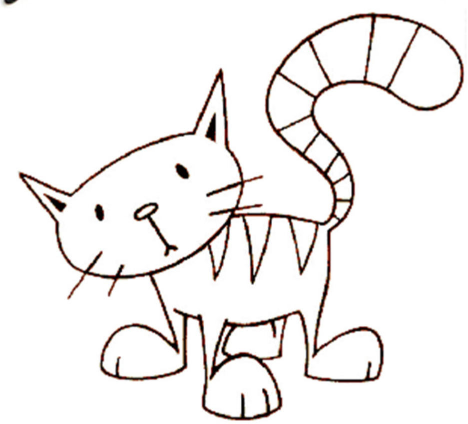
Lecture 4

The Schrödinger Equation and its Interpretation

In this lecture you will learn:

- **Schrödinger equation: the time-dependent form**
- **Schrödinger equation: the probabilistic interpretation**
- **Breakdown of determinism in quantum physics**

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$



The Quantum Physics of Photons

We know that light obeys the following wave equation in free-space:

$$\nabla^2 \vec{E} = \frac{1}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2} \xrightarrow{\text{In 1D}} \frac{\partial^2 \vec{E}}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2}$$

What if we didn't know this wave equation, and didn't even know Maxwell's equations, and wished to "reverse engineer" the above wave equation from what we know about photons

1) According to Planck, the energy of a light packet or light quantum or light photon is related to its frequency by:

$$E = \hbar\omega$$

2) The momentum magnitude of a photon is related to its wavelength via:

$$p = \frac{2\pi\hbar}{\lambda} \qquad \left\{ p^2 = \vec{p}.\vec{p} \right.$$

3) We also know something else about photons:

$$\omega = \frac{2\pi c}{\lambda} \Rightarrow \hbar\omega = \frac{2\pi\hbar c}{\lambda} \Rightarrow E = pc$$

Profound!!

Energy goes linearly with the momentum magnitude

Wave Equation for Photons: An Example of Reverse Engineering

Lets rewrite the last one as: $E = pc$

$$\Rightarrow \hbar\omega = \frac{2\pi\hbar}{\lambda}c \qquad \left\{ k = \frac{2\pi}{\lambda} \right.$$

$$\Rightarrow \boxed{\omega = kc} \Rightarrow \boxed{\omega^2 = k^2c^2} \qquad \left\{ k^2 = \vec{k}.\vec{k} \right.$$

Suppose light wave could be written as:

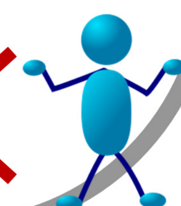
$$\vec{E}(\vec{r},t) = \vec{E}_o e^{i\vec{k}.\vec{r}} e^{-i\omega t}$$

So how about we try the following wave equation for photons and see if any work:

1) $\dfrac{\partial \vec{E}}{\partial t} = \text{constant} \times \nabla^2 \vec{E}$ $\xrightarrow{\text{Plug in the wave above}}$ $i\omega = \text{constant} \times k^2$

2) $\dfrac{\partial^2 \vec{E}}{\partial t^2} = \text{constant} \times \nabla^2 \vec{E}$ $\xrightarrow{\text{Plug in the wave above}}$ $\omega^2 = \text{constant} \times k^2$

2) $\dfrac{\partial \vec{E}}{\partial t} = \text{constant} \times \left(\nabla \times \vec{E}\right)$ $\longrightarrow$ $\vec{E}.\dfrac{\partial \vec{E}}{\partial t} = \dfrac{\partial\left(\vec{E}.\vec{E}\right)}{\partial t} = 0$



Wave Equation for Photons: An Example of Reverse Engineering

2) $$\frac{\partial^2 \vec{E}}{\partial t^2} = \text{constant} \times \nabla^2 \vec{E} \xrightarrow{\text{Plug in the wave above}} \omega^2 = \text{constant} \times k^2$$

And so the constant must be c^2 and we get:

$$\frac{\partial^2 \vec{E}}{\partial t^2} = c^2 \nabla^2 \vec{E}$$

And this is just the wave equation obtained from Maxwell's equations!!

The Classical (Newtonian) Physics of Particles

$$m \longrightarrow \vec{p} = m\vec{v}$$

Classical Physics:

1) A particle with mass *m* and velocity $\vec{v}$ has momentum given by:

$$\vec{p} = m\vec{v}$$

2) The (kinetic) energy of the particle is:

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} \qquad \begin{cases} v^2 = \vec{v}.\vec{v} \\ p^2 = \vec{p}.\vec{p} \end{cases}$$

For a massive particle, energy momentum relationship is quadratic

Note how difference the above energy-momentum relation for particle with non-zero mass is compared to that for a photons which is:

$$E = pc \longrightarrow$$

Massless photons (energy momentum relationship is linear)

The De Broglie Hypothesis for Massive Particles

1) De Broglie assumed that "associated" with a particle of momentum $p=mv$, there is a wave of some sort with a wavelength λ equal to:

$$\lambda = \frac{2\pi\hbar}{p}$$

Basically, he just extended the relation known previously for light particles to matter particles

2) De Broglie further assumed that "associated" with a particle of energy E, there is a wave of some sort with a frequency ω equal to:

$$\omega = \frac{E}{\hbar}$$

Again, he just extended the relation known previously for light particles to matter particles

3) There is also something else we know about a massive particle:

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

$$\begin{cases} v^2 = \vec{v}.\vec{v} \\ p^2 = \vec{p}.\vec{p} \end{cases}$$

Energy momentum relationship is quadratic

The Schrödinger Equation - I

Statement of the Problem:

We would like to drive a wave equation for particles with mass, so that the amplitude of the wave, or the wavefunction , can be written as:

$$\psi(\vec{r},t) = A\, e^{i\vec{k}.\vec{r}} e^{-i\omega t} \qquad \left\{ k = \frac{2\pi}{\lambda} \right.$$

We start with:

$$E = \frac{p^2}{2m} \qquad \left\{ p^2 = \vec{p}.\vec{p} \right.$$

De Broglie second hypothesis

$$\Rightarrow \hbar\omega = \frac{p^2}{2m}$$

De Broglie first hypothesis

$$\Rightarrow \hbar\omega = \frac{\left(\frac{2\pi\hbar}{\lambda}\right)^2}{2m} \qquad \left\{ k = \frac{2\pi}{\lambda} \right. \longleftrightarrow \quad p = \frac{2\pi\hbar}{\lambda} = \hbar k$$

$$\Rightarrow \hbar\omega = \frac{\hbar^2 k^2}{2m} \qquad \left\{ k^2 = \vec{k}.\vec{k} \right.$$

The Schrödinger Equation: Reverse Engineering

Need to find an equation for the wave amplitude (or the wavefunction):

$$\psi(\vec{r},t) = A\, e^{i\vec{k}.\vec{r}} e^{-i\omega t}$$

that satisfies:

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} \qquad \left\{ k^2 = \vec{k}.\vec{k} \right.$$

You have now enough experience to figure out that the desired equation must be first order in time and second order in space:

$$\frac{\partial \psi(\vec{r},t)}{\partial t} = \text{constant}\ \nabla^2 \psi(\vec{r},t)$$

The constant term can be figured out to get:

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

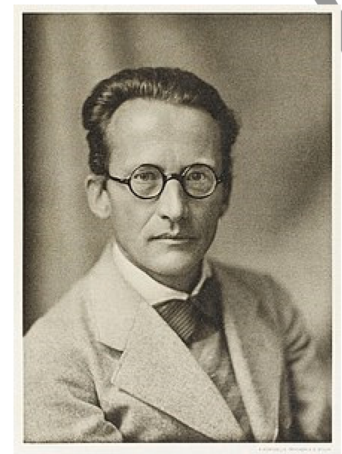
This is one form of the celebrated Schrödinger equation (published in 1926) !!!

Notice how different it is from the wave equation for photons:

$$\frac{\partial^2 \vec{E}}{\partial t^2} = c^2 \nabla^2 \vec{E}$$

The Schrödinger Equation - III

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t)$$ ⟶ It is complex!!



