ECE162A
Homework #3

Problem 1

Consider a particle in a box with:

$$V(x) = \begin{cases} 0 & \text{for} \quad -L/2 \le x \le L/2 \\ \infty & \text{for} \quad |x| > L/2 \end{cases}$$

Part A The potential $V(x)$ can be drawn as follows:

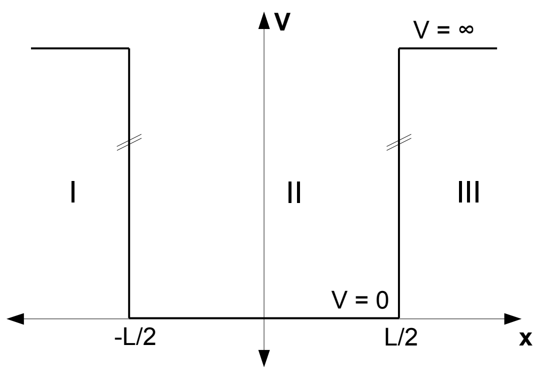

Figure 1: Potential $V(x)$ for an infinite well.

Part B Since $V(x) = \infty$ for $|x| > L/2$, the wave function for regions outside the well must be 0. From the continuity boundary condition, we can say that:

$$\psi_I(x = -L/2^-) = \psi_{II}(x = -L/2^+)$$
$$\psi_{II}(x = L/2^-) = \psi_{III}(x = L/2^+)$$

where ψ_I is the wave function for region 1, ψ_{II} is the wave function for region 2, and ψ_{III} is the wave function for region 3. Since $\psi_I(x) = \psi_{III}(x) = 0$, we can rewrite the boundary conditions as:

$$\psi_{II}(x = -L/2^+) = 0$$
$$\psi_{II}(x = L/2^-) = 0$$

The wave function for region 2 can be represented as a standing wave, as $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$ has fixed nodes at $-d/2$ and $d/2$. The general solution to the Schroedinger equation[1] for a standing wave is:

$$\psi_{II}(x) = A\sin(kx) + B\cos(kx) \quad \text{where} \quad k = \frac{\sqrt{2mE}}{\hbar} \tag{1}$$

[1] For the derivation, see Section 6-7 in Eisberg and Resnick

Part C After applying the boundary conditions at $x = \pm d/2$ to equation 1, we obtain the following equations:

$$A\sin\left(\frac{kL}{2}\right) + B\cos\left(\frac{kL}{2}\right) = 0 \quad \text{when} \quad x = L/2$$
$$-A\sin\left(\frac{kL}{2}\right) + B\cos\left(\frac{kL}{2}\right) = 0 \quad \text{when} \quad x = -L/2$$

By adding these two equations, we find:

$$2B\cos\left(\frac{kL}{2}\right) = 0 \tag{2}$$

Subtracting these two equations results in another relationship:

$$2A\sin\left(\frac{kL}{2}\right) = 0 \tag{3}$$

For a valid solution to the time-independent Schroedinger equation (TISE), we need values for A, B, and k that satisfy equations 2 and 3. Since there is no single value of k that causes both $\cos\left(\frac{kL}{2}\right)$ and $\sin\left(\frac{kL}{2}\right)$ to equal 0, we can separate the general solution (Equation 1) into two forms:

$$\psi(x) = B\cos(kx) \quad \text{and} \quad \cos\left(\frac{kL}{2}\right) = 0 \tag{4}$$
$$\psi(x) = A\sin(kx) \quad \text{and} \quad \sin\left(\frac{kL}{2}\right) = 0 \tag{5}$$

where $A = 0$ in equation 1 to obtain the first case and $B = 0$ to find the second.

