Quantum Mechanics and Atomic Physics

Lecture 7:

Potential Barriers

http://www.physics.rutgers.edu/ugrad/361

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Last Time

- We covered the finite potential well and looked at the graphical form of the quantization of energy states, which are a function of

$$\xi = k_2 L = L\sqrt{\frac{2mE}{\hbar^2}}$$

- We found that there are even parity and odd parity solutions.

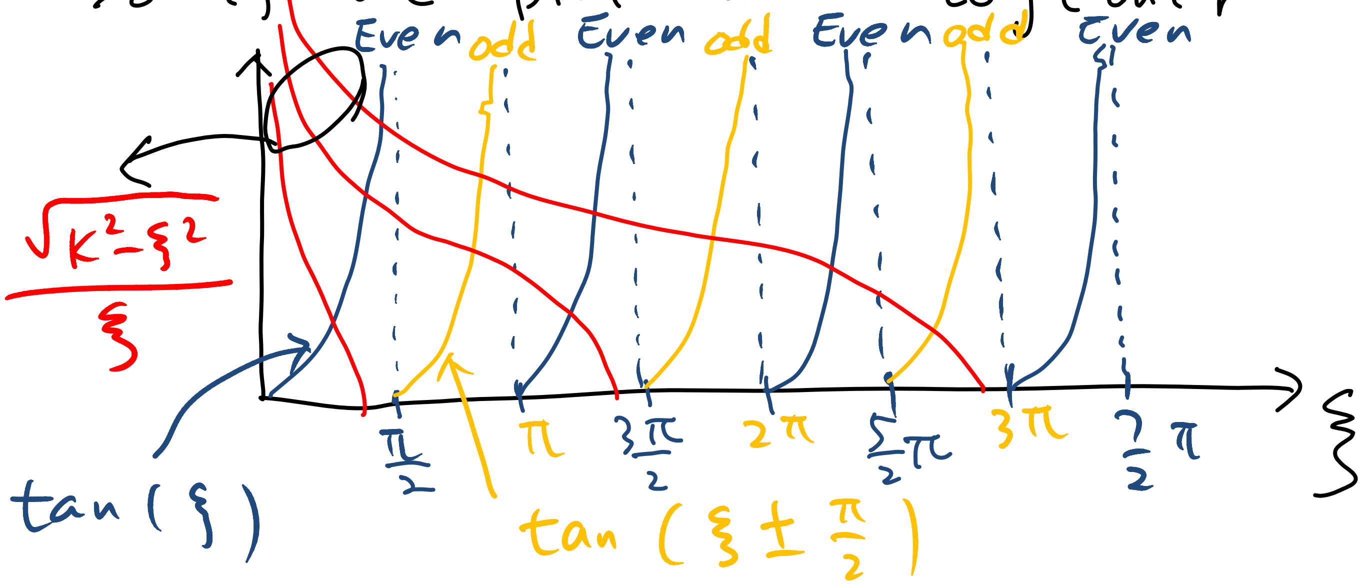
Number of bound states in a finite potential well

Note : $\xi^2 + \eta^2 = K^2 \left(\equiv \frac{2mV_0L^2}{\hbar^2} \right)$

Even solution : $\tan(\xi) = \frac{\eta}{\xi} = \frac{\sqrt{K^2 - \xi^2}}{\xi}$

odd solution ; $\tan(\xi \pm \frac{\pi}{2}) = \frac{\eta}{\xi} = \frac{\sqrt{K^2 - \xi^2}}{\xi}$

So if we plot them together



Number of bound states Cont'd

\# of Bound states $\equiv N$

If $0 \leq K < \frac{\pi}{2}$ $\left(\Leftrightarrow 0 \leq \frac{2K}{\pi} < 1 \right) \Rightarrow N = 1$

$\frac{\pi}{2} \leq K < \pi$ $\left(\Leftrightarrow 1 \leq \frac{2K}{\pi} < 2 \right) \Rightarrow N = 2$

$\pi \leq K < \frac{3}{2}\pi$ $\left(\Leftrightarrow 2 \leq \frac{2K}{\pi} < 3 \right) \Rightarrow N = 3$

$\vdots$

$$\therefore \quad N(K) = 1 + \underbrace{\left[\frac{2K}{\pi} \right]}$$

largest integer less than or equal to $\frac{2K}{\pi}$

Example: CCD

- Finite potential wells are used in everyday devices!
  - Digital cameras: two-dimensional grid of potential wells
    - This is called a charge-coupled-device or CCD
      - Each well can be thought of as a "pixel" or a picture element

- Example: We have a camera with "9micron pixels"; this means each potential well is 9 by 9microns in size (1micron = 10^{-6}m). Let's assume it can hold 60,000 electrons before becoming full (each energy level can hold two electrons of opposite spin). If we assume that the pixels are one-dimensional finite square wells, what must be their depth V_0?

