Some Basic Notions of Quantum Mechanics

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Some Classical Mechanics

Isaac Newton

• Lagrangian formulation: particle wants to minimize the total of the *Lagrangian* $\mathfrak{I} = T - V = \mathfrak{I}(x, \dot{x}, t)$, where:

$$T = \text{kinetic energy}$$

$$V = \text{potential energy}$$

$$x = \text{location}$$

$$\dot{x} = \text{velocity}\,(dx/dt)$$

$$t = \text{time}$$

• Given initial and final location/time $(x_i, t_i), (x_f, t_f)$, the path $x(t)$ classically taken minimizes (extremizes) the *action*

$$S[x(t)] = \int_{t_i}^{t_f} \mathfrak{I}(x, \dot{x}) dt \quad (\text{here } V \text{ is time independent})$$

• Why? ????

• Via calculus of variations, this leads to the following equation, which holds in the classical path for every t:

$$\frac{\partial \mathfrak{I}}{\partial x_i(t)} = \frac{d}{dt}\left[\frac{\partial \mathfrak{I}}{\partial \dot{x}_i(t)}\right]$$

• Often, the following notations are used:

$$x_i \equiv q_i \qquad F_i \equiv \frac{\partial \mathfrak{I}}{\partial q_i} \quad \text{(force)} \qquad p_i \equiv \frac{\partial \mathfrak{I}}{\partial \dot{q}_i} \quad \text{(momentum)}$$

• And so

$$F_i = \frac{dp_i}{dt} \left(ma = m\frac{dv}{dt} = \frac{d(mv)}{dt} = \frac{dp}{dt}\right)$$

↑

Force

• In the continuous case, often $\mathfrak{I} = \mathfrak{I}(f,\dot{f},f',t)$ and one minimizes $\iint \mathfrak{I}(f,\dot{f},f',t)dxdt \Rightarrow$

$$\frac{\partial \mathfrak{I}}{\partial f} - \frac{d}{dt}\frac{\partial \mathfrak{I}}{\partial \dot{f}} - \frac{d}{dx}\frac{\partial \mathfrak{I}}{\partial f'} = 0.$$

f' **Stands for the coupling of "infinitely close particles" (e.g. points of a string).**

The Hamiltonian

- We have $\quad p = \dfrac{\partial \Im}{\partial \dot{q}}$

- Suppose we want to find an expression, call it **H**, such that

$$\dfrac{\partial H}{\partial p} = \dot{q}. \qquad \text{So :}$$

$$H = \int 1 \cdot \dot{q}\, dp = p\dot{q} - \int p \dfrac{d\dot{q}}{dp}\, dp =$$

$$p\dot{q} - \int \dfrac{\partial \Im}{\partial \dot{q}} \dfrac{d\dot{q}}{dp}\, dp = p\dot{q} - \Im$$

- What is **H** in physical terms? Look at a particle moving under a simple potential:

$$H = p\dot{q} - \Im = (mv)\dot{x} - \left(\dfrac{mv^2}{2} - mgx \right) = \dfrac{mv^2}{2} + mgx$$

- So **H** is the **TOTAL ENERGY** (kinetic + potential).

- What are the Hamiltonian equations? As we saw

$$\frac{\partial H}{\partial p} = \dot{q}$$

- And also

$$\frac{\partial H}{\partial q} = \frac{\partial (p\dot{q} - \mathfrak{I})}{\partial q} = -\frac{\partial \mathfrak{I}}{\partial q} = -\dot{p}$$

- So

$$\frac{\partial H}{\partial p} = \dot{q} \qquad \frac{\partial H}{\partial q} = -\dot{p}$$

Example: Free Fall
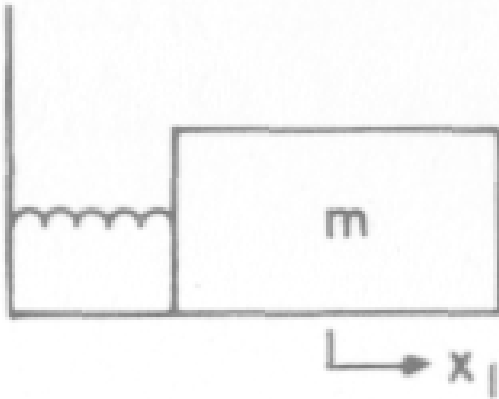
$$H = \frac{mv^2}{2} + mgx = \frac{p^2}{2m} + mgx$$

• Note that we have to write the energy as a function of the momentum and the coordinates, as opposed to the coordinate and its time derivatives (the latter is appropriate for the Lagrangian formulation).

• The equations are (remember: $q = x, \dot{q} = v$)

$$\frac{\partial H}{\partial p} = \dot{q} \Rightarrow \frac{p}{m} = v \quad \text{(nothing new)}$$

$$\frac{\partial H}{\partial q} = -\dot{p} \Rightarrow mg = -(m\dot{v}) = -ma \Rightarrow a = -g$$

Which is indeed the free fall equation.

Example: Harmonic Oscillator

• The point at which the spring is at zero potential energy will be taken to be $x = 0$. The Hamiltonian is then
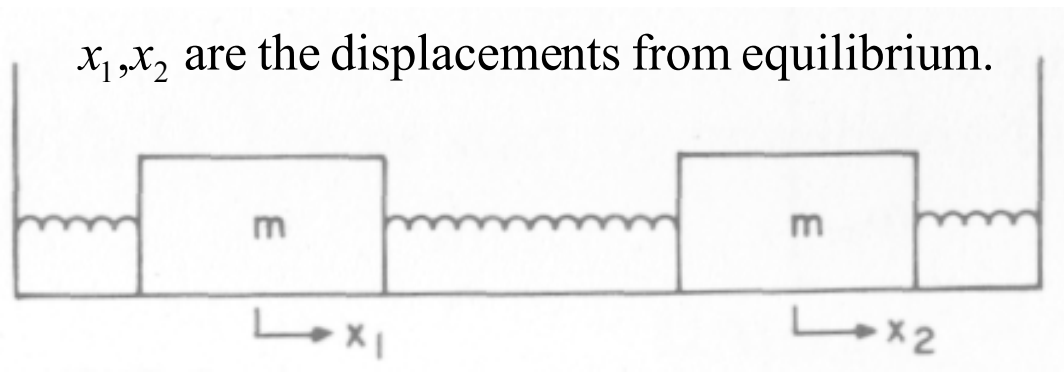
$$H = \frac{p^2}{2m} + \frac{kx^2}{2}, \quad \frac{\partial H}{\partial q} = -\dot{p} \Rightarrow$$

$$kx = -m\dot{v} = -m\ddot{x} \Rightarrow \ddot{x} = -\frac{k}{m}x \Rightarrow$$

$$x = A\cos\left(\sqrt{\frac{k}{m}}\,t\right) + B\sin\left(\sqrt{\frac{k}{m}}\,t\right)$$

• *A,B* are determined by the initial conditions.

Example: Coupled Harmonic Oscillator

x_1, x_2 are the displacements from equilibrium.

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{k}{2}\left[x_1^2 + x_2^2 + (x_1 - x_2)^2\right] \Rightarrow$$

$$\ddot{x}_1 = \frac{-2k}{m}x_1 + \frac{k}{m}x_2 \;,\; \ddot{x}_2 = \frac{k}{m}x_1 - \frac{2k}{m}x_2$$

- Let us discuss differential equations of the form

$$\Omega x = \ddot{x}$$

Where:

- x is a vector of functions.

- Ω is Hermitian with negative eigenvalues $-\lambda_1^2, -\lambda_2^2$ and eigenvectors e_1, e_2

$$\text{Denote } E \equiv \begin{pmatrix} e_1 \\ e_2 \end{pmatrix} \quad (E \text{ is a } 2 \times 2 \text{ matrix})$$

$$\Omega x = \ddot{x} \implies E\Omega E^t y = \ddot{y}$$

$$E\Omega E^t = D, \, x = E^t y, \, y = Ex$$

$$D = \begin{pmatrix} -\lambda_1^2 & 0 \\ 0 & -\lambda_2^2 \end{pmatrix}, \, E \text{ is unitary}$$

- After diagonalizing, the system is easy to solve. If we assume that the initial velocity is zero,

$$y = \cos(\lambda_1 t), \cos(\lambda_2 t)$$

- Initial conditions:

$$x_1(0) = a, \, x_2(0) = b, \, \dot{x}_1(0) = 0, \, \dot{x}_2(0) = 0$$

- For y, the initial conditions are then $E\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a' \\ b' \end{pmatrix}$
  so the solution is

$$y = \begin{pmatrix} \cos(\lambda_1 t) & 0 \\ 0 & \cos(\lambda_2 t) \end{pmatrix} \begin{pmatrix} a' \\ b' \end{pmatrix} \equiv C\begin{pmatrix} a' \\ b' \end{pmatrix}$$

- To return to x,

$$x = E^t C E \begin{pmatrix} a \\ b \end{pmatrix} = E^t \left[\begin{pmatrix} c_{11}(t) & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & c_{22}(t) \end{pmatrix} \right] E \begin{pmatrix} a \\ b \end{pmatrix} =$$

$$\left[c_{11}(t) e_1 e_1^t + c_{22}(t) e_2 e_2^t \right] \begin{pmatrix} a \\ b \end{pmatrix} \Rightarrow$$

$$\left| x(t) \right\rangle = U(t) \left| x(0) \right\rangle, \, U(t) = c_{11}(t) \left| I \right\rangle\!\left\langle I \right| + c_{22}(t) \left| II \right\rangle\!\left\langle II \right|$$

Where we have taken the opportunity to introduce a common QM notation, Dirac's famous *bra* and *ket:*

- $\left| ? \right\rangle, \left\langle ? \right|$ stand for column and row vectors.

- $\left| I \right\rangle, \left| II \right\rangle$ stand for Ω's eigenvectors.

- $c_{11}(t), c_{22}(t)$ are solutions to the differential equations *with one variable,* $\ddot{f} = \omega_1 f, \ddot{f} = \omega_2 f$ where ω_1, ω_2 are Ω's eigenvalues.

- $U(t)$ is called the ***propagator*** and is of fundamental importance in QM.

Example: Vibrating String

• Once we realize that the propagator formulation carries over to the infinite dimensional case, we can write down in a straightforward manner the solution to more general problems, such as the vibrating string:
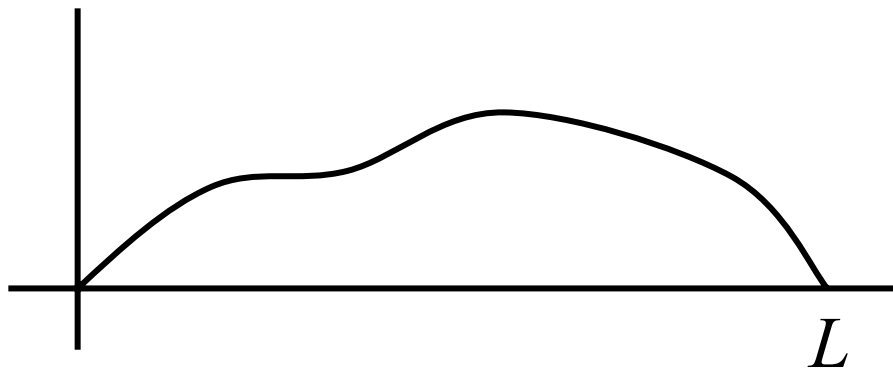
• First, we have to write down the corresponding differential equation. Think of the string as being composed of many small springs, that is, the limiting case of many masses coupled by springs:
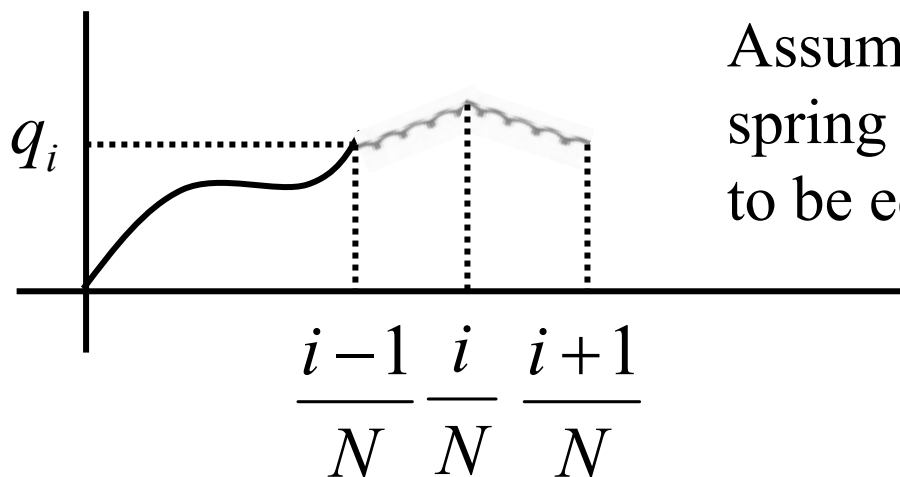
Assume the spring constant k to be equal to 1.

- The Lagrangian is the limit of $\left(\text{denote } \dfrac{L}{N} \equiv h\right)$

$$...+\frac{1}{2}m\dot{q}_i^2+...-\frac{1}{2}\left[...+h^2+(q_i-q_{i-1})^2+h^2+(q_{i+1}-q_i)^2+...\right]$$

hence the equations are $\dfrac{q_{i-1}-2q_i+q_{i+1}}{m}=\ddot{q}_i$

but in the limit, $q_{i-1}-2q_i+q_{i+1}$ is just the well-known approximation to the second derivative, so – ignoring constants – the spring equation is

$$\frac{\partial^2 f(x,t)}{\partial x^2}=\frac{\partial^2 f(x,t)}{\partial t^2}$$

- To solve $\dfrac{\partial^2 f(x,t)}{\partial x^2} = \dfrac{\partial^2 f(x,t)}{\partial t^2}$, proceed as before:

- First, find the (normalize) eigenvectors/eigenvalues

  of the operator $\dfrac{\partial^2 f}{\partial x^2}$. Since they're restricted to be

  zero at 0 and L, they are

$$I_m = \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin\left(\frac{m\pi}{L}x\right),\ \text{eigenvalue} = -\frac{m^2\pi^2}{L^2}$$

- What are the equivalents of $c_{11}(t), c_{22}(t)$?

  As before, if we restrict the initial velocity to be 0,

  the solutions are $\cos\left(\dfrac{m\pi}{L}t\right)$, and $-$ also as

  before $-$ the general solution can be written with

  a propagator:

$$U(t) = \sum_{m=1}^{\infty} \cos\left(\frac{m\pi}{L}t\right) I_m I_m^t,\ f(x,t) = U(t)f(x,0) \Rightarrow$$

$$|\psi(x,t)\rangle = \left[\sum_{m=1}^{\infty} \cos\left(\frac{m\pi}{L}t\right) |I_m\rangle\langle I_m|\right]|\psi(x,0)\rangle =$$

$$\sum_{m=1}^{\infty} \cos\left(\frac{m\pi}{L}t\right)\langle I_m|\psi(x,0)\rangle|I_m\rangle$$

But in the limit the internal product is just an integral, so

$$f(x,t) = \sum_{m=1}^{\infty} \cos\left(\frac{m\pi}{L}t\right)\left(\int_0^L f(x,0)I_m\, dx\right)I_m$$

Why all this?....

• Later, we will see that in QM, every single particle has a function – the *probability amplitude* – associated with it, and the main goal is to determine how it changes over time. It turns out that this function satisfies a first order (in time) differential equation (as opposed to our examples which had a second time derivative), called *Schrödinger's equation,* and one seeks the propagator which – given the probability amplitude at $t = 0$ – computes it for every t:

$$\left|\psi(x,t)\right\rangle = U(t)\left|\psi(x,0)\right\rangle$$

Poisson Brackets and Canonical Transformations

Let $\omega(p,q)$ be some function of the state variables p,q, where we assume no explicit dependence on t. Then its change over time is given by

$$\frac{d\omega}{dt} = \sum_i \left(\frac{\partial \omega}{\partial q_i} \dot{q}_i + \frac{\partial \omega}{\partial p_i} \dot{p}_i \right) =$$

$$\sum_i \left(\frac{\partial \omega}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial \omega}{\partial p_i} \frac{\partial H}{\partial q_i} \right) \equiv \{\omega, H\}$$

• For any two $\omega(p,q), \lambda(p,q)$ define the *Poisson bracket* by

$$\{\omega, \lambda\} = \sum_i \left(\frac{\partial \omega}{\partial q_i} \frac{\partial \lambda}{\partial p_i} - \frac{\partial \omega}{\partial p_i} \frac{\partial \lambda}{\partial q_i} \right)$$

• Note that

$$\{q_i, q_j\} = 0 \quad \{p_i, p_j\} = 0 \quad \{q_i, p_j\} = \delta_{ij}$$

- We may want to define new variables

$$q \rightarrow \overline{q}(p,q), \, p \rightarrow \overline{p}(p,q)$$

A straightforward calculation yields that if we want Hamilton's equations to hold in the new coordinates, we must have

$$\{\overline{q}_i, \overline{q}_j\} = 0 \quad \{\overline{p}_i, \overline{p}_j\} = 0 \quad \{\overline{q}_i, \overline{p}_j\} = \delta_{ij}$$

Such a transformation is called *canonical.*

Note the similarity: in classical mechanics

$$\frac{d\omega}{dt} = \{\omega, H\}$$

And in quantum mechanics

$$\frac{d\langle \Omega \rangle}{dt} = \frac{-i}{\hbar} \langle [\Omega, H] \rangle$$

Examples:

• Rotation is a canonical transformation (check it).

• Important: the two body problem. Assume we have two bodies in space, with locations and masses given by $(m_1, r_1), (m_2, r_2)$. Assume also that there's a potential which depends only on their relative distance, $V(r_1 - r_2)$. We can then define a canonical transformation that reduces the analysis to that of two *independent* bodies:

$$r_{CM} = \frac{m_1 r_1 + m_2 r_2}{m_1 + m_2}, \, m_{CM} = m_1 + m_2, V_{CM} = 0 \text{ (the center of mass)}$$

$$r = r_1 - r_2, m = \frac{m_1 m_2}{m_1 + m_2} \equiv \mu, V = V(r) \text{ (the reduced mass)}$$

• Thus the center of mass is a free particle, and the reduced mass moves under the potential V. One can then solve for them separately. One such system, for example, is the hydrogen atom.

• We will later show how one can guess such a transformation; it follows from the requirement that the Hamiltonian be diagonal in the new coordinates.

The Electromagnetic Lagrangian

• The force acting on a charge q, moving at speed $\mathbf{v}$, due to an electric field $\mathbf{E}$ and a magnetic field $\mathbf{B}$, is

$$F=q\left(E+\frac{v}{c}\times B\right),\text{ with the potentials A,}\phi$$

satisfying $\nabla\times A=B$, $E=-\nabla\phi-\frac{1}{c}\frac{\partial A}{\partial t}$.

Next, define a Lagrangian $\Im=\frac{1}{2}m\mathbf{v}\cdot\mathbf{v}-q\phi+\frac{q}{c}\mathbf{v}\cdot A$

We have to check that $\dfrac{d}{dt}\left(\dfrac{\partial\Im}{\partial v_i}\right)=\dfrac{\partial\Im}{\partial x_i}$, it yields

$$\frac{d}{dt}\left(\underbrace{m\mathbf{v}+\frac{qA}{c}}_{\substack{\text{"canonical}\\\text{momentum"}}}\right)=-q(\nabla\phi)+\frac{q}{c}\nabla(\mathbf{v}\cdot A)\Rightarrow\frac{d}{dt}(m\mathbf{v})=$$

$$-q(\nabla\phi)+\frac{q}{c}\left[-\underbrace{\frac{dA}{dt}}_{\frac{\partial A}{\partial t}+(\mathbf{v}\cdot\nabla)A}+\nabla(\mathbf{v}\cdot A)\right]=q(-\nabla\phi)+q\left(-\frac{1}{c}\frac{\partial A}{dt}\right)+$$

$$\frac{q}{c}\left[\underbrace{\nabla(\mathbf{v}\cdot A)-(\mathbf{v}\cdot\nabla)A}_{\mathbf{v}\times(\nabla\times A)=\mathbf{v}\times B}\right]=q\left(E+\frac{v}{c}\times B\right).\text{ Note however that}$$

$q\phi-\dfrac{q}{c}\mathbf{v}\cdot A$ is not really a potential.