If $\cos\left(\frac{kL}{2}\right) = 0$, then k must take the following values in equation 4:

$$\frac{kL}{2} = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \ldots$$
$$k = \frac{n\pi}{L} \quad \text{where} \quad n = 1, 3, 5, \ldots$$

For $\sin\left(\frac{kL}{2}\right) = 0$, k must take the following values in equation 5:

$$\frac{kL}{2} = \pi, 2\pi, 3\pi, \ldots$$
$$k = \frac{n\pi}{L} \quad \text{where} \quad n = 2, 4, 6, \ldots$$

Therefore, k is a discrete quantity and $\psi(x)$ can be written as:

$$\psi(x) = B_n\cos(k_n x) \quad \text{where} \quad k_n = \frac{n\pi}{L} \quad n = 1, 3, 5, \ldots \tag{6}$$
$$\psi(x) = A_n\sin(k_n x) \quad \text{where} \quad k_n = \frac{n\pi}{L} \quad n = 2, 4, 6, \ldots \tag{7}$$

Part D The wave functions for the first three eigen states ($n = 1, 2, 3$) are:

$$\psi_1(x) = B_1 \cos\left(\frac{\pi x}{L}\right)$$
$$\psi_2(x) = A_2 \cos\left(\frac{2\pi x}{L}\right)$$
$$\psi_3(x) = B_3 \cos\left(\frac{3\pi x}{L}\right)$$

The wave functions are plotted in Figure 2.

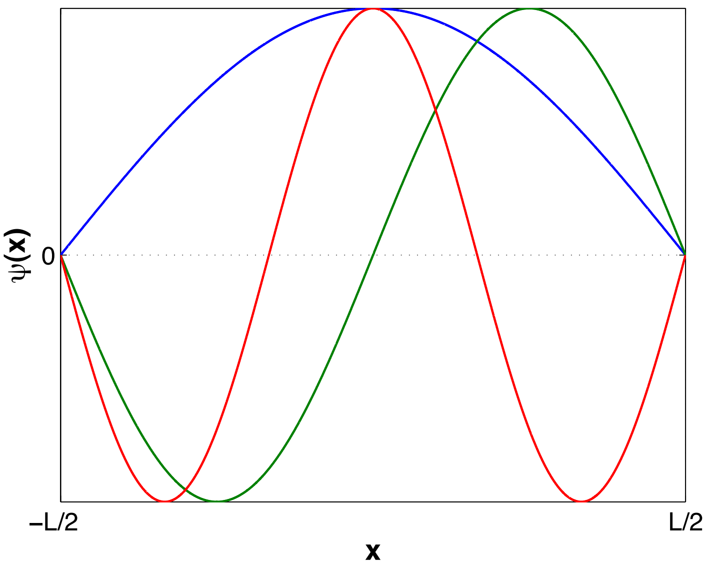

Figure 2: Wave function $\psi(x)$ for $n = 1$ (red), $n = 2$ (green), and $n = 3$ (blue).

Part E The first wave function can be normalized by determining the value for B_1 that satisfies the following condition:

$$\int_{-L/2}^{L/2} B_1^2 \cos^2(k_1 x)\, dx = 1 \quad \text{where} \quad k_1 = \frac{\pi}{L}$$

By simplifying the expression and chugging through the integration:

$$B_1^2 \int_{-L/2}^{L/2} B_1^2 \cos^2\left(\frac{\pi x}{L}\right) dx = 1$$
$$B_1^2 \int_{L/2}^{L/2} \left[\frac{\cos\left(\frac{2\pi x}{L}\right) + 1}{2}\right] dx = 1$$
$$\frac{B_1^2}{2}\left[\frac{L}{2\pi}\sin\left(\frac{2\pi x}{L}\right) + x\right]_{-L/2}^{L/2} = 1$$
$$\frac{B_1^2}{2}(L/2 + L/2) = 1$$

$$\boxed{B_1 = \sqrt{\frac{2}{L}}}$$

The normalized wave function can then be written as:

$$\psi_1(x) = \sqrt{\frac{2}{L}} \cos\left(\frac{\pi x}{L}\right)$$

Part F Energy and k are related by the following expression from Part B:

$$k = \frac{\sqrt{2mE}}{\hbar}$$

Rearranging an solving for energy gives:

$$E = \frac{\hbar^2 k^2}{2m}$$

Since we have already shown that k is quantized, the same can be said for energy E by plugging in valid values for k:

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2} \quad \text{where} \quad n = 1, 2, 3, ...$$

Energy is quantized when a particle is confined by a potential, limiting the particle to a certain region in space ($E < V_{barrier}$).