Number of eigenvalues $N = 30{,}000$

$$\therefore \quad N = 1 + \frac{2K}{\pi} \approx \frac{2K}{\pi}$$

$$\Rightarrow K = \frac{\pi}{2} N = \sqrt{\xi^2 + \eta^2} = \sqrt{\frac{2mV_0 L^2}{\hbar^2}}$$

$$\left(\frac{\pi}{2} N\right)^2 = \frac{2mV_0 L^2}{\hbar^2}$$

$$V_0 = \frac{(N\pi\hbar)^2}{8mL^2} \quad ; \quad L = \frac{9\,\text{microns}}{2} = 4.5\,\text{microns}$$

½ the width of well

$$V_0 = \frac{\left((30{,}000)\pi \cdot 1.055\times10^{-34}\,\text{J}\cdot\text{s}\right)^2}{8(9.11\times10^{-31}\,\text{kg})(4.5\times10^{-6}\,\text{m})^2} = 6.7\times10^{-19}\,\text{J}$$

$$\approx \underline{4.2\,\text{eV}}$$

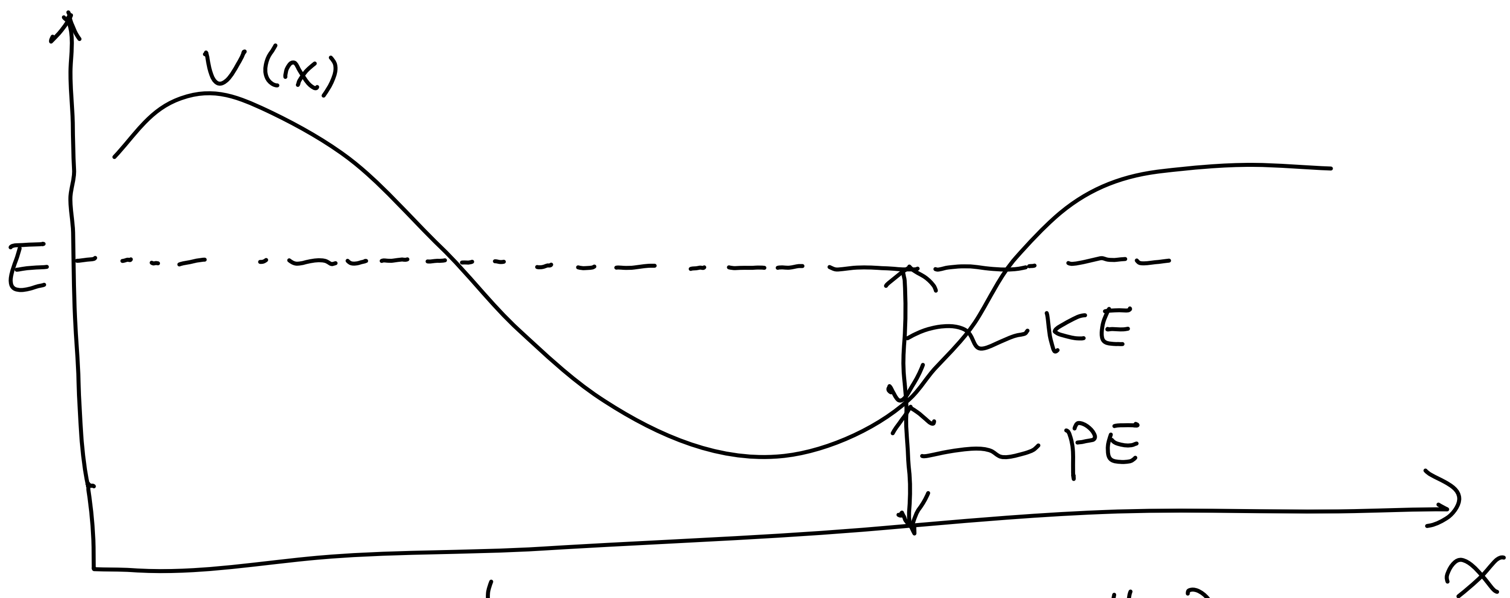
- Which is a device that can be easily powered with batteries!

Example 2

- Do the previous CCD camera problem, using the infinite well formula we found earlier, but simply using the approximate criterion that $E_N < V_0$.

Answer: Your answer should be identical to that of the previous example; be careful on the definition of "L".

