Schroedinger Eq as a wave equation

If no forces, no potential energy:

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} \quad , \quad \hbar \approx 10^{-34}\ \mathrm{J \cdot s}$$

Guess: $\Psi(x,t) = A e^{i(kx - \omega t)}$

Then $i\hbar(-i\omega) A e^{i(kx-\omega t)} = \frac{-\hbar^2}{2m} (ik)^2 A e^{i(kx-\omega t)}$

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

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

Because of (i) in the Schroedinger Eq., $\Psi(x,t)$ must be complex.

$\therefore$ A general soln: $\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, A(k) e^{i\left(kx - \frac{\hbar k^2}{2m} t\right)} dk$

This system has dispersion. Group velocity $\frac{\partial \omega}{\partial k} = \frac{\hbar k}{\cancel{2}m}$

A gaussian pulse spreads out. Phase velocity $= \frac{\omega}{k} = \frac{\hbar k}{2m}$

~~If forces are present, let the potential energy by $V(x)$ $\left(F = -\frac{dV}{dx}\right)$. Then the Schroedinger Eq. is~~

$$\cancel{i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi(x)}$$

Group velocity interpretation: classical Velocity $= \frac{\text{momentum}}{\text{mass}} = \frac{p}{m}$

$\therefore$ $\hbar k \rightarrow$ Momentum

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To solve the Schroedinger Eq we guess solutions like

$$\Psi(x,t) = \psi(x) e^{-i\omega t}$$

interpretation : $\omega = \frac{\text{Energy}}{\hbar}$

$\hbar \approx 10^{-34}$ J·s

Any solution of this type is called an "energy eigenstate".

$$= \psi(x) e^{-i\frac{E}{\hbar}t}$$

Then ~~(iℏ) ...~~

Then $(i\hbar)\left(\frac{-iE}{\hbar}\right)\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$

$$\boxed{\psi''(x) = -\frac{2mE}{\hbar^2}\psi(x)}$$

For positive E, Curvature of ψ is opposite sign from ψ.

or

or $\psi''(x) + \frac{2mE}{\hbar^2}\psi(x) = \emptyset$

or $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$ ← Time Independent Schroedinger Eq.

"Normal Mode" in classical physics (Phys 273)

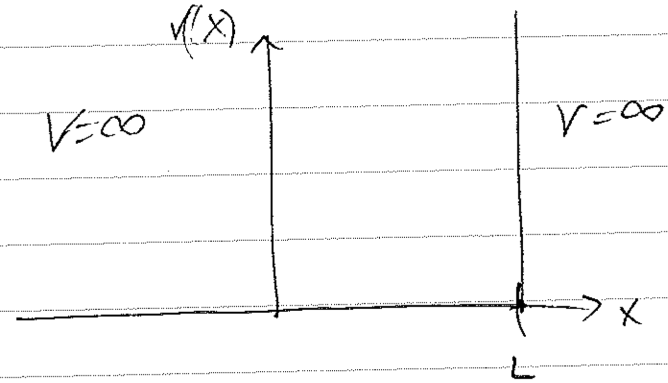
$\Longrightarrow$ "Energy Eigenstate" in Quantum Mechanics

More quantum interpretation. The wavefunction squared is the probability to find the particle at position x. $P(x) = |\psi(x)|^2$

Total probability must be 1:

$$\Rightarrow \int_{-\infty}^{\infty} |\psi(x)|^2 dx \equiv 1.$$

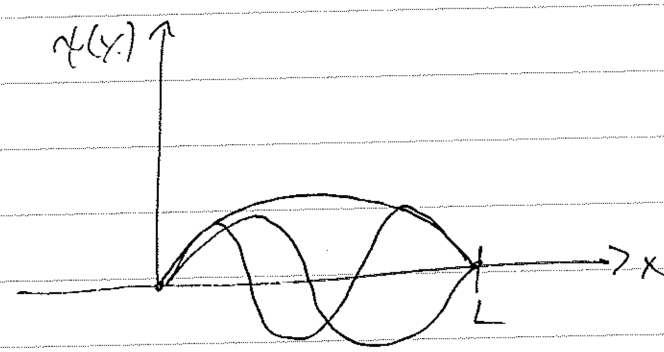
Simple case: Particle in a box.



$V = \emptyset$ between $\emptyset < x < L$
$V = \infty$ outside.

It turns out the ψ must be zero where $V = \infty$, and that ψ must be continuous. This is very ~~precisely~~ similar to the case where a rope is fixed btw two walls at $x = \emptyset$ and $x = L$.