Erwin Schrödinger
(1887-1961)
Nobel Prize 1933

Note that the equation has these three ingredients built into it:

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \qquad \omega = \frac{E}{\hbar} \qquad p = \frac{2\pi\hbar}{\lambda} = \hbar k$$

Schrödinger suffered from tuberculosis and several times in the 1920s stayed at a sanatorium in Arosa. It was there that he formulated his wave equation.

As a check, we take a wave solution: $\psi(\vec{r},t) = A\,e^{i\vec{k}.\vec{r}}e^{-i\omega t}$

And plug it into the Schrödinger equation to get:

$$\hbar\omega A\,e^{i\vec{k}.\vec{r}}e^{-i\omega t} = \frac{\hbar^2 k^2}{2m}A\,e^{i\vec{k}.\vec{r}}e^{-i\omega t}$$

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

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

The Schrödinger Equation: Adding the Potential Energy

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

Plugging in the solution:

$$\psi(\vec{r},t) = A\, e^{i\vec{k}.\vec{r}} e^{-i\omega t}$$

gives:

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

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

But what if the energy *E* of the particle consists of the kinetic energy $\frac{p^2}{2m}$ plus some potential energy *V*, i.e.:

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

The Schrödinger Equation: Adding the Potential Energy

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

There is a problem with the equation: only kinetic energy of the particle is taken into account in the expression used for deriving it:

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2k^2}{2m} = \text{KE}$$

But particle might also have a potential energy ……!! How do we fix this??

We want: $E = \text{KE} + \text{PE}$

Right Hand Side:

The right hand side differential operator, $-\frac{\hbar^2}{2m}\nabla^2$, when it acts on the wave amplitude (or the wavefunction), it gives the kinetic energy of the particle:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) = -\frac{\hbar^2}{2m}\nabla^2 Ae^{i\vec{k}.\vec{r}}e^{-i\omega t} = \underbrace{\frac{\hbar^2k^2}{2m}}_{\text{Kinetic energy}} Ae^{i\vec{k}.\vec{r}}e^{-i\omega t}$$

The Schrödinger Equation: Adding the Potential Energy

Right Hand Side:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) = -\frac{\hbar^2}{2m}\nabla^2 A e^{i\vec{k}.\vec{r}} e^{-i\omega t} = \frac{\hbar^2 k^2}{2m} A e^{i\vec{k}.\vec{r}} e^{-i\omega t}$$

Suppose the potential energy of the particle is a function of position and is given by: $V(\vec{r})$

For example: **if the particle has charge** e **and is in a uniform electric field** $\vec{E}$ **then its potential energy (i.e. the electrostatic potential energy) will be:**

$$V(\vec{r}) = -e\vec{E}.\vec{r} = e\phi(\vec{r})$$

We try to change the right hand side so that it gives the total energy of the particle and not just the kinetic energy. In other words,

$$-\frac{\hbar^2}{2m}\nabla^2 \xrightarrow{\text{change to}} -\frac{\hbar^2}{2m}\nabla^2 + \boxed{??}$$

so that

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \boxed{??}\right)\psi(\vec{r},t) = [\mathrm{KE} + \mathrm{PE}]\psi(\vec{r},t)$$

The Schrödinger Equation: Adding the Potential Energy

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \boxed{??}\right)\psi(\vec{r},t) = [\text{KE} + \text{PE}]\psi(\vec{r},t)$$

Try the simplest choice: $V(\vec{r})$

So we have:

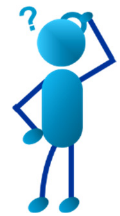
$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right)\psi(\vec{r},t)$$

This is the final form of the celebrated Schrödinger equation (published in 1926) !!!

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

This is the wave equation for a massive particle!!

But what the heck does this wave equation mean??



The Schrödinger Equation: Time-Dependent Potential Energy

The potential energy could be a function of time as well, so more generally:

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

In this course, we will spend most of the time on time-independent potential energies

The Schrödinger Equation: 3D and 1D Versions

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

3D version

The 1D version below works if the problem is one dimensional – meaning all the action in the problem is in one dimension and everything is uniform in the other two dimensions

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

1D version

Also good for building intuition in quantum physics!

The Schrödinger Equation: What Does it mean??

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t) \longrightarrow$$ It is complex!!

Here are the questions that the scientific community was thinking when Schrödinger published his wave equation:

1) **What is the wave equation about? Meaning, what is oscillating? This $\psi(\vec{r},t)$ is the amplitude of what exactly?**

2) **Is the electron, or for that matter any other particle to which the Schrödinger equation applies, a wave or a particle? And is then ψ the amplitude of this wave?**

3) **Or is it that the particle is really a particle but it is somehow guided by this wave? Like a surfer riding a wave!!!**

4) **Normally, all other wave equations are real and are for real amplitudes. Complex notation is used only for convenience and the real part taken at the end to get physical results. But the Schrödinger equation is complex, and the wavefunction is complex too, so how can it represent physical reality!!**

The Schrödinger Equation: The Probability Interpretation

In 1926, Max Born offered the following interpretation of the wavefunction $\psi(\vec{r},t)$ of a particle:

Max Born
(1882-1970)
Nobel Prize: 1954

The real quantity $|\psi(\vec{r},t)|^2$ is equal to the a-priori probability of finding the particle at location $\vec{r}$ at time t if a measurement is made to find the position of the particle

$$|\psi(\vec{r},t)|^2 = \psi^*(\vec{r},t)\psi(\vec{r},t)$$

What this means is that:

1) One cannot know with pure certainty, nor can one calculate with complete certainty, where a particle might be found BEFORE a measurement is actually made to locate the particle

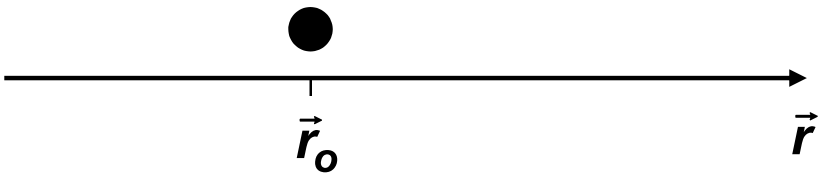
2) Schrödinger equation allows one to calculate only the a-priori probabilities of finding the particle at any place (BEFORE a measurement is made to locate it)

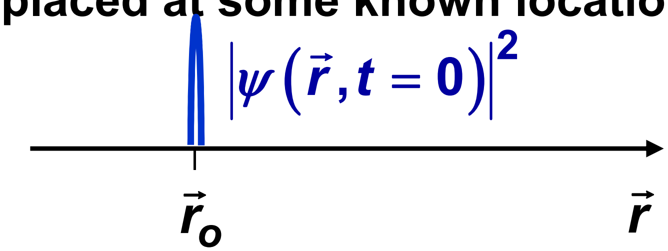
What happened to determinism?? 

The Statistical Interpretation and the Breakdown of Determinism

The probabilistic interpretation of $\psi(\vec{r},t)$ has the following statistical interpretation with respect to experiments:

1) Initial condition: Suppose at time t=0, a particle is placed at some known location:





2) Time evolution: Its subsequent dynamics and evolution are governed by the Schrödinger equation:

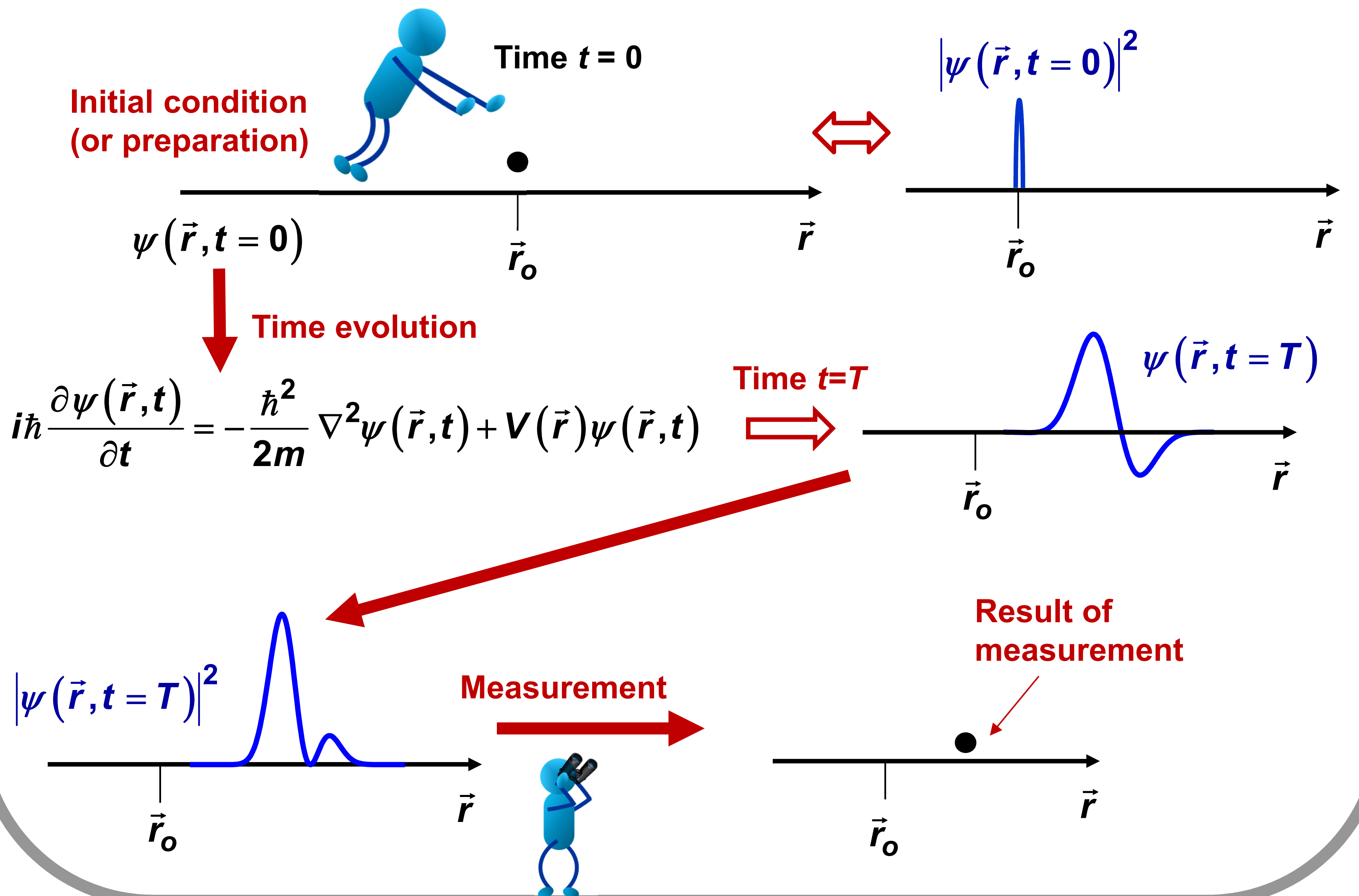
$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t)$$

3) Measurement: At a later time t=T, the location of the particle is measured. The a-priori probability of finding the particle at location $\vec{r}$ at time t=T is given by:

$$\left|\psi(\vec{r},T)\right|^2 = \psi^*(\vec{r},T)\psi(\vec{r},T)$$

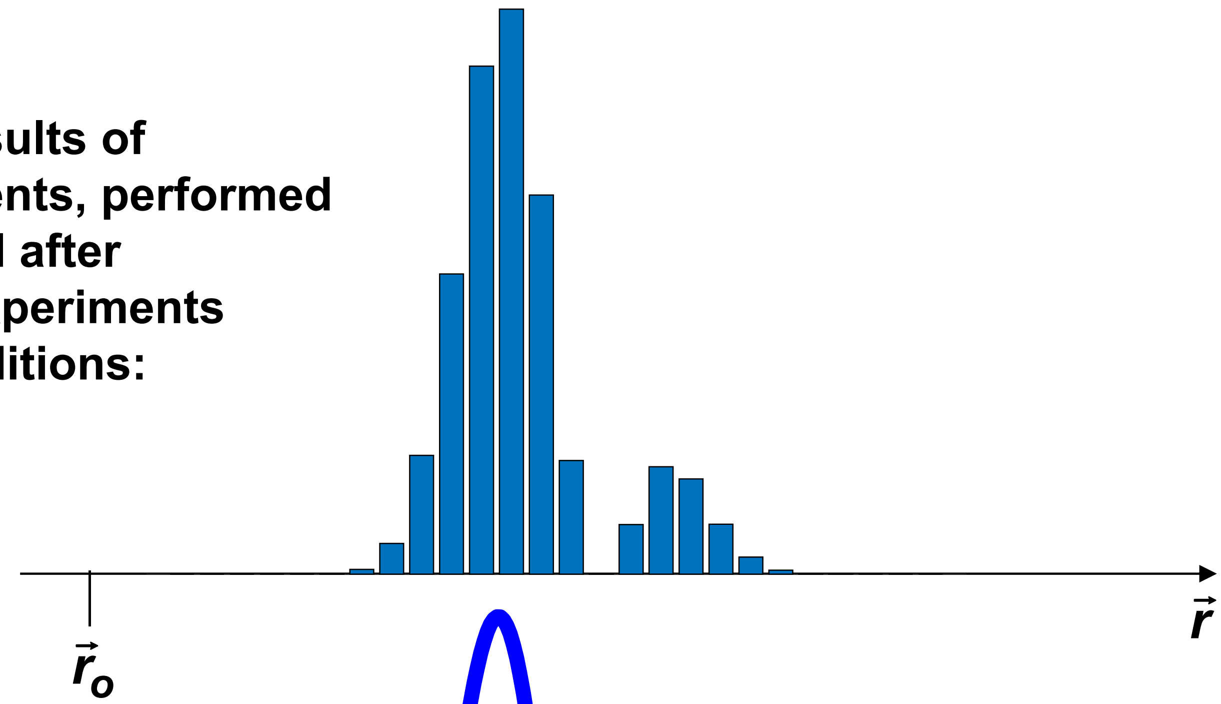
4) The above experiment (1 through 3) is then repeated many times under exactly the same conditions. But the measured location at time t=T would be different each time the experiment is conducted (notice the breakdown of determinism!). However, the measured probabilities of finding the particle will agree with the Born probability rule!

The Statistical Interpretation and the Breakdown of Determinism

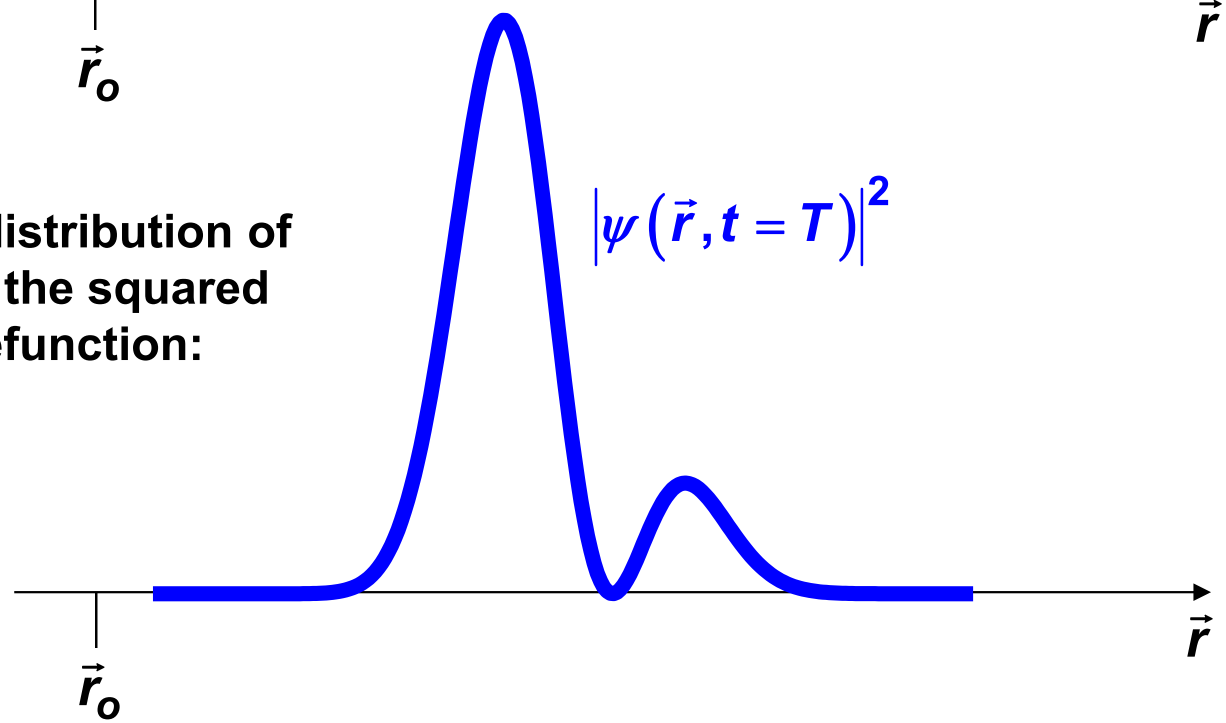


The Statistical Interpretation of Quantum Probabilities

Histogram of the results of position measurements, performed at time *t*=*T*, obtained after conducting many experiments under identical conditions:



A-priori probability distribution of position as given by the squared modulus of the wavefunction:



The Schrödinger Equation: The Probability Interpretation

The real quantity $\left|\psi(\vec{r},t)\right|^2$ is equal to the a-priori probability of finding the particle at location $\vec{r}$ at time t

$$\left|\psi(\vec{r},t)\right|^2 = \psi^*(\vec{r},t)\,\psi(\vec{r},t)$$

So if $\left|\psi(\vec{r},t)\right|^2$ is really a probability distribution, then it must be properly normalized:

$$\iiint dV\,\left|\psi(\vec{r},t)\right|^2 = \int d^3\vec{r}\,\left|\psi(\vec{r},t)\right|^2 = 1 \qquad \text{(in 3D)}$$

$$\int_{-\infty}^{\infty} dx\,\left|\psi(x,t)\right|^2 = 1 \qquad \text{(in 1D)}$$

The probability of finding the particle in the entire universe must be unity

The Schrödinger Equation: A Free Particle in 3D

Assume a <u>free-particle</u> (zero potential):

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + \cancelto{0}{V}(\vec{r})\psi(\vec{r},t)$$

$$\left\{\ V(\vec{r}) = 0\right.$$

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

Plane wave is a solution:

$$\psi(\vec{r},t) = A\,e^{i\vec{k}.\vec{r}}e^{-i\frac{E}{\hbar}t}$$

<u>Plane wave solution works only when:</u>

$$V(\vec{r}) = \text{constant}$$

Plug the solution into the Schrodinger equation:

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

$$EA\,e^{i\vec{k}.\vec{r}}e^{-i\frac{E}{\hbar}t} = \frac{\hbar^2k^2}{2m}A\,e^{i\vec{k}.\vec{r}}e^{-i\frac{E}{\hbar}t}$$

$$\Rightarrow E = \frac{\hbar^2k^2}{2m}$$

Plane Wave Solutions: A Free Particle in 3D

Plane wave is a solution:

$$\psi(\vec{r},t) = A\, e^{i\vec{k}.\vec{r}}\, e^{-i\frac{E}{\hbar}t}$$

$$\left\{ E = \hbar\omega = \frac{\hbar^2 k^2}{2m} \right.$$

We must have:

$$\iiint dV\, \left|\psi(\vec{r},t)\right|^2 = \int d^3\vec{r}\, \left|\psi(\vec{r},t)\right|^2 = 1$$

$$\Rightarrow \iiint dV \left| A\, e^{i\vec{k}.\vec{r}}\, e^{-i\frac{E}{\hbar}t} \right|^2 = |A|^2 \iiint dV = |A|^2\, V = 1$$

$$\Rightarrow |A| = \frac{1}{\sqrt{V}}$$ → **V is the volume of the universe!**

$$\Rightarrow \psi(\vec{r},t) = \frac{1}{\sqrt{V}}\, e^{i\vec{k}.\vec{r}}\, e^{-i\frac{E}{\hbar}t}$$ → **Properly normalized solution!**

So the a-priori probability of finding the particle at any location is:

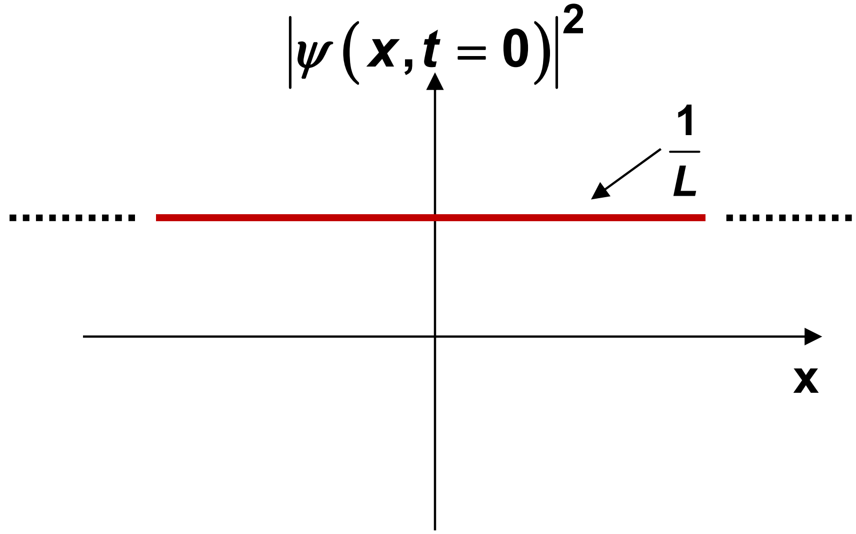
$$\left|\psi(\vec{r},t)\right|^2 = \frac{1}{V}$$ → **The a-priori probability of finding the particle at any place is the same because the wavefunction is spread over all space**

A Plane Wave Solution for a Free Particle in 1D

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + \cancelto{0}{V}(x)\psi(x,t)$$

Consider a wave-like solution
in a 1D universe of length *L*:

$$\psi(x,t) = \frac{1}{\sqrt{L}}e^{ikx}e^{-i\frac{E}{\hbar}t} \Longrightarrow \left\{ E = \frac{\hbar^2 k^2}{2m} \right.$$



The a-priori probability of finding the particle is constant in space (i.e. the particle can be anywhere ?!).

This does not correspond to our notion of a localized particle in classical physics ………….!

A Localized Free Particle in 1D: A Wavepacket

1D:

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} + \cancelto{0}{V(x)}\psi(x,t) \qquad \left\{ V(x) = 0 \right.$$

Plane wave is a solution:

$$\psi(x,t) = A\, e^{ikx} e^{-i\frac{E}{\hbar}t} \qquad \left\{ E = \frac{\hbar^2 k^2}{2m} \right.$$

Or more appropriately,

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

Now consider a superposition solution of many different plane waves:

$$\psi(x,t) = \sum_n A_n\, e^{ik_n x} e^{-i\frac{E(k_n)}{\hbar}t}$$

If the superposition consists of plane waves with wavevectors that are very close to each other we can write the above sum as an integral:

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} A(k)\, e^{ikx} e^{-i\frac{E(k)}{\hbar}t} \rightarrow \int_{-\infty}^{\infty} \frac{dk}{2\pi} \psi(k)\, e^{ikx} e^{-i\frac{E(k)}{\hbar}t}$$

A Localized Free Particle in 1D: A Wavepacket

Consider the 1D wavepacket solution (a superposition of plane waves):

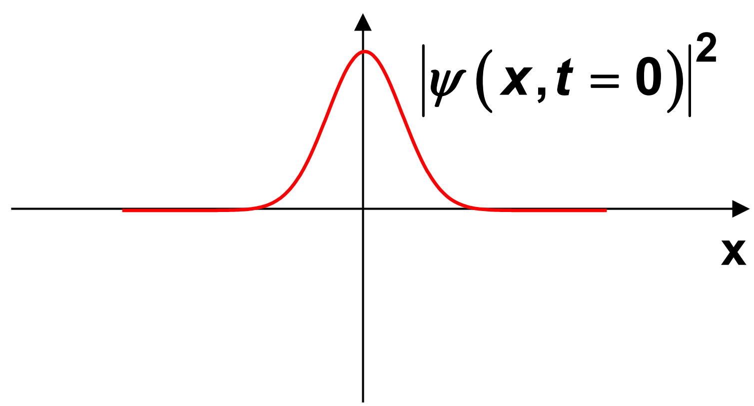
$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\psi(k)\, e^{ikx} e^{-i\frac{E(k)}{\hbar}t} \qquad \left\{ E(k) = \frac{\hbar^2 k^2}{2m} \right.$$

We must have:

$$\int_{-\infty}^{\infty} dx \left|\psi(x,t)\right|^2 = 1$$

$$\Rightarrow \int_{-\infty}^{\infty} dx \left| \int_{-\infty}^{\infty} \frac{dk}{2\pi}\psi(k)\, e^{ikx} e^{-i\frac{E(k)}{\hbar}t} \right|^2 = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\left|\psi(k)\right|^2 = 1$$

The probability of finding the particle is now non-zero only in a finite section of space
The particle is localized !