Sketching Wavefunctions



large KE ⇒ large p ⇒ small λ

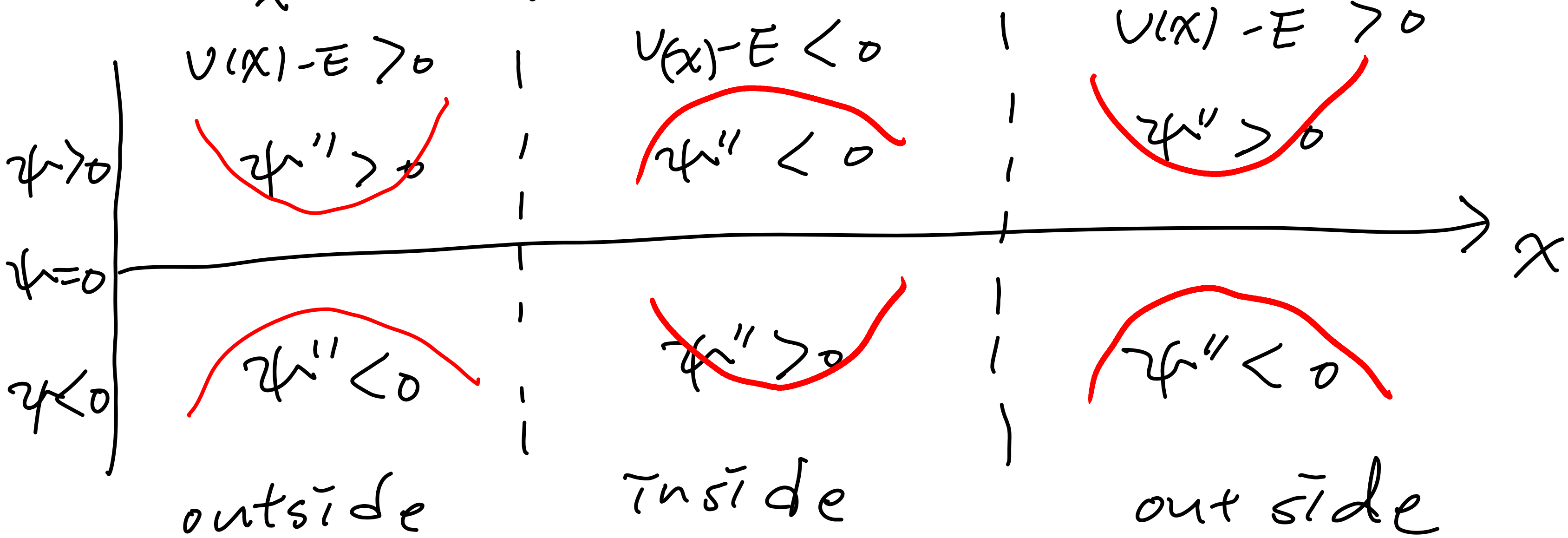
$\left(\lambda = \frac{h}{p}\right)$

large KE ⇒ large speed ⇒ spend less time in deeper well

⇒ smaller amplitude

Continued

$$\frac{d^2\psi}{dx} = \frac{2m}{\hbar^2}[U(x) - E)\psi(x)$$



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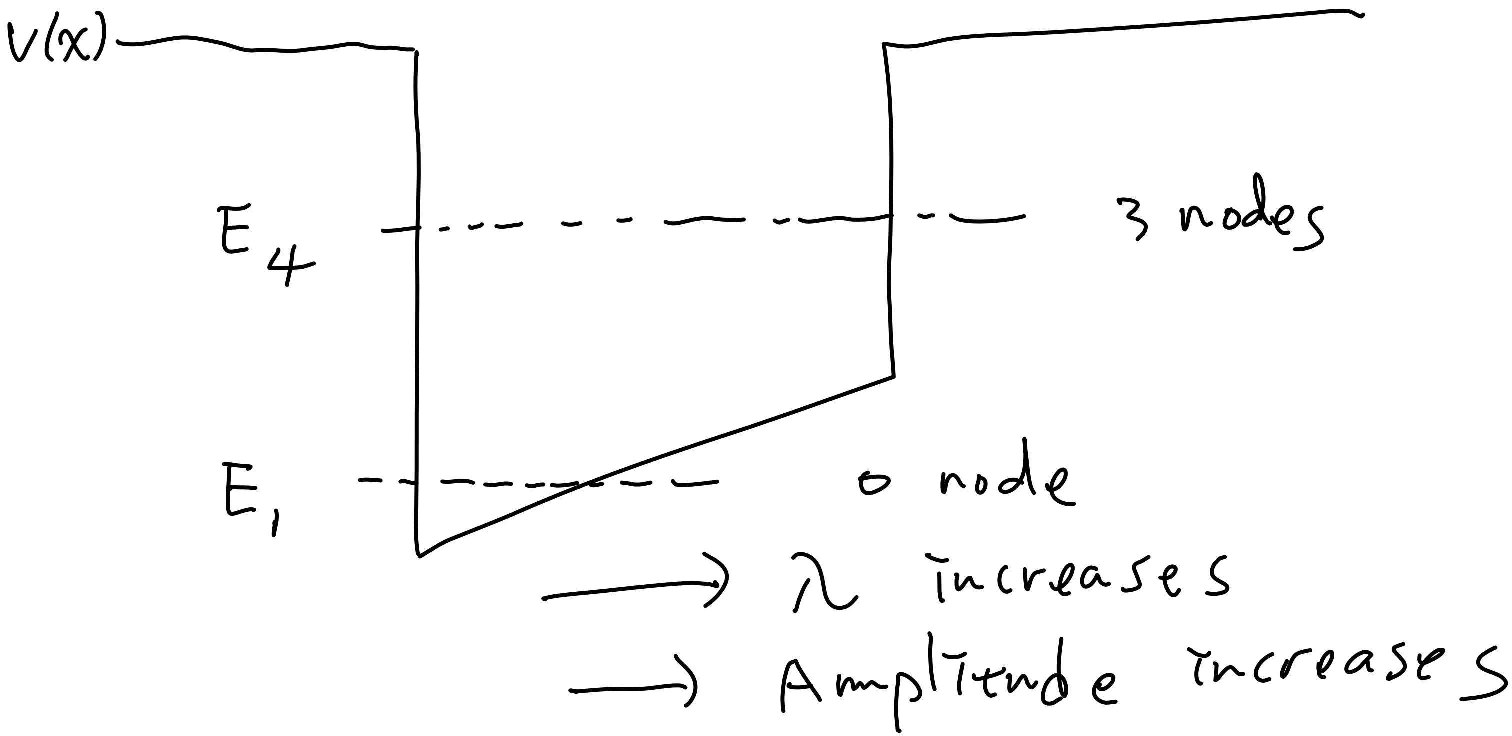
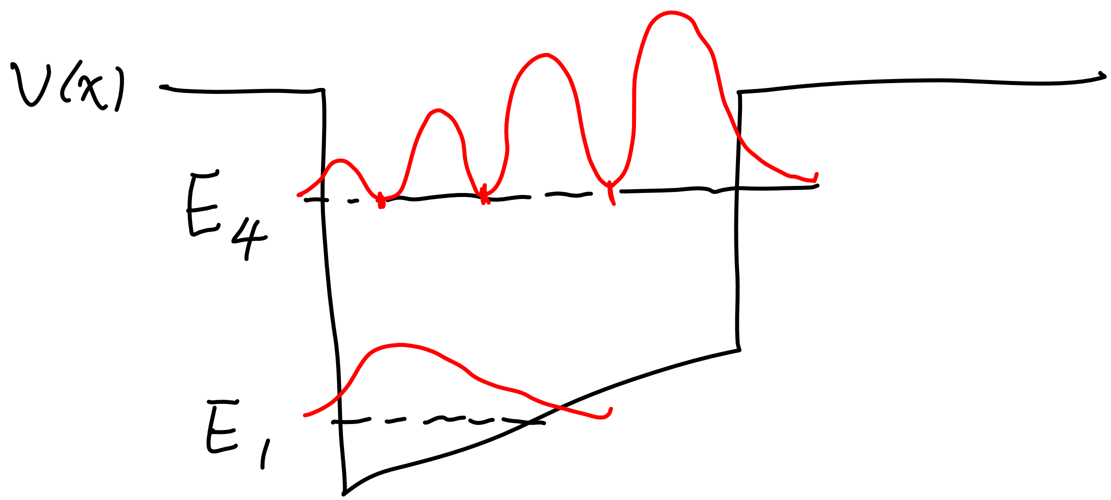
