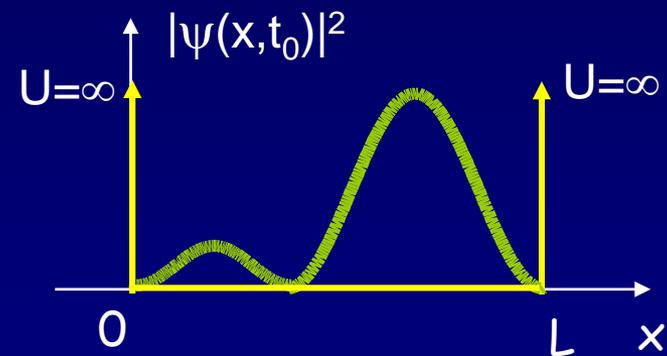
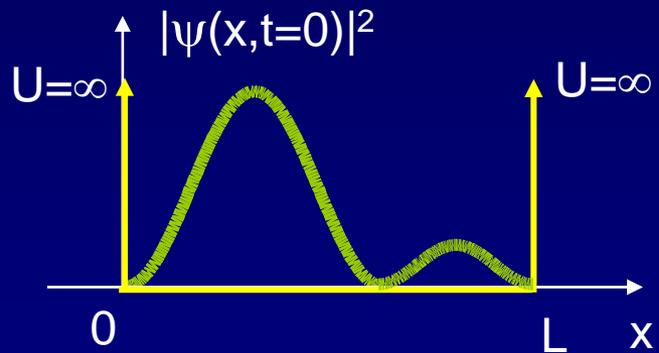


Lecture 14: Superposition & Time-Dependent Quantum States



Last Week

Time-independent Schrodinger's Equation (SEQ):

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

- It describes a particle that has a definite energy, E .
- The solutions, $\psi(x)$, are time independent (stationary states).

We considered three potentials, $U(x)$:

Infinite square well

- Boundary conditions \rightarrow only certain allowed energies (and corresponding “energy eigenstates”)

Finite-depth square well

- Particle can “leak” into forbidden region.
- Comparison with infinite-depth well.

Harmonic oscillator

- Energy levels are equally spaced.
- A good approximation in many problems.

Today

Time dependent SEQ:

Superposition of states and particle motion

Measurement in quantum physics

(Time-energy uncertainty principle)

Time-Dependent SEQ

To explore how particle wave functions evolve with time, which is useful for a number of applications as we shall see, we need to consider the **time-dependent SEQ**:

$$-\frac{\hbar^2}{2m} \frac{d^2 \Psi(x,t)}{dx^2} + U(x)\Psi(x,t) = i\hbar \frac{d\Psi(x,t)}{dt}$$

Changes from the time-independent version:

- $E\psi \rightarrow i\hbar d\Psi/dt$ We no longer assume a definite E .
- $\psi(x) \rightarrow \Psi(x,t)$ The solutions will have time dependence.
- $i = \sqrt{-1}$ appears The solutions will be complex.

This equation describes the complete time and space dependence of a quantum particle in a potential $U(x)$.

It replaces the classical particle dynamics law, $F=ma$.

The SEQ is linear in Ψ , and so the **Superposition Principle** applies:

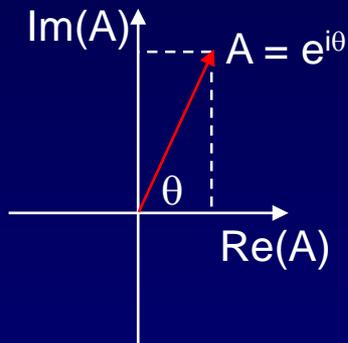
If Ψ_1 and Ψ_2 are solutions to the time-dependent SEQ, then so is any linear combination of Ψ_1 and Ψ_2 (example: $\Psi = 0.6\Psi_1 + 0.8i\Psi_2$)

Review of Complex Numbers

The equation, $re^{i\theta} = r(\cos\theta + i\sin\theta) = r\cos\theta + ir\sin\theta$, might be new to you. It is a convenient way to represent complex numbers like $x + iy$. It also (once you are used to it) makes trigonometry simpler.