Part G The condition for continuity of $d\psi(x)/dx$ across the boundary is violated in Figure 2. This is acceptable because we are using an infinite potential, which is only an approximation to a large potential and is not physically realizable. If the potential were large but finite, we would have continuity of $d\psi(x)/dx$.

Part H If the potential well has the following properties:

$$V(x) = \begin{cases} V_o & \text{for} \quad -L \leq x \leq L \\ \infty & \text{for} \quad |x| > L/2 \end{cases}$$

we can find k and both $\psi_n(x)$ and E_n for $n = 1, 2, 3$. Since the length of the cavity has doubled, we can write k as:

$$k = \frac{n\pi}{2L} \quad \text{where} \quad n = 1, 2, 3, ... \tag{8}$$

The first three wave functions ($n = 1, 2, 3$) are then:

$$\psi_1(x) = B_1 \cos\left(\frac{\pi x}{2L}\right)$$
$$\psi_2(x) = A_2 \cos\left(\frac{\pi x}{L}\right)$$
$$\psi_3(x) = B_3 \cos\left(\frac{3\pi x}{2L}\right)$$

where B_1 is

$$B_1 = \sqrt{\frac{2}{2L}} = \sqrt{\frac{1}{L}}$$

Finally, the expression for $k = \frac{\sqrt{2mE}}{\hbar}$ from Part B is no longer since $V_o \neq 0$. We must take V_o into account within the well, which can be done with a familiar equation:

$$k = \frac{\sqrt{2m(E - V_o)}}{\hbar}$$

Rearranging to solve for E and plugging in k from equation 8 gives us an expression for the eigen energy values (E_n):

$$E = \frac{\hbar^2}{2m} + V_o$$
$$E_n = \frac{n^2\hbar^2\pi^2}{8mL^2} + V_o \quad \text{where} \quad n = 1, 2, 3, ...$$

The first three eigen values ($n = 1, 2, 3$) are then:

$$E_1 = \frac{\hbar^2\pi^2}{8mL^2} + V_o$$
$$E_2 = \frac{\hbar^2\pi^2}{2mL^2} + V_o$$
$$E_3 = \frac{9\hbar^2\pi^2}{8mL^2} + V_o$$

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Problem 2

Figure 3 represents the finite potential well system used in the Problem 2.

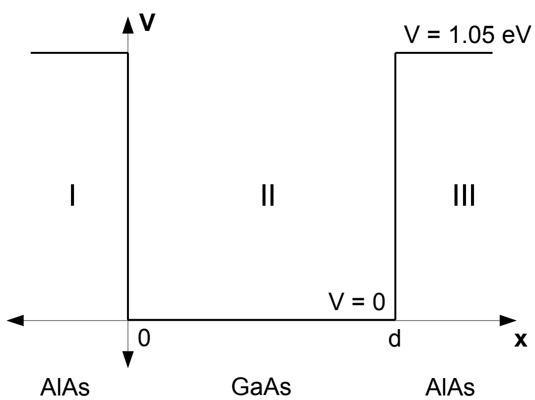

Figure 3: AlAs/GaAs/AlAs hetero junction quantum well for Problem 2.

Part A The wave functions in regions I and III will take the form of a decaying exponential since $E < V_o$ for particles confined in the well. The wave function in region II will represent waves traveling in $+x$ and $-x$ due to reflection off the potential barriers, and has fixed nodes similar to the infinite well analyzed in Problem 1. Due to the fixed nodes at $x = 0$ and $x = d$, we can use the solution for a standing wave. Wave functions for regions I, II, and III can be written:

$$\psi_I(x) = C\exp(k_I x) + D\exp(-k_I x)$$
$$\psi_{II}(x) = A\sin(k_{II}x) + B\cos(k_{II}x)$$
$$\psi_{III}(x) = E\exp(k_{III}x) + F\exp(-k_{III}x)$$

where

$$k_I = k_{III} = \frac{\sqrt{2m(V_o - E)}}{\hbar}$$
$$k_{II} = \frac{\sqrt{2mE}}{\hbar}$$

Since k_I and k_{II} are positive, we can also set $D = 0$ since $\psi(x) \to \infty$ for a particle traveling towards $x \to -\infty$. We also can set $E = 0$ by the same argument.

