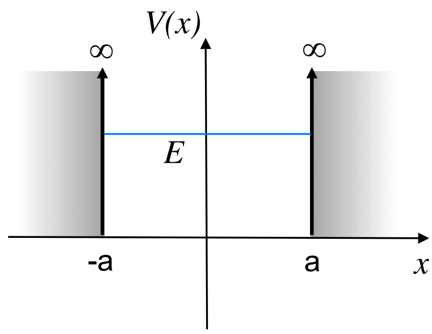
Quantum Mechanics (P304H)
Part 2 – Lecture 13

Dr. Dan Protopopescu, Room 524
dan.protopopescu@glasgow.ac.uk

5. Potential Well

- Third example: Infinite Potential Well
  - The potential is defined as:

$$V(x) = \begin{cases} 0 & \text{if} \quad -a < x < a \\ \infty & \text{if} \quad |x| > a \end{cases}$$



  - The 1D Schrödinger equation is:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = 0 \qquad \text{for} \qquad -a < x < a$$

  - The solution is the sum of the two plane waves propagating in opposite directions, which is equivalent to the sum of a cosine and a sine (i.e. standing waves), with wave number k:

$$\psi(x) = A' e^{ikx} + B' e^{-ikx} = A\cos kx + B\sin kx \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

5. Potential Well

The wave function must be zero at both walls of well:

$$\left.\begin{array}{l} A\cos(ka)+B\sin(ka)=0 \\ A\cos(-ka)+B\sin(-ka)=0 \quad\Rightarrow\quad A\cos(ka)-B\sin(ka)=0 \end{array}\right\}\Rightarrow$$

$$\Rightarrow \quad A\cos(ka)=0 \quad \text{and} \quad B\sin(ka)=0$$

We look at each condition separately

$$\cos(\mathrm{ka})=0 \Rightarrow k_n=\frac{n\pi}{2a}=\frac{n\pi}{L}, \quad n=1,3,5,\ldots$$

$$\sin(\mathrm{ka})=0 \Rightarrow k_n=\frac{n\pi}{2a}=\frac{n\pi}{L}, \quad n=2,4,6,\ldots$$

Quantization of the wave number

Normalization condition:

$$\int_{-a}^{a}\psi_n{}^*(x)\psi_n(x)dx=1\Rightarrow\int_{-a}^{a}|A|^2\cos^2 kx\,dx=|A|^2\frac{1}{2}(a-(-a))=1 \overset{e.g.}{\Rightarrow} A=\frac{1}{\sqrt{a}}$$

5. Potential Well

- Solutions:

$$\psi_n(x)=\frac{1}{\sqrt{a}}\cos\left(\frac{n\pi}{2a}x\right), \quad n=1,3,5,\ldots$$

symmetric (even function)

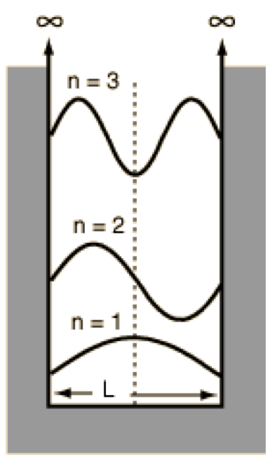
$$\psi_n(x)=\psi_n(-x)$$

$$\psi_n(x)=\frac{1}{\sqrt{a}}\sin\left(\frac{n\pi}{2a}x\right), \quad n=2,4,6,\ldots$$

antisymmetric (odd function)

$$\psi_n(x)=-\psi_n(-x)$$

The solution has to have a definite *parity* (either odd or even).