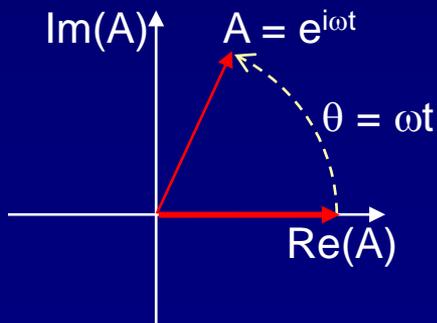
a. Draw an Argand diagram of $e^{i\theta}$.

(Just like Cartesian vs polar coordinates)



The Argand diagram of a complex number, A , puts $\text{Re}(A)$ on the x-axis and $\text{Im}(A)$ on the y-axis. Notice the trig relation between the x and y components. θ is the angle of A from the real axis. In an Argand diagram, $e^{i\theta}$ looks like a vector of length 1, and components $(\cos\theta, \sin\theta)$.

b. Suppose that θ varies with time, $\theta = \omega t$. How does the Argand diagram behave?



At $t = 0$, $\theta = 0$, so $A = 1$ (no imaginary component).

As time progresses, A rotates counterclockwise with angular frequency ω .

This is the math that underlies phasors.

The quantity, $ce^{i\theta}$ (c and θ both real), is a complex number of magnitude $|c|$. The magnitude of a complex number, A , is $|A| = \sqrt{A^*A}$, where A^* is the complex conjugate of A .

Act i

$$i \equiv \sqrt{-1}$$

1. What is $(-i)i$?

- a. $-i$ b. -1 c. $+1$

2. What is $1/i$?

- a. -1 b. $-i$ c. $+i$

3. What is $|e^{i\phi}|^2$?

- a. 0 b. $e^{2i\phi}$ c. 1

Relationship between Time-Independent and Time-Dependent SE

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

$$-\frac{\hbar^2}{2m} \frac{d^2 \Psi(x,t)}{dx^2} + U(x)\Psi(x,t) = i\hbar \frac{d\Psi(x,t)}{dt} \quad \Psi(x,t)$$

Try to see if separable solutions can be found:

$$\Psi(x,t) = \psi(x) f(t) \quad \frac{1}{\psi(x)} \left[-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + U(x)\psi(x) \right] = \text{const.} = \frac{1}{f(t)} \left[i\hbar \frac{df(t)}{dt} \right]$$

From time-independent SEQ we see that **const. = E = E_n**

How many energy eigenstates? Infinite number!

Infinite number of separable solutions. Label with *n*

$$\Psi_n(x,t) = \psi_n(x) f_n(t)$$

Now what about the general case, not just energy eigenstates?

Superposition! **Any** time dependent state can be written as a weighted sum of normalized separable-states: $\Psi_n(x,t) = \psi_n(x) f_n(t)$

Final Result: $\Psi(x,t) = \sum_{n=1}^{\infty} a_n \Psi_n(x,t) = \sum_{n=1}^{\infty} a_n \psi_n(x) f_n(t)$

What is $f_n(t)$?

Any state of atom 

Time-dependence of Energy Eigenstates

The time-independent SEQ is just a special case of the time-dependent SEQ.

So, if $\Psi(\mathbf{x},t)$ is a state with definite energy, it is a solution to both equations.

Both equations have the same left-hand side, so the right sides must be equal:

RHS of time
ind. SEQ

$$E\Psi(\mathbf{x},t) = i\hbar \frac{d\Psi(\mathbf{x},t)}{dt}$$

RHS of time
dep. SEQ

This equation has the solution:

$$\Psi(\mathbf{x},t) = \psi(\mathbf{x})e^{-i\omega t} \text{ with } \omega = \frac{E}{\hbar}$$

Notes:

- $\psi(\mathbf{x})$ is a solution to the time ind SEQ with energy E .
- $E = \hbar\omega = hf$, as expected.

Ψ is complex. However, we are interested in $|\Psi|^2$, because that's what we **measure**.

$$|\Psi(\mathbf{x},t)|^2 = (\psi^*(\mathbf{x})e^{+i\omega t})(\psi(\mathbf{x})e^{-i\omega t}) = |\psi(\mathbf{x})|^2$$

This is *always* a real number.

So, for an energy eigenstate:
the probability density, $|\Psi|^2$, has no time dependence! (i.e., it's a “stationary state”).

We don't actually need the time-independent SEQ, but if we know we're dealing with energy eigenstates, the math is simpler.

