1. 1D ionization. This problem is from the January, 2007, prelims. Consider a non-relativistic mass m particle with coordinate x in one dimension that is subject to an attractive delta-function potential at $x = 0$, *i.e.*, a potential $V(x) = -V_0\delta(x/a)$, with $V_0 > 0$.

(a) The ground state of the particle is a bound state. Find its wave function and binding energy.

Solution

The ground state will be even and of the form $\psi = A\exp(-\kappa|x|)$ where $\hbar^2\kappa^2/2m = -E_0$. Plugging ψ into the Schroedinger equation we get

$$-\nabla^2\psi + \frac{2m}{\hbar^2}V\psi = -\kappa^2\psi\ .$$

Now integrate from $-\epsilon$ to $+\epsilon$,

$$-2\left.\frac{d\psi}{dx}\right|_{+\epsilon} - \frac{2m}{\hbar^2}V_0 a\psi = 0\ ,$$

from which we learn

$$\kappa = \frac{mV_0 a}{\hbar^2}\ ,$$

and

$$-E_0 = \frac{mV_0^2 a^2}{2\hbar^2}\ .$$

The normalization constant is found from

$$1 = 2\int_0^\infty A^2 e^{-2\kappa x}\,dx\ ,$$

which gives

$$A = \sqrt{\kappa}\ ,$$

and

$$\psi(x,t) = \sqrt{\kappa}e^{-\kappa x + iE_0 t/\hbar}\ ,$$

where E_0 and κ are as given above.

End Solution

(b) The particle is now perturbed by a weak time-dependent potential $V(x,t) = Fx\cos\omega t$. Find the transition rate from the bound state to the continuum. (It may help to confine the particle in a large box $|x| < L/2$ and take the limit $L \to \infty$.)

Solution

We want to use time dependent perturbation theory to calculate the transition rate. For this we need to know the continuum states. If we think of a free particle plane wave, we note there will be a "kink" in the plane wave at the origin due to the delta-function. However, if we use the large box trick, the continuum states will be odd or even, $\sin kx$ or $\cos(k|x|+\phi_k)$. Note that in the absence of the delta-function potential, the wave functions would be sin or cos, but the even functions will see the potential and be somewhat different. As it turns out the ground state is even and the perturbing potential is odd, so the final state must be odd (in first order). We don't need to worry about the cosine states! So, we're concerned with states in the continuum of the form $\sqrt{2/L}\sin(2\pi nx/L)$ where n is an integer greater than 0. Note that the energy of this state is $E_n = 2\pi^2\hbar^2 n^2/mL^2$. The perturbation is $(Fx/2)(\exp(i\omega t) + \exp(-i\omega t))$ and only the second term will drive transitions to the continuum. By the Golden Rule, the transition rate is

$$\Gamma = \frac{2\pi}{\hbar}\rho(E_n) \mid \langle n \mid Fx/2 \mid \psi\rangle \mid^2 ,$$

where $\rho(E_n)$ is the density of states at the continuum energy, $E_n = -E_0+\hbar\omega$. The number of odd continuum states with energy less than E_n is n,

$$\rho(E) = \frac{dn}{dE} = \left(\frac{dE}{dn}\right)^{-1} = \frac{mL^2}{4\pi^2\hbar^2 n} = \frac{L}{2\pi\hbar}\sqrt{\frac{m}{2E_n}} .$$

Next we need to evaluate the matrix element

$$\langle n \mid Fx/2 \mid \psi\rangle = 2\sqrt{\kappa}\sqrt{\frac{2}{L}}\frac{F}{2}\int_0^{L/2} xe^{-\kappa x}\sin(2\pi nx/L)\,dx .$$

Recall that we will be taking the limit as $L \to \infty$. If $L \gg 1/\kappa$, we make no error in extending the integral to ∞. Also, we can evaluate a simpler integral and differentiate the result with respect to $-\kappa$ to get the integral we need. The simpler integral is

$$\begin{aligned}
\int_0^\infty e^{-\kappa x}\sin k_n x\,dx &= \frac{1}{2i}\int_0^\infty \left(e^{-(\kappa - ik_n)x} - e^{-(\kappa + ik_n)x}\right) dx \\
&= \frac{1}{2i}\left(\frac{1}{\kappa - ik_n} - \frac{1}{\kappa + ik_n}\right) \\
&= \frac{k_n}{\kappa^2 + k_n^2} .
\end{aligned}$$