We can evaluate the de Broglie wavelength:

$$k_n=\frac{n\pi}{2a}\Rightarrow \quad \lambda_n=\frac{2\pi}{k_n}=\frac{2L}{n} \quad n=1,2,3,4,\ldots.$$

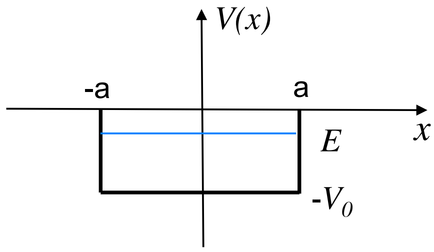
Only half integer and integer wavelengths fit in the box.
The energy is quantized, i.e. only certain energy values are allowed (*energy eigenvalues*)

$$E_n=\frac{p^2}{2m}=\frac{\hbar^2 k_n{}^2}{2m}=\frac{\hbar^2\pi^2 n^2}{8ma^2}=\frac{\hbar^2\pi^2 n^2}{2mL^2}$$

5. Potential Well

- Fourth example: Finite square well

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



- Case 1: $E < 0$, (*bound state*) with $-V_0 \leq E < 0$. Inside the well:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0$$

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} + \alpha^2\psi(x) = 0, \quad |x| < a$$

$$\alpha = \sqrt{\frac{2m}{\hbar^2}(V_0 + E)} = \sqrt{\frac{2m}{\hbar^2}(V_0 - |E|)}$$

- Outside the well:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = 0 \qquad \text{with} \quad \beta = \sqrt{-\frac{2m}{\hbar^2}E} = \sqrt{\frac{2m}{\hbar^2}|E|}$$

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} - \beta^2\psi(x) = 0, \quad |x| > a$$

The energy: $|E| = -E$ is the *binding energy* of the particle.

5. Potential Well

- Like for the infinite potential, solution is either odd or even:

1) Even function:

$$\psi(x) = \begin{cases} A\cos(\alpha x), & 0 < |x| < a \\ Ce^{-\beta|x|}, & |x| > a \end{cases} \qquad (\text{since } De^{\beta|x|} \xrightarrow{x\to\infty} \infty \;\Rightarrow\; D = 0)$$

- Continuity of $\psi(x)$ and $d\psi/dx$:

$$\begin{aligned} A\cos(\alpha a) &= Ce^{-\beta a} \\ -\alpha A\sin(\alpha a) &= -\beta Ce^{-\beta a} \end{aligned} \quad \Rightarrow \alpha a \tan(\alpha a) = \beta a \quad (1)$$

2) Odd function:

$$\psi(x) = \begin{cases} B\sin(\alpha x), & 0 < |x| < a \\ Ce^{-\beta|x|}, & |x| > a \end{cases}$$

- Continuity of $\psi(x)$ and $d\psi/dx$:

$$\begin{aligned} B\sin(\alpha a) &= Ce^{-\beta a} \\ \alpha B\cos(\alpha a) &= -\beta Ce^{-\beta a} \end{aligned} \quad \Rightarrow \alpha a \cot(\alpha a) = -\beta a \quad (2)$$

The energy levels of the bound states are found by solving the *transcendental* equations (1) and (2). These equations can not be solved analytically and have to be solved graphically or numerically.

5. Potential Well

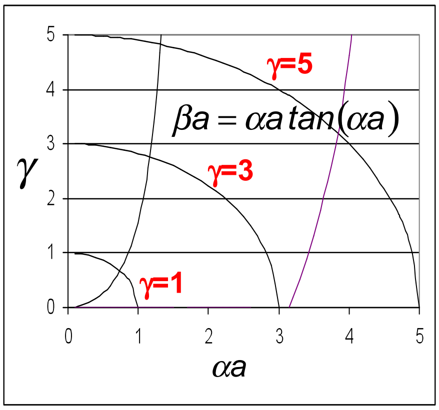
- If we define the dimensionless quantity γ (*strength parameter*):

$$\gamma^2 \equiv (\alpha a)^2 + (\beta a)^2 = \frac{2m}{\hbar^2}(V_0 + E)a^2 - \frac{2m}{\hbar^2}Ea^2 = \frac{2m}{\hbar^2}V_0 a^2$$