Example: Motion of a Free Particle

A free particle moves without applied forces; so set $U(x) = 0$.

The SEQ is now reasonably simple:

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

The second x -derivative is proportional to the first t -derivative.

Here's one solution:

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

This is a traveling wave. The particle has

Momentum: $p = \hbar k = h/\lambda$

Energy: $E = \hbar\omega = hf$

Not a surprise. Same classical result.

Check it. Take the derivatives:

$$\frac{\partial \Psi}{\partial x} = ik Ae^{i(kx - \omega t)}$$

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

$$\frac{\partial \Psi}{\partial t} = (-i\omega) Ae^{i(kx - \omega t)}$$

So, it works if:

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

That's the same as:

$$\frac{p^2}{2m} = E$$

Time-dependence of Superpositions

A particle can be in a superposition of states that have different energies.

This superposition is still a solution of the time-dependent SEQ, but not of the time-independent SEQ, because two different E 's are involved.

Two questions:

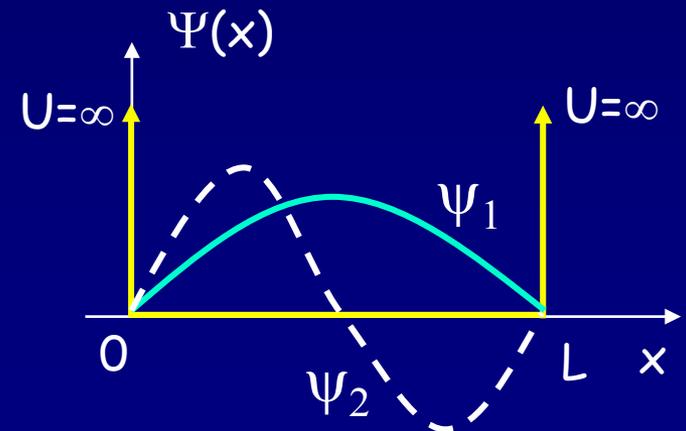
- How does this superposition evolve with time?
For example, is the probability density still stationary?
- What happens if we measure the particle's energy?

First, look at the time dependence. Consider the first two energy states in an infinite well. Here's the superposition:

$$\Psi(x, t) = \psi_1(x)e^{-i\omega_1 t} + \psi_2(x)e^{-i\omega_2 t}$$

$$\omega_1 = \frac{E_1}{\hbar}, E_1 = \frac{\hbar^2}{8mL^2}$$

$$\omega_2 = \frac{E_2}{\hbar}, E_2 = 4E_1$$



The two terms have different frequencies, so they oscillate in and out of phase.

Particle Motion in a Well

The probability density is given by: $|\Psi(x,t)|^2$:

$$|\Psi(x,t)|^2 = \psi_1^2 + \psi_2^2 + 2\psi_1\psi_2 \cos((\omega_2 - \omega_1)t)$$

Interference term

We used the identity:

$$e^{i\theta} + e^{-i\theta} = 2\cos\theta$$

$$\Psi(x,t) = \psi_1(x)e^{-i\omega_1 t} + \psi_2(x)e^{-i\omega_2 t}$$

$$|\Psi(x,t)|^2 = \left| \psi_1(x)e^{-i\omega_1 t} + \psi_2(x)e^{-i\omega_2 t} \right|^2$$

$$|\Psi(x,t)|^2 = \left(\psi_1(x)e^{-i\omega_1 t} + \psi_2(x)e^{-i\omega_2 t} \right) \left(\psi_1(x)e^{+i\omega_1 t} + \psi_2(x)e^{+i\omega_2 t} \right)$$

$$|\Psi(x,t)|^2 = |\psi_1(x)|^2 + |\psi_2(x)|^2 + \underbrace{\psi_1(x)\psi_2(x) \left(e^{i(\omega_2 - \omega_1)t} + e^{-i(\omega_2 - \omega_1)t} \right)}_{e^{i\theta} + e^{-i\theta} = 2\cos\theta}$$

$$e^{i\theta} + e^{-i\theta} = 2\cos\theta$$

Particle Motion in a Well

The probability density is given by: $|\Psi(x,t)|^2$:

$$|\Psi(x,t)|^2 = \psi_1^2 + \psi_2^2 + 2\psi_1\psi_2 \cos((\omega_2 - \omega_1)t)$$