- Number of nodes excluding the boundaries is equal to “n-1”, with ground state corresponding to n=1.



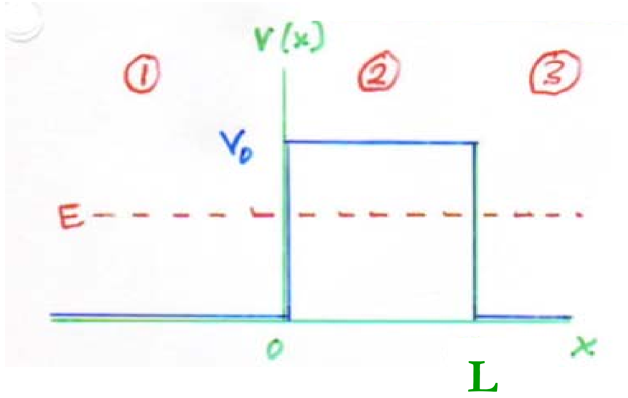
Example

- Sketch $|\Psi|^2$ for E_1 and E_4

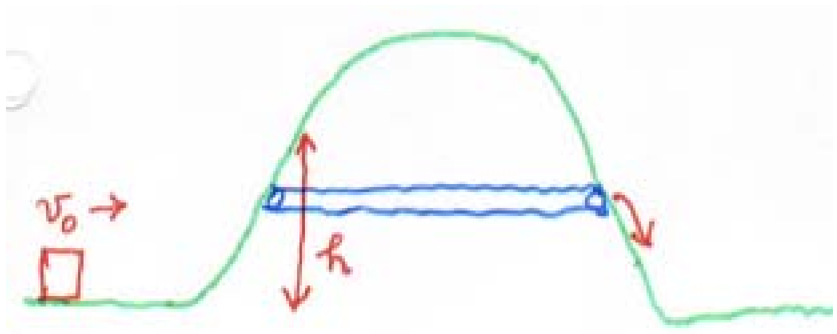


Potential Barriers

- A potential barrier can be thought of as an "inside-out" potential well.
- The possibility of finding the particle in region (3) is called *tunneling*.