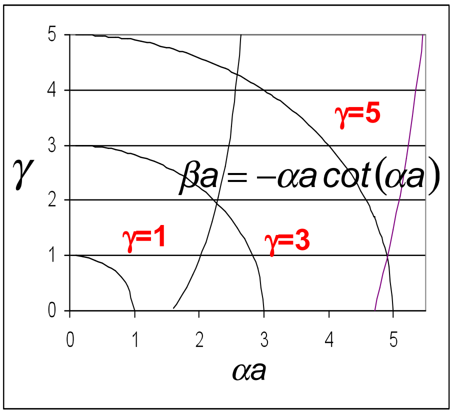
($mV_o a$ defines the value of γ) then we can solve the equations graphically:

$$\beta a = \alpha a \tan(\alpha a) \quad \text{(for even states)}$$

$$\beta a = -\alpha a \cot(\alpha a) \quad \text{(for odd states)}$$



Even states



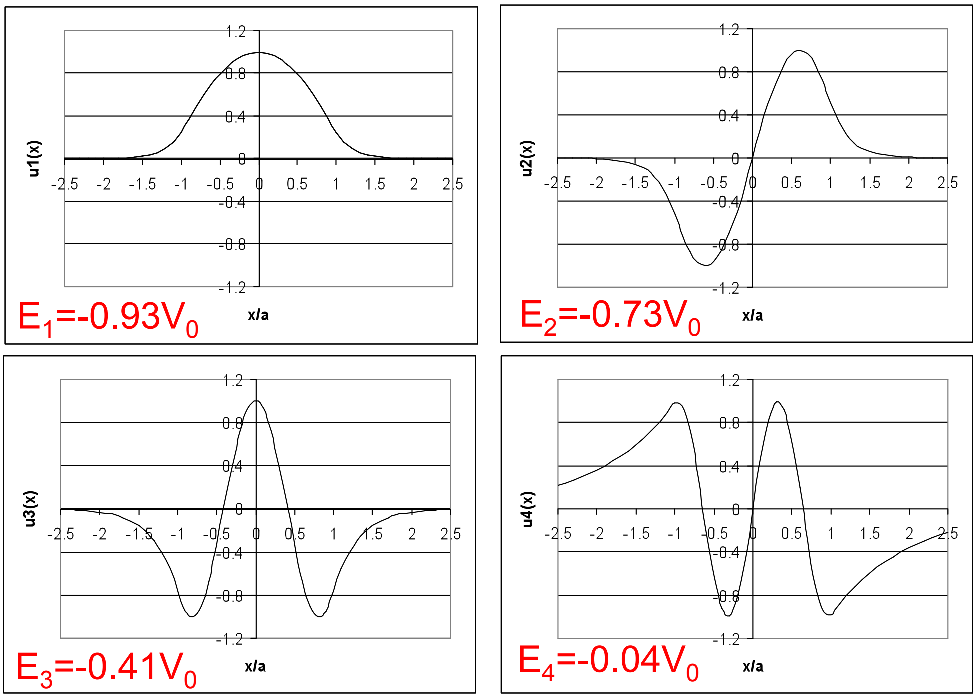
Odd states

5. Potential Well

Solutions: odd and even states alternate

- For $\gamma = 1$ we have one even state; for $\gamma = 3$: two states (one odd, one even); and for $\gamma = 5$: four states (two odd, two even)

Case $\gamma = 5$:



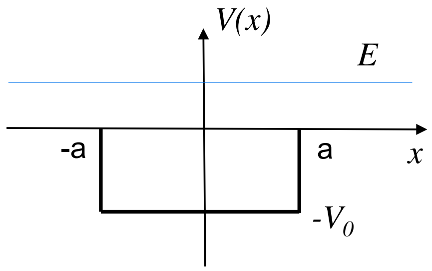
For $V_0 \to \infty \Rightarrow \gamma \to \infty$ and we recover the infinite well solution with:

$$\alpha a = n\frac{\pi}{2}, \quad n = 1, 2, \ldots$$

$$\Rightarrow E_n = \frac{\hbar^2}{8m}\frac{\pi^2 n^2}{a^2}$$

5. Potential Well

- Case 2: $E > 0$, scattering in the potential well
  - The 1D Schrodinger equation is:



$$\frac{d^2\psi(x)}{dx^2}+\frac{2m}{\hbar^2}\left[E-V(x)\right]\psi(x)=0$$

  - The solution:

$$\psi(x)=\begin{cases} Ae^{ikx}+Be^{-ikx} & ,x<-a \\ Fe^{i\alpha x}+Ge^{-i\alpha x} & ,-a<x<a \\ Ce^{ikx}, & x>a \end{cases}$$

with $k=\sqrt{\frac{2mE}{\hbar^2}}$, $\alpha=\sqrt{\frac{2m(V_0+E)}{\hbar^2}}$

  - Similar to the potential barrier ($E>V_0$) but $V_0 \rightarrow -V_0$, $k' \rightarrow \alpha$ and $a \rightarrow L=2a$