Before determining the coefficients to the wave equations, we can simplify the boundary conditions by "shifting" the finite well over by $d/2$ and the coordinates symmetric around 0. This can be done by setting $x' = x - d/2$, resulting in boundary conditions at $x' = \pm d/2$. This is shown in Figure 4

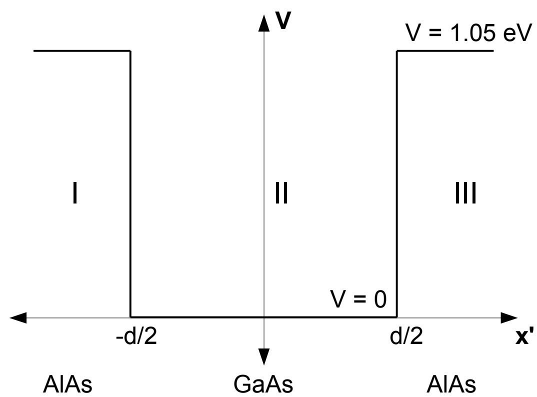

Figure 4: Potential well after shifting the position along x by $d/2$.

Applying continuity of $\psi(x')$ and $d\psi(x')/dx'$ at $x' = d/2$, we have the following equations:

$$A\sin\left(k_{II}\frac{d}{2}\right) + B\cos\left(k_{II}\frac{d}{2}\right) = F\exp\left(-\alpha\frac{d}{2}\right) \tag{9}$$
$$Ak_{II}\cos\left(k_{II}\frac{d}{2}\right) - Bk_{II}\sin\left(k_{II}\frac{d}{2}\right) = -\alpha F\exp\left(-\alpha\frac{d}{2}\right) \tag{10}$$

where $\alpha \equiv k_I = k_{III}$. Also, at $x' = -d/2$ we have:

$$A\sin\left(-k_{II}\frac{d}{2}\right) + B\cos\left(-k_{II}\frac{d}{2}\right) = C\exp\left(-\alpha\frac{d}{2}\right) \tag{11}$$
$$Ak_{II}\cos\left(-k_{II}\frac{d}{2}\right) - Bk_{II}\sin\left(-k_{II}\frac{d}{2}\right) = \alpha C\exp\left(-\alpha\frac{d}{2}\right) \tag{12}$$

By manipulating the expressions above, we can obtain:

$$
\begin{aligned}
2A\sin\left(k_{II}\frac{d}{2}\right) &= (F-C)\exp\left(-\alpha\frac{d}{2}\right) && \text{from} \quad 9-11 \\
2B\cos\left(k_{II}\frac{d}{2}\right) &= (F+C)\exp\left(-\alpha\frac{d}{2}\right) && \text{from} \quad 9+11 \\
2Bk_{II}\sin\left(k_{II}\frac{d}{2}\right) &= -\alpha(F+C)\exp\left(-\alpha\frac{d}{2}\right) && \text{from} \quad 10-12 \\
2Ak_{II}\cos\left(k_{II}\frac{d}{2}\right) &= \alpha(F-C)\exp\left(-\alpha\frac{d}{2}\right) && \text{from} \quad 10+12
\end{aligned}
$$

These equations have two different solutions, where $A = 0$ and $(F - C) = 0$ or $B = 0$ and $(F + C) = 0$.

Taking $A = 0$, we have:

$$B\cos\left(k_{II}\frac{d}{2}\right) = F\exp\left(-\alpha\frac{d}{2}\right) \tag{13}$$

$$-Bk_{II}\sin\left(k_{II}\frac{d}{2}\right) = -\alpha F\exp\left(-\alpha\frac{d}{2}\right) \tag{14}$$

Dividing these two equations results in the energy condition for the symmetric case:

$$k_{II}\tan\left(k_{II}\frac{d}{2}\right) = \alpha$$

We can also solve for F and C in terms of B using equation 13:

$$F = C = B\cos\left(k_{II}\frac{d}{2}\right)\exp\left(\alpha\frac{d}{2}\right)$$

Taking $B = 0$, we have:

$$A\sin\left(k_{II}\frac{d}{2}\right) = F\exp\left(-\alpha\frac{d}{2}\right) \tag{15}$$

$$Ak_{II}\cos\left(k_{II}\frac{d}{2}\right) = -\alpha F\exp\left(-\alpha\frac{d}{2}\right) \tag{16}$$

