \frac{1}{2}\, p\,(m(x))^{-1} p + V(x)\,,$$

where $[x, p] = i\hbar$.

(a) The standard continuity conditions (continuity of $\psi(x)$ and $\psi'(x) = d\psi(x)/dx$) only apply at $x = 0$ if $m_1 = m_0$. Derive the modified continuity conditions that apply at points where the mass is discontinuous.

Solution

The left momentum operator operates on both the mass and right momentum operator (which operates on the wave function). Writing things out, we have

$$-\frac{1}{2}\hbar^2 \left(\frac{d}{dx}\frac{1}{m}\right)\frac{d\psi}{dx} - \frac{1}{2}\hbar^2 \frac{1}{m}\frac{d^2\psi}{dx^2} + V\psi - E\psi = 0\,.$$

Since $1/m$ has a step discontinuity, its derivative is a δ-function. This must be canceled by a δ-function elsewhere in the equation. We certainly don't want ψ to contain a δ-function, because then its derivatives would contain the first and second derivatives of a δ-function which would not be canceled by other terms in the equation. Also, ψ' should not contain a δ-function, else ψ'' would be the derivative of a δ-function and not canceled by other terms in the equation. Thus, ψ'' must contain a δ-function which cancels that from the derivative of $1/m$. This means ψ' has a step discontinuity and ψ is continuous.

It remains to express the discontinuity in ψ' in terms of the discontinuity in $1/m$. We do this by integrating from $-\epsilon$ to $+\epsilon$. In the limit $\epsilon \longrightarrow 0$, the terms containing V and E drop out. Also we can cancel the $\hbar^2/2$. So we are left with

$$\int_{-\epsilon}^{+\epsilon} \frac{1}{m}\frac{d^2\psi}{dx^2}\,dx = -\int_{-\epsilon}^{+\epsilon} \left(\frac{d}{dx}\frac{1}{m}\right)\frac{d\psi}{dx}\,dx\,.$$

Both integrals contain the product of a function with a step at $x = 0$ and a δ-function centered on $x = 0$, so the question is, how do we treat this? That is, what's a *delta*-function times a step? If we imagine that the δ-function is not quite infinitely narrow but is spread out over a very small distance, then the step will also be spread out over that same distance. If we do things symmetrically, then the δ-function is an even function and the step is a constant plus an odd function. The constant is just the average values on either side of the step. The integral of the δ-function times the constant gives the constant and the δ-function times the odd function gives 0. So

$$\frac{1}{2}\left(\frac{1}{m_0} + \frac{1}{m_1}\right)\left(\frac{d\psi(x_+)}{dx} - \frac{d\psi(x_-)}{dx}\right) = -\frac{1}{2}\left(\frac{1}{m_0} - \frac{1}{m_1}\right)\left(\frac{d\psi(x_+)}{dx} + \frac{d\psi(x_-)}{dx}\right)\,,$$

$x_\pm$ indicates the function should be evaluated just to the right or left of $x = 0$. Simplifying, we get the conditions for ψ'

$$\frac{1}{m_0}\frac{d\psi(x_+)}{dx} = \frac{1}{m_1}\frac{d\psi(x_-)}{dx} ,$$

and of course we already mentioned that ψ is continuous,

$$\psi(x_+) = \psi(x_-) .$$

Note that if $m_1 = m_0$, our conditions reduce to continuity of both ψ and ψ' as expected.

——— End Solution ———

(b) The (unnormalized) wavefunction of an eigenstate of the Hamiltonian with an energy $E < V_0$ is given by $\psi(x) = A\sin k(x - x_0)$ for $x > 0$. Find k, x_0 and $\psi(x)$ for $x < 0$. Make a sketch of the function $\psi(x)$, indicating its essential features.