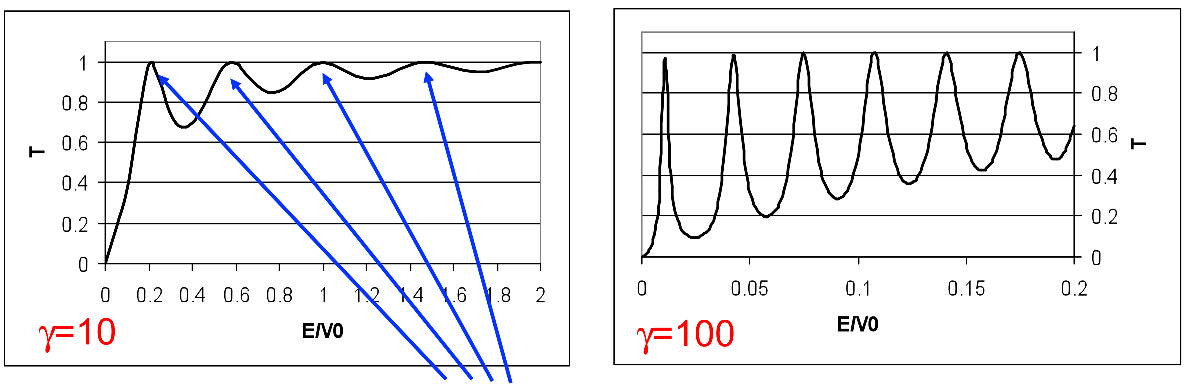
$$R=\frac{|B|^2}{|A|^2}=\left[1+\frac{4k^2\alpha^2}{\left(k^2-\alpha^2\right)^2\sin^2(\alpha L)}\right]^{-1}=\left[1+\frac{4E\left(E+V_0\right)}{V_0^2\sin^2(\alpha L)}\right]^{-1}$$

$$T=\frac{|C|^2}{|A|^2}=\left[1+\frac{\left(k^2-\alpha^2\right)^2\sin^2(\alpha L)}{4k^2\alpha^2}\right]^{-1}=\left[1+\frac{V_0^2\sin^2(\alpha L)}{4E\left(E+V_0\right)}\right]^{-1}$$

$$R+T=1$$

5. Potential Well

- Transmission coefficients for $\gamma=10$ and $\gamma=100$:



$\alpha L=n\pi$

  - Transition maxima ($T=1$) occur when $\alpha L=n\pi$, i.e. when L is an integral or half-integral number of the de Broglie wavelength $2\pi/\alpha$.
  - As E becomes large compared to V_0, the transmission tends asymptotically to 1.
  - For larger values of γ the minima become deeper.

6. Examples and applications

Ramsauer effect: 1D Potential Well

- Scattering of low energy electrons from atoms (normally noble gases such as Xenon or Krypton).
- Investigated by Ramsauer and Townsend independently in the 1920s
- Classically, it was expected that the probability of interaction would diminish with energy.

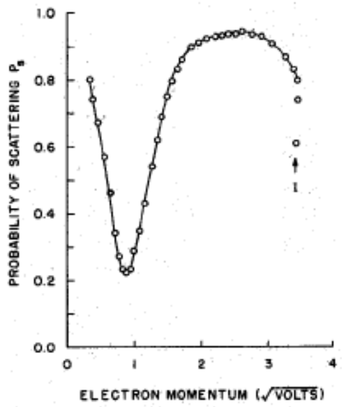


FIG. 4. The probability of scattering P_s as a function of $(V-V_s)^{1/2}$, where $V-V_s$ is the electron energy. Ionization occurs at "I".