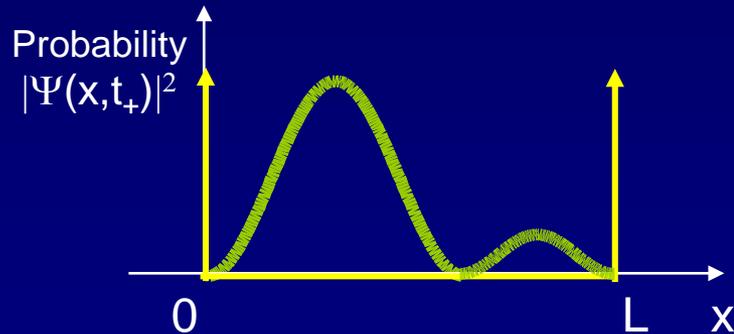
Interference term

So, $|\Psi(x,t)|^2$ oscillates between:

In phase: ($\cos = +1$)

$$|\Psi(x,t)|^2 = (\psi_1 + \psi_2)^2$$

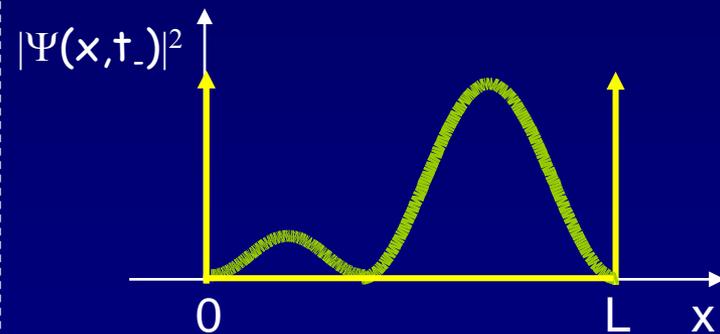
Particle localized on left side of well:



Out of phase: ($\cos = -1$)

$$|\Psi(x,t)|^2 = (\psi_1 - \psi_2)^2$$

Particle localized on right side of well:



The frequency of oscillation is $\omega = \omega_2 - \omega_1 = (E_2 - E_1)/\hbar$, or $f = (E_2 - E_1)/h$. This is precisely the frequency of a photon that would make a transition between the two states.

Interference Beats

The motion of the probability density comes from the changing interference between terms in Ψ that have different energy.

The beat frequency between two terms is the frequency difference, $f_2 - f_1$.

So energy differences are important: $E_1 - E_2 = hf_1 - hf_2$, etc.

Just like in Newtonian physics: **absolute energies aren't important** (you can pick where to call $U=0$ for convenience), only energy differences.

Normalizing Superpositions

We want the total probability to equal 1, even when the particle is in a superposition of states:

$$P_{tot} = \int |\psi|^2 dx = \int |a\psi_1 + b\psi_2|^2 dx = 1$$

This looks like a mess. However, we're in luck. Multiply it out:

$$\begin{aligned} \int |a\psi_1 + b\psi_2|^2 dx &= \int |a\psi_1|^2 dx + \int |b\psi_2|^2 dx + \int (a\psi_1)^* (b\psi_2) dx + \int (b\psi_2)^* (a\psi_1) dx \\ &= |a|^2 \int |\psi_1|^2 dx + |b|^2 \int |\psi_2|^2 dx + a^* b \int (\psi_1)^* (\psi_2) dx + b^* a \int (\psi_2)^* (\psi_1) dx \\ &= |a|^2 + |b|^2 + 0 + 0 \end{aligned}$$

If ψ_1 is normalized If ψ_2 is normalized It is a mathematical theorem that these integrals always = 0 if the energies are different.

Math
415

A normalized superposition must have $|a|^2 + |b|^2 = 1$.

$\psi = 0.8\psi_1 + 0.6\psi_2$ is normalized.
 $\psi = 0.5\psi_1 + 0.5\psi_2$ is not normalized.

Act 2

Consider a particle in an infinite square well. At $t = 0$ it is in the state:

$$\Psi(x, t) = 0.5\psi_2(x) + A_2\psi_4(x)$$

with $\psi_2(x)$ and $\psi_4(x)$ both normalized.