Dividing these two equations results in the energy condition for the antisymmetric case:

$$-k_{II}\cot\left(k_{II}\frac{d}{2}\right) = \alpha$$

We can also solve for F and C in terms of A using equation 15:

$$F = -C = A\sin\left(k_{II}\frac{d}{2}\right)\exp\left(\alpha\frac{d}{2}\right)$$

We now have two independent solutions: a symmetric solution with $A = 0$ and an antisymmetric solution with $B = 0$. The symmetric solution is:

$$\begin{aligned}
\psi_I(x) &= B\cos\left(k_{II}\frac{d}{2}\right)\exp\left(\alpha\frac{d}{2}\right)\exp\left(\alpha\left(x-\frac{d}{2}\right)\right) \\
\psi_{II}(x) &= B\cos\left(k_{II}\left(x-\frac{d}{2}\right)\right) \\
\psi_{III}(x) &= B\cos\left(k_{II}\frac{d}{2}\right)\exp\left(\alpha\frac{d}{2}\right)\exp\left(-\alpha\left(x-\frac{d}{2}\right)\right)
\end{aligned}$$

or more simply:

$$\begin{aligned}
\psi_I(x) &= B\cos\left(k_{II}\frac{d}{2}\right)\exp\left(\alpha x\right) \\
\psi_{II}(x) &= B\cos\left(k_{II}\left(x-\frac{d}{2}\right)\right) \\
\psi_{III}(x) &= B\cos\left(k_{II}\frac{d}{2}\right)\exp\left(-\alpha\left(x-d\right)\right)
\end{aligned}$$

Similarly, for the antisymmetric case, we have:

$$\begin{aligned}
\psi_I(x) &= -A\sin\left(k_{II}\frac{d}{2}\right)\exp\left(\alpha x\right) \\
\psi_{II}(x) &= A\sin\left(k_{II}\left(x-\frac{d}{2}\right)\right) \\
\psi_{III}(x) &= A\sin\left(k_{II}\frac{d}{2}\right)\exp\left(-\alpha\left(x-d\right)\right)
\end{aligned}$$

Part B See Figure 6-26 in Eisberg and Resnick. While this is for a finite well between $\pm a/2$, the results for this problem will be similar if $-a/2$ is taken to be 0 and $a/2$ is taken to be d.

Part C The maximum energy of the lowest energy state (E_1) occurs when $V_o = \infty$. For $d = 5$nm and $m_{eff} = 0.067m_e$, we can find E_1 for an infinite well:

$$\begin{aligned}
E_1 &= \frac{\hbar^2\pi^2}{2mL^2} \\
&= \frac{(1.0545\times10^{-34})^2\pi^2}{2(0.067\cdot 9.1\times10^{-31})(5\times10^{-9})^2} \\
&= 3.60\times10^{-20}\text{ J} \\
&= \frac{3.60\times10^{-20}\text{ J}}{1.602\times10^{-19}\text{ J/eV}} = 0.2247\text{ eV}
\end{aligned}$$

■

Problem 3

The general expression for the phase component of a value x is:

$$\theta = \arctan\left(\frac{\Im[x]}{\Re[x]}\right)$$

where $\Im[x]$ is the imaginary component of x and $\Re[x]$ is the real component.

Part A: E < V We know that the $+x$ and $-x$ traveling waves have the the following coefficients from boundary conditions:

$$\begin{aligned} A &= \frac{1}{2}\left(1 + i\frac{\alpha}{k}\right)C \quad (+x) \\ B &= \frac{1}{2}\left(1 - i\frac{\alpha}{k}\right)C \quad (-x) \end{aligned}$$

We can express reflection as B/A, or:

$$\begin{aligned} \frac{B}{A} &= \frac{k - i\alpha}{k + i\alpha} \\ &= \frac{k^2 - \alpha^2 - i(2k\alpha)}{k^2 + \alpha^2} \end{aligned}$$