Tunneling



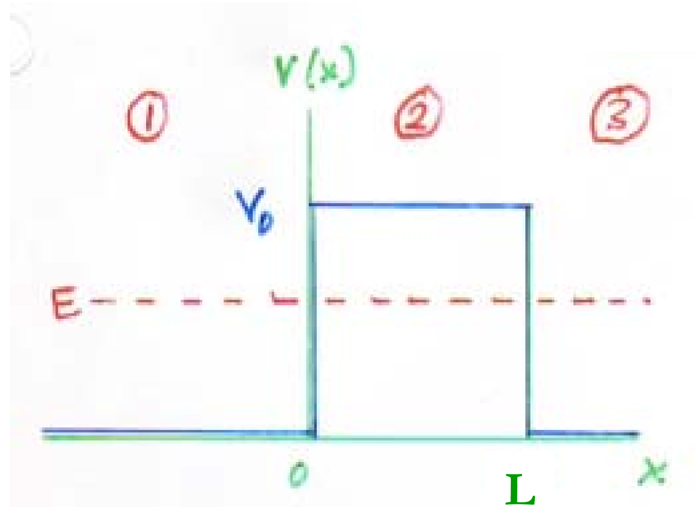
- A mass m has speed v_0. How high up the frictionless hill can it go?

$$\frac{1}{2}mv_0^2 + mgh \Rightarrow h = \frac{v_0^2}{2g}$$

- If h is less than the height of the hill, the block can't get over the hill.
- But if there is a tunnel at height < h, the block can get through.
- **In QM it goes through anyway!**

Barrier Potential

- Regions (1) and (3):
  $V=0$ for $x<0$ and $x>L$
- Region (2):
  $V=V_0$ for $0<x<L$



- V_0 is the height of the barrier
- L is the width of the barrier

Barrier Potential: $E<V_0$

- Case I: $E<V_0$

In regions ① & ③:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - E\psi = 0$$

General Solutions:

$$\psi_1 = A_0 e^{ik_1x} + A e^{-ik_1x}$$

$$\psi_3 = D e^{ik_1x} + F e^{-ik_1x}$$

w/ $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

If particle gets into region (3) it must Keep going right (nothing to reflect it). So F=0.

In region ②:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (V_0-E)\psi = 0$$

$$\psi_2 = B e^{-k_2x} + C e^{k_2x}, \quad k_2 = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

$A_0^*A_0$ is the incident wave.
A^*A is the reflected wave.
D^*D is the transmitted wave.

Boundary Conditions

- $\psi_1 = \psi_2$ at $x=0 \Rightarrow A_0 + A = B + C$
- $\left.\frac{d\psi_1}{dx}\right|_0 = \left.\frac{d\psi_2}{dx}\right|_0 \Rightarrow ik_1 A_0 - ik_1 A = -k_2 B + k_2 C$
- $\psi_2 = \psi_3$ at $x=L \Rightarrow B e^{-k_2 L} + C e^{k_2 L} = D e^{ik_1 L}$
- $\left.\frac{d\psi_2}{dx}\right|_L = \left.\frac{d\psi_3}{dx}\right|_L \Rightarrow -k_2 B e^{-k_2 L} + k_2 C e^{k_2 L} = ik_1 D e^{ik_1 L}$

- With lots of algebra we can eliminate A, B and C.

$$\frac{D}{A_0} = \frac{4i\frac{k_1}{k_2} e^{-ik_1 L}}{-g^{*2} e^{k_2 L} + g^2 e^{-k_2 L}}$$

$$g = 1 + i\frac{k_1}{k_2} \quad \text{and} \quad g^* = 1 - i\frac{k_1}{k_2}$$

D/A_0 is the amplitude of transmitted wave probability density as a fraction of that of the incident wave

Transmission coefficient

- Let's define the probability flux as the probability per unit area per second of finding the particle.
  - Flux = v * n $\propto$ v*$|\Psi|^2$ = (p/m)*$|\Psi|^2$

    $\propto \kappa$*$|\Psi|^2$

  where n=#particles/volume

Transmission coefficient

- Transmission coefficient (T) is defined as

  Transmitted flux/Incident flux =

$$T = \frac{v_{out}|\Psi_{out}|^2}{v_{in}|\Psi_{in}|^2} = \frac{k_{out}|\Psi_{out}|^2}{k_{in}|\Psi_{in}|^2} = \frac{|D|^2}{|A_0|^2}$$