The Electromagnetic Hamiltonian

As before, $H = p \cdot v - \mathfrak{I} = \frac{1}{2} m v \cdot v + q\phi = T + q\phi$

But in order to write it correctly, it has to be

expressed in terms of $p = mv + \frac{q}{c} A$, so

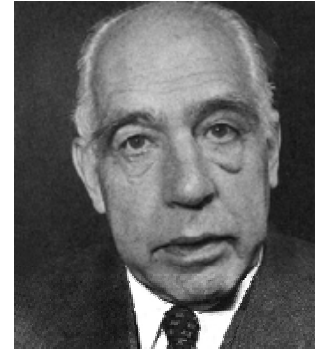$$H = \frac{\left\| p - \frac{q}{c} A \right\|^2}{2m} + q\phi.$$

QM was developed in order to explain physical phenomena which were not consistent with classical physics.

Max Planck
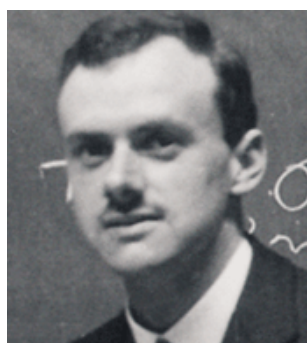
Albert Einstein

Niels Bohr
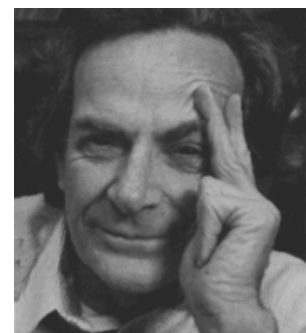
Werner Heisenberg

Erwin Schrödinger
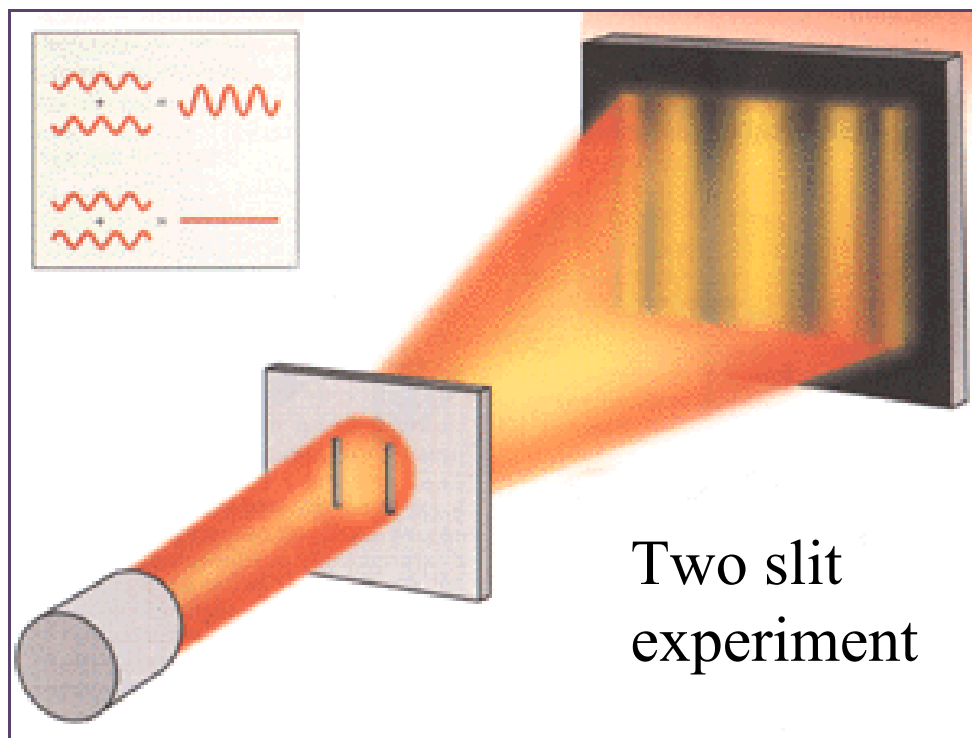
Max Born

Louis de Broglie

Paul Dirac

Richard Feynman

Part I: Physical Intuition and the Finite-Dimensional Case

Prelude: The Nature of Light

Light was thought to be made of particles, which move in a straight line. Later, light *interference* was discovered (Young, 1801), which led to the conclusion that light is a wave:


Two slit experiment

The mathematics behind this: a wave can be described by the equation $e^{i(kx-\omega t)}$. Such a wave moves through space at a speed of ω/k. ω is the **frequency**, k the **wave number**. If another wave is Δ behind, their sum is

$$\left| e^{i(kx-\omega t)} + e^{i(k(x+\Delta)-\omega t)} \right| = \left| e^{i(kx-\omega t)}(1 + e^{ik\Delta}) \right| = \left| 1 + e^{ik\Delta} \right|$$

which peaks/is zero when $k\Delta = 2n\pi \,/\, k\Delta = (2n+1)\pi$. Denoting $\lambda = 2\pi/k$ (the **wavelength**), there is a maximum if $\Delta = n\lambda$, which is hardly surprising – it means that if the lag between the two waves is a multiple of the wavelength, they contribute to each other (they are **in phase**).

(a) ... (b)
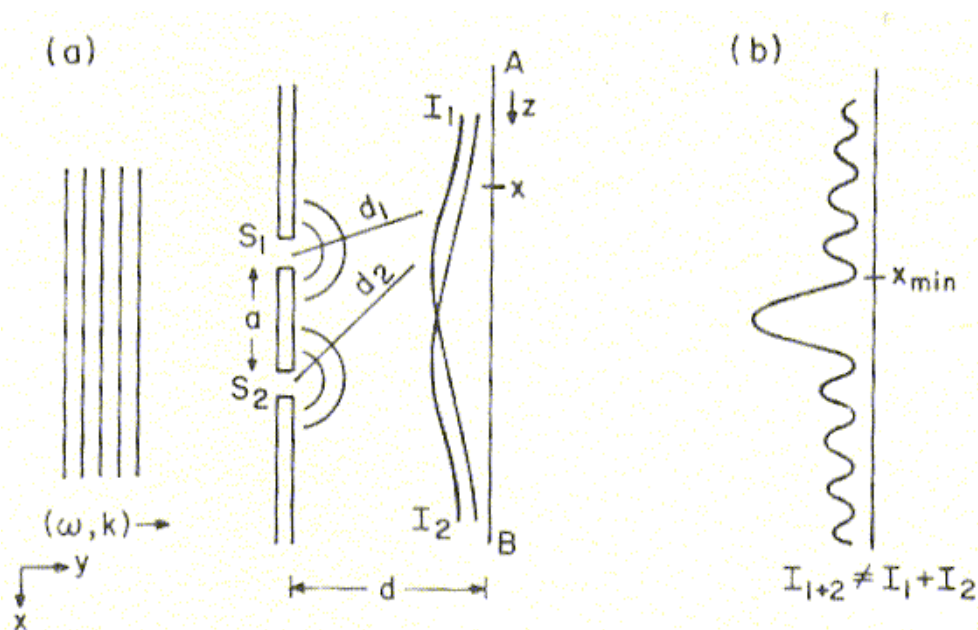
Wave interference: as opposed to the drawing, assume $d \gg a, x$. Then the lag between the two waves is $\sqrt{d^2 + x^2} - \sqrt{d^2 + (x-a)^2} \approx \dfrac{ax}{d} = \Delta.$

so, the maxima correspond to $ax/d = n\lambda$, which implies that the distance between adjacent maxima is $\lambda d/a$ (this can actually be used to measure the light's wavelength).

• Mathematically, if the (complex) wave functions are h_1, h_2, then the energy arriving when slit i is open is $|h_i|^2$, and the energy arriving when both are
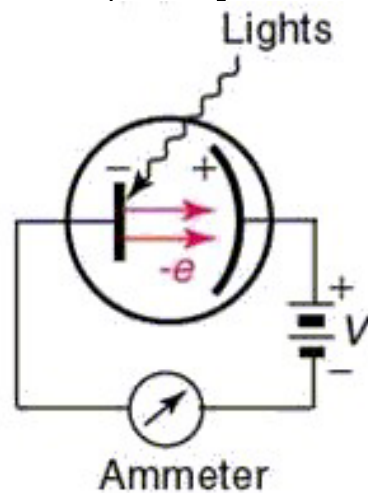
open is **NOT** $|h_1|^2 + |h_2|^2$, but

$$|h_1 + h_2|^2 = |h_1|^2 + |h_2|^2 + \underbrace{2|h_1||h_2|\cos(\delta)}_{\text{interference term}}$$
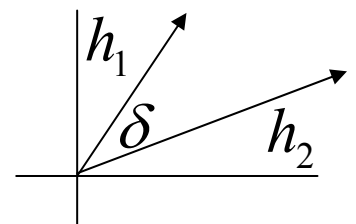
So far so good – but it turns out that the wave model fails to explain certain phenomena.

When you shine light upon certain metals, electrons are emitted (the **photoelectric effect**).

Lights

It turns out that

Ammeter

• The emitted electrons move with greater speed if the light has a higher frequency.

• No electron is emitted until the light passes a threshold frequency – no matter how strong the light is.

• The electrons are emitted too quickly.

All this contradicts the hypothesis about the wavelike nature of light.

• Einstein solved this problem (and was awarded the Nobel prize for that), by suggesting that light is composed of little "quanta", which impact like "baseballs", and not like waves. These were later termed **photons**, and it turned out that a photon with frequency ω has an energy and momentum given by

$\hbar$ is a very small constant.

$$E = \hbar\omega$$
$$p = \hbar k$$

note: $E = pc$.

It also turns out that not only don't the lightwaves behave like waves – also, particles don't behave like particles.

Let's go back to the two slit experiment. How will it look with particles (electrons)? We may assume it will look like
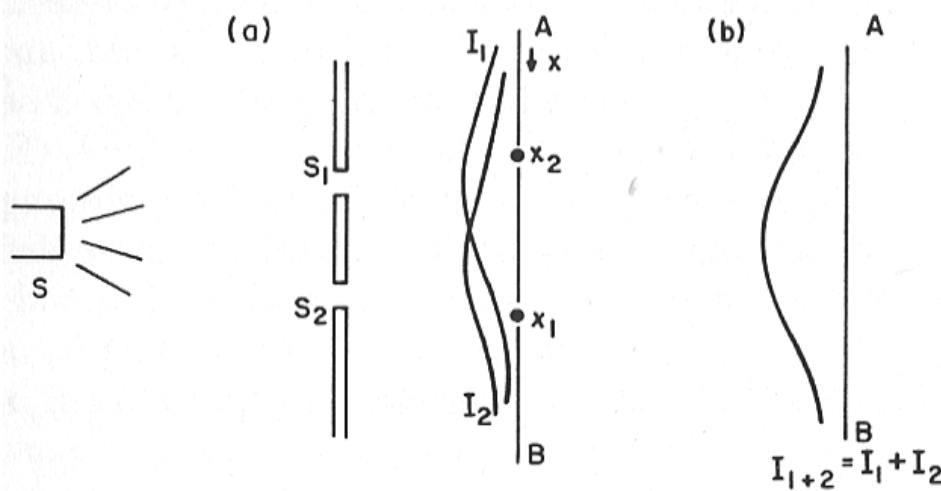
i.e., the number of electrons hitting any specific point on the wall when both slits are open, will be the sum of the numbers when only the first/second slit is open.

But that doesn't happen; the electrons also interfere. That is, at some points, LESS electrons hit when BOTH slits are open!! This happens even if the electrons are fired very slowly (one at a time).

There is no way to explain this – it just happens.

• Note: we can immediately realize that each electron cannot go through one slit. However, they don't "break", because when they arrive at the wall, the energy corresponds to a "whole" electron.

• Fortunately, the simple model that describes wave interference ($|h_1 + h_2|^2$) also explains particle interference. The problem is, of course, to compute the so-called "probability amplitudes" h_1, h_2.

There are h_1, h_2 such that $P_i = |h_i|^2$ and $P_{12} = |h_1 + h_2|^2$.
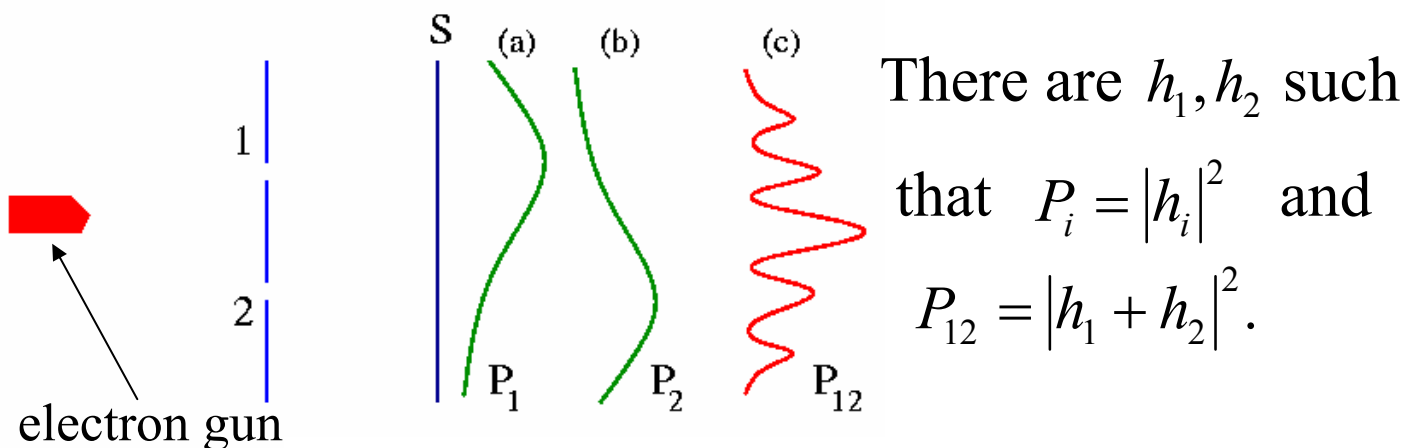
What happens if we try to watch the electrons? If we see them all, there's no interference!

To be explained later. Intuitively, the measurement *forces* the particle to assume a definite position.
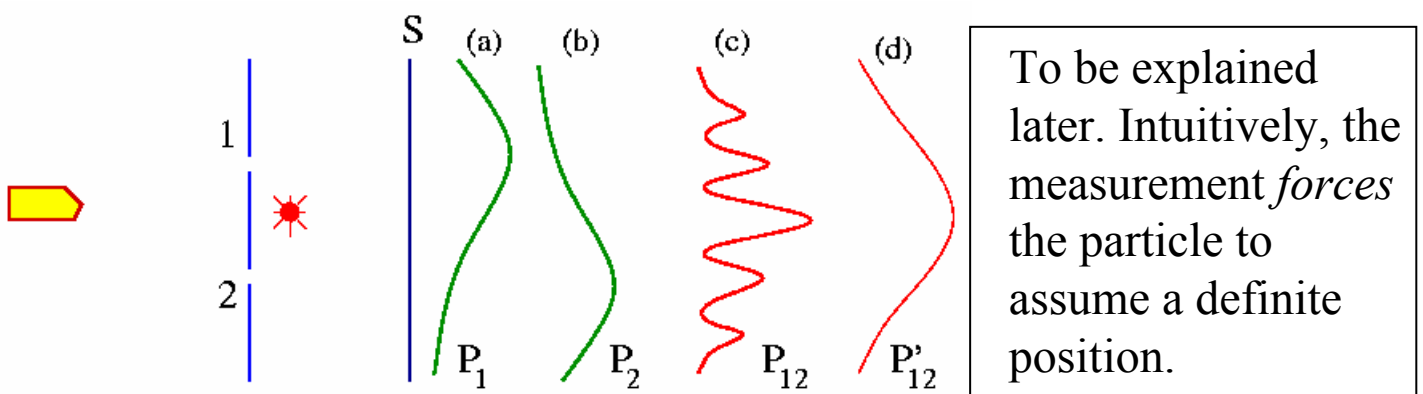
Some QM axioms:

• Probability is the squared absolute value of the amplitude.

• If there are several possibilities for an event to happen, the amplitudes for these possibilities are summed. So, to get the total probability, you first sum and then take absolute value squared – thus there is interference.

• When it is possible to decide what alternative was taken, you sum the probabilities (as usual – no interference).

• There is uncertainty; we cannot predict what will happen, even if we know everything in advance. This uncertainty is reflected, for example, in the inability to exactly describe both a particle's position and momentum – the famous Heisenberg uncertainty principle. All we can do is provide probability distributions. But, as opposed to our standard understanding of what uncertainty is, here it's much deeper; it's not "I know the particle is somewhere, I just don't know where" – the particle isn't anywhere, so to say. And if we try to nail it down, we lose its momentum. There's no way out of this.

It's strange – but it works.

To quote Feynman…

"That's how it is. If you don't like it, go to a different universe, where the laws are simpler" – R.P Feynman, NZ, 1979.

The Heisenberg Uncertainty Principle

• Take the limiting case of a wave with amplitude $e^{i(kx-\omega t)}$. It has exact momentum ($\hbar k$) and energy ($\hbar \omega$) but there's no information on its location, because for every x the probability is 1.

• Real particles have amplitudes that are not uniform in space. They may look like a Gaussian, meaning that there's a far higher probability to find the particle near the Gaussian's center. But in order to get a Gaussian, you have to add many "pure waves". Each "pure wave" has definite momentum – but when you mix them, the uncertainty in the momentum increases. The narrower the "position Gaussian", the broader the "momentum Gaussian" (more later).