The phase difference between B and A then:

$$\theta = \arctan\left(\frac{-2k\alpha/(k^2+\alpha^2)}{(k^2-\alpha^2)/(k^2+\alpha^2)}\right)$$

$$\boxed{\theta = -\arctan\left(\frac{2k\alpha}{k^2 - \alpha^2}\right)}$$

Part B: E > V We know that the $+x$ and $-x$ traveling waves have the the following coefficients from boundary conditions:

$$\begin{aligned} A &= \frac{1}{2}\left(1 + \frac{k_{II}}{k_I}\right)C \quad (+x) \\ B &= \frac{1}{2}\left(1 - \frac{k_{II}}{k_I}\right)C \quad (-x) \end{aligned}$$

We can express reflection as B/A, or:

$$\frac{B}{A} = \frac{k_I - k_{II}}{k_I + k_{II}}$$

Since $\Im(B/A) = 0$,

$$\boxed{\theta = \arctan(0) = 0}$$

Part C: E < V(∞) In the region where $V(x) = \infty$, the wave function will be 0. The wave equation for the region where $V(x) = 0$ is:

$$\psi_{V=0} = A\exp(ikx) + B\exp(-ikx)$$

The continuity of $\psi(x)$ at the boundary ($x = 0$) insists that:

$$A + B = 0$$
$$A = -B$$

The wave equation can then be written as:

$$\begin{aligned}\psi_{V=0} &= A\left(\exp(ikx) - \exp(-ikx)\right)\\ &= A\left(\exp(ikx) + \exp(-i(kx - \pi))\right)\end{aligned}$$

since $\exp(i\pi) = -1$. Therefore, the phase difference θ between the incident and reflected wave for a step with $V(x) = \infty$ is:

$$\boxed{\theta = \pi}$$

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Problem 4

Small angle scattering of α particles disagrees with the Rutherford formula because the formula only takes into consideration scattering due to the coulombic force of the atomic nucleus/nucleii on the α particle. As a result, scattering due to the α particle interacting with electrons around the nucleus are effectively ignored. This form of scattering typically results in small angles, while scattering due to the coulombic force of the nucleus can result in large angles. ■

Problem 5

Figure 6 represents the system discussed in Part A.

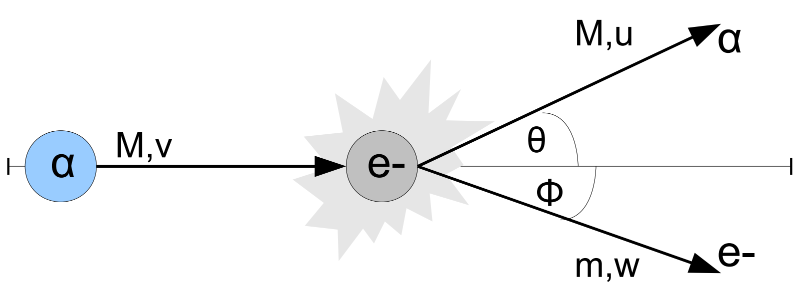

Figure 5: α particle scattered from an e^-

Part A We can start with momentum conservation and kinetic energy conservation of the α particle and stationary electron. For momentum conservation in x and y, we have:

$$Mv = Mu\cos\theta + mw\cos\phi$$
$$Mu\sin\theta = mw\sin\phi$$

Conservation of kinetic energy gives:

$$\frac{1}{2}Mv^2 = \frac{1}{2}Mu^2 + \frac{1}{2}mw^2$$

Rearranging the momentum equations give:

$$mw\cos\phi = M\left(v - u\cos\theta\right)$$
$$mw\sin\phi = Mu\sin\theta$$

Squaring both sides and adding the two momentum equations results in:

$$m^2w^2\left(\cos^2\phi + \sin^2\phi\right) = M^2\left(v^2 - 2vu\cos\theta + u^2\cos^2\theta + u^2\sin^2\theta\right) \quad (17)$$
$$m^2w^2 = M^2\left(v^2 - 2uv\cos\theta + u^2\right) \quad (18)$$

The kinetic energy equation can also be written in terms of m^2w^2:

$$m^2w^2 = Mm\left(v^2 - u^2\right) \quad (19)$$

Once we equate the expressions from equations 18 and 19:

$$M^2\left(v^2 - 2uv\cos\theta + u^2\right) = Mm\left(v^2 - u^2\right) \quad (20)$$
$$cos\theta = \frac{v}{2u}\left(1 - \frac{m}{M}\right) + \frac{u}{2v}\left(1 + \frac{m}{M}\right) \quad (21)$$