Now differentiate with respect to $-\kappa$ and find that the integral we need for the matrix element is

$$\int_0^{L/2} xe^{-\kappa x}\sin(2\pi nx/L)\,dx = \frac{2\kappa k_n}{(\kappa^2 + k_n^2)^2} .$$

Putting it all together,

$$\Gamma = \frac{2\pi}{\hbar}\frac{L}{2\pi\hbar}\sqrt{\frac{m}{2E_n}}\frac{2\kappa F^2}{L}\frac{4\kappa^2 k_n^2}{(\kappa^2 + k_n^2)^4} = \frac{2\hbar F^2}{m}\frac{(-E_0)^{3/2}(E_n)^{1/2}}{(-E_0 + E_n)^4} .$$

Note that the energies in the denominator sum to $\hbar\omega$. Also, note that for $E_n \to 0$, the rate goes to 0 and also, for $E_n \to \infty$, the rate goes to 0. The maximum seems to be at $E_n = -E_0/7$.

End Solution

2. Spherical Square Potential. Consider low energy scattering of a particle of mass m from a spherical potential of radius a:

$$V(r) = \begin{cases} V_0 & r < a \\ 0 & r > a \end{cases} ,$$

where V_0 may be either positive or negative.

(a) Calculate the s-wave phase shift for incident energy E. Note that low energy scattering means $ka \ll 1$.

Solution

The s-wave phase shift is particular easy to calculate because there are no angular terms in the Schroedinger equation which takes the form

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}(rR(r)) + V(r)R(r) = ER(r) ,$$

where $R(r)$ is the radial wave function (aside from $1/\sqrt{4\pi}$, all there is for an s-wave!). Multiply through by r and let $u(r) = rR(r)$. Then the Schroedinger equation becomes

$$\frac{d^2u}{dr^2} - \frac{2m}{\hbar^2}Vu + k^2u = 0 ,$$

with $k = \sqrt{2mE/\hbar^2}$. For $r > a$, the potential term is 0 and the solution is

$$u_o = -e^{-ikr} + e^{+ikr + 2i\delta_0} ,$$

where δ_0 is the s-wave phase shift we want to calculate. Note the minus sign in front of the first exponential. This makes the solution proportional to the two Hankel functions, so that δ_0 has the proper definition. To start with let's suppose $V_0 > E$. Then the interior solution is

$$u_i(r) = \sinh(\kappa r) , \qquad \kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} .$$

We match the interior and exterior solutions at $r = a$, by matching the logarithmic derivatives. The result is

$$\frac{1}{\kappa a}\tanh(\kappa a) = \frac{1}{ka}\tan(ka + \delta_0) ,$$

which gives

$$\delta_0 = \tan^{-1}\left(\frac{ka}{\kappa a}\tanh(\kappa a)\right) - ka \bmod \pi \; .$$

In the limit $\kappa a \gg 1$, the potential approaches that of a hard sphere and

$$\delta_0 \to -ka \bmod \pi \; ,$$

as discussed in lecture. At the other extreme, $V_0 \to E$, $\kappa a \to 0$,

$$\delta_0 \to \tan^{-1} ka - ka \bmod \pi \to -\frac{(ka)^3}{3} \bmod \pi \; .$$

Now suppose $V_0 < E$. The interior solution is

$$u_i(r) = \sin(qr) \; , \qquad q = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} \; .$$