Some Math

Show that:

$$\int_{-\infty}^{\infty} dx \left|\psi(x,t)\right|^2 = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\left|\psi(k)\right|^2$$

Parseval's Theorem

Proof:

$$\int_{-\infty}^{\infty} dx \left|\psi(x,t)\right|^2$$

$$= \int_{-\infty}^{\infty} dx \left| \int_{-\infty}^{\infty} \frac{dk}{2\pi}\psi(k)\, e^{ikx} e^{-i\frac{E(k)}{\hbar}t} \right|^2$$

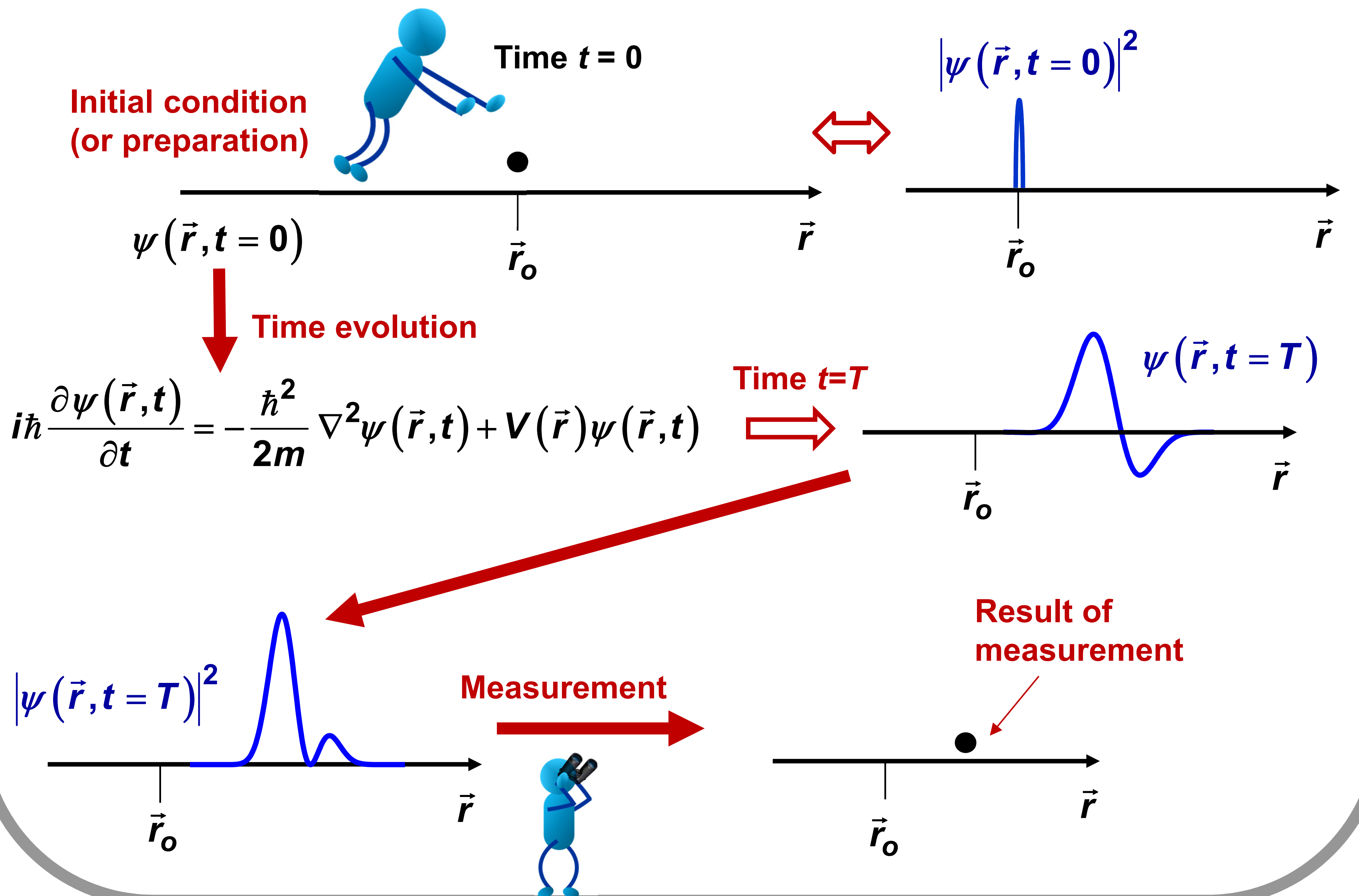
$$= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} \frac{dk}{2\pi}\psi^*(k)\, e^{-ikx} e^{+i\frac{E(k)}{\hbar}t} \int_{-\infty}^{\infty} \frac{dk'}{2\pi}\psi(k')\, e^{ik'x} e^{-i\frac{E(k')}{\hbar}t}$$

$$= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \psi(k') e^{-i\frac{E(k')}{\hbar}t} \psi^*(k) e^{+i\frac{E(k)}{\hbar}t} \underbrace{\int_{-\infty}^{\infty} dx \;\; e^{-ikx} e^{ik'x}}$$

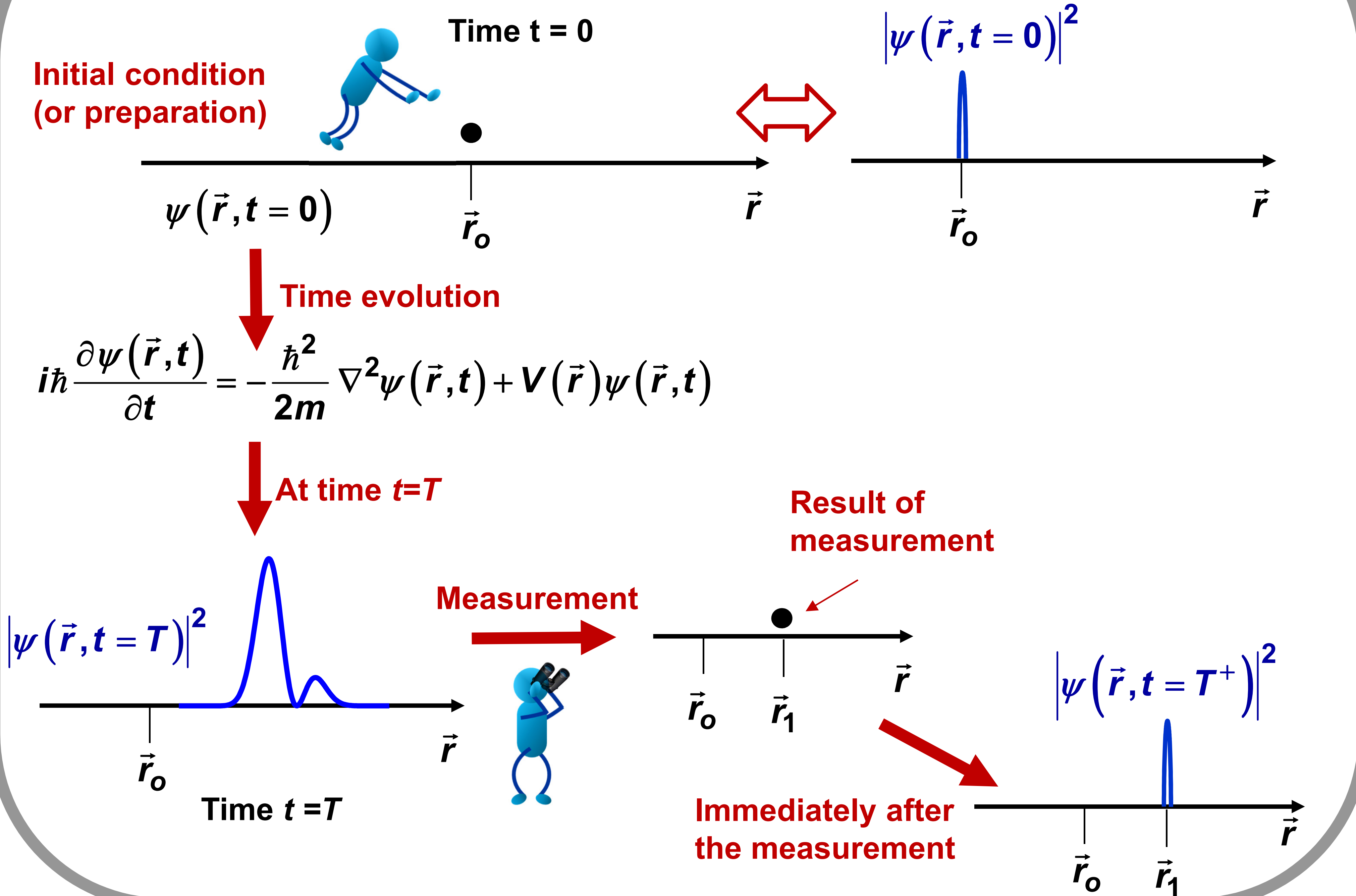
$$= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \psi(k') e^{-i\frac{E(k')}{\hbar}t} \psi^*(k) e^{+i\frac{E(k)}{\hbar}t} \underbrace{(2\pi)\,\delta(k-k')}$$