Need $\psi(x) = A \sin\left(\frac{n\pi x}{L}\right)$, $n =$ integer



$$k_n = \frac{n\pi}{L}$$

$$\omega_n = \frac{\hbar k_n^2}{2m} = \frac{\hbar n^2 \pi^2}{2mL^2} \qquad E_n = \hbar\omega_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

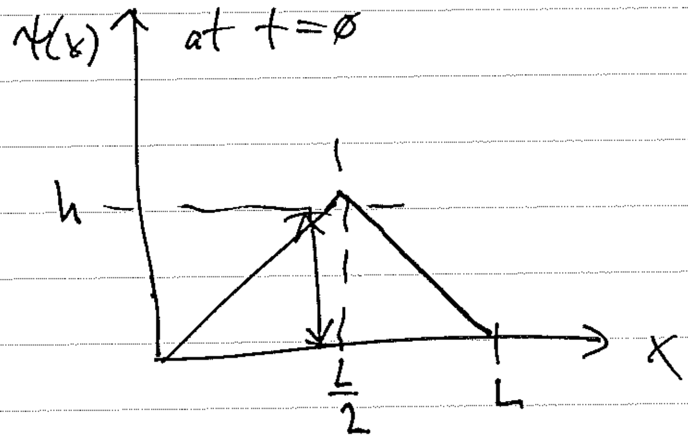
$$\psi(x,t) = A \sin\left(\frac{n\pi x}{L}\right) e^{i\omega_n t} = A \sin\left(\frac{n\pi x}{L}\right) e^{i\hbar n^2 \pi^2 t/(2mL^2)}$$

General solution $= \psi(x,t) = \sum_{n=1}^{\infty} \underbrace{A_n}_{a_n} \sin\left(\frac{n\pi x}{L}\right) e^{i\omega_n t}$

Suppose we are told what $\psi(x,t)$ looks like at $t=\emptyset$. How do we calculate the correct expansion coefficients $\{a_n\}$? Answer: Fourier's Trick.

$$a_n = \frac{2}{L}\int_{\emptyset}^{L} \psi(x,t=\emptyset)\,\sin\left(\frac{n\pi x}{L}\right)dx$$

Example: Triangle function at $t=\emptyset$:



Then $a_n = \frac{8h}{(n\pi)^2}(-1)^{(n-1)/2}$, $n=$ odd only.

$$\psi(x,t) = \sum_{n=1}^{\infty} \frac{8h}{(n\pi)^2}(-1)^{(n-1)/2}\sin\left(\frac{n\pi x}{L}\right)e^{i\hbar n^2\pi^2 t/(2mL^2)}$$

Need to choose the constant h so that $\int|\psi|^2dx=1$.

The primary distinction with the rope system is that in for the rope

$$\omega_n = \sqrt{\frac{T}{\rho}}\,\frac{n\pi}{L}$$

In QM the expansion coefficients have a profound physical interpretation: They are proportional to the probability of observing energy values:

$$|a_n|^2 \sim \text{probability to observe energy } E_n \text{ where for the particle in a box}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

This means $\sum_{n=1}^{\infty} |a_n|^2 = 1$

~~Ex: Suppose $\Psi(x,t)$~~

In general, let $\{\phi_n(x)\}$ be the set of energy eigenfunctions ($\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$ in this case).

Then $\Psi(x,t) = a_1\phi_1(x)e^{-i\omega_1 t} + a_2\phi_2(x)e^{-i\omega_2 t}$

$$+ a_3\phi_3(x)e^{-i\omega_3 t} + \ldots$$

Then $|a_1|^2$ = Probability to observe energy $= E_1 = \hbar\omega_1$

$|a_2|^2 =$ " $= E_2 = \hbar\omega_2$

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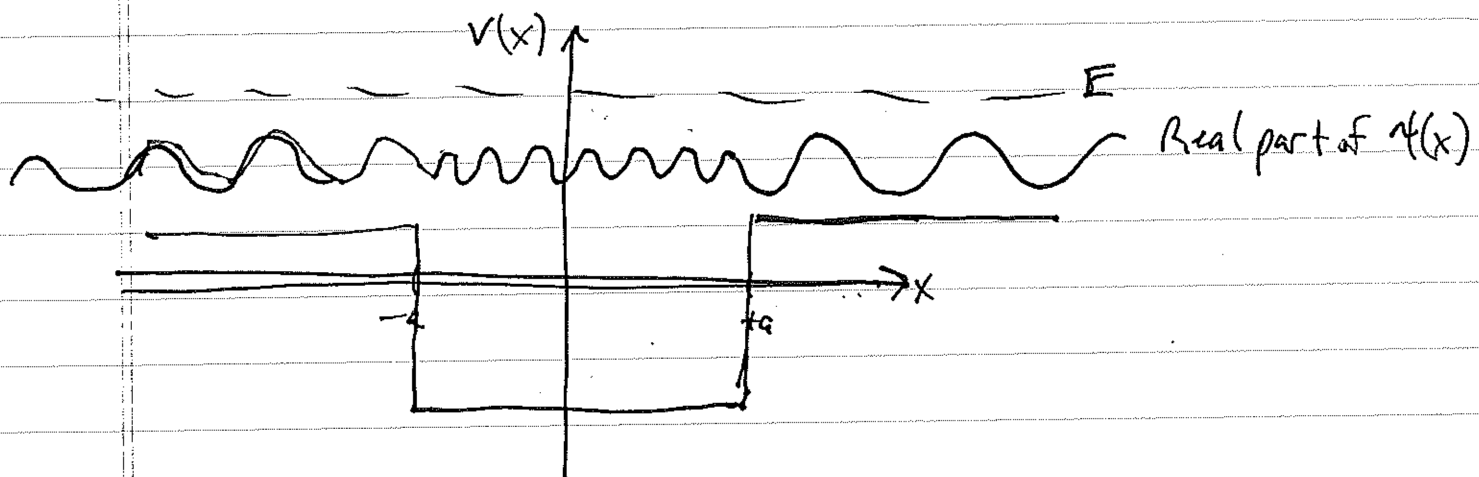
If $V(x) = \text{constant} = V_0$, then again