Again, we match logarithmic derivatives,

$$\frac{1}{qa}\tan(qa) = \frac{1}{ka}\tan(ka + \delta_0) \; ,$$

or

$$\delta_0 = \tan^{-1}\left(\frac{ka}{qa}\tan(qa)\right) - ka \bmod \pi \; .$$

When the potential is larger than E, the phase is negative. When the potential is less than E, the phase is positive. If you work out what this does to the wave, you'll see that the wave is pushed out by a repulsive potential and pulled in by an attractive potential. We can carry this a little farther by considering bound states. If we look for a bound state with energy $\epsilon < 0$ and define

$$q_1 = \sqrt{\frac{2m(\epsilon - V_0)}{\hbar^2}} \; , \qquad \kappa_1 = \sqrt{-\frac{2m\epsilon}{\hbar^2}} \; ,$$

then the matching condition for a bound state gives

$$\frac{1}{q_1 a}\tan(q_1 a) = -\frac{1}{\kappa_1 a} \; .$$

If the bound state energy is small, then $q_1 \approx q$ and the left hand side of the bound state matching condition is almost the same as the left hand side of the scattering matching condition, so we see that the phase shift is determined by the bound state energy (provided it's small). In fact, we imagine a thought experiment where we start with V_0 small and increase it's magnitude (that is make it more negative) until we just have a bound state,

$\kappa_1 = 0$ when the state is bound with 0 energy. In this case, $\tan(q_1 a)$ is such that $q_1 a$ is just past $\pi/2$ and qa will be just less than $\pi/2$. If we crank up V_0 some more, eventually a second bound state appears. At this point, $q_1 a$ is just slightly greater than $\pi/2 + \pi$ and qa slightly less. As we make the well deeper and deeper to produce more bound states, the scattering phase increases, so that it's $\delta_0 = \pi/2 + n\pi$ as bound state $n + 1$ is added.

End Solution

(b) Can the s-wave phase shift be a multiple of π? What happens in this case? Hint: Google "Ramsauer Effect."

Solution

From the discussion in the previous part, it's easy to see that if the potential is deep enough to produce several bound states, there's enough room to adjust ka to get a phase shift of $n\pi$. In this case, $\sin\delta_l = 0$ and there is no scattering. A target that was opaque suddenly becomes transparent when the correct incident energy is reached. This is called the "Ramsauer Effect," and is observed in the scattering of low energy electrons from noble gases.

End Solution

3. A really, really square potential! This problem appeared on the May, 2004 prelims. A beam of particles of mass m and energy E propagates along the z axis of a coordinate system and scatters from the cubic potential

$$V = \begin{cases} v & \text{if } |x| \le L,\ |y| \le L, \text{ and } |z| \le L, \\ 0 & \text{otherwise} \end{cases}$$

where v is a small constant energy.

(a) Use the Born approximation to find an explicit formula for the scattering cross section $\sigma = \sigma(\theta, \phi)$ as a function of the angles θ and ϕ. Recall that spherical coordinates of a point in space are related to the Cartesian coordinates (x, y, z) by $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, and $x = r\cos\theta$. The Born approximation is easy to evaluate in one coordinate system and hard in the other.

Solution

The Born approximation is a prefactor times the Fourier transform of the potential evaluated at the difference in input and output wavevectors. The scattering amplitude is

$$f(\theta, \phi) = -\frac{m}{2\pi\hbar^2}\int d^3\boldsymbol{x} V(\boldsymbol{x}) e^{-i\Delta\boldsymbol{k}\cdot\boldsymbol{x}} \ .$$

Since the boundaries of the potential are easy to describe in Cartesian coordinates and a bear to describe in spherical coordinates, that should be a clue that we want to do the integral in Cartesian coordinates.

$$f(\theta, \phi) = -\frac{mv}{2\pi\hbar^2} I_x I_y I_z \ ,$$

where

$$I_x = \int_{-L}^{+L} e^{-ik_x x}\,dx = \frac{2}{k_x}\sin(k_x L)\,,$$

$$I_y = \int_{-L}^{+L} e^{-ik_y y}\,dy = \frac{2}{k_y}\sin(k_y L)\,,$$

$$I_z = \int_{-L}^{+L} e^{-i(k_z - k)z}\,dz = \frac{2}{(k_z - k)}\sin((k_z - k)L)\,.$$

