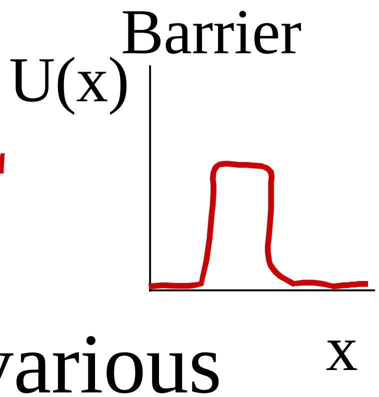
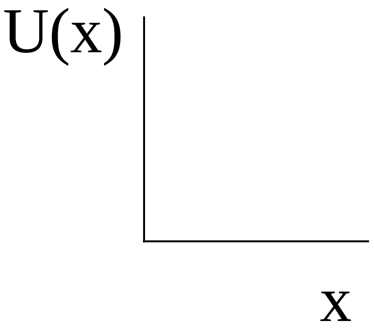
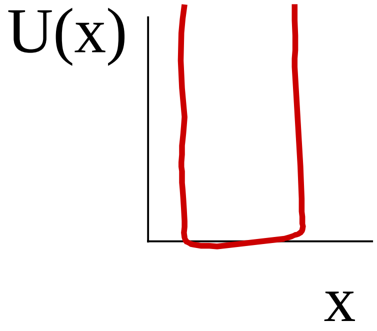
Time-Independent SE



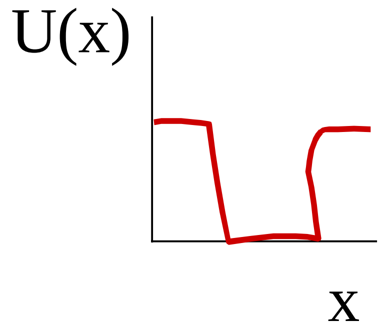
- Solve the time-independent SE for various potential energy functions



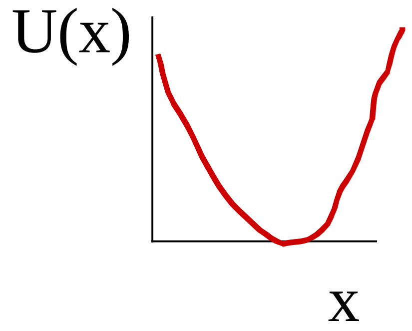
Free particle



Infinite Square Well



Finite Square Well



Harmonic Oscillator

Time-Independent SE

- Solution to time-independent SE in 3-dimensions uses Spherical Harmonics (generalization of Legendre Polynomials)
- Identical particles requires symmetric (anti-summetric) wave function depending on whether particles are bosons (fermions)

Free Particle

$$H\varphi(x) = E\varphi(x)$$

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

$$U(x) = 0$$

$$\frac{d^2\varphi}{dx^2} + \frac{2m}{\hbar^2}E\varphi(x) = 0$$

$$\frac{d^2\varphi}{dx^2} + k^2\varphi(x) = 0$$

Same as harmonic oscillator equation

Free Particle

$$k^2 = \frac{2mE}{\hbar^2} = \frac{p^2}{\hbar^2}$$

$$p = \hbar k, \quad k = \frac{2\pi}{\lambda}$$

$$p = \frac{h}{\lambda}$$

SE includes deBroglie hypothesis

Wave Function

$$\varphi(x) = Ae^{\pm ikx}$$

$$\Psi(x,t) = Ae^{\pm i(kx \pm \omega t)}$$

Free Particle

- Solution to SE for a free particle is a travelling wave with angular frequency and wave number k
- The constant *A* is determined by the normalization condition

$$E = h\upsilon = \hbar\omega$$

$$p = \frac{h}{\lambda} = \hbar k$$

$$\int_{all\ \ space} \varphi^* \varphi = 1$$

$U(x) \neq 0$

- Key to solving SE for $U(x) \neq 0$ is to impose boundary conditions at points where $U(x)$ has significant changes.
- Wave function must be continuous everywhere
- For realistic potentials, first derivative of wave function must also be continuous

Infinite Square Well

- $U = \infty$ for $x < -a$ and $x > a$
- $U = 0$ for $-a \leq x \leq a$
- Probability that particle exists at x where $U = \infty$ is 0
- So, wave function is 0 for $x < -a$ and $x > a$ and wave function has some finite value with a probability integral of one in well

Infinite Square Well

- Infinite square well is a first approximation to a case where particle is bound in some region
- Example: electron bound in an atom

Infinite Square Well

- Wave function is zero outside square well and on boundary
- Inside square well, SE is the same as for a free particle
- Time-independent wave function for a free particle is $\varphi = Ae^{\pm ikx}$
- How can we make free particle wave function satisfy boundary conditions?

Infinite Square Well

$$Ae^{\pm ikx} = B\cos kx + iC\sin kx$$

$$\varphi = B\cos kx$$

$$ka = \frac{n\pi}{2}, \quad n = 1, 3, 5, \ldots$$

$$p = \hbar k = \frac{hn\pi}{(2\pi)2a} = \frac{nh}{4a}$$

$$E = \frac{p^2}{2m} = \frac{n^2 h^2}{32ma^2}$$

Infinite square well has quantized energy levels

Infinite Square Well

$$E = \frac{p^2}{2m} = \frac{n^2 h^2}{32ma^2} = \frac{(6.6\times 10^{-34})^2}{(32)(9.1\times 10^{-31})(10^{-10})^2}$$

$$E = 1.5\times 10^{-18} = \ 9 \ \ eV$$

Correct order of magnitude for atomic energy levels

Infinite Square Well

Normalization condition to determine B

$$\int_{-a}^{a} B^2 \cos^2 kx = B^2 a = 1$$

$$B = \frac{1}{\sqrt{a}}$$

$$\varphi = \frac{1}{\sqrt{a}} \cos \frac{2mE}{\hbar^2} x$$

Particle most likely found in middle of well