

# The Schrödinger equation

## Announcements:

- Next homework assignment is available
- I will be giving a public talk about physics at the Large Hadron Collider (LHC) at 2pm tomorrow in G1B30. If you are interested in particle physics, you may find it interesting.
- I have decided to cancel the class scheduled for Friday, March 20.



Erwin Schrödinger  
(1887 – 1961)

We begin working with the Schrödinger equation. Today will be free particle and Monday will be the infinite square well (particle in a box).

# Getting to Schrödinger's wave equation

$$\frac{\partial^2 E}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2}$$

Works for light (photons), why doesn't it work for electrons?

We found that solutions to this equation are

$$y = A \cos(kx) \sin(\omega t) + B \sin(kx) \cos(\omega t)$$

or  $y = C \sin(kx - \omega t) + D \sin(kx + \omega t)$

with the constraint  $k = \frac{\omega}{c}$  which can be written  $\omega = kc$

Multiplying by  $\hbar$  we get  $\hbar\omega = \hbar kc$  which is just  $E = pc$

But we know that  $E=pc$  only works for massless particles so this equation can't work for electrons.

# Getting to Schrödinger's wave equation

$\frac{\partial^2 E}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2}$  doesn't work for electrons. What does?

$$y = A \cos(kx) \sin(\omega t) + B \sin(kx) \cos(\omega t)$$

or  $y = C \sin(kx - \omega t) + D \sin(kx + \omega t)$

Note that each derivative of  $x$  gives us a  $k$  (momentum) while each derivative of  $t$  gives us an  $\omega$  (energy).

Equal numbers of derivatives result in  $E = pc$

For massive particles we need  $K = \frac{p^2}{2m}$

So we need two derivatives of  $x$  for  $p^2$  but only one derivative of  $t$  for  $K$ .

If we add in potential energy as well we get the Schrödinger equation...

# The Schrödinger equation

**The Schrodinger equation for a matter wave in one dimension  $\Psi(x,t)$ :**

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

Kinetic energy + Potential energy = Total energy

This is the *time dependent* Schrödinger equation (TDSE) (discussed in 7.11) and is also the most general form.

Note, we now use  $V$  instead of  $U$  for the potential energy.

This potential energy is a function of  $x$  and  $t$ . It gives the potential energy of the particle for any  $x$  and  $t$ . It is not intrinsic to the particles but something from the problem at hand.

# Deriving time independent Schrödinger equation

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

In most physics situations (like hydrogen atom) the potential function  $V$  does not change in time so can write  $V(x,t) = V(x)$ .

In this case, we can separate  $\Psi(x,t)$  into  $\psi(x)\phi(t)$ :  $\Psi(x,t) = \psi(x)\phi(t)$

Can prove that  $\phi(t)$  is always the same:  $\phi(t) = e^{-iEt/\hbar}$

Text uses  $\phi(t) = e^{-i\omega t}$  which is exactly the same since  $E = \hbar\omega$

Putting  $\Psi(x,t) = \psi(x)\phi(t)$  with  $\phi(t) = e^{-iEt/\hbar}$ , into the TDSE gives the time independent Schrödinger equation (TISE):

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

HW problem 8 takes you through these steps in detail.

# Solving quantum mechanics problems

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

1. Determine  $V(x)$  for the problem.
2. Guess (or lookup) the functional form of the solution
3. Plug in solutions to check that solution is correct and find any constraints on constants
4. Figure out boundary conditions and apply them to the general solution to get more constraints
5. Use the normalization constraint  $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$  to normalize the spatial wave function.
6. Multiply by time dependence for full solution:  $\Psi(x, t) = \psi(x)e^{-iEt/\hbar}$
7. Use solution to obtain information like graphs of  $\psi(x)$  and  $|\psi(x)|^2$ , energy levels, probabilities on positions, etc.

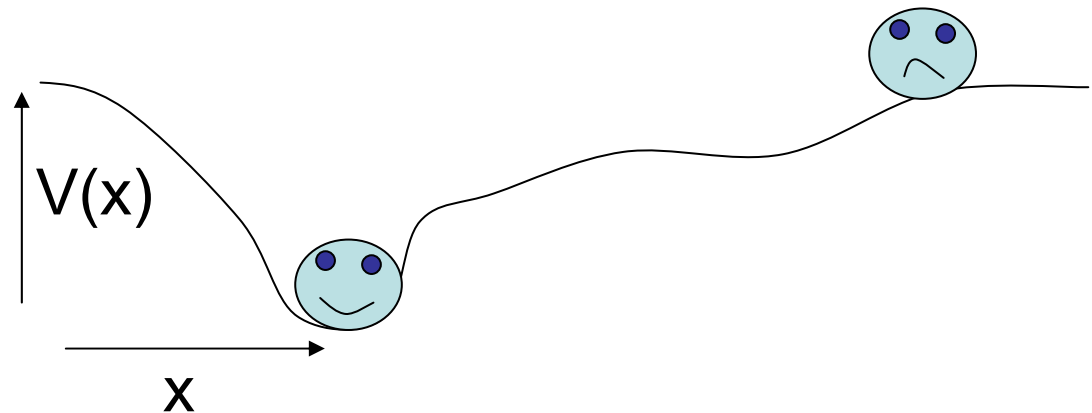
# Clicker question 1

## Set frequency to DA

Given a potential energy function  $V(x)$ , where would a particle naturally want to be?