$k_x = k\sin\theta\cos\phi$, $k_y = k\sin\theta\sin\phi$, and $k_z - k = k(\cos\theta - 1) = -2k\sin^2\theta/2$. Plug it all in and square to get

$$\sigma(\theta,\phi) = \frac{4m^2v^2}{\pi^2\hbar^4k^6}\,\frac{\sin^2(kL\sin\theta\cos\phi)\sin^2(kL\sin\theta\sin\phi)\sin^2(2kL\sin^2\theta/2)}{\sin^4\theta\sin^4(\theta/2)\cos^2\phi\sin^2\phi}\,.$$

Recall, $\hbar^2k^2/2m = E$ so the factor out in front can be simplified to give

$$\sigma(\theta,\phi) = \frac{v^2}{\pi^2E^2k^2}\,\frac{\sin^2(kL\sin\theta\cos\phi)\sin^2(kL\sin\theta\sin\phi)\sin^2(2kL\sin^2\theta/2)}{\sin^4\theta\sin^4(\theta/2)\cos^2\phi\sin^2\phi}\,,$$

where it's easy to see that the expression has the dimensions of an area. (Recall v is an energy!)

——— End Solution ———

(b) Under what circumstances is this approximation for the scattering cross section valid? Explain.

——— Solution ———

The Born approximation is obtained by writing the wave function as $\psi = \psi_0 + \psi_s$ where ψ_0 is the incident plane wave and ψ_s is the scattered wave. This wave function is inserted in the Schroedinger equation and one obtains the inhomogeneous wave equation for ψ_s with source terms involving the scattering potential times ψ_0 and ψ_s. The assumption leading to the Born approximation is that the ψ_s can be ignored as a source term or that ψ_s is very small compared to ψ_0. (One could make an expansion in which $V\psi_0$ produces the first order ψ_{s1}, $V\psi_{s1}$ produces a second order ψ_{s2}, etc. The Born approximation cuts off the expansion after the first term.) Recall that the outgoing wave is $f(\theta,\phi)\exp(ikr)/r$. Translated to our problem, the Born approximation will be valid when the outgoing wave is small at the edge of the potential. This means $EkL \gg |v|$.

——— End Solution ———

4. Neutron capture. (Based on a problem in Dicke and Witke, *Introduction to Quantum Mechanics*.) For a particular nucleus, the neutron absorption cross section, for 0.1 eV neutrons, is $\sigma_a = 2.5 \times 10^{-18}\,\mathrm{cm}^2$. What are the upper and lower bounds on the 0.1 eV neutron elastic scattering cross section?

Solution

Very low energy scattering will be pure s-wave. In this case,

$$\sigma_a = \frac{\pi}{k^2}\left(1 - \left|e^{2i\delta_0}\right|^2\right) ,$$

and

$$\sigma_s = \frac{\pi}{k^2}\left|1 - e^{2i\delta_0}\right|^2 .$$

The wavenumber for 0.1 eV neutrons can be found from $k = \sqrt{2mE/\hbar^2}$, with $mc^2 = 939.5\,\mathrm{MeV}$ for a neutron and $\hbar c = 1.975 \times 10^{-5}\,\mathrm{eV\,cm}$. Then $\pi/k^2 = 6.52 \times 10^{-18}\,\mathrm{cm}^2$. If we write $\exp(2i\delta_0) = \exp(ia)\exp(-b)$, then the absorption cross section is

$$\sigma_a = \frac{\pi}{k^2}\left(1 - e^{-2b}\right) ,$$

from which we learn $\exp(-b) = 0.7852$. Then the scattering cross section is

$$\sigma_s = \frac{\pi}{k^2}\left(1 - 2e^{-b}\cos a + e^{-2b}\right) .$$

As a can be anything, the limits on the scattering cross section are

$$\sigma_s = \frac{\pi}{k^2}\left(1 \pm e^{-b}\right)^2 = 0.30 \times 10^{-18}\,\mathrm{cm}^2 \text{ to } 20.8 \times 10^{-18}\,\mathrm{cm}^2 .$$

End Solution