1. What is A_2 ? a. 0.5 b. 0.707 c. 0.866 d. - 0.866

2. At some later time t ,
what is the probability density at the center of the well?
a. 0 b. 1 c. It depends on the time t .

Measurements of Energy

Fundamentals of Measurement Theory in Quantum Mechanics

What happens when we measure the energy of a particle whose wave function is a superposition of more than one energy state?

If the wave function is in an energy eigenstate (E_1 , say), then we know with certainty that we will obtain E_1 (unless the apparatus is broken).

If the wave function is a superposition ($\psi = a\psi_1 + b\psi_2$) of energies E_1 and E_2 , then *we aren't certain what the result will be*. However:

We know with certainty that we will only obtain E_1 or E_2 !!

REALLY??

YES!!!

To be specific, we will never obtain $(E_1 + E_2)/2$, or any other value.

What about a and b ? (In general these will be complex numbers.)

$|a|^2$ and $|b|^2$ are the probabilities of obtaining E_1 and E_2 , respectively.

That's why we normalize the wave function to make $|a|^2 + |b|^2 = 1$.

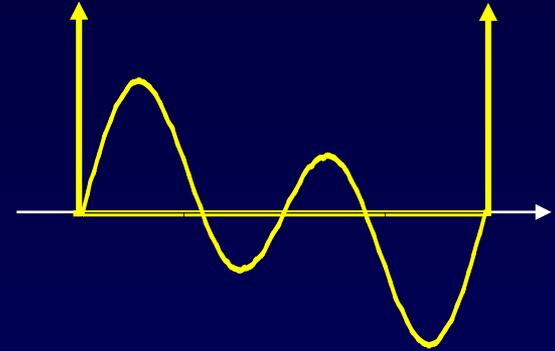
We can't prove this statement. It is one of the fundamental postulates of quantum theory. Treat it as an empirical fact.

Act 3

Consider a particle in an infinite well.
It is in the state:

$$\Psi(x, t) = 0.5\Psi_2(x, t) + 0.866\Psi_4(x, t)$$

with $\psi_2(x)$ and $\psi_4(x)$ both normalized.



We now measure the energy of the particle. What value is obtained?

- a. E_2 b. E_4 c. $0.25 E_2 + 0.75 E_4$ d. It depends on when we measure the energy.

Not part of this act, but an important question, nevertheless:

If E_2 is observed, what is the state of the particle after the measurement?

The "Collapse" of the Wave Function

If E_2 is observed, what is the state of the particle after the measurement?

We start out with this wave function:

$$\Psi(x, t) = 0.5\Psi_2(x, t) + 0.866\Psi_4(x, t)$$

Before we make the measurement, we can't predict the result of an energy measurement with certainty.

However, after the measurement, we know with certainty that $E = E_2$.
To be specific: We know that a second measurement will yield E_2 . (Why?)

Therefore, after obtaining E_2 , the wave function must now be:

$$\Psi(x, t) = \Psi_2(x, t)$$

That is, the wave function has "collapsed" to the state that corresponds with the result we obtained.

This is one of the weirder features of QM, and is the principal reason that Einstein never accepted QM as a complete theory.

("God does not place dice!")

Supplement: Time-Energy Uncertainty Principle

Now that we are considering time-dependent problems, it is a good time to introduce another application of the Heisenberg Uncertainty Principle, based on measurements of energy and time. We start from our previous result and consider what happens for photons:

$$\Delta p \Delta x \geq \hbar \Rightarrow (c\Delta p) \left(\frac{\Delta x}{c} \right) \geq \hbar \Rightarrow \Delta E \Delta t \geq \hbar$$

Sometimes this is further transformed as follows:

$$\Delta E \Delta t \geq \hbar \Rightarrow (\hbar\Delta\omega) \Delta t \geq \hbar$$

$$\Delta\omega \Delta t \geq 1 \Rightarrow \Delta f \Delta t \geq 1/2\pi$$

The last line is a *standard result* from **Fourier wave analysis**; this should not surprise us – the Uncertainty Principle arises simply because particles behave as waves that are oscillating in time as well as in space.