Momentum certain, but zero knowledge on position

Position certain, but zero knowledge on momentum

Momentum uncertainty

Position uncertainty
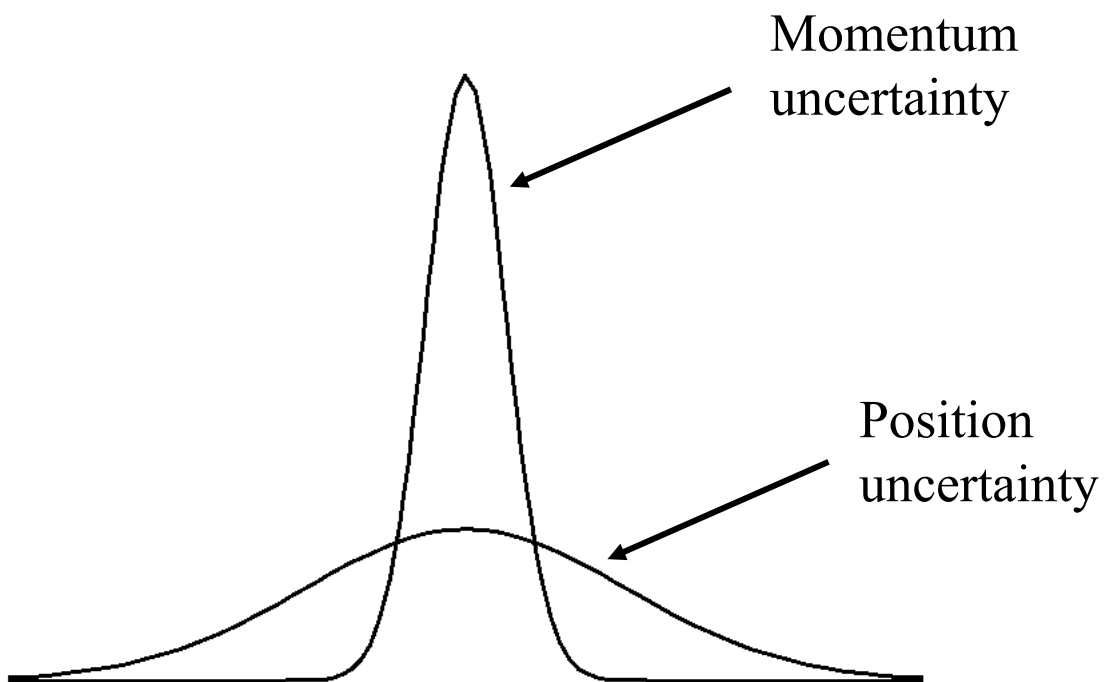
Trying to measure both location and momentum
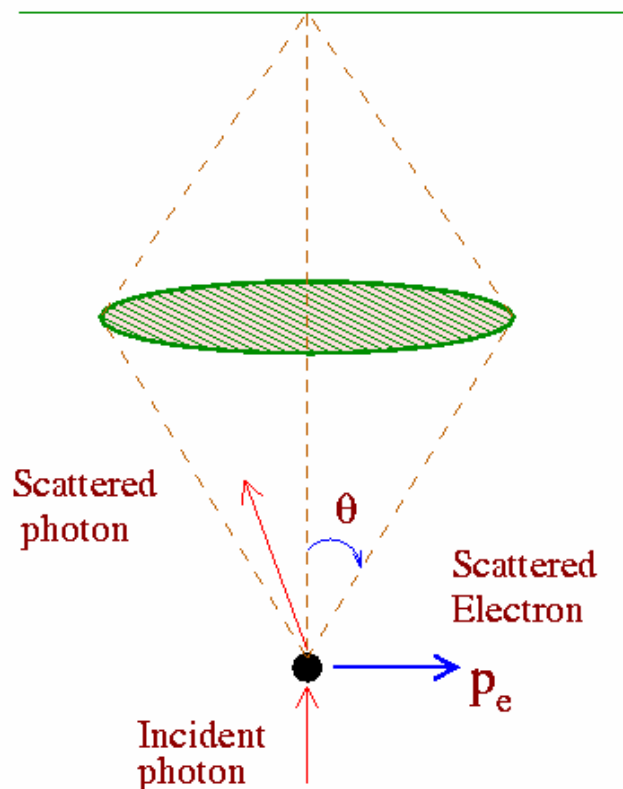
The smallest distance between two points in an object that will produce separated images is $\Delta_x \approx \lambda/\sin(\theta)$. If a photon has energy $\hbar\omega$, it possesses momentum $\hbar/\lambda$. To be collected by the lens, the photon must be scattered through any angle between $-\theta$ to θ. So, the x-component of the momentum may have any value between $-\hbar\sin(\theta)/\lambda$ to $\hbar\sin(\theta)/\lambda$. Thus the uncertainty in the electron's momentum is $\approx \hbar\sin(\theta)/\lambda$. So, the product of the uncertainties is $\approx \hbar$.

Intuitively, we need a "powerful" photon (high frequency) to get good position measurements; but the higher the energy, the more it knocks off the electron, hence the momentum uncertainty becomes larger.

Interlude – the Resolution of a Microscope

Airy Patterns and the Limit of Resolution

Figure 1
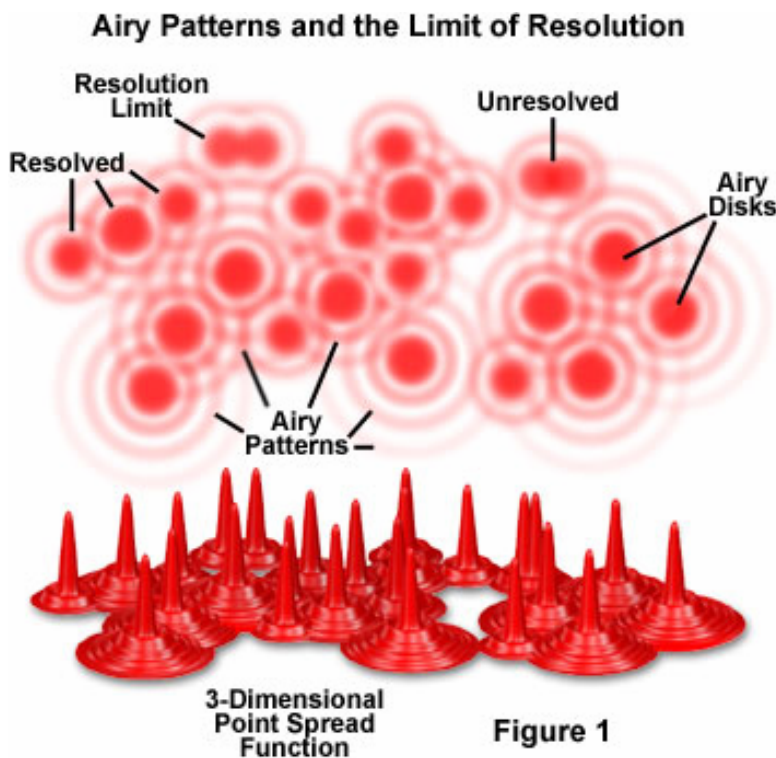
The resolution of an optical microscope is defined as the shortest distance a between two points on a specimen that can still be distinguished by the observer or camera system as separate entities. When λ becomes close to a, it's impossible to distinguish. That's why electron microscopes are used (much smaller wavelength).
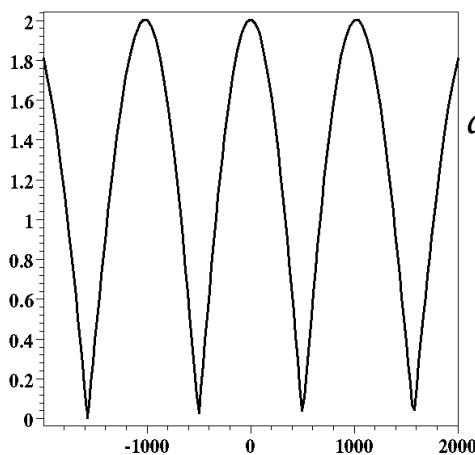
$d = 10^4, a = 0.005, \lambda = 0.01$

Distance between peaks should be $\lambda d/a = 2 \cdot 10^4$

$d = 10^4, a = 0.1, \lambda = 0.01$

Distance between peaks should be $\lambda d/a = 10^3$

$d = 10^4, a = 0.01, \lambda = 0.01$

Distance between peaks should be $\lambda d/a = 10^4$
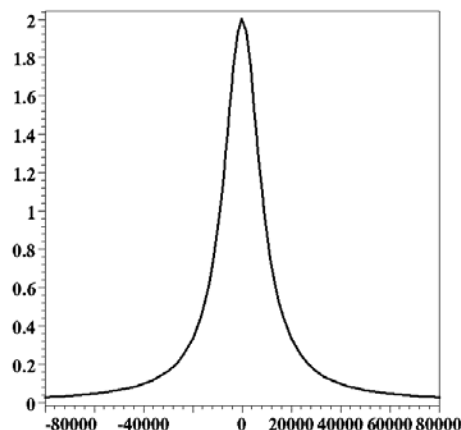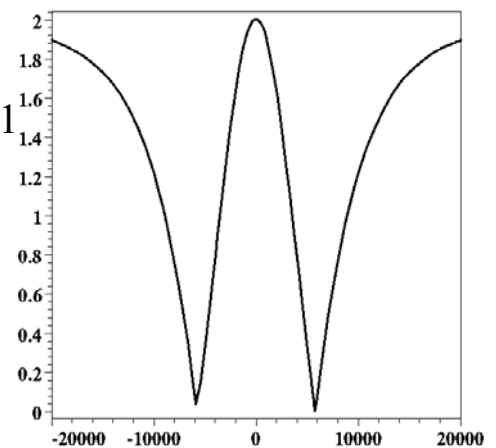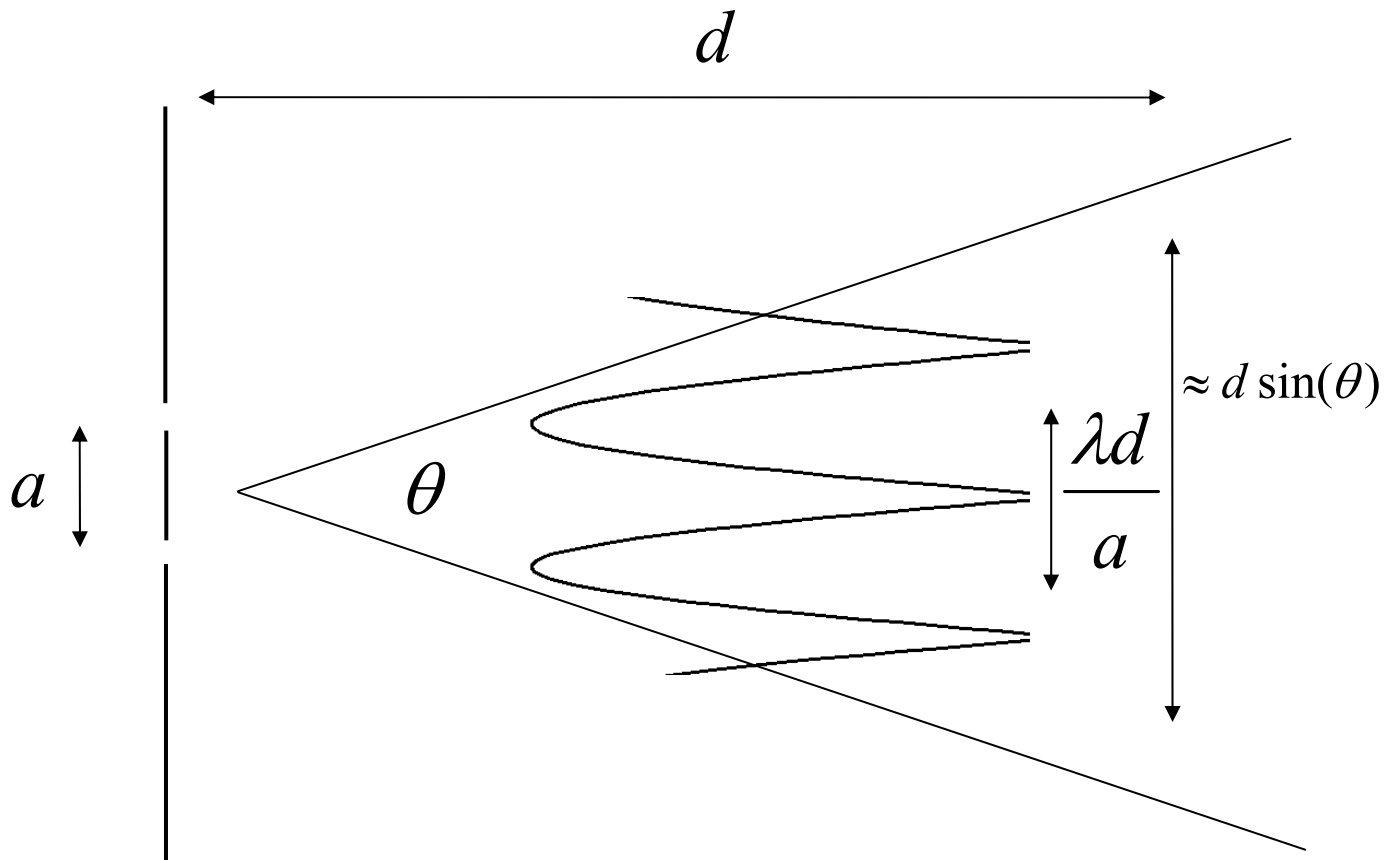
In order to distinguish the objects, the two maxima should fall in the view area, so we must have

$$d \sin(\theta) \geq \frac{\lambda d}{a} \Rightarrow a \geq \frac{\lambda}{\sin(\theta)}$$

Another experimental demonstration of the uncertainty principle – shooting a particle through a single slit (Fraunhofer diffraction):

wavelength = λ

Single Slit Diffraction

Incident plane wave

One can prove that

$$\theta \approx \lambda/W.$$

θ

y

slit width = W
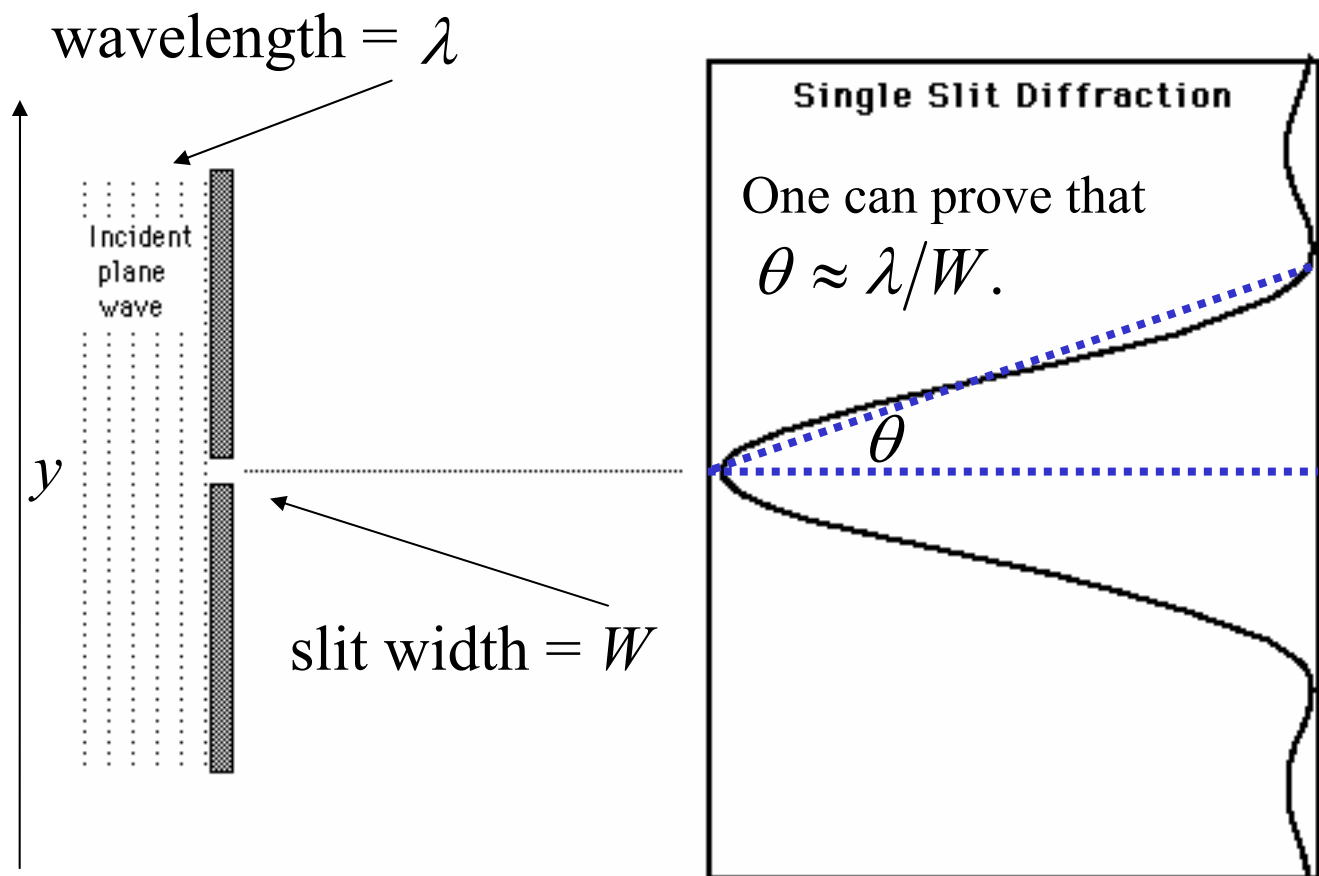
Before the particle (wave) hits the barrier, we can assume that its y-momentum is zero. After it passes the slit, we know its position with an accuracy of $\Delta y \approx W$, but there's an uncertainty in the y-momentum, $\Delta p_y \approx p\lambda/W$ (where p is the original momentum). So, $\Delta y \Delta p_y \approx p\lambda$, but QM tells us that $p\lambda = h (= 2\pi\hbar)$.

• The narrower we make the slit, the more confident we are about the location; but then the diffraction pattern becomes wider, and we lose confidence in the momentum.

De Broglie Waves: The Wavy Nature of Particles

In the previous slide, we adapted to particles a result connecting the wavelength and momentum of a photon. This is based on De Broglie's ingenious "hunch" in 1924: "if waves (light) behave also like particles, then particles should also behave like waves". It turns out that a moving body behaves in certain ways as though it has a wavy nature. Its wavelength λ is defined, just like

for a photon, by $\lambda = \dfrac{h}{p} = \dfrac{h}{mv}.$

If so, electrons for example must diffract. This was proved experimentally by Davisson and Germer in 1927: they shot electrons at a crystal made of layers. An electron is scattered from different layers, hence there's a phase difference, hence there's diffraction.
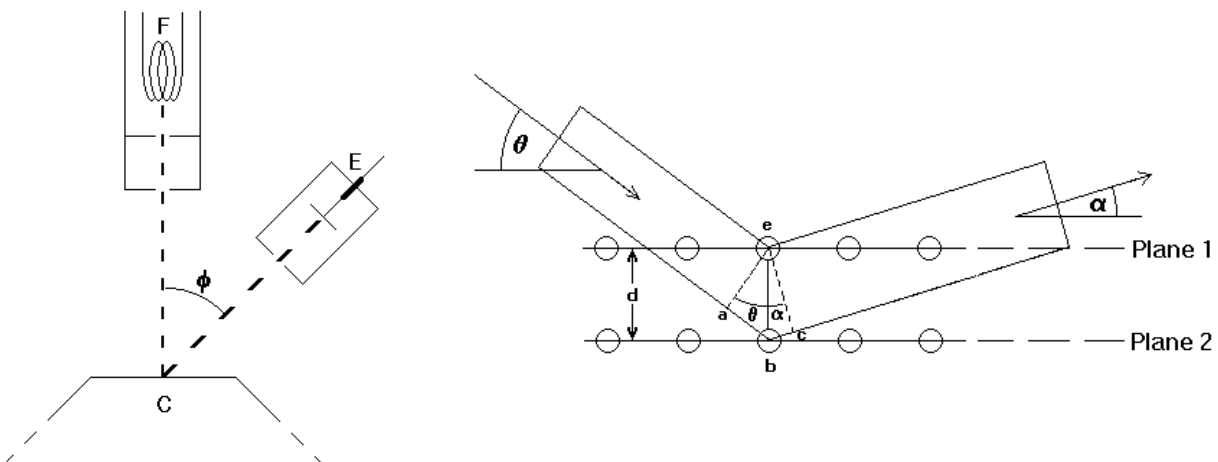
Note: larger objects (baseballs) also show interference, but λ is so small that the interference pattern is practically impossible to create and observe.

Application: the Radius of an Atom

• Let the "average radius" of the hydrogen atom be denoted by a.

• The momentum p should be, on the average, h/a. this implies that the average kinetic energy is

$$\frac{p^2}{2m} = \frac{h^2}{2ma^2}$$

• The potential energy is $-e^2/a$, where e is the electron charge. Hence the total energy is

$$E = \frac{h^2}{2ma^2} - \frac{e^2}{a}$$

• It's easy now to find the a minimizing this expression, and it's indeed pretty close to the true radius.

• Why then can't we squash an atom, and why doesn't the electron collapse onto the nucleus? Because then the uncertainty in the position will go to zero, and the uncertainty – and hence the average – of the momentum (and the energy) will go to infinity.