- However, it was observed that there were minima in the probability of interaction at ~0.7eV for Xe.
- No classical explanation was available, and it could only be explained through QM.
- Assume the atoms are like potential wells. The minimum of probability (i.e. max T) should be at:

$$\alpha = \frac{n\pi}{L} \quad \Rightarrow \quad E_k = \frac{\hbar^2\alpha^2}{2m} = \frac{h^2}{8mL^2} \quad \text{for} \quad n = 1$$

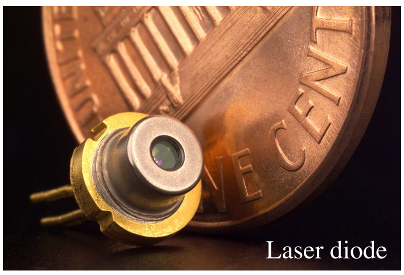
$$\text{For } L \sim 10^{-10}\,m \quad \Rightarrow E_k = \frac{\left(6.6\times10^{-34}\right)^2}{32\times9.1\times10^{-31}\left(10^{-10}\right)^2} = 1.6\times10^{-18}\,J \sim 10\,eV$$

(More accurate result if done in 3D)

6. Applications

Quantum wells:

- Semiconductor material with small energy gap (e.g. GaAs) is sandwiched between energy barriers from material with a larger energy gap (e.g. AlGaAs). A quantum well is formed between the barriers.
- Typical layer thicknesses ~ *1-10 nm*.
- Quantization effects result in allowed energy bands, whose energy positions are dependent on the height and width of the barrier.
- This is used in the fabrication of specialised semiconductor devices such as: laser diodes, high electron mobility transistors (HFET or MODFET), quantum well infrared photodetectors (QWIP arrays).

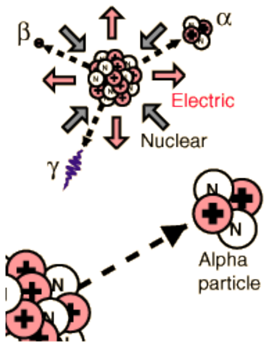


Laser diode

False color image from a far IR
1 megapixel GaAs QWIP camera

Image credits: Wikipedia and NASA

6. Alpha decay



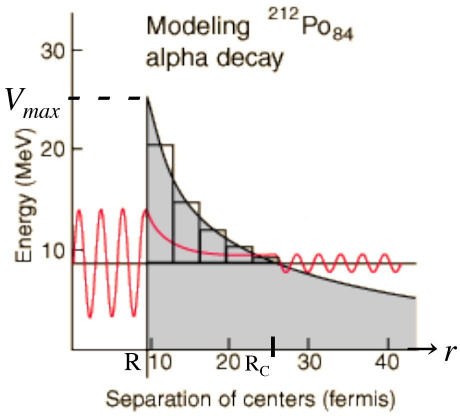
Energy of the alpha particle is lower than the Coulomb potential barrier in the nucleus → tunnelling occurs

$$V(r) = \frac{2(Z_1 - 2)e^2}{4\pi\varepsilon_0 r}, \quad r > R$$

– Example: ^{212}Po $(Z_1{=}84)$, $E_\alpha = 8.78\ MeV$
  Coulomb barrier $V_{max} = 26\ MeV$, $R \simeq 9\ fm$,
  Distance where $E_{barrier} = E_\alpha$ is $R_c \simeq 27\ fm$
  and $M = 3727\ MeV$

The transmission coefficient can be approximated by a product of potential step transmission coefficients:

$$T \simeq \prod_i T_i(V_i, a)$$



6. Examples of 1-D Potentials: α decay

Alpha decay (continued):

- The time between two attempts at the barrier walls is:

$$\Delta t = \frac{2R}{v} = 2R\sqrt{\frac{M}{2E_\alpha}}$$

- For small values of the transmission, T and the number of attempts n before the probability to escape is ½ are related by

$$nT \approx \frac{1}{2}$$

- The corresponding half-life for the α decay is

$$t_{1/2} \approx n\Delta t \approx \frac{\Delta t}{2T}$$

- For ^{212}Po, for example, we can calculate: $\Delta t = 0.88{\times}10^{-21} s$, $T = 1.5{\times}10^{-15}$ so we can estimate $n = 0.33x10^{15}$ and $t_{1/2} \simeq 0.29\ \mu s$

↖ in good agreement with the measured value (in this case)