To find the maximum scattering angle, we can evaluate $d\cos\theta/du = 0$ and solve for u:

$$\frac{d}{du}\left[\frac{v}{2u}\left(1 - \frac{m}{M}\right) + \frac{u}{2v}\left(1 + \frac{m}{M}\right)\right] = 0$$
$$\therefore u = v\sqrt{\frac{M-m}{M+m}} \quad (u > 0)$$

Substituting this expression for u back into equation 21 gives:

$$\cos\theta_{max} = \sqrt{1 - \frac{m^2}{M^2}}$$

Since $m << M$, we can utilize the second-order taylor series expansion for $\cos\theta$ and $\sqrt{1+x}$ where $|x| < 1$:

$$\cos\theta_{max} \approx 1 - \frac{\theta_{max}^2}{2}$$
$$\sqrt{1 - \frac{m^2}{M^2}} \approx 1 + \frac{-m^2/M^2}{2}$$

Equating these expressions and solving for θ_{max} gives:

$$\boxed{\cos\theta_{max} \approx \frac{m}{M} = \frac{1}{7400} \approx 1 \times 10^{-4}\ \text{rad}}$$

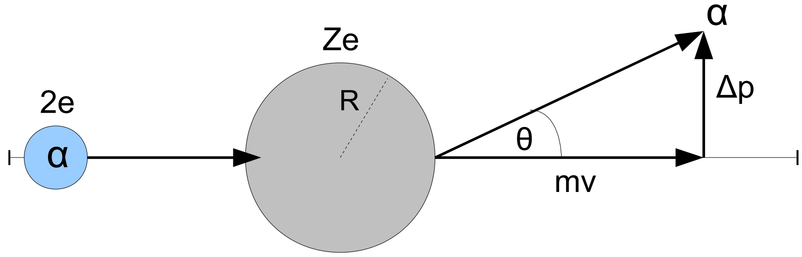

Figure 6: α particle scattered from an Thompson atom.

Part B The incident α particle interacts with positive charge that is dispersed within an atomic radius of $1\mathring{A}$. For an arbitrary atom with Z protons, the maximum force felt by the α particle in passage through the atom occurs at the atom's surface:

$$F_{max} = \frac{(Ze)(2e)}{4\pi\epsilon_o R^2}$$

where e is the charge of an electron. If the particle is deflected by the atom, a certain momentum Δp (perpendicular to the direction of motion) is associated with the deflection angle. This can be written as:

$$\Delta p = \int F dt = F_m \Delta t$$

where Δt is the time that the α particle is subjected to the atomic forces and equals $2R/v$. In this expression, R is the atomic radius and v is the α particle velocity. Combining equations, we now have:

$$\Delta p = \frac{4Ze^2}{4\pi\epsilon_o R v}$$

Since we expect the scattered angle to be small, we can use the small angle approximation that $\tan\theta \approx \theta$. We can then show that:

$$\begin{aligned}\theta \approx \frac{\Delta p}{mv} &= \frac{4Ze^2}{4\pi\epsilon_o R m v^2} \\ &= \frac{2Ze^2}{4\pi\epsilon_o R\left(\frac{1}{2}mv^2\right)}\end{aligned}$$

This is simply the potential energy of the atomic surface, divided by the kinetic energy of the incident α particle.

As an example, gold has an atomic number $Z = 79$ and let the kinetic energy of the α particle be 5 MeV. We then have:

$$\theta = 8.988 \times 10^9 \cdot \frac{2 \cdot 79\left(1.602 \times 10^{-19}\right)^2}{10^{-10} \cdot 5 \times 10^6 \cdot 1.602 \times 10^{-19}} = 4.55 \times 10^{-4}\text{ rad}$$

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Problem 6

The angular momentum L is:

$$L = n\hbar = \frac{nh}{2\pi}$$

Solving for n:

$$n = \frac{2\pi L}{h} = \frac{2\pi\left(7.382 \times 10^{-34}\right)}{6.626 \times 10^{-34}}$$

$$\boxed{n = 7}$$

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