E. Time-dependent Schrödinger Equation is the governing Wave Equation

- A breakthrough – Cannot be derived from classical physics
- Like Newton's law in classical mechanics, Schrödinger Equation is a fundamental principle
- What does time-dependent Schrödinger Equation refer to?
  - A particle of mass m
  - Under the influence of a potential energy function, which is a function of position (of the particle) and possibly a function of time

1D problems: $U(x,t)$; 2D: $U(x,y,t)$; 3D: $U(x,y,z,t)$

- Time-dependent Schrödinger Equation (TDSE)

1D Problems: $$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + U(x,t)\,\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)} \quad \text{(TDSE)}$$

- No one can derive it
- It is right because its answers to various problems are right
- 2^{nd} derivative w.r.t. x (space), 1^{st} derivative in t (time)
  [this is different from classical wave equations]
- Work for $U(x,t)$ in general, $U(x)$ (does not depend on t) is easier to handle and provides a systematic way of finding a system's [i.e. given $U(x)$] allowed energies and solving how $\Psi(x,t)$ evolves in time.

- TDSE makes sense for <u>free particle</u> case

Free particle : $U(x) = 0$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)$$

Try $\Psi_p(x,t) = A\,e^{i\left(\frac{px}{\hbar} - \frac{E}{\hbar}t\right)}$

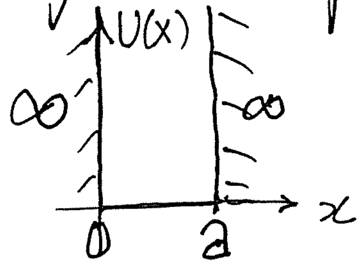
$$\begin{cases} LHS = -\frac{\hbar^2}{2m}\left(\frac{ip}{\hbar}\right)^2 A\,e^{i\left(\frac{px}{\hbar} - \frac{E}{\hbar}t\right)} = \frac{p^2}{2m}\Psi_p(x,t) \\ RHS = i\hbar\left(-\frac{iE}{\hbar}\right) A\,e^{i\left(\frac{px}{\hbar} - \frac{E}{\hbar}t\right)} = E\,\Psi_p(x,t) \end{cases}$$

$\therefore\ E = \frac{p^2}{2m}$ the correct dispersion $(E\text{-}p)$ relation

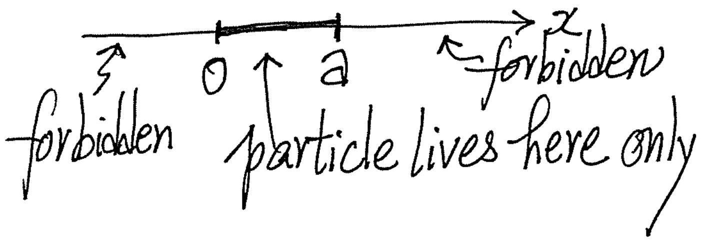
[This is <u>not</u> a proof. This shows that TDSE gives sensible result] for free particle.

- TDSE is not one equation
- <u>It is an equation, one for each physical system</u>

E.g. $U(x,t) = U(x) = \begin{cases} 0 & 0<x<a \\ \infty & \text{otherwise} \end{cases}$

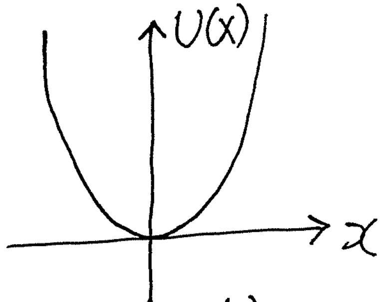


particle confined in $0<x<a$



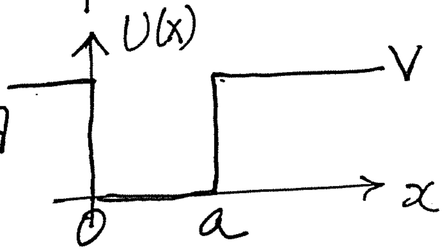
(particle-in-a-box)

E.g. $U(x,t) = U(x) = \frac{1}{2}kx^2$



1D harmonic oscillator

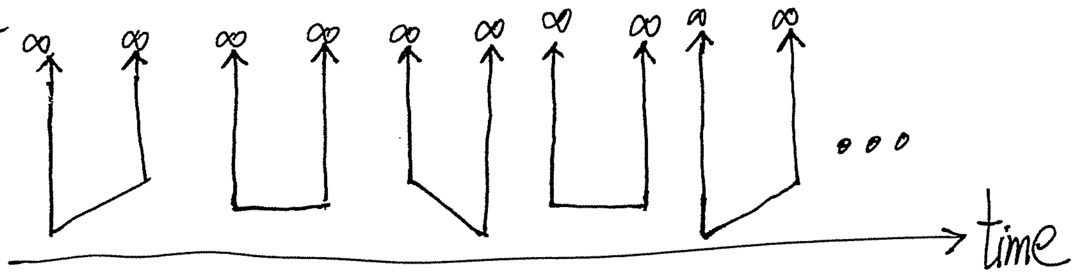
E.g. $U(x,t) = U(x) = \begin{cases} 0 & 0<x<a \\ V & x<0,\ x>a \end{cases}$



1D finite (square) well

E.g. $U(x,t) = \begin{cases} x\cos\omega t & -a<x<a \\ \infty & |x|>a \end{cases}$

(Harder problem)



- These $U(x)$ OR $U(x,t)$ go into $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + U(x,t)\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)$

- We will focus on $U(x)$ cases
  - How TDSE leads to TISE (time-<u>in</u>dependent Schrödinger Equation) and what does TISE do?
  - Time evolution?

2D Problems:

$$\boxed{-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\Psi(x,y,t)+\underbrace{U(x,y,t)}_{\text{specifies the problem}}\Psi(x,y,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,y,t)}$$

2D

E.g.: 2D particle-in-a-box; 2D circular well; 2D harmonic oscillator
2D rectangular box [What are $U(x,y)$?]

3D Problems:

$$\boxed{-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Psi(x,y,z,t)+\underbrace{U(x,y,z,t)}_{\text{specifies the problem}}\Psi(x,y,z,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,y,z,t)}$$

3D

E.g.: 3D box, 3D $a\times b\times c$ box, 3D spherical infinite well,
3D spherical finite well, Hydrogen atom (Coulomb potential energy),
3D harmonic oscillator [What are $U(x,y,z)$?]

- Try to write down TDSE for 2D/3D problems
  E.g. 2D Hydrogen atom

- (Harder) Helium atom?

Summary

- Mass (m) + dimension (1D, 2D, 3D) + What is $\left\{ \begin{matrix} U(x,t) \\ U(x,y,t) \\ U(x,y,z,t) \end{matrix} \right\}$

defines the wave equation

- 3D: $\dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2} \equiv \nabla^2$ (Laplacian)

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t) + U(\vec{r},t)\,\Psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t)}$$

The is the usual form of TDSE