More on Probability Amplitudes

Two slit experiment again:
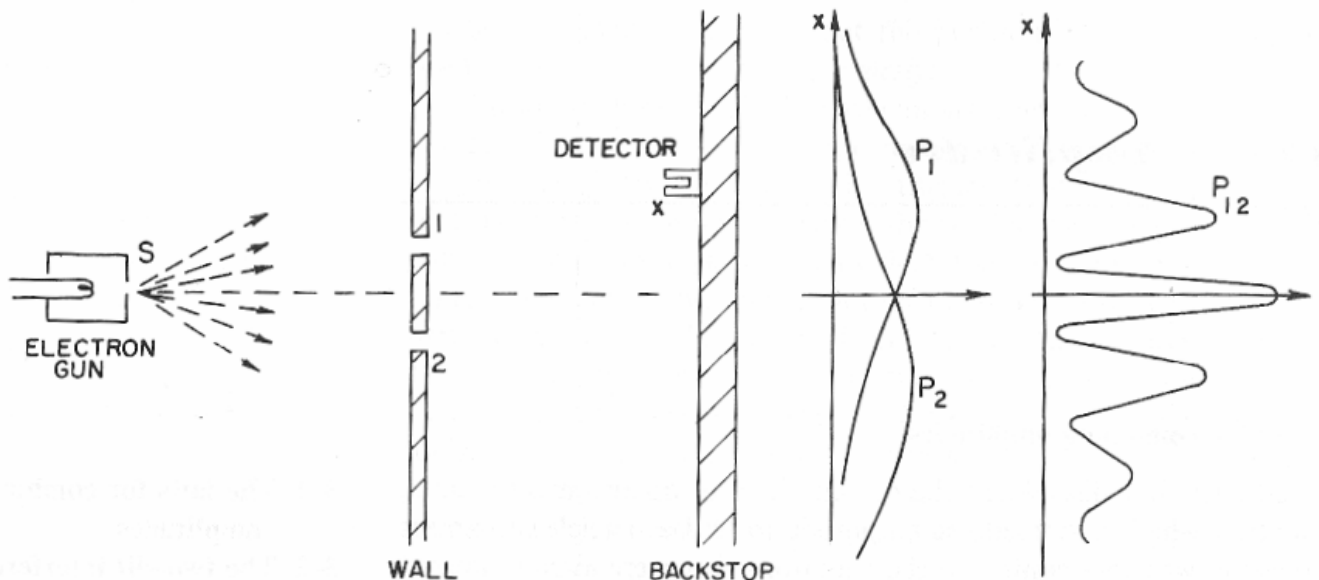
Denote the amplitude that a particle from s will arrive at x by Dirac's "bra and ket" notation:

$$\langle \text{particle arrives at } x | \text{particle leaves } s \rangle \equiv \langle x | s \rangle$$

We will later see that it's just an inner product.

We know that the probability is the square of the amplitude. We also know that amplitudes add:

$$\langle x | s \rangle_{\text{both slits open}} = \langle x | s \rangle_{\text{slit 1 open}} + \langle x | s \rangle_{\text{slit 2 open}}$$

Another law about amplitudes: the amplitude for a path is the product of the amplitudes to go part of the way and the rest of the way.
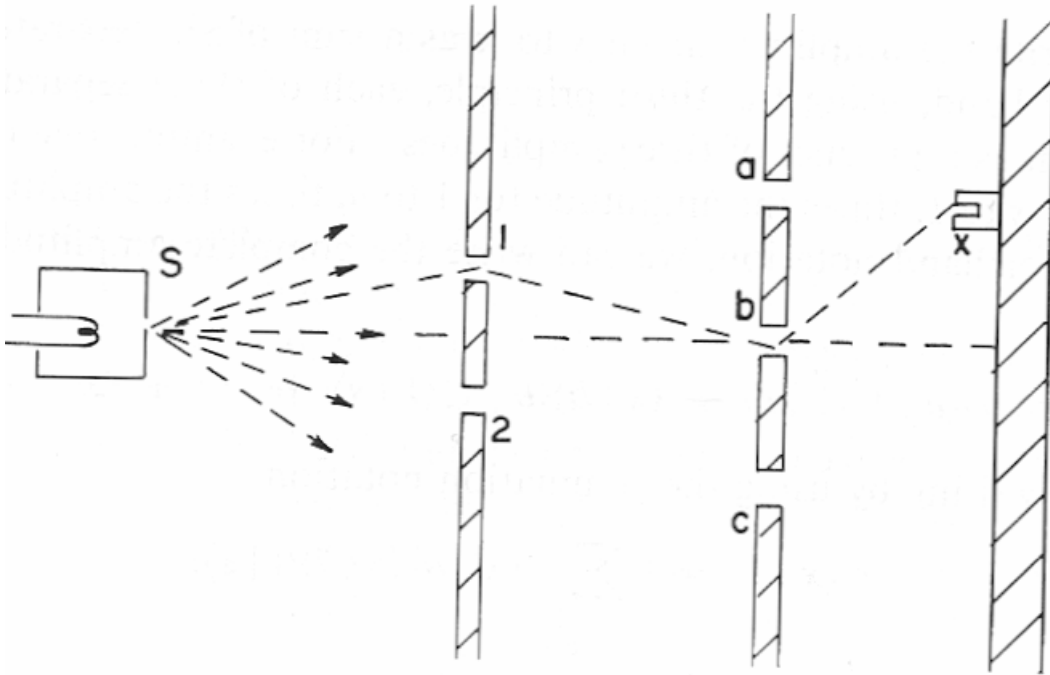
$$\langle x|s \rangle = \sum_{\substack{i=1,2 \\ \alpha=a,b,c}} \langle x|\alpha \rangle \langle \alpha|i \rangle \langle i|s \rangle$$

• We will later address amplitudes with a time variable (e.g. what is the amplitude for a particle to be somewhere at a given time).

• Another amplitude rule – if two particles don't interact, the amplitude for them to do two things is the product of the individual amplitudes.

Applying the amplitude rules to the two-slit experiment with a light source (trying to find what slit the electron went through)
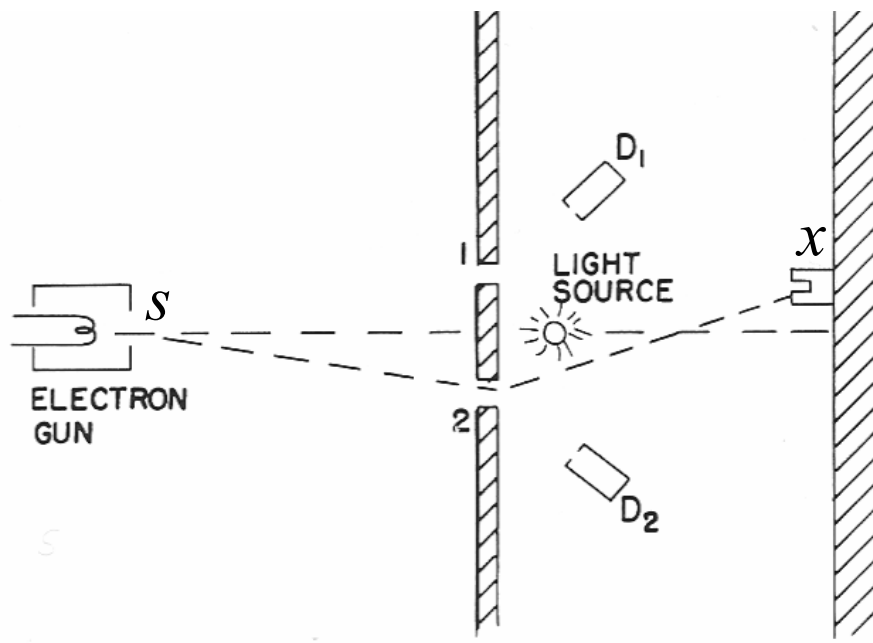
If there's no light, $\langle x|s\rangle = \phi_1 + \phi_2 = \langle x|1\rangle\langle 1|s\rangle + \langle x|2\rangle\langle 2|s\rangle$

If there's light, there are certain amplitudes for a photon to arrive at $D_1(D_2)$ if the electron went through 1 – call these amplitudes $a(b)$. Applying the principles and some symmetry considerations:

$$\Pr(\text{electron at } x) = \overbrace{|a\phi_1 + b\phi_2|^2}^{\text{photon at } D_1} + \overbrace{|a\phi_2 + b\phi_1|^2}^{\text{photon at } D_2}$$

If we can detect the slit via which the electron went with total certainty, then $b=0$ and the probability is $|\phi_1|^2 + |\phi_2|^2$, hence no interference at all. If we try to decrease the photon energy, we will have to increase its wavelength, hence b will grow and we'll have more and more interference.

Question: how can a light source affect the interference of baseballs?

Another Example: Scattering from a Crystal

neutron source → crystal → θ → neutron counter
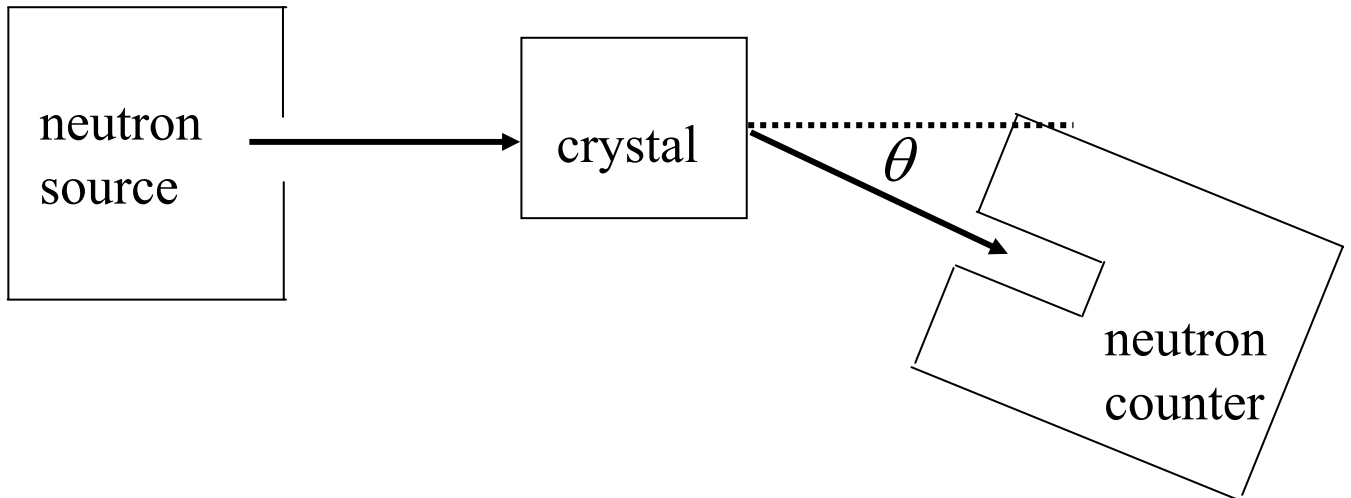
There are some crystals for which the scattering has both "classical" and interference components:

number of neutrons

θ
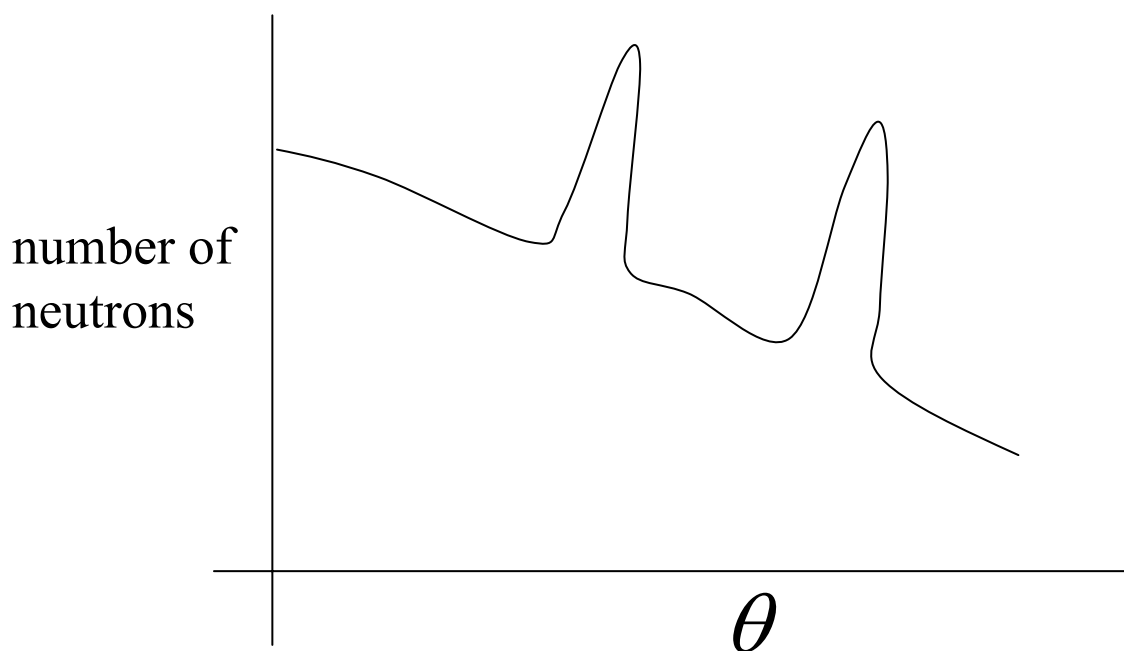
Why does this happen?

• Sometimes the crystal nuclei have a property called "spin" (they may be "spin up" or "spin down" – more later).

• Usually, the neutron is scattered without "leaving a mark" on the specific atom which scattered it. That case is like the two slit experiment without light, and we get interference.

• But sometimes the neutron can "leave a mark" on the atom that it scattered from – by changing the latter's spin (and also its own spin). That is equivalent to the two-slit experiment with light; in that case, we *can* distinguish what path the neutron took, and therefore we should add *probabilities* and not *amplitudes* (so no interference).

• In this crystal the neutron sometimes changes the nuclei spin and sometimes it doesn't – hence we have a mixture of both distributions: interference and no interference. **Note: it makes no difference whether we try or don't try to find the atom from which the neutron scattered!**

result   spin changed   Spin not changed
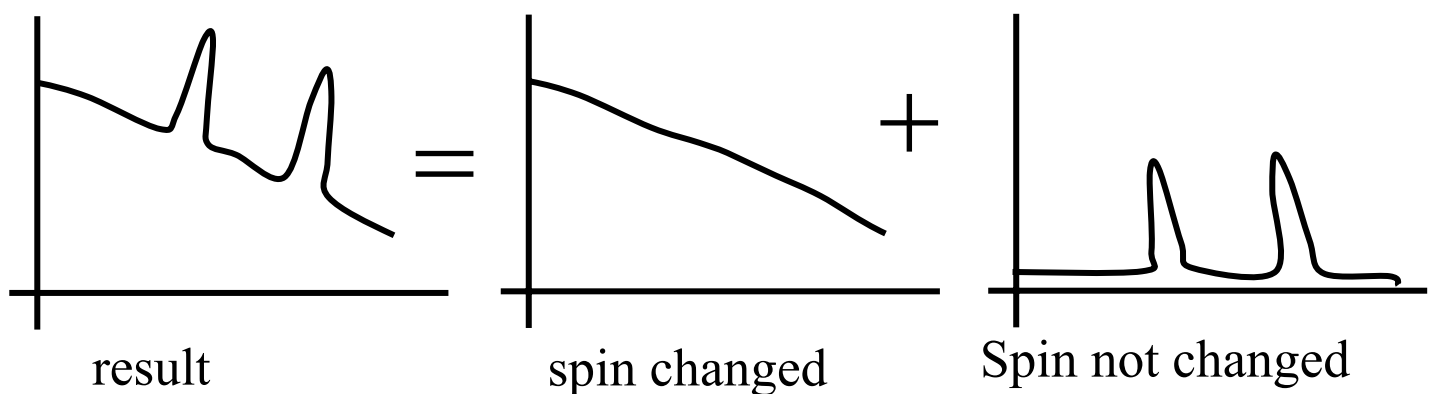
Bosons and Fermions

Let's look at a scattering of two particles:
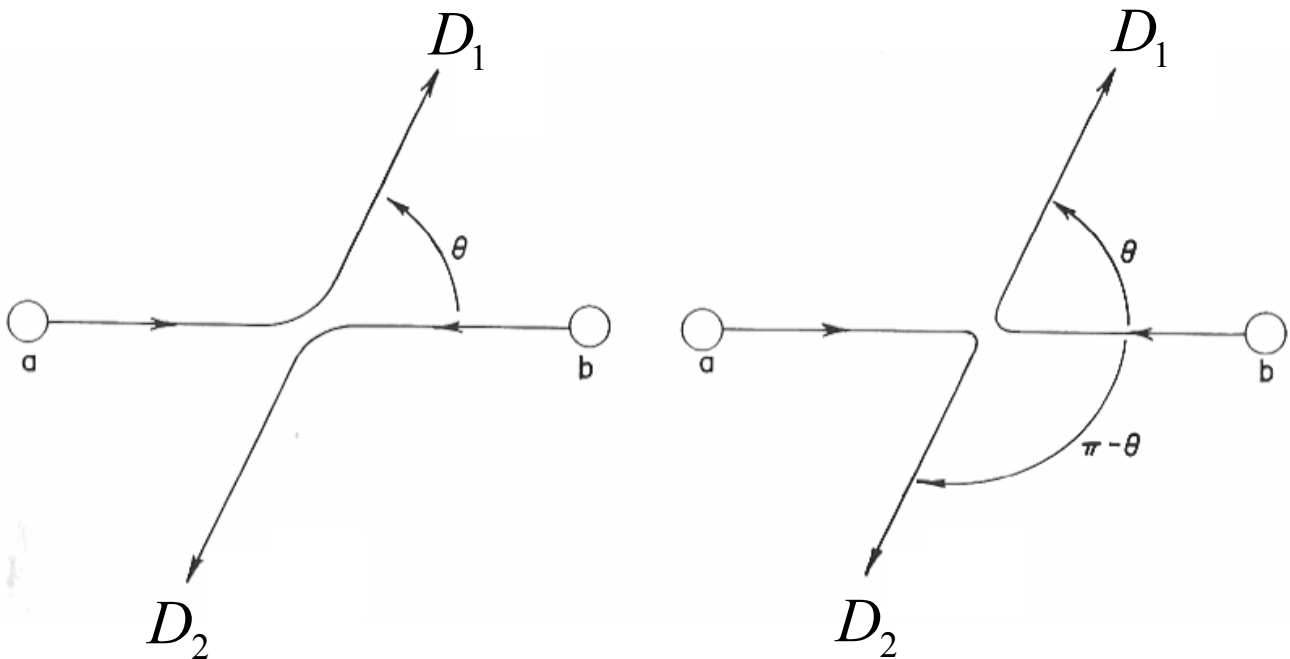
• If the amplitude for the left event is $f(\theta)$, then the probability of *any* particle arriving at the detector D_1 is

$$\text{Pr} = \left|f(\theta)\right|^2 + \left|f(\pi - \theta)\right|^2 : \theta = \frac{\pi}{2} \Rightarrow \text{Pr} = 2\left|f\left(\frac{\pi}{2}\right)\right|^2$$

• But what if the particles are *identical*? Then we cannot differentiate between the left and right events, and we have to add amplitudes before taking the squared absolute value to find the probability.

•. Exchanging the particles does not change the physics (probabilities), but it may change the phase. Since exchanging again brings us back to the original system, the amplitude must either remain the same or be multiplied by -1. It turns out that there are two types of particles: for *Bosons* the amplitudes are the same, for *Fermions* they are inverse.