$\Delta E \Delta t$ Uncertainty Principle Example*

A particular optical fiber transmits light over the range 1300-1600 nm (corresponding to a frequency range of 2.3×10^{14} Hz to 1.9×10^{14} Hz). How long (approximately) is the shortest pulse that can propagate down this fiber?

$$\Delta \omega \Delta t \geq 1 \Rightarrow 2\pi \Delta f \Delta t \geq 1$$

$$\Delta t \geq 1/2\pi \Delta f$$

$$\geq 1/(2\pi \cdot 0.4 \times 10^{14} \text{ Hz})$$

$$= 4 \times 10^{-15} \text{ s} = \boxed{4 \text{ fs}}$$

Note: This means the upper limit to data transmission is $\sim 1/(4\text{fs}) = 2.5 \times 10^{14}$ bits/second = 250 Tb/s

*This problem obviously does not require “quantum mechanics” *per se*. However, due to the Correspondence Principle, QM had better give a consistent result.

Next Week

3-Dimensional Potential Well

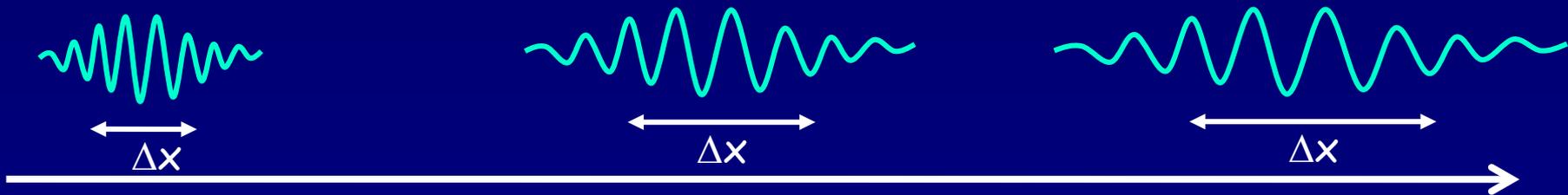
Schrödinger's Equation for the Hydrogen Atom

Supplement: Quantum Information References

- Quantum computing
 - Employs superpositions of quantum states - astoundingly good for certain parallel computation, may use entangled states for error checking
 - www.wired.com/2014/05/quantum-computing/#slide-id-914531
 - www.theguardian.com/science/2012/oct/09/physics-nobel-prize-quantum-computing
- Quantum entanglement
 - Quantum systems that have interacted with each other can be in states where each system individually has no information – all information is shared *nonlocally* between the two pieces, no matter how far apart they are.
 - library.lanl.gov/cgi-bin/getfile?00783354.pdf
- Quantum cryptography
 - Employs single photons or entangled pairs of photons to generate a secret key. Can determine if there has been eavesdropping in information transfer
 - www.csa.com/discoveryguides/crypt/overview.php
 - library.lanl.gov/cgi-bin/getfile?00783355.pdf
- Quantum teleportation
 - Employs an entangled state to produce an exact replica of a third quantum state at a different point in space
 - quantumfrontiers.com/2012/08/19/how-to-build-a-teleportation-machine-intro-to-entanglement/
 - www.livescience.com/49028-farthest-quantum-teleportation.html
 - www.cnet.com/news/scientists-achieve-reliable-quantum-teleportation-for-the-first-time/

Supplement: Free particle motion

- It turns out (next slide) that the constructive interference region for a matter wavepacket moves at the “group velocity”
$$v = h/\lambda m = p/m$$
- So there’s a simple correspondence between the quantum picture and our classical picture of particles moving around with momentum $p = mv$.
- But the quantum packet will spread out in the long run, since it has a range of p , so the correspondence is never perfect.



Position of maximum probability moves
and the width of probability distribution spreads out

Supplement: Group velocity

- Say a wave-packet starts out at $x=0$ at $t=0$.
 - meaning each harmonic component has the same phase there.
- After time t
 - the harmonic component at ω_1 will have changed phase by $\omega_1 t$
 - the harmonic component at ω_2 will have changed phase by $\omega_2 t$
 - The phase difference between these components at $x=0$ will now be $(\omega_2 - \omega_1) t$

To find the point x where they're in phase, we need to find where the phase difference from moving downstream by x cancels that:

 - $(\omega_2 - \omega_1) t = (k_2 - k_1) x$ Or for small differences in ω, k : $t d\omega = x dk$

Result

$$v_g = x/t = d\omega/dk$$

$$\text{In this case } v_g = p/m$$