$$= \int_{-\infty}^{\infty} \frac{dk}{2\pi}\left|\psi(k)\right|^2$$

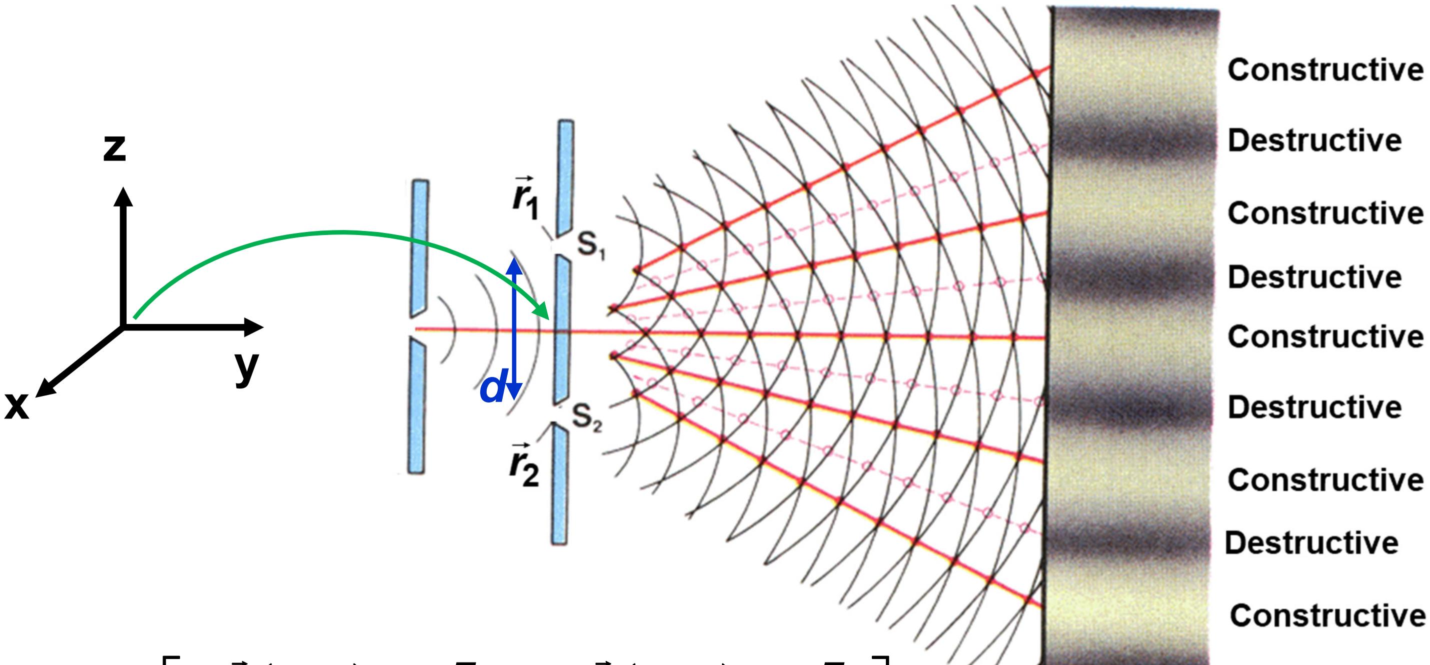
The Statistical Interpretation and the Breakdown of Determinism



The Collapse of the Wavefunction upon Measurement



The Schrödinger Equation: Interference Explained



$$\psi(\vec r,t) \approx U_o \left[\frac{e^{i\vec k.(\vec r-\vec r_1)}}{r} e^{-i\frac{E}{\hbar}t} + \frac{e^{i\vec k.(\vec r-\vec r_2)}}{r} e^{-i\frac{E}{\hbar}t} \right]$$

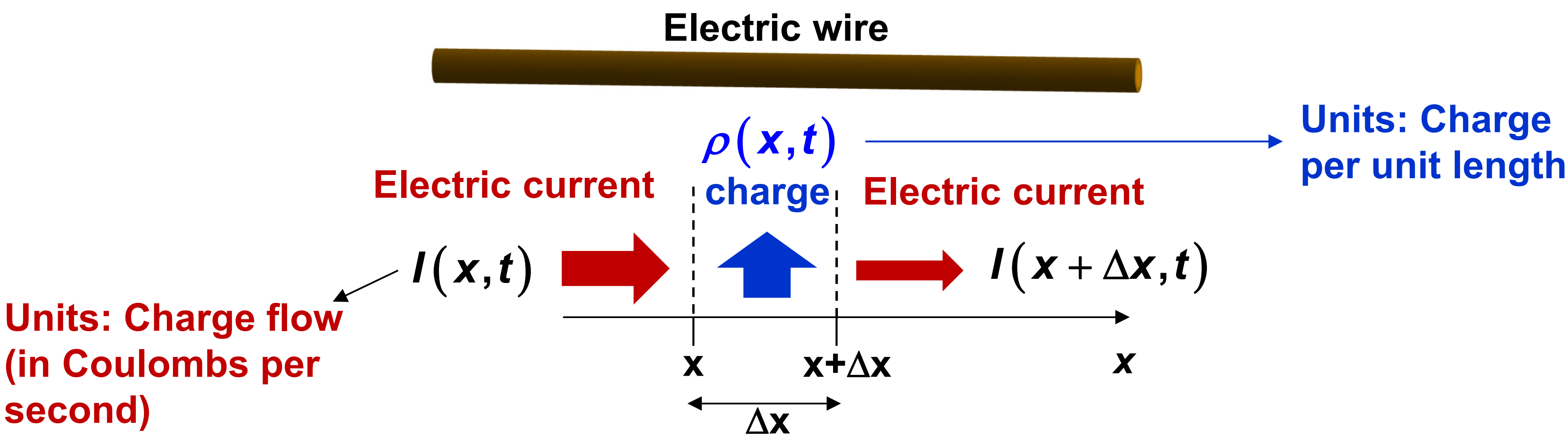
$$\left|\psi(\vec r,t)\right|^2 \approx \left|U_o\right|^2 \left| \frac{e^{i\vec k.(\vec r-\vec r_1)}}{r} e^{-i\frac{E}{\hbar}t} + \frac{e^{i\vec k.(\vec r-\vec r_2)}}{r} e^{-i\frac{E}{\hbar}t} \right|^2$$

$$\left\{ \begin{array}{l} \vec r_1 - \vec r_2 = d e_z \\ \vec k = k\left[\sin\theta\cos\phi e_x + \sin\theta\sin\phi e_y + \cos\theta e_z\right] \\ \hbar\omega = E = \dfrac{\hbar^2 k^2}{2m} \\ k = \dfrac{2\pi}{\lambda} \end{array} \right.$$

$$= \frac{\left|U_o\right|^2}{r^2} \left| e^{i\vec k.(\vec r-\vec r_1)} + e^{i\vec k.(\vec r-\vec r_2)} \right|^2 = 2\frac{U_o^2}{r^2}\left[1+\cos\left(\vec k.(\vec r_1-\vec r_2)\right)\right]$$

$$= 2\frac{U_o^2}{r^2}\left[1+\cos(kd\cos\theta)\right] = 2\frac{U_o^2}{r^2}\left[1+\cos\left(\frac{2\pi}{\lambda}d\cos\theta\right)\right]$$