——— Solution ———

For $x > 0$, solutions are $\exp(\pm ikx)$ with $E = \hbar^2k^2/2m_0$. Of course, these can be combined into the real functions $\cos(kx)$ and $\sin(kx)$, and the two can be converted into a single sine function with an amplitude and phase, $\psi(x) = A\sin(k(x - x_0))$. For $x < 0$, solutions are $\exp(\pm\kappa x)$ with $V_0 - E = \hbar^2\kappa^2/2m_1$. Since x can be arbitrarily large and negative, only the solution $\exp(\kappa x)$ is acceptable. We write it as $\psi(x) = B\exp(\kappa x)$. Continuity of ψ at $x = 0$ gives,

$$B = -A\sin(kx_0) .$$

Applying the condition on ψ' gives

$$\frac{1}{m_1}\kappa B = \frac{1}{m_0}kA\cos(kx_0) .$$

Solving for the tangent gives

$$x_0 = -\frac{1}{k}\tan^{-1}\left(\frac{k}{\kappa}\frac{m_1}{m_0}\right) .$$

With the expressions for k and κ in terms of E and $V_0 - E$, we have

$$\frac{k}{\kappa} = \sqrt{\frac{m_0}{m_1}\frac{E}{V_0 - E}} ,$$

and

$$x_0 = -\sqrt{\frac{\hbar^2}{2m_0E}}\,\tan^{-1}\left(\sqrt{\frac{m_1}{m_0}\frac{E}{V_0 - E}}\right) .$$

We can solve for B by isolating the cosine and the sine and squaring and adding.

$$\left(1 + \frac{m_0^2}{m_1^2}\frac{\kappa^2}{k^2}\right) B^2 = A^2 \; ,$$

or

$$B = \frac{1}{\sqrt{1 + \frac{m_0}{m_1}\frac{V_0 - E}{E}}} A \; .$$

The essential features on the plot would be the continuity of ψ, the change in slope, the exponential decay towards negative x and the wave towards positive x.

End Solution

2. Non-square Potential Barrier. In Homework 2, Problem 5, you solved the case of a plane wave incident on a barrier or well of width a. In this problem, we want to consider penetration of a barrier, so we will start out by assuming a wave of energy E is incident on a square barrier of height V_0 and width a. In your previous solution for this case, you should have discovered that the transmission probability is

$$t = \frac{4k^2\kappa^2}{(k^2 - \kappa^2)^2 \sinh^2(\kappa a) + 4k^2\kappa^2 \cosh^2(\kappa a)} \; ,$$

where $k = \sqrt{2mE/\hbar^2}$ and $\kappa = \sqrt{2m(V_0 - E)/\hbar^2}$.

(a) Show that for a high, wide barrier, this can be written as

$$t = \frac{16E(V_0 - E)}{V_0^2} e^{-2\sqrt{2m(V_0 - E)/\hbar^2}\, a} \; .$$

Solution

The main thing is that for big enough $\kappa \propto \sqrt{V_0}a$, the hyperbolic functions become $\exp(\kappa a)/2$. Plugging this in for both sinh and cosh and substituting $k^2 = 2mE/\hbar^2$ and $\kappa^2 = 2m(V_0 - E)/\hbar^2$ gives the desired result.

End Solution

It's an interesting fact that the argument of the exponent above depends on the width of the potential but the factor out in front (sometimes called the *prefactor*) doesn't. One might have thought that if one had two square barriers, each of height V_0 and width $a/2$, and these occurred one after the other with no gap, that the probability for transmission through both barriers would be the product of the probabilities for transmission through one and then the next. That is, $t(a) = t(a/2) \times t(a/2)$. This is correct for the exponential, but not for the prefactor! This can be understood in a qualitative way by noting that the exponential gives the decrease in the wave function through the barrier while the prefactor has to do with the matching (reflecting and transmitting) at the front and back ends of the barrier.

(b) Consider a barrier in which the potential depends on x, $V(x)$ and where the barrier extends from x_1 to x_2. That is $V(x_1) = V(x_2) = E$ and for $x_1 < x < x_2$, $V(x) > E$. This potential is envisioned as more or less smooth with no sudden steps. Give arguments to support the idea that the transmission probability through this barrier is roughly

$$t \approx e^{-2\int_{x_1}^{x_2} \sqrt{2m(V(x)-E)/\hbar^2}\,dx} .$$

Solution

First of all, there's no prefactor. If the potential is smooth on the scale of a wavelength, then one expects very little reflection due to the "impedance mismatch." So, the prefactor has just been dropped. Also, if there is a step, the prefactor is small in the ratio E/V_0 where V_0 must be the height of the barrier just after the step. This can be small, but for the usual barrier penetration problem, the exponential is much, much smaller!