- A. Where  $V(x)$  is highest
- B. Where  $V(x)$  is lowest**
- C. Where  $V(x) <$  kinetic energy
- D. Where  $V(x) >$  kinetic energy
- E. Does not depend on  $V(x)$

Particles want to go to position of lowest potential energy, like a ball going downhill.



Mathematically we know this because  $\vec{F} = -\vec{\nabla}U$

# Free particle

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

Start with simplest case of a free particle (no forces acting on it).

What is  $V(x)$  for a free particle?

Constant. Smart (easy) choice is  $V(x)=0$ .

What are the boundary conditions for a free particle?

None.

So we need to find what functions satisfy  $-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x)$

but we don't need to apply boundary conditions.

## Clicker question 2

## Set frequency to DA

Which of the following are possible solutions to  $-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x)$

A.  $A \cos(kx)$

B.  $Ae^{-kx}$

C.  $A \sin(kx)$

D. A and C

E. None of A,B,C

Try answer B:  $\frac{d^2\psi(x)}{dx^2} = A(-k)(-k)e^{-kx} = k^2\psi(x)$

This gives us  $-\frac{\hbar^2 k^2}{2m} \psi(x) = E\psi(x)$

This works as long as  $k^2 = -\frac{2mE}{\hbar^2}$

But  $k$  is a real measurable thing so it cannot be complex and therefore  $k^2$  is positive.

Since the only energy we have is kinetic, it must also be positive so the quantity  $2mE/\hbar^2$  must be positive.

So answer B does not work. Answers A and C both work.

For A:  $\frac{d^2\psi(x)}{dx^2} = -Ak^2 \cos(kx) = -k^2\psi(x)$  which gives  $\frac{\hbar^2 k^2}{2m} \psi(x) = E\psi(x)$

### Clicker question 3

### Set frequency to DA

Putting either  $\psi(x)=A\cos(kx)$  or  $\psi(x)=A\sin(kx)$  into the TISE we end up with  $\frac{\hbar^2 k^2}{2m} \psi(x) = E \psi(x)$

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

This works as long as  $\frac{\hbar^2 k^2}{2m} = E$  Since  $p = \hbar k$  this just means the total energy is the kinetic energy

Based on this, what can we say about the free particle energy?

- A. Quantized as  $E_n = E_0 n^2$
- B. Quantized as  $E_n = E_0 n$
- C. Quantized as  $E_n = E_0 / n^2$
- D. Quantized in some other way
- E. Not quantized**

The only requirement is  $E = p^2 / 2m$ . There is no quantization.

**The energy of a free particle is not quantized!**

# Free particle

The general (spatial part) solution for a free particle is:

$$\psi(x) = A \cos(kx) + B \sin(kx)$$

Using some identities you will be proving in the homework, this can also be written as

$$\psi(x) = C e^{ikx} + D e^{-ikx}$$

To get the full wave function we multiply by the time dependence:

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

This is the sum of two traveling waves, each with momentum  $\hbar k$  and energy  $\hbar\omega$ .

The  $C$  wave is moving right and the  $D$  wave is moving left.

Lets pick the right going wave and check it one more time.

# Check free particle solution in TDSE

$$\text{TDSE: } -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}$$

For a free particle,  $V(x,t)=0$  and the solution for a particle moving to the right is  $\Psi(x,t) = C e^{i(kx - \omega t)}$

If we plug this into the TDSE, what do we get?

$$\frac{\partial^2 \Psi(x,t)}{\partial x^2} = C(ik)(ik)e^{i(kx - \omega t)} = -Ck^2 e^{i(kx - \omega t)} = -k^2 \Psi(x,t)$$

$$\frac{\partial \Psi(x,t)}{\partial t} = -Ci\omega e^{i(kx - \omega t)} = -i\omega \Psi(x,t)$$

Putting it all together gives:  $\frac{\hbar^2 k^2}{2m} \Psi(x,t) = \hbar \omega \Psi(x,t)$

**It all works!**

↓  
Kinetic  
energy

=

↓  
Total  
energy