A Detour: Charge Conservation Law in an Electric Wire



Conservation of charge requires:

$$I(x,t) - I(x+\Delta x,t) = \frac{\partial}{\partial t}\left[\rho(x,t)\,\Delta x\right]$$

Divide both sides by Δx :

$$\frac{I(x,t) - I(x+\Delta x,t)}{\Delta x} = \frac{\partial}{\partial t}\left[\rho(x,t)\right]$$

Rearrange and take the limit Δx goes to zero:

$$\frac{d\rho(x,t)}{dt} = -\frac{\partial I(x,t)}{\partial x} \longrightarrow \text{Charge conservation law}$$

The Schrödinger Equation: The Probabilistic Interpretation

$$\psi(x,t=0) \Rightarrow i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \Rightarrow \psi(x,t)$$

Question: Does Schrödinger equation preserve the probability norm as time progresses?? It better ….!!!

Suppose at time t= 0:

$$\int_{-\infty}^{\infty} dx\,\left|\psi(x,t=0)\right|^2 = 1$$

Then is it true that at any time t > 0 (conservation of probability) we have:

$$\int_{-\infty}^{\infty} dx\,\left|\psi(x,t)\right|^2 = 1 \longrightarrow$$

This better not get violated !! Otherwise, the probability interpretation would go down the drain!

The Schrödinger Equation: The Probabilistic Interpretation

We must have:

$$\boxed{\frac{d}{dt}\int_{-\infty}^{\infty} dx\,\left|\psi(x,t)\right|^2 = 0}$$

$$\left\{ \text{Since } \int_{-\infty}^{\infty} dx\,\left|\psi(x,t)\right|^2 = 1 \right.$$

Start from:

$$\frac{\partial}{\partial t}\left|\psi(x,t)\right|^2 = \frac{\partial}{\partial t}\left[\psi^*(x,t)\psi(x,t)\right] = \psi^*(x,t)\frac{\partial\psi(x,t)}{\partial t} + \frac{\partial\psi^*(x,t)}{\partial t}\psi(x,t)$$

Use the Schrodinger equation and its complex conjugate:

$$\left\{\begin{aligned} i\hbar\frac{\partial\psi(x,t)}{\partial t} &= -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \\ -i\hbar\frac{\partial\psi^*(x,t)}{\partial t} &= -\frac{\hbar^2}{2m}\frac{\partial^2\psi^*(x,t)}{\partial x^2} + V(x)\psi^*(x,t) \end{aligned}\right.$$

To get:

$$\frac{\partial}{\partial t}\left|\psi(x,t)\right|^2 = \psi^*(x,t)\,i\frac{\hbar}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} - \psi(x,t)\,i\frac{\hbar}{2m}\frac{\partial^2\psi^*(x,t)}{\partial x^2}$$

The Schrödinger Equation: The Probability Current

$$\frac{\partial}{\partial t}\left|\psi(x,t)\right|^2 = \psi^*(x,t)\, i\frac{\hbar}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} - \psi(x,t)\, i\frac{\hbar}{2m}\frac{\partial^2\psi^*(x,t)}{\partial x^2}$$

$$= -\frac{\partial}{\partial x}\left[\psi^*(x,t)\frac{\hbar}{2im}\frac{\partial\psi(x,t)}{\partial x} - \psi(x,t)\frac{\hbar}{2im}\frac{\partial\psi^*(x,t)}{\partial x}\right]$$

$$= -\frac{\partial I(x,t)}{\partial x}$$

Where:

$$I(x,t) = \psi^*(x,t)\frac{\hbar}{2im}\frac{\partial\psi(x,t)}{\partial x} - \psi(x,t)\frac{\hbar}{2im}\frac{\partial\psi^*(x,t)}{\partial x}$$

We showed that:

$$\frac{\partial}{\partial t}\left|\psi(x,t)\right|^2 = -\frac{\partial I(x,t)}{\partial x}$$

This is a conservation law for probability

Where:

$$I(x,t) = \psi^*(x,t)\frac{\hbar}{2im}\frac{\partial\psi(x,t)}{\partial x} - \psi(x,t)\frac{\hbar}{2im}\frac{\partial\psi^*(x,t)}{\partial x}$$

This is the probability current

The Conservation of Probability

We showed that:

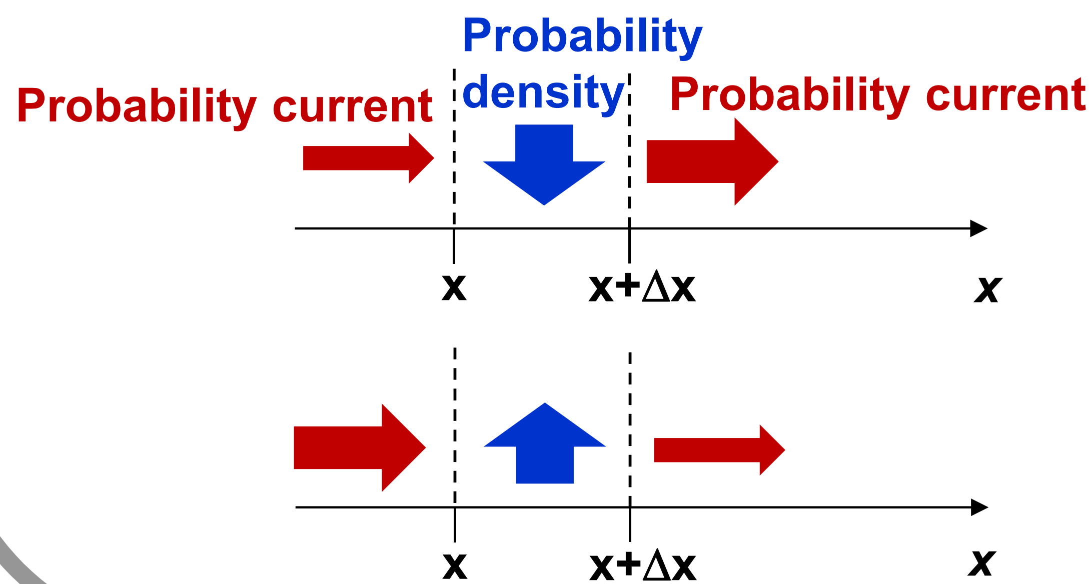
$$\frac{\partial}{\partial t}\left|\psi(x,t)\right|^2 = -\frac{\partial I(x,t)}{\partial x}$$

This is a conservation law for probability

Where:

$$I(x,t) = \psi^*(x,t)\frac{\hbar}{2im}\frac{\partial \psi(x,t)}{\partial x} - \psi(x,t)\frac{\hbar}{2im}\frac{\partial \psi^*(x,t)}{\partial x}$$

This is probability current



Units: probability flow

$$\frac{\partial}{\partial t}\left|\psi(x,t)\right|^2 = -\frac{\partial I(x,t)}{\partial x}$$

Units: probability per unit length

The Schrödinger Equation: The Conservation of Probability

We showed that:

$$\frac{\partial}{\partial t}\left|\psi(x,t)\right|^2 = -\frac{\partial I(x,t)}{\partial x}$$

Integrate both sides over all space:

$$\frac{\partial}{\partial t}\int_{-\infty}^{+\infty} dx \left|\psi(x,t)\right|^2 = -\int_{-\infty}^{+\infty} dx \frac{\partial I(x,t)}{\partial x}$$

$$= \cancelto{0}{I(-\infty,t)} - \cancelto{0}{I(+\infty,t)} = 0$$

Assuming the wavefunction goes to zero as $x \rightarrow \pm\infty$

Therefore:

$$\frac{\partial}{\partial t}\int_{-\infty}^{\infty} dx \left|\psi(x,t)\right|^2 = 0$$

The Schrödinger Equation: The Probabilistic Interpretation (3D)

$$\psi(\vec{r},t=0) \Rightarrow i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t) \Rightarrow \psi(\vec{r},t)$$

Question: Does Schrödinger equation preserve the probability norm as time progresses?? It better ….!!!

