5. Potential Well

- Third example: Infinite Potential Well
  - The potential is defined as:
    \[
    V(x) = \begin{cases} 
    0 & \text{if } -a < x < a \\
    \infty & \text{if } |x| > a
    \end{cases}
    \]
  - The 1D Schrödinger equation is:
    \[
    \frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = 0 \quad \text{for} \quad -a < x < a
    \]
  - 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 \( k \):
    \[
    \psi(x) = A' e^{ikx} + B' e^{-ikx} = A \cos kx + B \sin kx
    \]
    \[
    k = \sqrt{\frac{2mE}{\hbar^2}}
    \]
The wave function must be zero at both walls of well:
\[ A \cos(ka) + B \sin(ka) = 0 \]
\[ A \cos(-ka) + B \sin(-ka) = 0 \quad \Rightarrow \quad A \cos(ka) - B \sin(ka) = 0 \]
\[ \Rightarrow \quad A \cos(ka) = 0 \quad \text{and} \quad B \sin(ka) = 0 \]

We look at each condition separately
\[ \cos(ka) = 0 \quad \Rightarrow \quad k_n = \frac{n\pi}{2a} = \frac{n\pi}{L}, \quad n = 1,3,5,... \]
\[ \sin(ka) = 0 \quad \Rightarrow \quad k_n = \frac{n\pi}{2a} = \frac{n\pi}{L}, \quad n = 2,4,6,... \]

Normalization condition:
\[ \int_{-a}^{a} |\psi_n(x)|^2 dx = 1 \quad \Rightarrow \quad A = \frac{1}{\sqrt{a}} \]

Quantization of the wave number

\[ \cos(ka) = 0 \quad \Rightarrow \quad k_n = \frac{n\pi}{2a} = \frac{n\pi}{L}, \quad n = 1,3,5,... \]
\[ \sin(ka) = 0 \quad \Rightarrow \quad k_n = \frac{n\pi}{2a} = \frac{n\pi}{L}, \quad n = 2,4,6,... \]

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- Solutions:
  \[ \psi_n(x) = \frac{1}{\sqrt{a}} \cos\left(\frac{n\pi}{2a} x\right), \quad n = 1,3,5,... \quad \text{symmetric (even function)} \]
  \[ \psi_n(x) = \frac{1}{\sqrt{a}} \sin\left(\frac{n\pi}{2a} x\right), \quad n = 2,4,6,... \quad \text{antisymmetric (odd function)} \]

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

We can evaluate the de Broglie wavelength:
\[ k_n = \frac{n\pi}{2a} \quad \Rightarrow \quad \lambda_n = \frac{2\pi}{k_n} = \frac{2L}{n}, \quad n = 1,2,3,4,... \]

Only half integer and integer wavelengths fit in the box.

The energy is quantized, i.e. only certain energy values are allowed (energy eigenvalues)
\[ E_n = \frac{p^2}{2m} = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{8ma^2} = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \]
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- 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:
  \[ \frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} E \psi(x) = 0 \quad \text{with} \quad \beta = \sqrt{-\frac{2m}{\hbar^2} E} = \sqrt{\frac{2m}{\hbar^2} |E|} \]
  \[ \Rightarrow \frac{d^2\psi(x)}{dx^2} - \beta^2\psi(x) = 0, \quad |x| > a \]

The energy: \(|E| = -E\) is the binding energy of the particle.

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- Like for the infinite potential, solution is either odd or even:
  1) Even function:
     \[ \psi(x) = \begin{cases} 
     A \cos(\alpha x), & 0 < |x| < a \\
     Ce^{-\beta |x|}, & |x| > a 
     \end{cases} \]
     (since \( De^{\beta |x|} \xrightarrow{x \to \infty} \infty \Rightarrow D = 0 \))
     - Continuity of \( \psi(x) \) and \( d\psi/dx \):
       \[ A \cos(\alpha a) = Ce^{-\beta a} \quad \Rightarrow \alpha a \tan(\alpha a) = \beta a \] (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 \( d\psi/dx \):
       \[ B \sin(\alpha a) = Ce^{-\beta a} \quad \Rightarrow \alpha a \cot(\alpha a) = -\beta a \] (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.
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- If we define the dimensionless quantity $\gamma$ (strength parameter):
  
  $$
  \gamma^2 \equiv (\alpha a)^2 + (\beta a)^2 = \frac{2m}{\hbar^2} (V_0 + E) a^2 - \frac{2m}{\hbar^2} E a^2 = \frac{2m}{\hbar^2} V_0 a^2
  $$