• So, for a scattering of two bosons, the probability of one of them arriving at D_1 is

$$\text{Pr} = \left| f(\theta) + f(\pi - \theta) \right|^2 : \theta = \frac{\pi}{2} \Rightarrow \text{Pr} = 4\left| f\left(\frac{\pi}{2}\right) \right|^2$$

• And for two Fermions it is

$$\text{Pr} = \left| f(\theta) - f(\pi - \theta) \right|^2 : \theta = \frac{\pi}{2} \Rightarrow \text{Pr} = 0$$

• So, two Fermions cannot scatter at an angle of $\frac{\pi}{2}$!
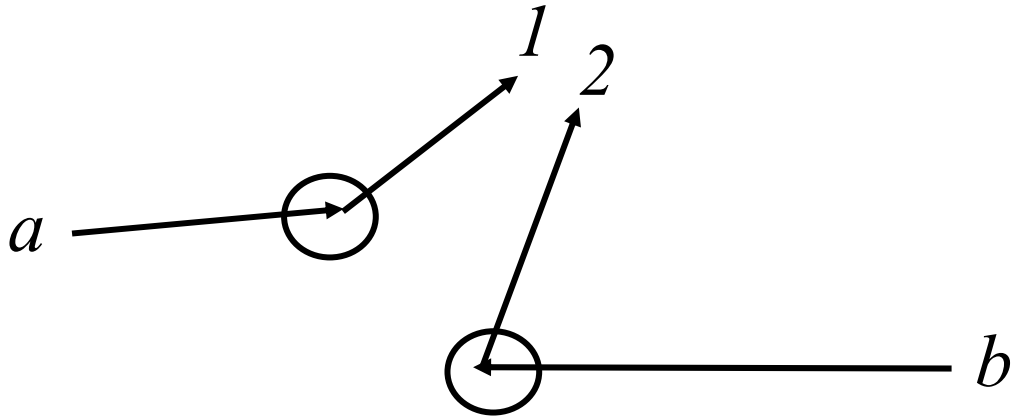
- Let's look at a double scattering. We know that the probability for this is $\left|\langle 1|a\rangle\right|^2\left|\langle 2|b\rangle\right|^2$.

- Assume that the particles are distinct. The probability for

$$(a \rightarrow 1 \wedge b \rightarrow 2) \vee (a \rightarrow 2 \wedge b \rightarrow 1)$$

is $\left|\langle 1|a\rangle\right|^2\left|\langle 2|b\rangle\right|^2 + \left|\langle 1|b\rangle\right|^2\left|\langle 2|a\rangle\right|^2$.

- If *1* approaches *2*, we can denote

$$\langle 1|a\rangle = \langle 2|a\rangle = a, \langle 1|b\rangle = \langle 2|b\rangle = b.$$

so the probability for both particles to go to *1* approaches $2|a|^2|b|^2$.

- But if they are Bosons, we cannot differentiate which went where, so we have to add amplitudes and then square:

$$\left|\langle 1|a\rangle\langle 2|b\rangle + \langle 1|b\rangle\langle 2|a\rangle\right|^2 \xrightarrow[1\rightarrow 2]{} 4|a|^2|b|^2$$

- This yields a probability two times bigger than for distinct particles. So: Bosons like to go to the same place, Fermions like to stay afar from each other. This is the *Pauli exclusion principle,* and without it atoms would have looked very different (electrons would stick together).

Light Polarization

Waves can be characterized by being either:

• **Transverse**: the thing that is "waving" is perpendicular to the direction of motion of the wave (light waves).

• **Longitudinal**: the thing that is "waving" is in the direction of motion of the wave (sound waves).
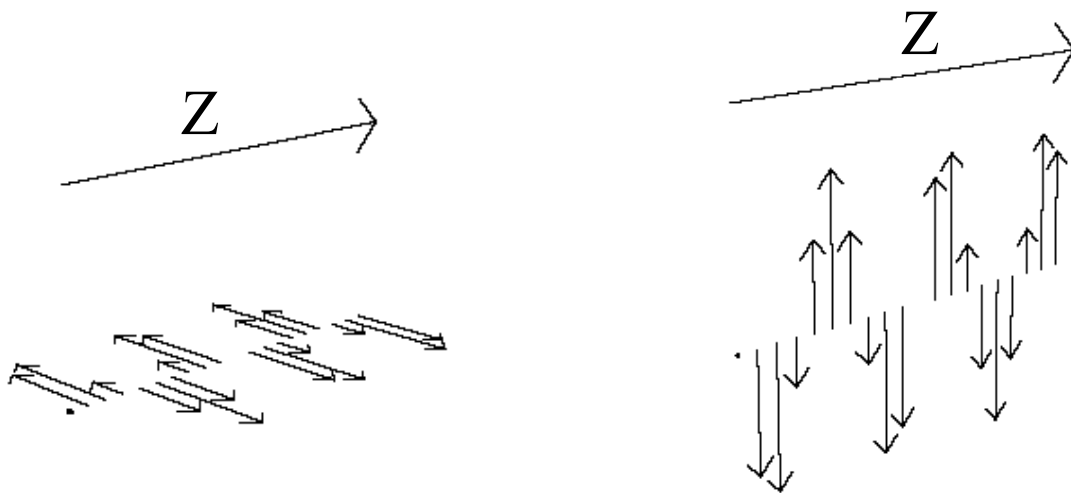
Two possible **polarizations** of light waves. The arrows depict the oscillations of the electromagnetic wave. These will be called x and y polarizations.

Polarizers:
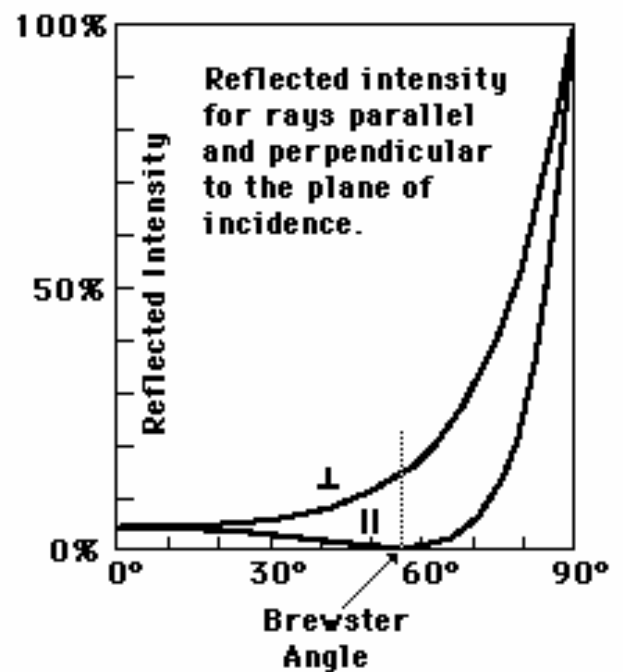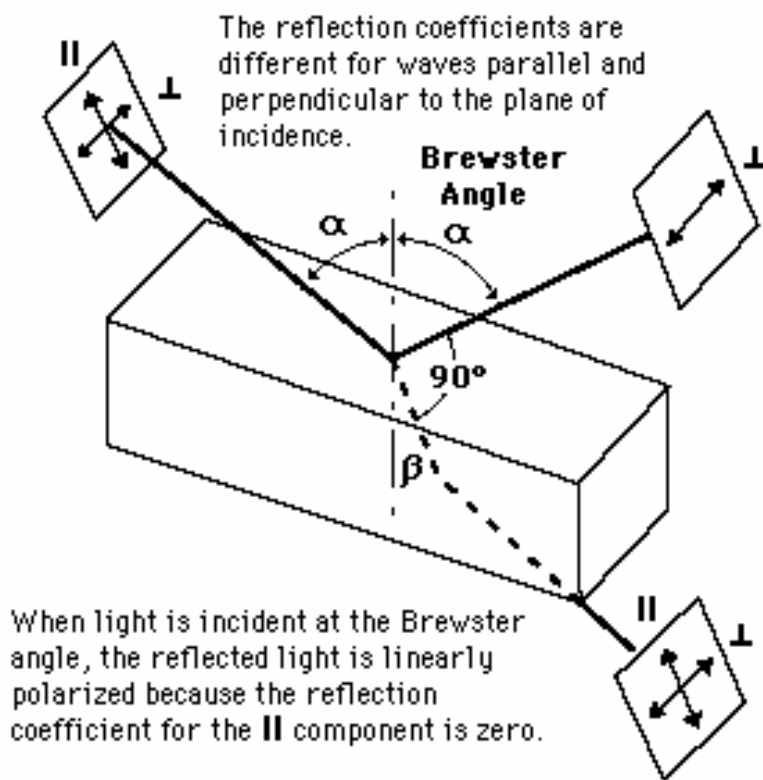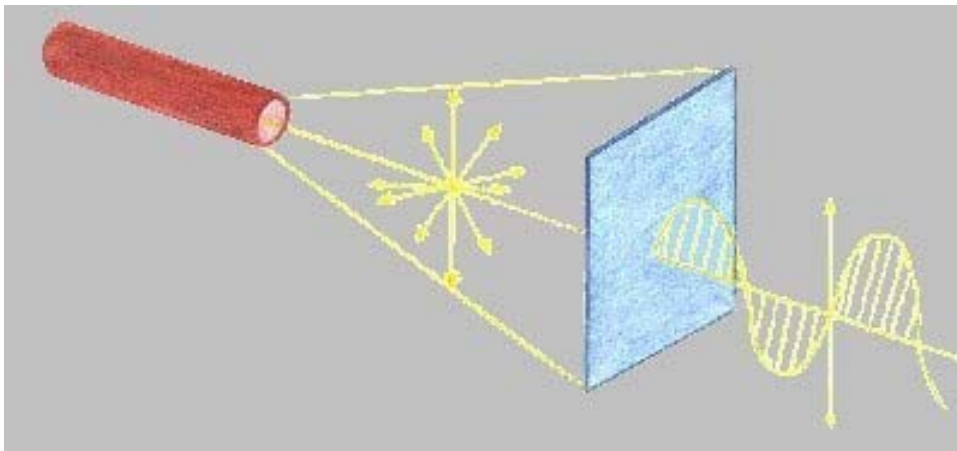
Polarization by reflection.

There are apparatuses that allow only light as a certain polarization to go through (LCD, polaroid sunglasses).

• From the QM point of view, *every single photon* has a mixture of the two polarizations associated with it, and we can only compute the probability that it goes through a certain polarizer.

• $|x\rangle$ and $|y\rangle$ resp. refer to the state of a single photon in an x resp. y beam which is polarized in the classical sense.

• Filtering with a polarizer in angle θ relative to x-y yields the state $|x'\rangle = \cos(\theta)|x\rangle + \sin(\theta)|y\rangle$.
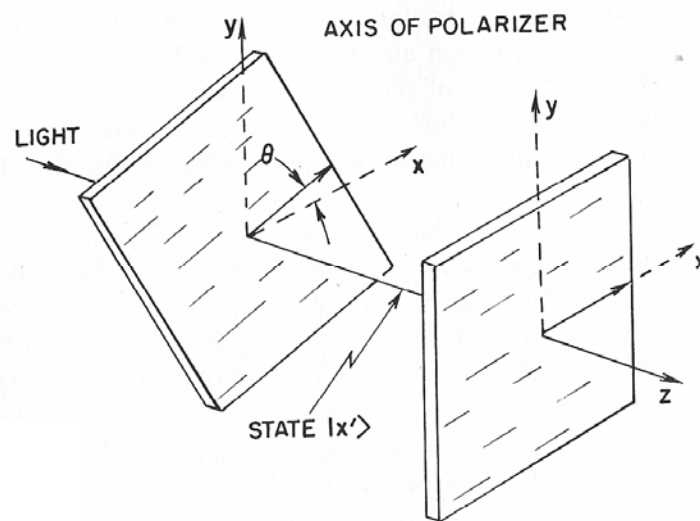
If we place a second polarizer at angle 0, then the probability that $|x'\rangle$ goes through is $\cos^2(\theta)$, which is in perfect accordance with classical physics – but here, it's not that the *wave* energy is decreased by this factor, but that only $\cos^2(\theta)$ of the photons go through – and those which do, don't lose any energy.

Thus – a classical, macro, continuous phenomena is explained by a (rather different) micro, discrete, QM phenomena.

Light is (classically) said to be *RHC polarized* if its *x* and *y* components are equal but $90°$ out of phase (in this case, the field is not linear as before, but oscillates in a circle which lies in the plane perpendicular to the light's direction). The QM interpretation for a single photon is

$$\left|RHC\right\rangle = \frac{1}{\sqrt{2}}\left(\left|x\right\rangle + i\left|y\right\rangle\right)$$

Where does the *i* come from? We know that a $90°$ phase shift, when repeated twice on $\left|y\right\rangle$, yields $-\left|y\right\rangle$. So, we can see why it is represented by a multiplication with *i*.

Interlude: Wiesner's Quantum Money

• Bank has a list of bills; each has a serial number and 20 photons embedded in the bill, each with one of four possible polarizations:
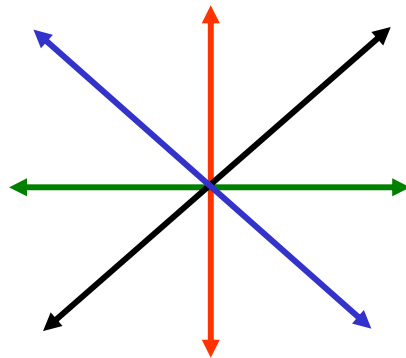
• A would-be counterfeiter cannot copy the bill, since any attempt to measure the polarization will not only probably destroy the original polarization, but will also leave too many possibilities. For example, if a photon measured with a green polarizer gives zero (the photon doesn't pass), it can be either a black, red, or blue photon. As with the electron, the measurement operation *changes the state;* this is why the method works.

• Note that the bank may say "yes" even if some photons are not correctly polarized – but the probability of the counterfeiter to obtain this can be made arbitrarily small.
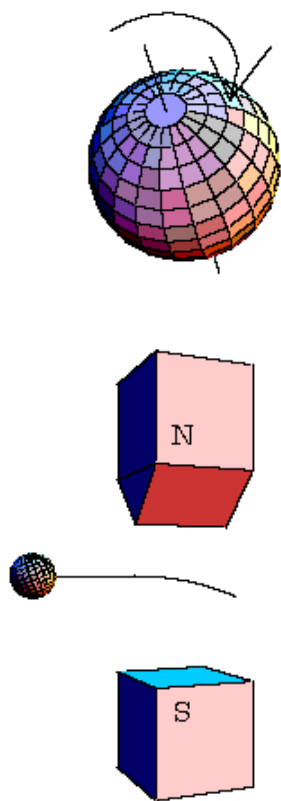
Introduction to base states: spin and the Stern-Gerlach experiment
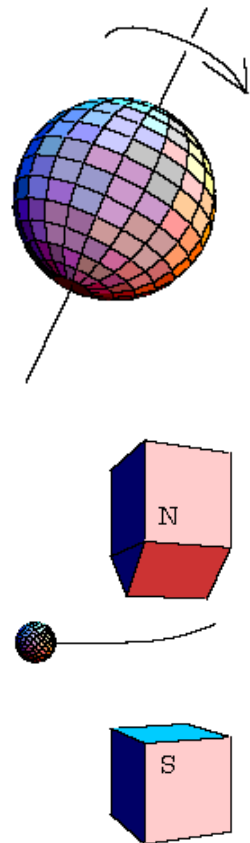
The total amount of deflection is a function of

• The total amount and distribution of electric charge on the ball.

• The orientation and rate of spin. As the rate of spin increases, so does the deflection. As the axis of the spin becomes more vertical, that amount of deflection also increases.

If the beam from the electron gun is directed to the magnets, as shown to the right, the beam is split into two parts. One half of the electrons in the beam are deflected up, the other half were deflected down. The amount of deflection up or down is exactly the same magnitude. Whether an individual electron is deflected up or down appears to be random. Stern and Gerlach did a version of this experiment in 1922.

This is very mysterious. It seems that the "spin" of electrons comes in only two states. If we assume, correctly, that the rate of spin, total charge, and charge distribution of all electrons is the same, then evidently the *magnitude* of the angle the spin axis makes with the horizontal is the same for all electrons. For some electrons, the spin axis is what we are calling "spin up", for others "spin down".

You should beware of the term "spin." If one uses the "classical radius of the electron" and the known total angular momentum of the electron, it is easy to calculate that a point on the equator of the electron is moving at about 137 times the speed of light! Thus, although we will continue to use the word "spin" it is really a shorthand for "intrinsic angular momentum." It has no classical counterpart.

Building a Spin Filter

spin up

spin down

electron gun
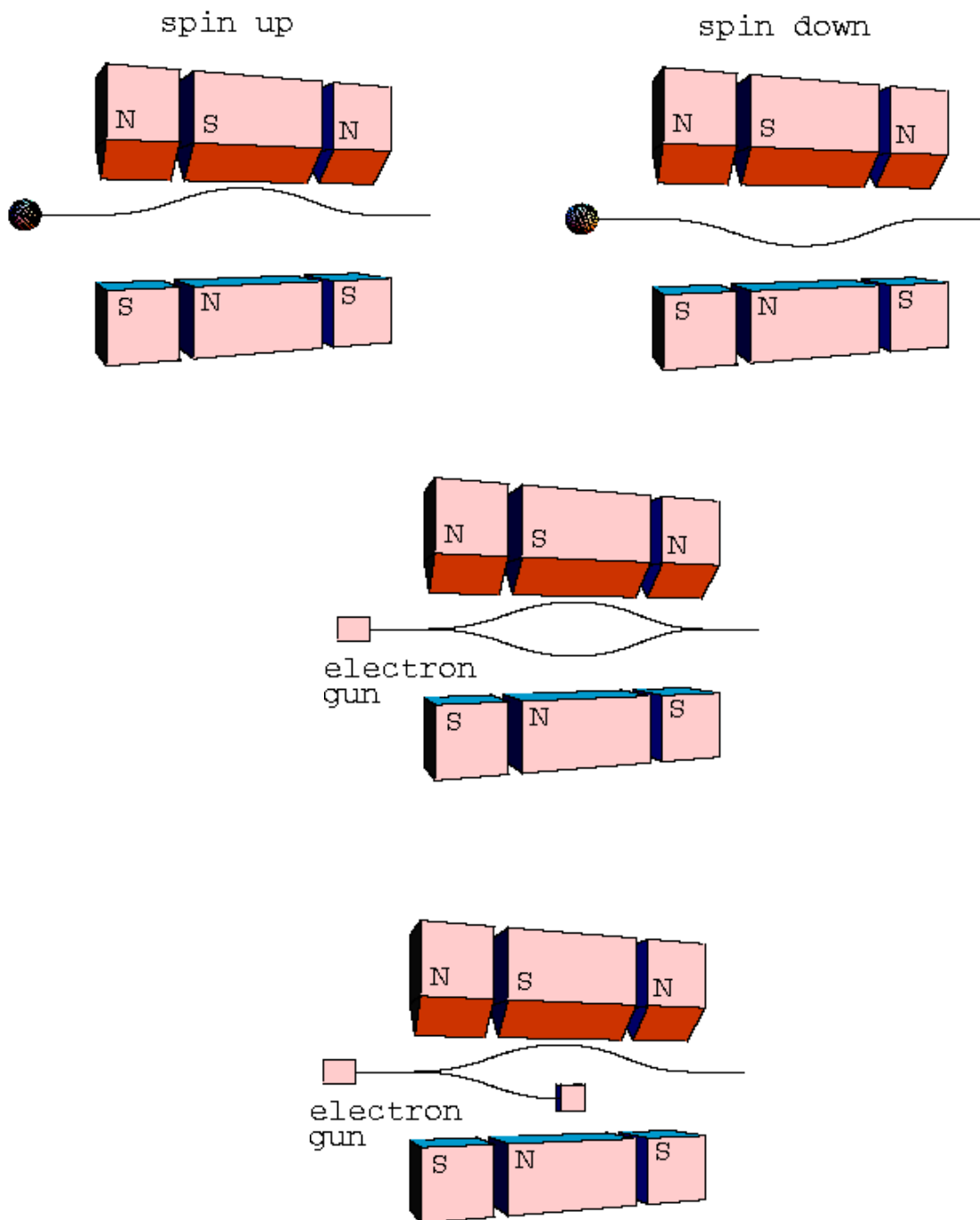
electron gun

The blocking mechanism is really a "filter" – allows only one spin type to go through.
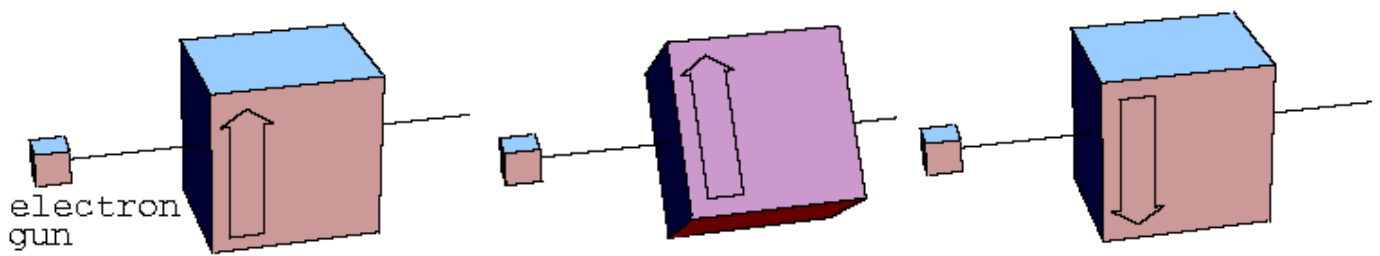
electron
gun

Shorthand notation for "spin up" filter. On the average, it allows half the electrons through. We can rotate the filter. Still, on the average, it allows half the electrons through.
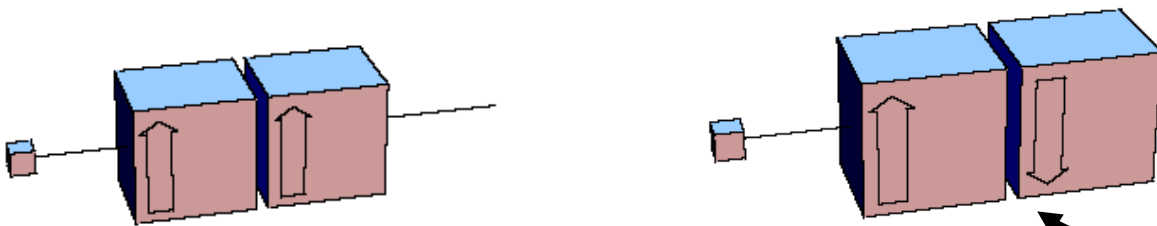
All those which passed the first will pass the second.