Suppose at time *t*= 0:

$$\int_{-\infty}^{\infty} d^3\vec{r}\,\left|\psi(\vec{r},t=0)\right|^2 = 1$$

Then is it true that at any time *t* > 0 (conservation of probability):

$$\int_{-\infty}^{\infty} d^3\vec{r}\,\left|\psi(\vec{r},t)\right|^2 = 1$$

This better not get violated !! Otherwise, the probability interpretation would go down the drain!

The Schrödinger Equation: The Probabilistic Interpretation (3D)

We must have:

$$\frac{\partial}{\partial t}\int d^3\vec{r}\,\left|\psi\left(\vec{r},t\right)\right|^2 = 0$$

Since $\int d^3\vec{r}\,\left|\psi\left(\vec{r},t\right)\right|^2 = 1$

Check:

$$\frac{\partial}{\partial t}\left|\psi\left(\vec{r},t\right)\right|^2 = \psi^*\left(\vec{r},t\right)\frac{\partial\psi\left(\vec{r},t\right)}{\partial t} + \frac{\partial\psi^*\left(\vec{r},t\right)}{\partial t}\psi\left(\vec{r},t\right)$$

Use:

$$\left\{\begin{aligned} i\hbar\frac{\partial\psi\left(\vec{r},t\right)}{\partial t} &= -\frac{\hbar^2}{2m}\nabla^2\psi\left(\vec{r},t\right) + V\left(\vec{r}\right)\psi\left(\vec{r},t\right) \\ -i\hbar\frac{\partial\psi^*\left(\vec{r},t\right)}{\partial t} &= -\frac{\hbar^2}{2m}\nabla^2\psi^*\left(\vec{r},t\right) + V\left(\vec{r}\right)\psi^*\left(\vec{r},t\right) \end{aligned}\right.$$

To get:

$$\frac{\partial}{\partial t}\left|\psi\left(\vec{r},t\right)\right|^2 = \psi^*\left(\vec{r},t\right) i\frac{\hbar}{2m}\nabla^2\psi\left(\vec{r},t\right) - \psi\left(\vec{r},t\right) i\frac{\hbar}{2m}\nabla^2\psi^*\left(\vec{r},t\right)$$

The Schrödinger Equation: The Probabilistic Interpretation (3D)

$$\frac{\partial}{\partial t}\left|\psi(\vec{r},t)\right|^2 = \psi^*(\vec{r},t)\, i\frac{\hbar}{2m}\nabla^2\psi(\vec{r},t) - \psi(\vec{r},t)\, i\frac{\hbar}{2m}\nabla^2\psi^*(\vec{r},t)$$

$$= -\nabla.\left[\psi^*(\vec{r},t)\frac{\hbar}{2im}\nabla\psi(\vec{r},t) - \psi(\vec{r},t)\frac{\hbar}{2im}\nabla\psi^*(\vec{r},t)\right]$$

$$= -\nabla.\vec{J}(\vec{r},t)$$

Where the probability current density is:

$$\vec{J}(\vec{r},t) = \psi^*(\vec{r},t)\frac{\hbar}{2im}\nabla\psi(\vec{r},t) - \psi(\vec{r},t)\frac{\hbar}{2im}\nabla\psi^*(\vec{r},t)$$

The conservation law for probability in 3D is expressed as:

$$\frac{\partial}{\partial t}\left|\psi(\vec{r},t)\right|^2 = -\nabla.\vec{J}(\vec{r},t)$$

Units: probability density per unit volume

Units: probability flow per unit time per unit area

The Schrödinger Equation: The Probabilistic Interpretation (3D)

The conservation law for probability in 3D is:

or

$$\frac{\partial}{\partial t}\left|\psi\left(\vec{r},t\right)\right|^2 = -\nabla .\, \vec{J}\left(\vec{r},t\right)$$

Stokes' theorem:

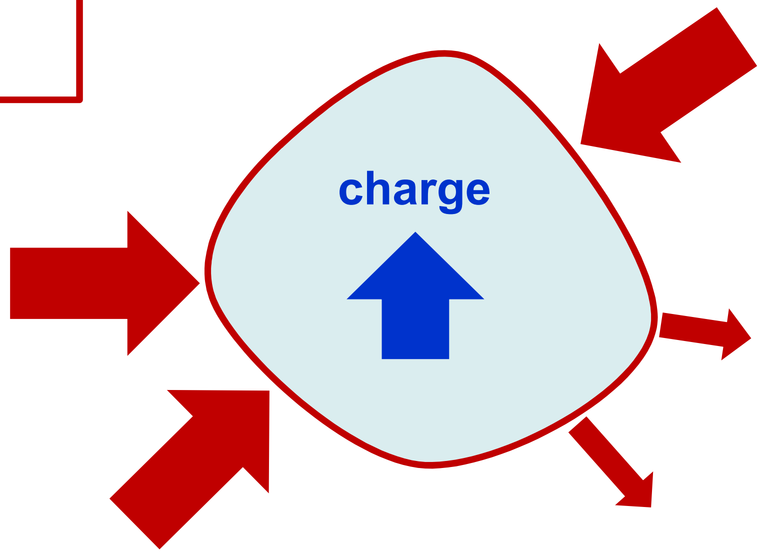
$$\iiint dV\, \nabla .\vec{A}\left(\vec{r},t\right) = \oiint d\vec{S}\, .\, \vec{A}\left(\vec{r},t\right)$$

Over a volume

Over a surface surrounding the volume

Using Stokes' theorem for any closed surface:

$$\frac{\partial}{\partial t}\iiint dV\, \left|\psi\left(\vec{r},t\right)\right|^2 = -\oiint d\vec{S} .\, \vec{J}\left(\vec{r},t\right)$$



If the surface is infinitely large:

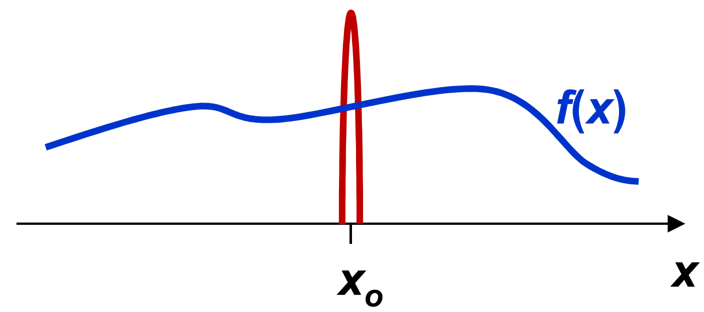
$$\frac{\partial}{\partial t}\int d^3\vec{r}\, \left|\psi\left(\vec{r},t\right)\right|^2 = -\int d\vec{S}\, .\, \vec{J}\left(\vec{r},t\right) = 0$$

Assuming the wavefunction goes to zero over the surface when the surface is at infinity

Some Math: Delta Functions in 1D and 3D

A delta function in 1D has the following property:

$$\int_{-\infty}^{\infty} dx\, f(x)\, \delta(x - x_o) = f(x_o)$$



Integration of plane waves over all space (in 1D):

$$\int_{-\infty}^{\infty} dx\, e^{i(k-k')x} = 2\pi\, \delta(k - k')$$

A delta function in 3D has the following property:

$$\int d^3\vec{r}\, f(\vec{r})\, \delta^3(\vec{r} - \vec{r}_o) = f(\vec{r}_o)$$

$$\left\{ \begin{array}{l} \int d^3\vec{r} \leftrightarrow \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \\ \delta^3(\vec{r} - \vec{r}_o) = \\ \quad \delta(x - x_o)\,\delta(y - y_o)\,\delta(z - z_o) \end{array} \right.$$

Integration of a plane waves over all space (in 3D):

$$\int d^3\vec{r}\, e^{i(\vec{k}-\vec{k}').\vec{r}} = (2\pi)^3\, \delta^3(\vec{k} - \vec{k}')$$