  ($mV_0 a$ defines the value of $\gamma$) then we can solve the equations graphically:

  $\beta a = \alpha a \tan(\alpha a)$ (for even states)
  
  $\beta a = -\alpha a \cot(\alpha a)$ (for odd states)

- 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:

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

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

  $E_1 = -0.93V_0$

  $E_2 = -0.73V_0$

  $E_3 = -0.41V_0$

  $E_4 = -0.04V_0$
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- Case 2: \( E > 0 \), scattering in the potential well
  - The 1D Schrodinger equation is:
    \[
    \frac{d^2 \psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \psi(x) = 0
    \]
  - The solution:
    \[
    \psi(x) = \begin{cases} 
    A e^{ikx} + B e^{-ikx}, & x < -a \\
    F e^{i\alpha x} + G e^{-i\alpha x}, & -a < x < a \\
    C e^{ikx}, & x > a
    \end{cases}
    \]
  - Similar to the potential barrier \((E>V_0)\) but \( V_0 \rightarrow -V_0 \), \( k' \rightarrow \alpha \) and \( a \rightarrow L=2a \)
    \[
    R = \frac{|B|^2}{|A|^2} = \left[ 1 + \frac{4k^2\alpha^2}{(k^2 - \alpha^2)^2 \sin^2(\alpha L)} \right]^{-1}
    \]
    \[
    T = \frac{|C|^2}{|A|^2} = \left[ 1 + \frac{(k^2 - \alpha^2)^2 \sin^2(\alpha L)}{4k^2\alpha^2} \right]^{-1}
    \]

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- Transmission coefficients for \( \gamma = 10 \) and \( \gamma = 100 \):
  - 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 \( \gamma \) the minima become deeper.
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.
- However, it was observed that there were minima in the probability of interaction at \( \sim 0.7 \text{eV} \) 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:

\[
\alpha = \frac{n\pi}{L} \Rightarrow E_n = \frac{\hbar^2 \alpha^2}{2m} = \frac{\hbar^2}{8mL^2} \quad \text{for } n = 1
\]

For \( L \sim 10^{-10} \text{m} \)
\[
E_n = \frac{(6.6 \times 10^{-34})^2}{32 \times 9.1 \times 10^{-31} (10^{-10})^2} = 1.6 \times 10^{-18} \text{J} \sim 10 \text{eV}
\]

(More accurate result if done in 3D)

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 \( \sim 1-10 \text{ nm} \).
- 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).
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: \(^{212}\text{Po}\) \((Z_1 = 84)\), \(E_{\alpha} = 8.78\ MeV\)

  Coulomb barrier \(V_{\text{max}} = 26\ MeV\), \(R \approx 9\ fm\),
  Distance where \(E_{\text{barrier}} = E_{\alpha}\) is \(R_c \approx 27\ fm\)
  and \(M = 3727\ MeV\)

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

\[ T \approx \prod_i T_i(V_i, a) \]

6. Examples of 1-D Potentials: \(\alpha\) decay

Alpha decay (continued):

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

  \[ \Delta t = \frac{2R}{\nu} = 2R \sqrt{\frac{M}{2E_{\alpha}}} \]

- For small values of the transmission, \(T\) and the number of attempts \(n\) before the probability to escape is \(\frac{1}{2}\) are related by

  \[ nT \approx \frac{1}{2} \]

- The corresponding half-life for the \(\alpha\) decay is

  \[ t_{1/2} \approx n\Delta t = \frac{\Delta t}{2T} \]

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

\(\checkmark\) in good agreement with the measured value (in this case)