None of those which passed the first will pass the second (**nothing** passes both of them).

Half of those which passed the first will pass the second: in general, it's $\cos^2\left(\dfrac{\alpha}{2}\right)$

One quarter will pass.

To realize that something strange is going on, think about a filter with both paths unblocked being here:

Correlation measurements in a radioactive substance that emits a pair of electrons in each decay:
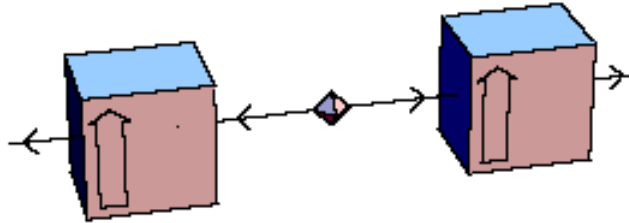
If the right electron passes, then its left hand companion does not pass its filter, and vice-versa. We say that each radioactive decay has a total spin of zero: if one electron is spin up its companion is spin down.
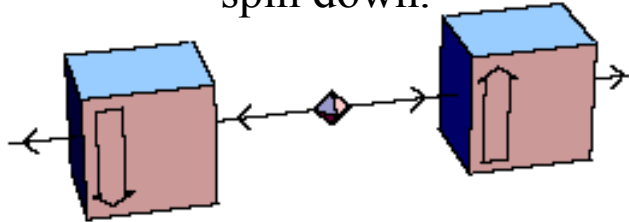
Again, one-half of the right hand electrons pass through their filter and one-half of the left hand electrons pass through their filter. But this time if a particular right hand electron passes its filter, then its companion left hand electron always passes its filter. Similarly, if the right hand electron does not pass its filter, its companion electron doesn't pass through its filter either.
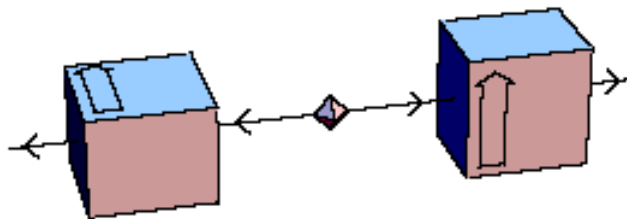
1. One-half of the right hand electrons emerge from their filter.

2. One-half of the left hand electrons emerge from their filter.

3. If a particular right hand electron passes its filter, one-half of the time its companion left hand electron will emerge from its filter, one-half of the time it will not.

It turns out that in the "world of Stern-Gerlach apparatuses" (SGA), the states U and D (denoting spin up and down) form something that resembles a basis in linear algebra. What does this mean? For example:

• If an electron is in one of these *base states* (B), we can predict the probability it goes through any SGA, *regardless* of its previous history.

• Every state and every transition amplitude can be describe as a mixture of these states:

$$\chi = \sum_{i \in B} \langle i | \chi \rangle | i \rangle \qquad \langle \chi | \phi \rangle = \sum_{i \in B} \langle \chi | i \rangle \langle i | \phi \rangle$$

• Since the base states are complete (i.e. they span all states), we must have that the sum of probabilities of a state to be in any of the base states is 1, or

$$\sum_{i \in B} \left| \langle i | \chi \rangle \right|^2 = \sum_{i \in B} \langle i | \chi \rangle \langle i | \chi \rangle^* = 1$$

But the probability of a state to go to itself must be 1, so according to ⬏ , we must have

$$\langle \chi | \chi \rangle = \sum_{i \in B} \langle \chi | i \rangle \langle i | \chi \rangle = 1 \Rightarrow \forall_{\chi, \phi} \langle \chi | \phi \rangle = \langle \phi | \chi \rangle^*$$

Just like in linear algebra, we have many sets of base states; e.g. the outputs of SGAs which are rotated in various angles, each time leaving only one beam unblocked. And just as in linear algebra, we can switch from description in $B_1 = \{i\}$ to a description in $B_2 = \{j\}$, if we know $\langle j | i \rangle$ for all i,j. For example, for spin ½, and for rotation around the longitudinal axis, the transition matrix is

$$\begin{pmatrix} \cos\left(\dfrac{\theta}{2}\right) & \sin\left(\dfrac{\theta}{2}\right) \\ -\sin\left(\dfrac{\theta}{2}\right) & \cos\left(\dfrac{\theta}{2}\right) \end{pmatrix}$$

Operators and base states

Suppose we do something to a particle – for example, make it go through a mess of SGAs. Let's call this mess A an *operator*.

• If we have such an operator, we may ask questions such as: given two states χ, ϕ , what is the amplitude for $\phi \rightarrow A \rightarrow \chi$, which will be denoted $\langle \chi | A | \phi \rangle$. We get another familiar result from linear algebra (remember that it makes more sense if you read from left to right):

$$\langle \chi | A | \phi \rangle = \sum_{i,j} \langle \chi | j \rangle \langle j | A | i \rangle \langle i | \phi \rangle$$

Where i,j range over base states.

• Other "linear algebra laws" follow – the composition of operators is the matrix product of their individual matrices, we have the usual laws for transforming between bases, etc.

• The matrix product representation encapsulates a rather strange result – composition of operators (like position and momentum) is not necessarily commutative, as opposed to classical physics. This has profound consequences.

Dependence of Amplitude on Time: The Hamiltonian

- How does the amplitude change with time?

- For a particle in a *state of definite energy* E_0, the amplitude is independent of position and is given by $ae^{-i(E_0/\hbar)t}$ (intuition: it's like a wave, and it has zero uncertainty in momentum, hence infinite uncertainty in position).

- Note that any *probability* question for such a particle is independent of time; hence such a particle is said to be in a *stationary state.*

- In order to have probabilities which change in time, the particle has to have more than one energy state: note that $\left| a_1 e^{-i(E_1/\hbar)t} + a_2 e^{-i(E_2/\hbar)t} \right|^2$ depends on the time t.

- The amplitude of a particle in uniform motion is $ae^{-(i/\hbar)(Et - p \cdot x)}$, where E is the particle's total energy.

Interlude: Jumping Over a Potential Barrier
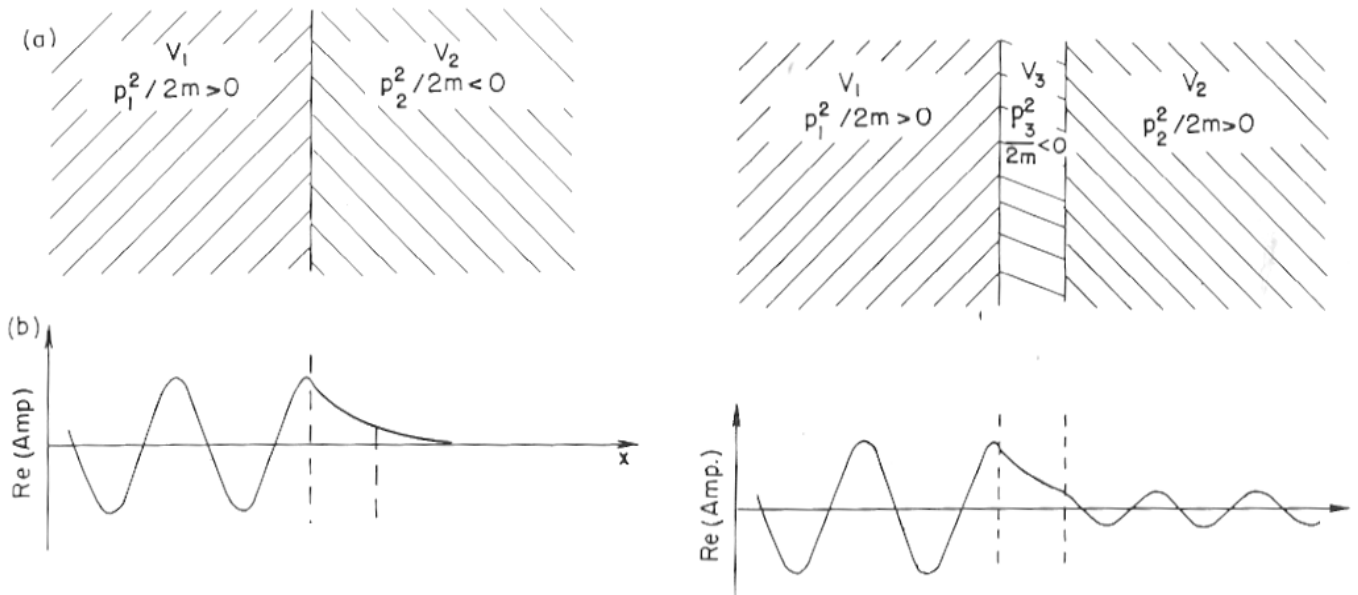
Suppose that a particle with a certain energy somehow goes over a potential barrier which is larger than its energy (this is, of course, impossible in classical physics). Its energy has to be negative, and since $E = p^2/2m$, its momentum has to be imaginary. Since the amplitude behaves like $ae^{-(i/\hbar)(Et - p \cdot x)}$, we may expect it to look like $e^{-\alpha x}$.

Incredibly enough, this is true. It explains, for example, particles getting into places which are forbidden by classical physics. More on this later.

A Little More on Bras and Kets

• Recall that if i ranges over base states, then

$$\langle \chi | \phi \rangle = \sum_i \langle \chi | i \rangle \langle i | \phi \rangle$$

• Inspired by this, we write $|\phi\rangle = \sum_i |i\rangle\langle i | \phi \rangle$

• And further: $| = \sum_i |i\rangle\langle i|$

• $\langle i |$ is a *bra* and $|i\rangle$ is a *ket* (these notations are valid not only for base states).

• If $|\phi\rangle = \sum_i |i\rangle C_i$ and $|\chi\rangle = \sum_i |i\rangle D_i$, then

$$\langle \chi | = \sum_i D_i^* \langle i | \text{ and } \langle \chi | \phi \rangle = \sum_i D_i^* C_i$$

• So it's just like an inner product. These notions extend naturally to an infinite number pf base states, with the L_2 structure $(f, g) = \int f^* g$ (plus some functions which are not in the classical L_2).

• For an operator A we have $A = \sum_{i,j} |i\rangle\langle i | A | j \rangle\langle j |$

• It's common in QM to denote the *state vector* $|\psi\rangle$ by anything which identifies it. For example, a state with a definite momentum p will be denoted by $|p\rangle$, etc.

How does the amplitude change under an apparatus, or operator? Passage of time is also an operator; denote by $U(t_2, t_1)$ the change which takes place between time t_1 and t_2. By that we mean that if a system is at state ϕ at time t_1, then its amplitude to be at state χ in time t_2 is $\langle \chi | U(t_2, t_1) | \phi \rangle$ So, it's enough to know $\langle i | U(t_2, t_1) | j \rangle$ for base states i, j.

Since $U(t_3, t_1) = U(t_3, t_2)U(t_2, t_1)$, it's enough to know $U(t + \Delta t, t)$. Denote as before $C_i(t) = \langle i | \psi(t) \rangle$, and $U_{i,j} = \langle i | U | j \rangle$. All this yields

$$C_i(t + \Delta t) = \sum_j U_{i,j}(t + \Delta t, t)C_j(t).$$

Letting $\Delta t \to 0$, guess that $U_{i,j} = \delta_{i,j} + K_{i,j}\Delta t$

For reasons to be explained, this is written as

$$U_{i,j}(t + \Delta t, t) = \delta_{i,j} - \frac{i}{\hbar}H_{i,j}(t)\Delta t$$

so $C_i(t + \Delta t) = \sum_j [\delta_{i,j} - \frac{i}{\hbar}H_{i,j}\Delta t]C_j(t)$

$$\frac{C_i(t + \Delta t) - C_i(t)}{\Delta t} = -\frac{i}{\hbar} \sum_j H_{i,j} C_j(t)$$

and

$$\boxed{i\hbar \frac{dC_i(t)}{dt} = \sum_j H_{i,j} C_j(t)}$$

H is called the *Hamiltonian.* It could also have been called the energy matrix: look at $C_1(t) = e^{-i(E_0/\hbar)t}$, the equation we saw for the amplitude for a particle at rest, with energy E_0. Then we have

$$i\hbar \frac{dC_1(t)}{dt} = E_0 C_1(t) = H_{1,1} C_1(t) \Rightarrow H_{1,1} = E_0$$

This is why H represents energy, and why the $-i/\hbar$ factor was inserted before. In classical mechanics, the function giving the total energy of the system is called the Hamiltonian, hence the name here.

Interlude: the Hamiltonian is Hermitian

Recall that the *adjoint* of a matrix A is defined by

$$[A^+]_{i,j} = A^*_{j,i} \quad \text{and that } A \text{ is } Hermitian \text{ if } A^+ = A.$$

Since $i\hbar \dfrac{dC(t)}{dt} = HC(t)$, we can write the solution as

$$|C(t)\rangle = e^{-iHt}|C(0)\rangle \quad \begin{array}{l}\text{(forget } \hbar \text{ for the moment,}\\ \text{it's only a constant).}\end{array}$$

so $\quad \langle C(t)| = \langle C(0)|e^{iH^+t}$

multiplying yields

$$1 = \langle C(t)|C(t)\rangle = \langle C(0)|e^{iH^+t}e^{-iHt}|C(0)\rangle$$

$$e^{iH^+t}e^{-iHt} = (I + iH^+t + \ldots)(I - iHt + \ldots) =$$
$$I + it(H^+ - H) + o(t^2)$$

So, we must have that $H^+ = H$.

Some useful facts: A Hermitian matrix has only real eigenvalues, and the eigenvectors corresponding to different eigenvalues are orthogonal. Also, if H is Hermitian, e^{-iH} $\left(\text{and therefore } e^{-iHt}\right)$ is unitary. So, the evolution of a state is actually a rotation.

A Two-State Example: the Ammonia Molecule
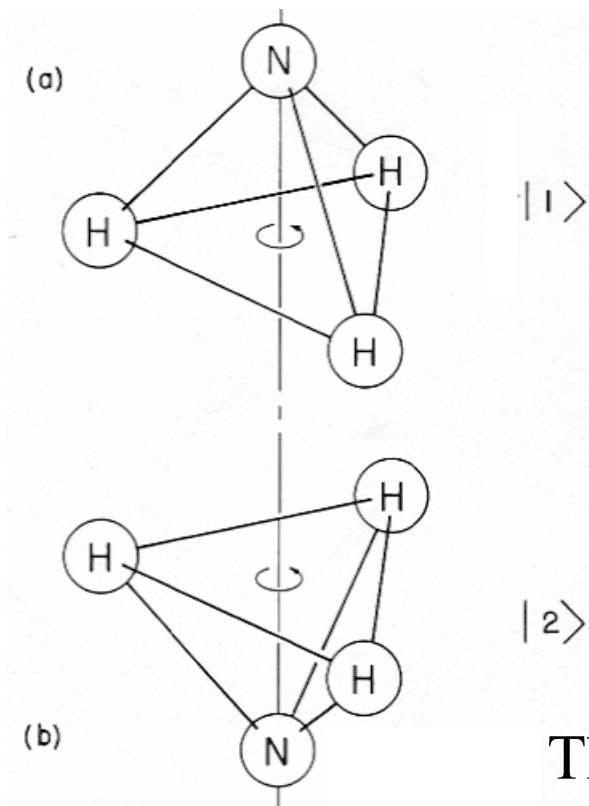
The molecule can flip, and every state is a combination of the "up" and "down" states:

$$\left|\psi\right\rangle = \left|1\right\rangle\left\langle 1 \middle| \psi\right\rangle + \left|2\right\rangle\left\langle 2 \middle| \psi\right\rangle =$$

$$\left|1\right\rangle C_1 + \left|2\right\rangle C_2$$

The question – what is the Hamiltonian? Based on symmetry considerations:

$$i\hbar\frac{dC_1}{dt} = E_0 C_1 - A C_2, \, i\hbar\frac{dC_2}{dt} = E_0 C_2 - A C_1 \Rightarrow$$

$$C_1(t) = \frac{a}{2}e^{-(i/\hbar)(E_0-A)t} + \frac{b}{2}e^{-(i/\hbar)(E_0+A)t}$$

$$C_2(t) = \frac{a}{2}e^{-(i/\hbar)(E_0-A)t} - \frac{b}{2}e^{-(i/\hbar)(E_0+A)t}$$

• What do these solutions mean? It's always useful to look for states with one frequency (or a definite energy). These occur in two cases: if $b = 0$ the energy is $E_0 - A$, and the amplitudes to be in $|1\rangle$ and $|2\rangle$ are the same. If $a = 0$, the energy is $E_0 + A$, and the amplitudes to be in $|1\rangle$ and $|2\rangle$ have opposite signs (but the probabilities are equal!).