Next, we notice that we can divide the interval from x_1 to x_2 into n smaller intervals of length Δx and, following the suggestion above, the transmission probability should just be the product of the probabilities for each "mini-barrier,"

$$\begin{aligned} t &= \prod_{i=1}^{n} e^{-2\sqrt{2m(V(x_i)-E)/\hbar^2}\,\Delta x} \\ &= e^{-2\sum_{i=1}^{n} -2\sqrt{2m(V(x_i)-E)/\hbar^2}\,\Delta x} \\ &\to e^{-2\int_{x_1}^{x_2} \sqrt{2m(V(x)-E)/\hbar^2}\,dx} . \end{aligned}$$

Of course, the exponential form of the transmission probability was derived on the assumption that $\kappa a \gg 1$ (so we could ignore the decaying exponentials in the sinh and cosh. For this approximation to make sense, the barrier height and width must be such that the decaying exponential can be ignored.

End Solution

3. Alpha Decay. In an alpha decay of a heavy nucleus, the alpha particle (^{4}He nucleus) is emitted with a typical kinetic energy of a few MeV. The half lives of alpha emitters range from a fraction of a second to billions of years. See R. D. Evans, *The Atomic Nucleus*, 1955, McGraw-Hill, p.78 for a plot in which the half life scale runs from 10^{-12} to 10^{+12} years while the decay energy runs from 4 to 7.5 MeV. The attempt to explain the large dynamic range in half life led to the tunneling explanation of alpha decay. We need a model

for the potential energy of interaction between the α particle and the daughter nucleus. To start with, there is the Coulomb interaction. The daughter nucleus has a positive charge $Z_1 e$ where e is the magnitude of the electron charge and Z_1 is typically 80-90. The α particle has charge $Z_2 e$, with $Z_2 = 2$. When the α particle is outside the nucleus, it feels only the Coulomb interaction and the potential is $Z_1 Z_2 e^2/r$ where r is the distance between the daughter nucleus and the α particle. A typical daughter nucleus has a total of $A \approx 220 - 240$ nucleons and its radius in fermis is $R \approx 1.5A^{1/3}$. (Over the interesting range of nuclei, the radius doesn't vary much!) As the α particle approaches the edge of the nucleus it feels the strong, but short range, force from the nearby nucleons which overwhelms the Coulomb force and so the potential drops suddenly. Inside the nucleus, the α particle feels a force only from the nearest nucleons which are more or less uniformly distributed around it, leading to no net force and a flat potential. So we are led to a model with two pieces: for $r < R$, $V(r) = -V_0$ and for $r > R$, $V(r) = Z_1 Z_2 e^2/r$. The Coulomb potential at the edge of the nucleus is $V(R) = Z_1 Z_2 e^2/R$.

(a) Estimate this potential height in MeV. Also estimate the radius at which the Coulomb potential is the same as the decay energy. To be definite, let's pick thorium ($Z = 90$, $A = 232$) decaying to radium ($Z = 88$, $A = 228$) with a decay energy $E \approx 4$MeV.

Solution

Well, this is pretty much plug and grind. If we do it in Gaussian units, we take $e = 4.8 \times 10^{-10}\,$statcoul, $A = 228$, so $R = 9 \times 10^{-13}\,$cm, and $Z_1 = 88$. This gives $V(R) = 45 \times 10^{-6}\,$erg $= 28\,$MeV. For the potential to be the same as the decay energy, the distance must be 7 times larger or $r_2 = 63 \times 10^{-13}\,$cm.

End Solution

(b) As a model, we assume the α particle exists as a particle within the nucleus and has the energy E. It is held within the nucleus by the barrier, but there's a chance for it to tunnel through. Calculate the transmission probability using the expression from problem 2. Be sure to make use of the fact that it's a high barrier!