$$\psi(x,t) = A e^{i(kx - \omega t)}$$

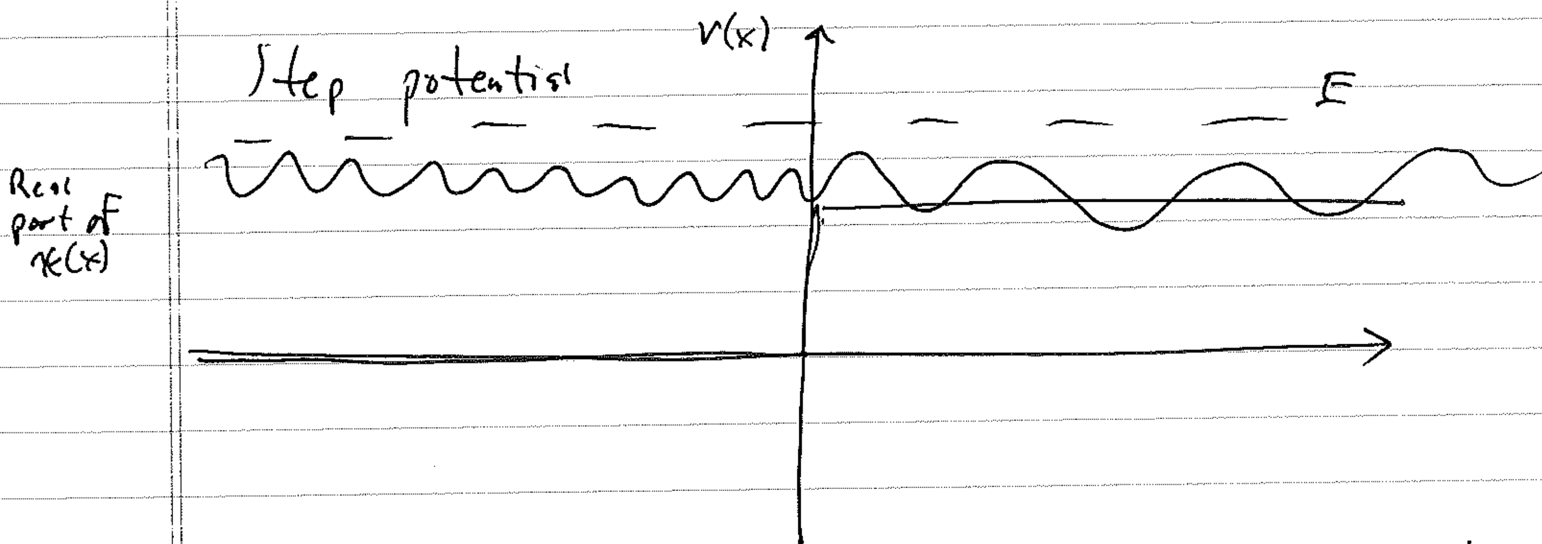
now k must be $k = \sqrt{\dfrac{2m(E - V_0)}{\hbar^2}}$

Where E is the particle energy, $E = \dfrac{(\hbar k)^2}{2m} + V_0$

Finite Square well:



Step potential



Calculate Transmission & Reflection coefficients for different types of potential steps.

Why "Quantum" Mechanics? What is quantized?

For free particles, nothing is quantized. For free particles ($V = \emptyset$), "quantum" mechanics is a misnomer. The name comes from the case of bound particles, like the particle in a box.

Then energy is quantized (discrete): $E_n = \hbar\omega_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$

For free particles, $E = \frac{\hbar^2 k^2}{2m}$, all k are allowed, because there are no boundary conditions.

~~For bound particles the Schrodinger Eq says.~~

$$\cancel{\psi''(x) = -\frac{2m\,(E - V(x))}{\hbar}}$$