• Suppose we know that when $t = 0$ the state is $|1\rangle$. This implies

$$C_1(0) = 1, C_2(0) = 0 \Rightarrow a = b = 1 \Rightarrow$$

$$C_1(t) = e^{-(i/\hbar)E_0 t} \left(\frac{e^{(i/\hbar)At} + e^{-(i/\hbar)At}}{2} \right) = e^{-(i/\hbar)E_0 t} \cos\left(\frac{At}{\hbar} \right)$$

$$C_2(t) = e^{-(i/\hbar)E_0 t} \left(\frac{e^{(i/\hbar)At} - e^{-(i/\hbar)At}}{2} \right) = ie^{-(i/\hbar)E_0 t} \sin\left(\frac{At}{\hbar} \right)$$

So $|C_2(t)|^2 = \sin^2(At/\hbar)$. Hence, if we *know* that at $t = 0$ the state is "up", we *also know* that at

$$t = \frac{\pi\hbar}{2A} \quad \text{the state is "down" (!!).}$$

Interlude: Symmetry and Conservation
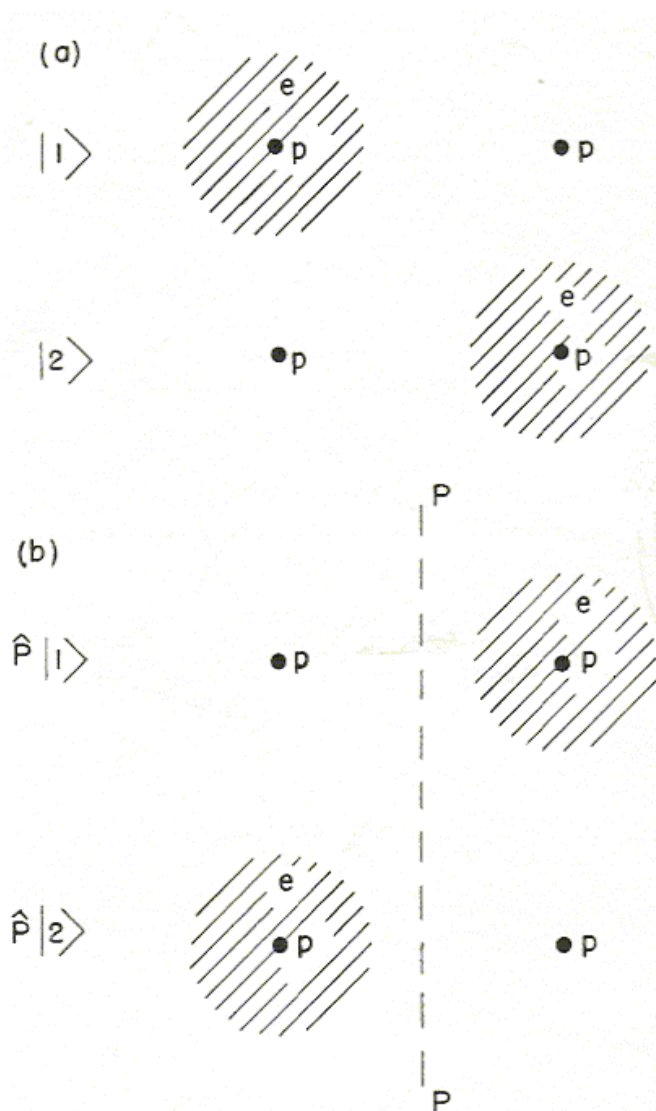
A hydrogen ion can be in one of the two states $|1\rangle$ and $|2\rangle$.

The operator P is defined by a reflection with the property

$$P|1\rangle = |2\rangle, \quad P|2\rangle = |1\rangle.$$

Assume that the physics of the ion is *symmetric* with respect to P. What does this mean? If we reflect by P, let the system evolve for some time, and reflect again, it will be just like letting the system evolve and then reflecting. If we denote, as before, the operation of "waiting" by U, it means that P and U commute: $PU = UP$. In general, an operator Q will be said to have a symmetry if it commutes with U.

Recall that $U = e^{\frac{-iHt}{\hbar}}$. So Q commutes with U iff Q commutes with H (remember that U is a sum of powers of H).

Suppose there's a state $|\psi\rangle$ such that $|\psi'\rangle = Q|\psi\rangle$ is physically the same state as $|\psi\rangle$; so, it differs from $|\psi\rangle$ only by a phase factor. For example, look at the two states

$$|I\rangle = \frac{|1\rangle + |2\rangle}{\sqrt{2}}, |II\rangle = \frac{|1\rangle - |2\rangle}{\sqrt{2}} : \ P|I\rangle = |I\rangle, \ P|II\rangle = -|II\rangle$$

so, the phase change is 0 for $|I\rangle$ and π for $|II\rangle$.

• Another example: look at an RHC polarized photon, and rotate it by an angle δ about the z-axis. Then its state is multiplied by $e^{i\delta}$.

• It's straightforward to see that if the symmetry operation of Q on a state $|\psi_0\rangle$ multiplies $|\psi_0\rangle$ by a phase factor $e^{i\delta}$, *then this is true forever*:

$$Q|\psi_0\rangle = e^{i\delta}|\psi_0\rangle \Rightarrow Q(U(t,0)|\psi_0\rangle) = U(t,0)(Q|\psi_0\rangle) =$$

$$U(t,0)(e^{i\delta}|\psi_0\rangle) = e^{i\delta}U(t,0)(|\psi_0\rangle) \Rightarrow Q|\psi_t\rangle = e^{i\delta}|\psi_t\rangle$$

But this is conservation!

Parity

Look at the operator $P(x, y, z) = (-x, -y, -z)$.

Since $P^2 = I$, it is immediate that if $P|\psi\rangle = e^{i\delta}|\psi\rangle$, then $e^{i\delta} = 1$ or $e^{i\delta} = -1$.

• P is called the *parity operator* and the two cases above correspond to states having even or odd parity. For the hydrogen ion, $|I\rangle$ has even parity, $|II\rangle$ has odd parity, and $|1\rangle$ has no definite parity.

• It turns out that parity is not always conserved; it is violated by β decay.

• If β decay is not involved, it turns out that any state with definite energy which is *not degenerate* (meaning that there are no other definite energy states that have the same energy) must have either even or odd parity. As a matter of fact, let Q be *any* symmetry operator, and let $|\psi\rangle$ be a non-degenerate state with energy E. So $H|\psi\rangle = E|\psi\rangle$, and

$$H(Q|\psi\rangle) = QH|\psi\rangle = QE|\psi\rangle = E(Q|\psi\rangle)$$

So, $Q|\psi\rangle$ is a state with definite energy E, but we assumed that $|\psi\rangle$ is the only such state. So we must have $Q|\psi\rangle = e^{i\delta}|\psi\rangle$, but as we saw before, if $Q = P$, then $e^{i\delta} = 1$ or -1.

The conservation laws in QM

• Various conservation laws can be expressed in QM as multiplication by a certain phase factor which depends on time, location etc. with a constant which equals the conserved quantity. Note: since there are states without a definite momentum for example, we cannot always talk about "conservation of momentum" as in classical physics (the most we can do for such states is hope that the *average* momentum is conserved). Some examples:

• Let $D_x(a)$ denote translation by a, and assume that there's a special state $|\psi_0\rangle$ such that $D_x(a)|\psi_0\rangle = e^{ika}|\psi_0\rangle$.

Then $k\hbar$ corresponds to the classical momentum. Similarly, there may be special states $|\psi_0\rangle$ such that after the passage of time τ, the state turns into $e^{-i\omega\tau}|\psi_0\rangle$. Then $\omega\hbar$ corresponds to the classical energy.

If you find this perplexing, check what happens to the wave equation $e^{i(kx-\omega t)}$ when $x \rightarrow x + a$ or $t \rightarrow t + \tau$ (and look again at the equations for a photon's momentum and energy).

• If $R_z(\phi)$ denotes rotation by ϕ around the *z-axis,* and

$R_z(\phi)|\psi_0\rangle = e^{im\phi}|\psi_0\rangle$, $m\hbar$ is the *angular momentum* for $|\psi_0\rangle$. It turns out that for an RHC/LHC photon this is equivalent to the classical notion of angular momentum, with values $\pm\hbar$. For linearly polarized light, there's equal amplitude to be in RHC or LHC, so a single photon doesn't have a definite angular momentum, and that's why (classically) a beam of linearly polarized light has zero angular momentum.

Infinitesimal Transformations

As in Lie group theory, it is customary in QM to study transformations with an infinitesimal displacement. For example, let $D_t(\tau) = U(t+\tau, t)$.

As we saw before, $\left|\psi(t)\right\rangle = e^{\frac{-iHt}{\hbar}}\left|\psi(0)\right\rangle$, so for a small Δt

$$\left|\psi(\Delta t)\right\rangle = U(\Delta t, 0)e^{\frac{-iH\Delta t}{\hbar}}\left|\psi(0)\right\rangle \approx \left(1 - \frac{-iH\Delta t}{\hbar}\right)\left|\psi(0)\right\rangle \Rightarrow$$

$$D_t(\Delta t) = 1 - \frac{i}{\hbar}(\Delta t)H.$$

But we know that for a state of definite energy E the passage of time multiplies the state by $e^{-i\omega\Delta t} \approx 1 - i\omega\Delta t \Rightarrow H = \omega\hbar = $ photon's energy. So, it makes sense to refer to H as the *energy operator* (more on this later).

- Similarly, for a small displacement $D_x(\Delta x)$, we may assume that the state changes linearly in $\Delta x : D_x(\Delta x)\left|\psi\right\rangle = \left(1 + \frac{i}{\hbar}p_x\Delta x\right)\left|\psi\right\rangle$

but $D_x(\Delta x)\left|\psi\right\rangle = e^{ik\Delta x}\left|\psi\right\rangle \approx \left(1 + ik\Delta x\right)\left|\psi\right\rangle \Rightarrow p_x = \hbar k$

for a definite momentum state; so, call p_x the *momentum operator.*
Note that $(i/\hbar)p_x$ behaves like $d\psi/dx$ should, so we can guess
That $p_x = -i\hbar\dfrac{d\left|\psi\right\rangle}{dx}$. That turns out to be true (more later).

- Similarly, we can define the angular momentum operator J_z by

$R_z(\Delta\phi)\left|\psi\right\rangle = e^{im\Delta\phi}\left|\psi\right\rangle = \left(1 + \frac{i}{\hbar}J_z\Delta\phi\right)\left|\psi\right\rangle \Rightarrow J_z\left|\psi\right\rangle = m\hbar\left|\psi\right\rangle$

And it immediately follows that J_z seems like $xp_y - yp_x.$

Part II: the Continuous (Infinite-Dimensional) Case: the Wave Function

The Wave Function and the Axiomatic Foundations of QM

• So far, we have dealt with a finite number of base states. That is, a system could be described by a finite linear combination of probability amplitudes.

• This does not always suffice. Think for example about the location of a particle along the x-axis. There is a continuum of possible locations, and they cannot be expressed as a finite linear combination of anything.

• Same holds for momentum.

• This led to the definition of the *wave function.* For a particle in a one-dimensional world, it is a continuous function which defines the amplitude to be, for example, at any location x.

• Next, we present the axioms of QM for what a wave function is and how it behaves over time. They are given side-by-side with the classical physics axioms, to emphasize both the similarity and difference between the two.

Classical	QM
The state of a particle at time t is given by its position $x(t)$ and momentum $p(t)$.	The state of a particle at time t is given by a vector (function) in Hilbert space, $\lvert \psi(t) \rangle$.
Every dynamical variable is a function of x and p. X and P are Hermitian.	The x of classical mechanics is replaced by the operator X, defined by $X\lvert f(x) \rangle = \lvert xf(x) \rangle$, and p is replaced by the operator P defined by $$P\lvert f(x) \rangle = -i\hbar \left\lvert \frac{df}{dx} \right\rangle.$$
A measurement of a dynamical variable $\Omega(x,p)$ yields a uniquely defined result, and the state is unchanged by the measurements.	If a particle is in the state $\lvert \psi \rangle$, a measurement of the variable Ω yields an eigenvalue ω of the operator $\Omega(X,P)$ with a probability $\Pr(\omega) \propto \lvert \langle \omega \vert \psi \rangle \rvert^2$, and the state changes from $\lvert \psi \rangle$ to $\lvert \omega \rangle$ ($\lvert \psi \rangle$ *collapses* to $\lvert \omega \rangle$).
The system changes with time according to Hamilton's equations, where $\mathbf{H}$ is the classical Hamiltonian (total energy): $$\dot{x} = \frac{\partial \mathbf{H}}{\partial p}, \quad \dot{p} = -\frac{\partial \mathbf{H}}{\partial x}$$	$\lvert \psi(t) \rangle$ changes according to *Schrödinger's equation:* $$i\hbar \frac{d}{dt}\lvert \psi(t) \rangle = H\lvert \psi(t) \rangle$$ where H is the quantum Hamiltonian, created by substituting $x \to X, p \to P$ In the classical Hamiltonian.

Points for Discussion:

- What is the wave function? Inner product: $\langle \psi | \phi \rangle = \int_{-\infty}^{\infty} \psi^* \phi$

- What are the X and P operators, and what are their eigenvectors and eigenvalues? Relation to Fourier transform!

$$\left\{ X: \ |x\rangle = \delta(x' - x), x \right\}, \left\{ P: \ |p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}}, p \right\}$$

- The meaning of the collapse of the state vector for the X and P operators. What happens if an eigenstate is measured? Reminder: two-slit experiment with measurement. Question: how can a photon cause the wave function of a battleship to collapse? Reminder: Stren-Gerlach experiment.

- The Schrödinger equation for a free particle as the limit of a finite dimensional state: where does the derivative come from? (Later).

Complications:

1. What does the classical xp go to: XP or PX? Answer: average.

2. What if Ω is degenerate? Answer: $\Pr(\omega) \propto \langle \psi | P_\omega | \psi \rangle$, where P_ω is the projection on the subspace of vectors with eigenvalue ω.

3. The eigenvalue spectrum of Ω is continuous. Answer: replace all sums by integrals, and "probability" by "probability density".

   Example: $\Omega = X$: $\Pr(a \leq \text{position} \leq b) = \int_a^b |\psi(x)|^2 dx$

   So we should have $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$ (normalization).

Expectation and Uncertainty

• We saw that the measurement process in QM is probabilistic. Yet, we can ask what the *average* result of measuring Ω in the state $|\psi\rangle$ is: following the usual definition of expectation, it equals

$$\langle\Omega\rangle \equiv \sum_{\omega} \omega \left|\langle\omega|\psi\rangle\right|^2 = \sum_{\omega} \omega\langle\omega|\psi\rangle\langle\psi|\omega\rangle = \langle\psi\left|\left[\sum_{\omega}\omega\,|\omega\rangle\langle\omega|\right]\right|\psi\rangle$$

where $\omega, |\omega\rangle$ range over the eigenvalues/eigenvectors of Ω. Since Ω is Hermitian, its (normalized) eigenvectors are orthonormal. It's easy to see that Ω can be resolved by

$$\Omega = \sum_{\omega} \omega\,|\omega\rangle\langle\omega|$$

(hint: verify that both sides are equal when operating on every $|\omega\rangle$, and use the fact that $\{|\omega\rangle\}$ span the entire space).

So, the expectation is $\langle\Omega\rangle = \langle\psi|\Omega|\psi\rangle$. This is nice, since we don't need to find $\Omega's$ eigenvalues and eigenvectors in order to compute the expectation.

• The average has a meaning only when computed over an ensemble of identical particles. It cannot be computed for a single particle, because the first measurement changes it.

• For an eigenstate, the expectation is equal to the corresponding eigenvalue. Thus, the Energy/Position /Momentum measurement of a state with definite EPM yields the "correct" and unique EPM result.

The uncertainty for Ω in a state $|\psi\rangle$ is also defined just like the classical variance:

$$(\Delta\Omega)^2 = \sum_{\omega} \Pr(\omega)(\omega - \langle\Omega\rangle)^2 = \left[\langle\psi|(\Omega - \langle\Omega\rangle)^2|\psi\rangle\right]^{1/2}$$

Example – the Gaussian centered at a with width Δ :

$$|\psi(x)\rangle = \frac{1}{(\pi\Delta^2)^{1/4}} e^{-(x-a)^2/2\Delta^2} \Rightarrow \Pr(x)dx = \frac{1}{(\pi\Delta^2)^{1/2}} e^{-(x-a)^2/\Delta^2}$$

The average of the position is

$$\langle X\rangle = \langle\psi|X|\psi\rangle = \int_{-\infty}^{\infty} \psi^*(x)x\psi(x)dx = a$$

which is hardly surprising. As for the uncertainty:

$$(\Delta X)^2 = \langle\psi|(X - \langle X\rangle)^2|\psi\rangle = \langle\psi|(X^2 - 2\langle X\rangle X + \langle X\rangle^2)|\psi\rangle =$$

$$\underbrace{\langle\psi|X^2|\psi\rangle - 2\langle X\rangle\langle\psi|X|\psi\rangle}_{\text{is just }\langle X\rangle} + \underbrace{\langle X\rangle^2}_{\substack{\text{expectation of a}\\\text{const. is the const.}}} = \langle\psi|X^2|\psi\rangle - \underbrace{\langle X\rangle^2}_{\text{this is }a^2}$$

So we have to compute

$$\langle\psi|X^2|\psi\rangle = \frac{1}{(\pi\Delta^2)^{1/2}} \int_{-\infty}^{\infty} e^{-(x-a)^2/2\Delta^2} x^2 e^{-(x-a)^2/2\Delta^2} dx = \frac{\Delta^2}{2} + a^2$$

and finally, $\Delta X = \dfrac{\Delta}{\sqrt{2}}$ (also hardly surprising).

What about the momentum operator *P*?

$$P|f(x)\rangle = -i\hbar \left| \frac{df}{dx} \right\rangle \Rightarrow \langle P \rangle = -i\hbar \int_{-\infty}^{\infty} \psi^* \psi' dx = 0$$

$$(\Delta P)^2 = -\hbar^2 \int_{-\infty}^{\infty} \psi^* \psi'' \, dx = \frac{\hbar^2}{2\Delta^2} \Rightarrow \Delta P = \frac{\hbar}{\sqrt{2}\Delta}$$

as can be directly verified by substituting and integrating. $\longrightarrow$ $$|\psi(x)\rangle = \frac{1}{(\pi\Delta^2)^{1/4}} e^{-(x-a)^2/2\Delta^2}$$

• It is instructive to see how $|\psi(x)\rangle$ looks in momentum space. Since the orthonormal basis corresponding to momentum space is given by $|p\rangle = (2\pi\hbar)^{-1/2} e^{ipx/\hbar}$, then $|\psi(x)\rangle$ is represented in momentum space by

$$\langle p|\psi\rangle = \int_{-\infty}^{\infty} p^* \psi \, dx = \left(\frac{\Delta^2}{\pi\hbar^2} \right)^{\frac{1}{4}} e^{-ipa/\hbar} e^{-p^2\Delta^2/2\hbar^2}$$

So, the narrower the position distribution (small Δ), the broader the momentum distribution. This not only agrees with the physics discussed before, it is also no surprise to anyone who studied the Fourier transform! Note: $\underbrace{\Delta P \cdot \Delta X = \hbar/2}_{\text{uncertainty principle}}$.

• This happens because P and X don't commute, and don't have common eigenvectors ("eigenkets"). Since only the eigenkets of an operator are unaffected by a measurement of the operator, we cannot have a system for which we know both the position and momentum.

• If two operators commute, there is a basis of common eigenkets, and the order of the measurements doesn't make a difference.