Solution

We need to calculate the argument of the exponential

$$a = 2\int_R^{r_2} \sqrt{2m(Z_1 Z_2 e^2/r - E)/\hbar^2}\, dr\ ,$$

where r_2 is the outer turning point, $r_2 = Z_1 Z_2 e^2/E$, calculated in part (a). We can factor to get

$$\begin{aligned} a &= 2\sqrt{2mE/\hbar^2}\int_R^{r_2}\sqrt{r_2/r-1}\,dr \\ &= 2\sqrt{2mE/\hbar^2}\,r_2\int_{R/r_2}^{1}\sqrt{1/x-1}\,dx \\ &= 2\sqrt{2mE/\hbar^2}\,r_2\left(-\cos^{-1}(\sqrt{x})+\sqrt{x-x^2}\right)\Big|_{R/r_2}^{1} \\ &= 2\sqrt{2mE/\hbar^2}\,r_2\left(\cos^{-1}(\sqrt{R/r_2})-\sqrt{R/r_2-(R/r_2)^2}\right)\,. \end{aligned}$$

(The integral can be done by substituting $\cos^2\theta = x$.) We've seen that R/r_2 is small (1/7). So we just go to first order in $\sqrt{R/r_2}$. The inverse cosine becomes $\pi/2-\sqrt{R/r_2}$ and the other term becomes just $\sqrt{R/r_2}$, so

$$\begin{aligned} a &= 2\sqrt{\frac{2mE}{\hbar^2}}\,r_2\left(\frac{\pi}{2}-2\sqrt{\frac{R}{r_2}}\right) \\ &= 2\sqrt{\frac{2mE}{\hbar^2}}\,\frac{Z_1Z_2e^2}{E}\left(\frac{\pi}{2}-2\sqrt{\frac{RE}{Z_1Z_2e^2}}\right) \\ &= \pi\sqrt{2m}\,\frac{Z_2e^2}{\hbar}\left(\frac{Z_1}{\sqrt{E}}-\frac{4}{\pi}\sqrt{\frac{Z_1R}{Z_2e^2}}\right)\,. \end{aligned}$$

Finally, the transmission probability is

$$t = e^{-\pi\sqrt{2m}\,\frac{Z_2e^2}{\hbar}\left(\frac{Z_1}{\sqrt{E}}-\frac{4}{\pi}\sqrt{\frac{Z_1R}{Z_2e^2}}\right)}\,.$$

Note that the prefactor in the exponent contains constants and parameters of the α particle. The first term inside the parentheses contains the energy dependence and also the charge number of the daughter nucleus (which sets the barrier height). The second term is a small correction. This says that if the log of the decay time is plotted against the inverse of the square root of the energy, for different isotopes (same Z_1), a straight line should result. Schwabl contains such a plot. Also see Evans referenced above. Sure enough, this dependence seems to hold.

——— End Solution ———

(c) Using the expression you derived above, determine a numerical value for the transmission probability in the decay of thorium to radium. You should get a very small number. I get 3.6×10^{-40}. Estimate the lifetime of thorium. You might want to make an estimate for the number of times per second the α particle hits the barrier. This times the transition probability (per collision) is the probability per second to decay (or the inverse of the lifetime).

Solution

To do this we need to make an estimate for the speed of the α particle. We know that nuclear binding energies are roughly 8 MeV per nucleon. Also, we know that the α particle is unbound by 4 MeV. We can estimate the speed of the particle within the nucleus as $v = \sqrt{2T/m}$, where T is the kinetic energy of the α particle within the nucleus. We might take $T = 20\,\mathrm{MeV}$. (Note that this does not appear in an exponent so any error we make in this estimate will only affect the lifetime as the square root!) Then $v = 3 \times 10^9\,\mathrm{cm\,s^{-1}}$. The diameter of the nucleus is $2R$ and each time the α particle traverses the nucleus, it gets another chance at the barrier, so

$$\frac{1}{\tau} = \frac{v}{2R} t = 6.1 \times 10^{-19}\,\mathrm{s^{-1}} ,$$

or

$$\tau = 5 \times 10^{10}\,\mathrm{yr} .$$

The measured value is about 2×10^{10} yr. Not bad for such a simple model! Actually, although the value is close, what's convincing about the model is that it gives the correct dependence of the lifetime on Z and E.