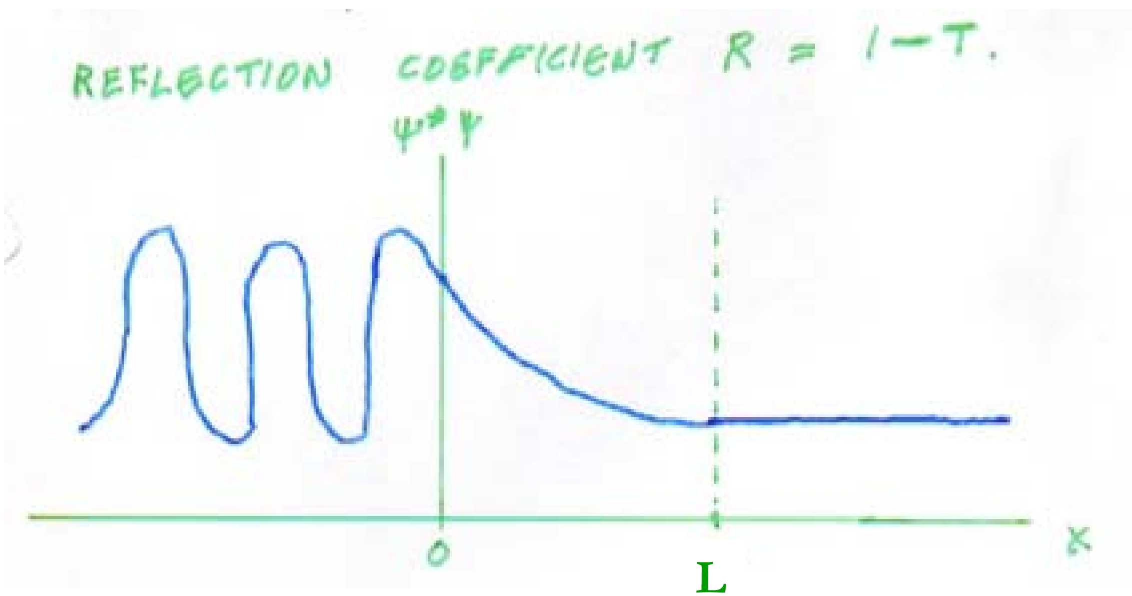
- **With lots of algebra:**

$$T = \frac{16k_1^2k_2^2 e^{-2k_2L}}{(k_1^2+k_2^2)^2(1+e^{-4k_2L}) - e^{-2k_2L}(2k_1^4-12k_1^2k_2^2+2k_2^4)}$$

$$= \left[1 + \frac{(e^{k_2L} - e^{-k_2L})^2}{16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)}\right]^{-1}$$

Probability of reflection

- Reflection coefficient R=1-T



- In region (3), D^*D is non-zero
- There is clear transmission of particles tunneling through the barrier!

Example

- An electron of energy E=3eV encounters a barrier of height V_0=10eV and width L=1.0 Angstrom. Find the probability of tunneling.

$$k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = 1.4\times10^{10}\, m^{-1}$$

Using numbers above and m = 9.11×10^{-31} kg

$$k_2L = (1.4\times10^{10}\, m^{-1})(1.0\times10^{-10}\, m) = 1.4$$

$$T = \left[1 + \frac{(e^{1.4} - e^{-1.4})^2}{16(\frac{3}{10})(1-\frac{3}{10})}\right]^{-1} = 0.19$$

So a 19% change.

Thick barrier approximation

- In the thick barrier limit ($k_2L >>1$),

$$T = \frac{16k_1^2k_2^2 e^{-2k_2L}}{(k_1^2+k_2^2)^2(1+e^{-4k_2L}) - e^{-2k_2L}(2k_1^4-12k_1^2k_2^2+2k_2^4)}$$

$$e^{-2k_2L} \simeq 0 \quad \text{and} \quad e^{-4k_2L} \simeq 0$$

$$T \simeq \frac{16k_1^2k_2^2}{(k_1^2+k_2^2)^2} e^{-2k_2L} = \boxed{16\left(\frac{E}{V_0}\right)\left(1-\frac{E}{V_0}\right)e^{-\frac{2L}{\hbar}\sqrt{2m(V_0-E)}}}$$

Thin Barrier Approximation

If $k_2 L \ll 1$, $e^{-4k_2L} \simeq 1$, $e^{-2k_2L} \simeq 1$, so

$$T = \frac{16 k_1^2 k_2^2 \, e^{-2k_2L}}{(k_1^2+k_2^2)^2(1+e^{-4k_2L}) - e^{-2k_2L}(2k_1^4 - 12k_1^2k_2^2 + 2k_2^2)}$$

$$\simeq \frac{16 k_1^2 k_2^2}{2(k_1^2+k_2^2)^2 - (2k_1^4 - 12k_1^2k_2^2 + 2k_2^2)} \cdot e^{-2k_2L}$$

$$= \frac{16k_1^2k_2^2}{16k_1^2k_2^2} e^{-2k_2L} = e^{-2k_2L}$$

$$= e^{-2\frac{L}{\hbar}\sqrt{2m(V_0-E)}}$$

(Reed 3.8)

$\Rightarrow$ For arbitrarily shaped barriers

$$P \sim e^{-2\int k(x)dx} = e^{-2\sqrt{\frac{2m}{\hbar}}\int\sqrt{U(x)-E}\,dx}$$

Alpha Decay

- In 1928, George Gamow showed that tunneling explains how alpha-decay radioactivity occurs.
  - Nucleus spontaneously decays by emitting an alpha-particle (He nucleus)
- Alpha-particles generally have only a few MeV of engery.   How can they "jump" from the well?
  - Alpha-particle *tunnels* out of nucleus over Coulomb barrier.