End Solution

4. Consider an infinitely deep well, $V(x) = 0$ for $-a < x < b$ and $V(x) = \infty$ for $x < -a$ or $x > b$. Within the well, there is a δ-function addition to the potential, $V = \lambda\delta(x)$. (Centered at the origin.) This may seem a little artificial, but it's possible to confine electrons in a plane where the motion perpendicular to the plane is the motion discussed in this problem. See Schwabl, chapter 3.

(a) Find the normalized eigenfunctions and a formula for the energy eigenvalues.

Solution

If the energy is E, then let $\hbar^2 k^2/2m = E$. The wavefunctions must vanish at $x = -a$ and $x = b$, so the solution for $x < 0$ is $\psi_- = A_- \sin(k(a + x))$ and the solution for $x > 0$ is $\psi_+ = A_+ \sin(k(b - x))$. Continuity of ψ yields $A_- \sin(ka) = A_+ \sin(kb)$. We can automatically satisfy the continuity conditions if we write

$$\psi_- = A\frac{\sin(k(a + x))}{\sin(ka)} \qquad \text{and} \qquad \psi_+ = A\frac{\sin(k(b - x))}{\sin(kb)} .$$

(This works unless ka or kb is an integral number of πs!) Then the normalization becomes

$$1 = |A|^2 \left(\int_a^0 \frac{\sin^2(k(a + x))}{\sin^2(ka)}\, dx + \int_0^b \frac{\sin^2(k(b - x))}{\sin^2(kb)}\, dx \right) .$$

Performing the integrals gives

$$1 = \frac{|A|^2}{2} \left(\frac{a - \sin(2ka)/2k}{\sin^2(ka)} + \frac{b - \sin(2kb)/2k}{\sin^2(kb)} \right) ,$$

This yields

$$A = \sqrt{2}\left(\frac{a - \sin(2ka)/2k}{\sin^2(ka)} + \frac{b - \sin(2kb)/2k}{\sin^2(kb)}\right)^{-1/2},$$

for the normalization constant. Special treatment is required if one of the sines in the denominator vanishes. The discontinuity in slope yields (dropping A since it's just a normalization constant)

$$\frac{\hbar^2}{2m}\left(-\frac{k\cos(kb)}{\sin(kb)} - \frac{k\cos(ka)}{\sin(ka)}\right) = \frac{\lambda}{2}\left(\frac{\sin(kb)}{\sin(kb)} + \frac{\sin(ka)}{\sin(ka)}\right).$$

Rearranging, we get the equation for determining the energies,

$$k\cot(kb) + k\cot(ka) = -\frac{2m\lambda}{\hbar^2},$$

and of course, care is required when ka or kb is near an integral multiple of π!

End Solution

(b) Discuss the special cases $\lambda \to 0$ and $\lambda \to \infty$.

Solution

The special case $\lambda = 0$ is just a well of length $a + b$ and we know that $k(a + b) = n\pi$. Does this come from our equation above?

$$k\left(\frac{\cos(kb)}{\sin(kb)} + \frac{\cos(ka)}{\sin(ka)}\right) = 0,$$

or $\sin(k(a + b) = 0$ which gives the desired result.

The special case $\lambda = \infty$ splits the well into two parts. The wave function must be 0 at the origin as well as at the two boundaries. This means $ka = n_1\pi$ and $kb = n_2\pi$ (which causes the denominators in some of the expressions above to vanish!). Essentially there are two independent wells and any eigenfunction from the left well can be paired with any eigenfunction in the right well to give an eigenfunction with the other. However to get stationary states (having only a single energy) one must take eigenfunctions in the left well with $\psi = 0$ in the right well and vice versa.

End Solution

(c) Discuss the special case $a = b$.

Solution

In this case, the well is an even function of x. If we think of the well without the δ-function, the odd functions $2ka = 2n\pi$ are zero at the location of the δ-function and these functions will be unchanged by the δ-function. Note also, that these are exactly the functions where our denominators above vanish. We don't need to use the expressions above, because we can use the odd functions for the infinite well without a δ-function. For the even functions, both the eigenfunctions and energies will be changed by the presence of the well, but we can use the expressions from part (a). In particular, k can be found from

$$2k\cot(ka) = -\frac{2m\lambda}{\hbar^2} .$$

——— End Solution ———