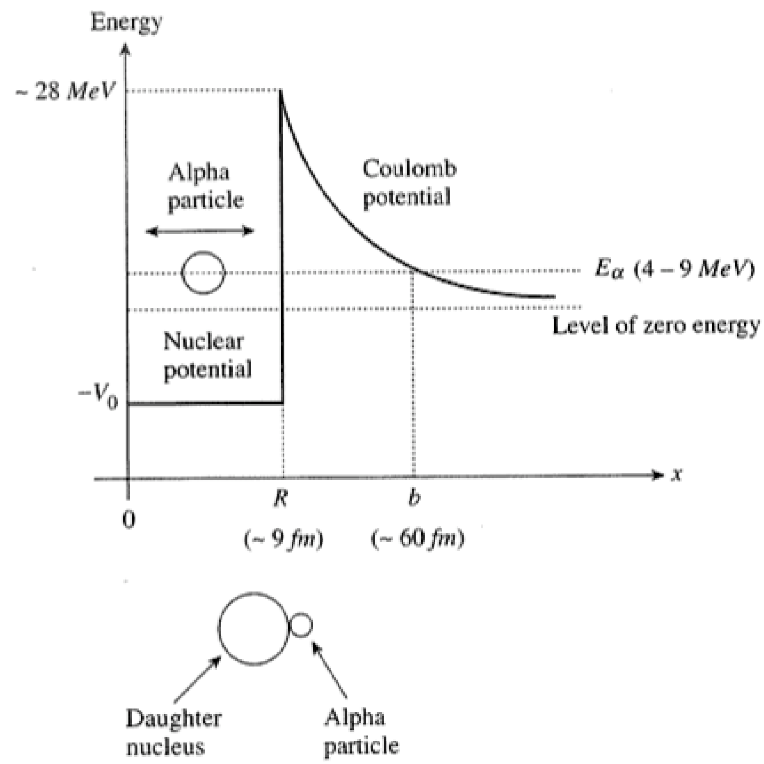


FIGURE 3.18 Alpha-decay.

$$V(r) = \frac{1}{4\pi\varepsilon_0}\frac{2Ze^2}{r}$$

Alpha Decay, con't

- To escape from the nucleus, the alpha particle must tunnel through the barrier.
- The probability to penetrate an arbitrarily shaped barrier (see Reed section 3.8):

$$P \approx e^{-2\int \sqrt{2m(V_0 - E)}/\hbar \, dx}$$

$$\Rightarrow \ln P \approx \left[-\frac{2}{\hbar} \int_R^b \sqrt{2m_\alpha \left(\frac{2Ze^2}{4\pi\varepsilon_0 r} - E \right)} \, dr \right]$$

$$\underset{KE}{E_\alpha} = \underbrace{\frac{2Ze^2}{4\pi\varepsilon_0 b}}_{PE} \Rightarrow \underline{b = \frac{2Ze^2}{4\pi\varepsilon_0 E_\alpha}}$$

$$\Rightarrow \ln P = -\frac{2}{\hbar} \sqrt{2m_\alpha E_\alpha} \int_R^b \sqrt{\frac{b}{r} - 1} \, dr$$

Change variable of integration

$r = b\sin^2\theta$

$$\Rightarrow \ln P \doteq -\frac{2}{\hbar}\sqrt{2m_\alpha E_\alpha}\, b\int_{\theta_R}^{\theta_b} 2\cos^2\theta\, d\theta$$

Use $\cos^2\theta = (1+\cos 2\theta)/2$

$$\int_{\theta_R}^{\theta_b}(1+\cos 2\theta)\,d\theta$$

$$= \left[\theta + \frac{1}{2}\sin 2\theta\right]_{\theta_R}^{\theta_b}$$

$b = b\sin^2\theta_b$

and

$\searrow$ $\theta_b = \pi/2$, $\theta_R = \sin^{-1}\left(\sqrt{\frac{R}{b}}\right)$

But $b >> R \Rightarrow \theta_R + \frac{1}{2}\sin 2\theta_R \approx 2\theta_R \approx 2\sqrt{\frac{R}{b}}$

$$\Rightarrow \ln P \approx -\frac{2}{\hbar}\sqrt{2m_\alpha E_\alpha}\, b\,\frac{\pi}{2} + \frac{4}{\hbar}\sqrt{2m_\alpha E_\alpha}\sqrt{Rb}$$

$$\approx -\frac{4\pi}{\hbar}\frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{v_\alpha} + \frac{4}{\hbar}\sqrt{\frac{4Ze^2 m_\alpha R}{4\pi\varepsilon_0}}$$

where $v_\alpha = \sqrt{\frac{2E}{m_\alpha}}$

The term: $-\frac{4\pi}{\hbar}\frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{v_\alpha}$ Gamow factor

$$\ln T_{1/2} \propto -\ln P \propto \frac{1}{v_\alpha}$$

- The *Gamow factor* determines the dependence of the probability on the speed (or energy) of the alpha particle.
- **This prediction of the half-life is in good agreement with observed half-lives of isotopes of heavy nuclei.**

Alpha-decay

Table 3.1 Thorium alpha-decays

Mass number A	E_α (MeV)	Half-life (sec)
220	8.95	10^{-5}
222	8.13	2.18×10^{3}
224	7.31	1.04
226	6.45	1854
228	5.52	6.0×10^{7}
230	4.77	2.5×10^{12}
232	4.08	4.4×10^{17}

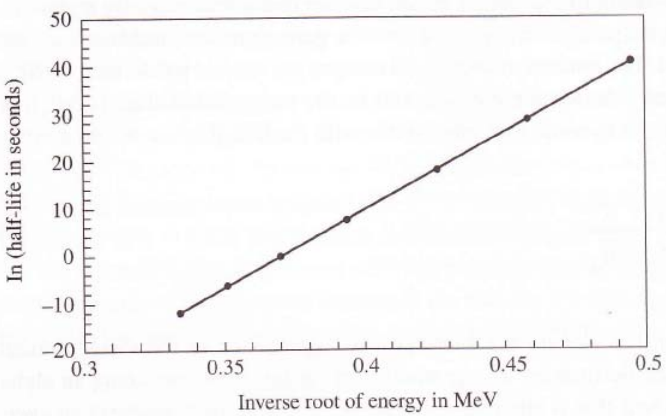


FIGURE 3.19 Observed and predicted thorium $t_{1/2}$ vs. E_α relationship.

$$\Rightarrow \ln P \approx -\frac{2}{\hbar}\sqrt{2m_\alpha E_\alpha}\, b\,\frac{\pi}{2} + \frac{4}{\hbar}\sqrt{2m_\alpha E_\alpha}\sqrt{Rb}$$

$$\approx -\frac{4\pi}{\hbar}\frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{v_\alpha} + \frac{4}{\hbar}\sqrt{\frac{4Ze^2 m_\alpha R}{4\pi\varepsilon_0}}$$

where $v_\alpha = \sqrt{\frac{2E}{m_\alpha}}$

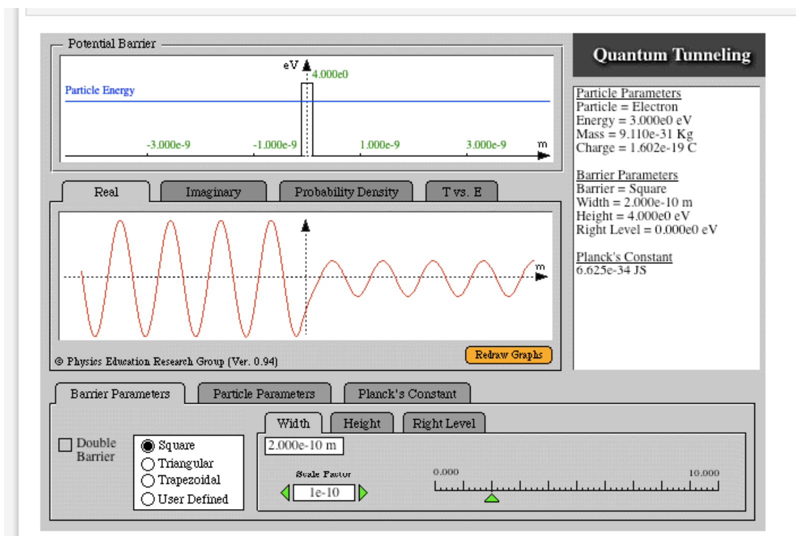
The term: $-\frac{4\pi}{\hbar}\frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{v_\alpha}$ Gamow factor

$$\ln T_{1/2} \propto -\ln P \propto \frac{1}{v_\alpha}$$

Animations

- There is a very nice educational website that allows you to try various quantum tunneling scenarios:

http://phys.educ.ksu.edu/vqm/html/qtunneling.html



Summary/Announcements

- We covered tunnelling through Potential Barriers ($E<V_0$)

- Next time:
  - We will discuss Scattering (Potential barriers with $E>V_0$)
  - Operators and Expectation Values

- Next homework due on Monday Oct 3