• The commutator of two operators is defined as

$$[\Omega, \Lambda] \equiv \Omega\Lambda - \Lambda\Omega$$

• It is straightforward to see that $[X, P] = i\hbar$

Interlude: Proof of Heisenberg's Uncertainty Theorem

We want to obtain a lower bound on

$$(\Delta X)^2 (\Delta P)^2 = \left\langle \psi \left| \left(X - \langle X \rangle \right)^2 \right| \psi \right\rangle \left\langle \psi \left| \left(P - \langle P \rangle \right)^2 \right| \psi \right\rangle$$

The trick is to reduce this to an expression depending on

$$[X, P] = XP - PX = i\hbar$$

define $A = X - \langle X \rangle$, $B = P - \langle P \rangle \Rightarrow AB - BA = XP - PX$

So we should bound

Since *A,B* are Hermitian

$$\left\langle \psi \left| A^2 \right| \psi \right\rangle \left\langle \psi \left| B^2 \right| \psi \right\rangle = \left\langle A\psi \mid A\psi \right\rangle \left\langle B\psi \mid B\psi \right\rangle$$

From the Cauchy-Schwartz inequality, this is larger than

$$\left| \left\langle A\psi \mid B\psi \right\rangle \right|^2 = \left| \left\langle \psi \left| AB \right| \psi \right\rangle \right|^2$$

Now comes the trick. Denote

$$C = \frac{AB - BA}{2}, D = \frac{AB + BA}{2} \Rightarrow AB = C + D$$

So we should bound $\left| \left\langle \psi \left| C + D \right| \psi \right\rangle \right|^2$

Now:

$$\left|\langle\psi|C+D|\psi\rangle\right|^2 = \left|\langle\psi|C|\psi\rangle+\langle\psi|D|\psi\rangle\right|^2 =$$

$$\left|\langle\psi|C|\psi\rangle\right|^2 + \left|\langle\psi|D|\psi\rangle\right|^2 +$$

$$\langle\psi|C|\psi\rangle\langle\psi|D|\psi\rangle^* + \langle\psi|C|\psi\rangle^*\langle\psi|D|\psi\rangle$$

But $C = \dfrac{i\hbar}{2}$, and since ψ is normalized, $\left|\langle\psi|C|\psi\rangle\right|^2 = \dfrac{\hbar^2}{4}$.

To get the inequality, we will throw away $\left|\langle\psi|D|\psi\rangle\right|^2$,

which is of course positive, and prove that

$$\underbrace{\langle\psi|C|\psi\rangle\langle\psi|D|\psi\rangle^* + \langle\psi|C|\psi\rangle^*\langle\psi|D|\psi\rangle}_{\text{Call this } G} = 0!$$

Ignoring the constant factor of 2, this last expression equals

$$G \equiv \langle\psi|AB-BA|\psi\rangle\langle\psi|AB+BA|\psi\rangle^* +$$

$$\langle\psi|AB-BA|\psi\rangle^*\langle\psi|AB+BA|\psi\rangle$$

Now we have to remember that $\forall_{\psi,\Omega} : \langle\psi|\Omega|\psi\rangle^* = \langle\psi|\Omega^+|\psi\rangle$

And that $A^+ = A, B^+ = B,$ and that $\forall_{\Lambda,\Omega} : (\Omega\Lambda)^+ = \Lambda^+\Omega^+$

And it immediately follows that G is indeed 0. Thus the proof is complete, and after taking roots: $(\Delta X)(\Delta P) \geq \hbar/2$

• Is the minimum attained? We can assume $\langle X \rangle = 0$. The Cauchy-Schwartz inequality is not strict only if the two vectors are linearly dependent, so we must have

$$\left(P - \langle P \rangle\right)\!|\psi\rangle = cX|\psi\rangle \Rightarrow \psi' = \frac{i}{\hbar}\left(\langle P \rangle + cx\right)\!\psi \Rightarrow$$

$$\psi(x) = \psi(0)e^{\frac{i}{\hbar}\left(\frac{cx^2}{2} + \langle P \rangle x\right)}$$

But to minimize, we must also have

$$\langle \psi |\left(P - \langle P \rangle\right)X + X\left(P - \langle P \rangle\right)\!|\psi\rangle = 0$$

but

$$\left(P - \langle P \rangle\right)\!|\psi\rangle = cX|\psi\rangle, \langle \psi |\left(P - \langle P \rangle\right) = c^*\langle \psi |X \Rightarrow$$

$$\langle \psi |\left(P - \langle P \rangle\right)X + X\left(P - \langle P \rangle\right)\!|\psi\rangle = \left(c + c^*\right)\!\langle \psi |X^2|\psi\rangle = 0$$

So c must be pure imaginary, $c = |c|i$ and so (after correcting by shifting with $\langle X \rangle$) we get

$$\psi(x) = \psi\!\left(\langle X \rangle\right)e^{i\langle P \rangle\left(\frac{x - \langle X \rangle}{\hbar}\right)}e^{-|c|\frac{\left(x - \langle X \rangle\right)^2}{2\hbar}}$$

That is, a Gaussian with a phase shift proportional to the momentum saturates the uncertainty.

Interlude: Finite-Dimensional Example: the effect of measurement (Shankar Ex. 4.2.1)

Consider the following operators on C^3 :

$$L_x = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, L_z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

- What are the possible values obtained if L_z is measured?

Answer: the L_z eigenvalues/normalized eigenvectors are

$$\left\{ 1, \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \right\}, \left\{ 0, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \right\}, \left\{ -1, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$$

So the possible results when L_z is measured are 0,1,-1.

- In the state in which $L_z = 1$, what are $\langle L_x \rangle, \langle L_x^2 \rangle, \Delta L_x$?

Answer: if $L_z = 1$, the state must be $(1,0,0)^t$. According to what we proved before:

$$\langle L_x \rangle = (1,0,0) L_x (1,0,0)^t = 0$$

$$\langle L_x^2 \rangle = (1,0,0) L_x^2 (1,0,0)^t = 1/2$$

$$\Delta L_x = \sqrt{\langle L_x^2 \rangle - \langle L_x \rangle^2} = 1/\sqrt{2}$$

Note: we should take conjugate transpose, but everything here's real.

• Find the eigenvalues and normalized eigenkets of L_x in the L_z basis.

Answer: the L_z basis is the standard one. An immediate computation yields that the L_x eigenvalues/normalized eigenvectors are

$$\left\{0, \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}\right\}, \left\{1, \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}\right\}, \left\{-1, \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}\right\}$$

• If a particle is in the state with $L_z = -1$, and L_x is measured, what are the possible outcomes and their probabilities?

Answer: if $L_z = -1$, the state must be $|\psi\rangle = (0,0,1)^t$. According to the axioms, the possible outcomes are the L_x eigenvalues, with probabilities equal to the square of the inner product of $|\psi\rangle$ with the corresponding eigenket. A straightforward calculation yields that we get 0 with probability $1/2$, 1 with probability $1/4$, and -1 with probability $1/4$.

• Consider the state $|\psi\rangle = \left(1/2, 1/2, 1/\sqrt{2}\right)^t$ in the L_z basis. If L_z^2 is measured in this state and the result is 1, what is the state after the measurement? If L_z is then measured, what are the possible outcomes and respective probabilities?

Answer:

$$L_z^2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

So, there's a degenerate eigenvalue, 1, with an eigenket subspace $V = \{(a,0,b)\}$, and a 0 eigenvalue with an eigenket (0,1,0). If 1 was measured, the result is the (normalized) projection of $|\psi\rangle$ on V, which equals $\left(1/\sqrt{3}\right)\left(1,0,\sqrt{2}\right)^t$.

Next, L_z is measured. The possible results, and their probabilities, are: 0 is measured with probability 0, 1 is measured with probability $1/3$, and -1 is measured with probability $2/3$.

NOTE: the measurement of L_z^2 does not determine the subsequent measurements of L_z!

• A particle is in a state for which the probabilities are

$$\Pr(L_z = 1) = 1/4, \Pr(L_z = 0) = 1/2, \Pr(L_z = -1) = 1/4.$$

note that the most general state with this property is

$$\left|\psi\right\rangle = \frac{e^{i\delta_1}}{2}\left|L_z = 1\right\rangle + \frac{e^{i\delta_2}}{\sqrt{2}}\left|L_z = 0\right\rangle + \frac{e^{i\delta_3}}{2}\left|L_z = -1\right\rangle$$

does this mean that one can choose arbitrary values of $\delta_1, \delta_2, \delta_3$ without affecting the physical state?

Answer: no. The physical state is immune only to *global* phase shifts: $\left|\psi\right\rangle$ and $e^{i\delta}\left|\psi\right\rangle$ are physically equivalent in the sense that they generate the same probability distribution for *any* observable. However, if for example $\delta_1 = \delta_2 = \delta_3 = 0$, then $\left|\psi\right\rangle = \left|L_x = 1\right\rangle$, and if $\delta_1 = \delta_3 = 0$ and $\delta_2 = \pi$, then $\left|\psi\right\rangle = \left|L_x = -1\right\rangle$.

A Note on the Position, Momentum, and Energy Operators

• We saw that for a state of definite position (delta function) the operator X indeed returns the position, and that for a state of definite momentum (a pure wave, $e^{i(kx-\omega t)}$) the operator P indeed returns the momentum.

• What about the other states? The most we can ask for is that the average of X (P) will be what we consider intuitively to be the average position (momentum). That is indeed the case.

• Let $|\psi\rangle$ be a state. The probability density to be at the position x is $|\psi(x)|^2 = \psi^*(x)\psi(x),$ so the average position is defined by $\int x\psi^*(x)\psi(x)dx,$ but the average of the X operator is defined by

$$\langle X\rangle = \langle\psi|X|\psi\rangle = \langle\psi|X\psi\rangle = \langle\psi|x\psi\rangle = \int x\psi^*(x)\psi(x)dx$$

And they are indeed equal.

Note: if the integration limits are unspecified, they are assumed to be $-\infty$ to $\infty.$

What about the momentum? Remember that the momentum operator is defined by

$$P|\psi\rangle = -i\hbar \left|\frac{d\psi}{dx}\right\rangle$$

and that its eigenkets, with eigenvalues p, are defined by

$$|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}}$$

So the probability for the state ψ to be with momentum p is

$$\left|\langle p|\psi\rangle\right|^2 = \langle p|\psi\rangle\langle\psi|p\rangle$$

So the average momentum is

$$\underbrace{\int p\langle p|\psi\rangle\langle\psi|p\rangle dp}_{I}.$$

We want to prove that this equals the average of the operator P, which is

$$\langle P\rangle = \langle\psi|P|\psi\rangle = \underbrace{(-i\hbar)\int \psi^*\psi' dx}_{II}$$

To prove that $I=II$, note that $\langle p|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int e^{\frac{-ipx}{\hbar}}\psi(x)dx$

Which is just ψ's Fourier transform (up to the $\hbar$ factor). Now, remember that (up to constants which we won't bother with here), the product of the Fourier transform with p is the transform of the derivative; this reduces $p\langle p|\psi\rangle$ in I to the transform of the derivative. Lastly, remember that the Fourier transform is unitary, so the inner product of the transforms equals the inner product of the respective functions. This immediately reduces I to II.

In very much the same way, the Hamiltonian H is the energy operator, and $\langle H \rangle = \langle \psi | H | \psi \rangle$ is the system's average energy.

- Example: Gaussian wave packet

$$|\psi\rangle = \frac{e^{ik_0(x+a)} e^{-(x+a)^2/2\Delta^2}}{\left(\pi\Delta^2\right)^{1/4}}$$

A straightforward calculation yields

- Average position = $\langle \psi | X | \psi \rangle = \int x \psi^* \psi \, dx = -a$

- Average momentum = $\langle \psi | P | \psi \rangle = \left(-i\hbar\right)\int \psi^* \psi' \, dx = k_0 \hbar$

- Average energy = (for a free particle)

$$\langle \psi | H | \psi \rangle = -\frac{\hbar^2}{2m} \int \psi^* \psi'' \, dx =$$

$$\frac{k_0^2 \hbar^2}{2m} + \frac{\hbar^2}{4m\Delta^2}$$

- Question: what happens to the average energy when $\Delta \to 0$, and why? It looks odd that the mass m is in the denominator – can you explain it?

Schrödinger's Equation

$$i\hbar \frac{d}{dt}\big|\psi(t)\big\rangle = H\big|\psi(t)\big\rangle \Rightarrow i\hbar \frac{d}{dt}\big|\psi(t)\big\rangle = -\frac{\hbar^2}{2m}\left|\frac{\partial^2 \psi}{\partial x^2}\right\rangle$$

For a free particle $(H = P^2/2m)$

• Tells us how a state changes over time, hence is very important. Where does it come from? There are various heuristics to justify the equation; for example, suppose a free electron is moving through a crystal, in which the atoms are close to each other:
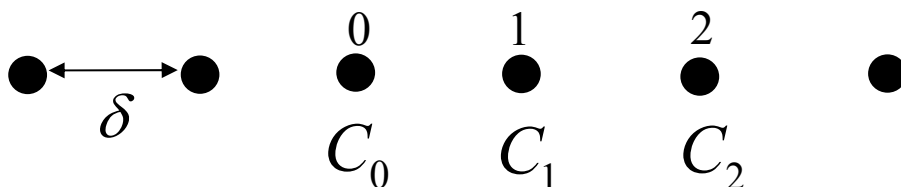
Let C_i be the amplitude to be at atom i at time t. Now look again at the equations for the ammonia molecule. Here, we have three states (if we assume that, as a very short time passes – remember, we're looking at the time derivative – the change in C_1 depends only on it and on C_0, C_2). So we can guess the following equation (up to constants):

$$i\hbar \frac{dC_1}{dt} = E_0 C_1 - A C_0 - A C_2$$

Now, use the well-known approximation for the second derivative at x:

$$f''(x) \approx \frac{f(x-\delta) - 2f(x) + f(x+\delta)}{\delta^2}$$

And thus the right-hand side equals, up to constants, the second derivative of the wave function by x.

• The simplest (and very common) case for a non-free particle has the Hamiltonian

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

Where V is some potential.

• **It is impossible to prove Schrödinger's equation. It does not follow from the axioms.**

Solving Schrödinger's Equation

$$i\hbar \frac{d}{dt}\left|\psi(t)\right\rangle = H\left|\psi(t)\right\rangle, \;\; i\hbar\left|\dot{\psi}\right\rangle = H\left|\psi\right\rangle$$

• This is a differential equation, which resembles equations in classical physics.

• The goal is to find the *propagator* $U(t)$ which satisfies

$$\left|\psi(t)\right\rangle = U(t)\left|\psi(0)\right\rangle.$$

• As often happens, a good direction to proceed is to first find the (normalized) eigenkets and eigenvalues of the Hermitian operator H.

• Since H is the energy operator, we will often denote the eigenkets/eigenvalues with the letter E:

$$H\left|E\right\rangle = E\left|E\right\rangle$$

• Suppose we have these eigenkets/eigenvalues. Since they are orthonormal and span the space, then for every state

$$\left|\psi(t)\right\rangle = \sum_{E}\left|E\right\rangle\left\langle E\middle|\psi(t)\right\rangle \equiv \sum_{E}\left|E\right\rangle a_{E}(t)$$

- Plugging this last form into the equation yields

$$i\hbar \dot{a}_E(t) = E a_E(t) \Rightarrow a_E(t) = a_E(0)e^{-iEt/\hbar}$$

- So, $\langle E | \psi(t) \rangle = a_E(t) = a_E(0)e^{-iEt/\hbar}$

- And

$$\left| \psi(t) \right\rangle = \sum_E a_E(t) \left| E \right\rangle = \sum_E a_E(0)e^{-iEt/\hbar} \left| E \right\rangle =$$

$$\sum_E \left\langle E | \psi(0) \right\rangle e^{-iEt/\hbar} \left| E \right\rangle = \sum_E \left\langle E | \psi(0) \right\rangle \left| E \right\rangle e^{-iEt/\hbar} =$$

$$\left[\sum_E \left| E \right\rangle \left\langle E \right| e^{-iEt/\hbar} \right] \psi(0) \Rightarrow \underline{U(t) = \sum_E \left| E \right\rangle \left\langle E \right| e^{-iEt/\hbar}}$$

- So we have a closed-form expression for the propagator. In the infinite dimensional case, the sum is replaced by an integral.

- The so-called *normal modes,* $\left| E(t) \right\rangle = \left| E \right\rangle e^{-iEt/\hbar}$, are also called *stationary modes,* because they change only by a phase factor, hence have the same probabilities to be in a certain state regardless of the time. They correspond to systems which start off in an eigenket of H (definite energy state).

• Another expression for the propagator is given by

$$U(t) = e^{-iHt/\hbar}$$

But it is not always manageable. Note that it implies that $U(t)$ is a unitary operator.

• Schrödinger's equation on the line is usually solved in the X-basis.

• Note that $U(t)$ is an operator. By $\left|\psi(t)\right\rangle = U(t)\left|\psi(0)\right\rangle$

we mean that $\quad \psi(x,t) = \int_{-\infty}^{\infty} \underbrace{U(x,t;x',0)}_{\text{propagator}} \ \underbrace{\psi(x',0)}_{\text{initial conditions}} \ dx'$

where $\quad U(x,t;x',0) = \sum_{E}\langle x|E\rangle\langle E|x'\rangle e^{-iHt/\hbar}$

Or, in the infinite dimensional case,

$$U(x,t;x',0) = \int_{E} \langle x|E\rangle\langle E|x'\rangle e^{-iEt/\hbar} dE$$

• How does one derive such equations? It's straightforward

from $U(t) = \sum_{E}|E\rangle\langle E|\,e^{-iEt/\hbar}$: multiply by $\langle x|$ on

the left and by $\left|x'\right\rangle$ on the right.

• The propagator as the evolution of simple states: let's look at the equation

$$\psi(x,t) = \int_{-\infty}^{\infty} \underbrace{U(x,t;x',0)}_{\text{propagator}} \ \underbrace{\psi(x',0)}_{\text{initial conditions}} \ dx'$$

And take $\psi(x',0)$ to be a state with definite position, that is, a delta function at a. Then

$$\psi(x,t) = \int_{-\infty}^{\infty} U(x,t;x',0)\delta(x'-a)dx' = U(x,t;a,0)$$

taking $x = b$ yields

$U(b,t;a,0) =$ The amplitude to be in b, at time t, when at $t = 0$ the state is a delta function at a.

• And in general, $U(x,t;x',0)$ is the factor weighing the contribution of the amplitude to be in x' at time 0 to the amplitude to be in x at time t.

Solving Schrödinger's Equation for a Free Particle

• If there's no potential, the equation is relatively simple:

$$i\hbar|\dot{\psi}\rangle = H|\psi\rangle = \frac{P^2}{2m}|\psi\rangle$$

• Is it trivial? Not at all; even for relatively simple initial states, the development of the wave function over time may be surprisingly complicated.

• To solve the equation, first find the eigenkets of *H:*

$$H|E\rangle = \frac{P^2}{2m}|E\rangle = E|E\rangle$$

• The kets $|p\rangle,$, which are eigenstates of *P,* suggest themselves. Remember that

$$|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ipx}{\hbar}}, \qquad P|p\rangle = p|p\rangle$$

and so

$$\frac{P^2}{2m}|p\rangle = \frac{p^2}{2m}|p\rangle = E|p\rangle \Rightarrow p = \pm\sqrt{2mE}$$

Hence for every E there are two corresponding eigenstates:

$$\left|E,+\right\rangle = \left|p = \sqrt{2mE}\right\rangle, \left|E,-\right\rangle = \left|p = -\sqrt{2mE}\right\rangle$$

• Physically, this means that a particle with energy E can be moving to the left or right. But in QM, the following state – which has no meaning in classical mechanics – also exists:

$$\left|E\right\rangle = \alpha\left|p = \sqrt{2mE}\right\rangle + \beta\left|p = -\sqrt{2mE}\right\rangle$$

Note that this is a *single* particle which can be caught moving either left or right!

• The next step is to compute the propagator. In the position eigenkets it equals

$$U(x, t; x', 0) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{ipx/\hbar} e^{-ipx'/\hbar} e^{-ip^2t/2m\hbar} dp$$

$$U(x, t; x', 0) = \int_{E} \langle x | E \rangle \langle E | x' \rangle e^{-iEt/\hbar} dE$$

The integral evaluates to $\left(\dfrac{m}{2\pi\hbar it} \right)^{\frac{1}{2}} e^{im(x-x')^2/2\hbar t}$

and so for an initial state $\psi(x',0)$, the state at time t is

$$\psi(x,t) = \left(\frac{m}{2\pi\hbar it}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{im(x-x')^2/2\hbar t}\,\psi(x',0)\,dx'$$

- What happens if $t \to 0$? We get the integral of a function multiplied by things like $\cos(Ax^2)$, where A is very large:
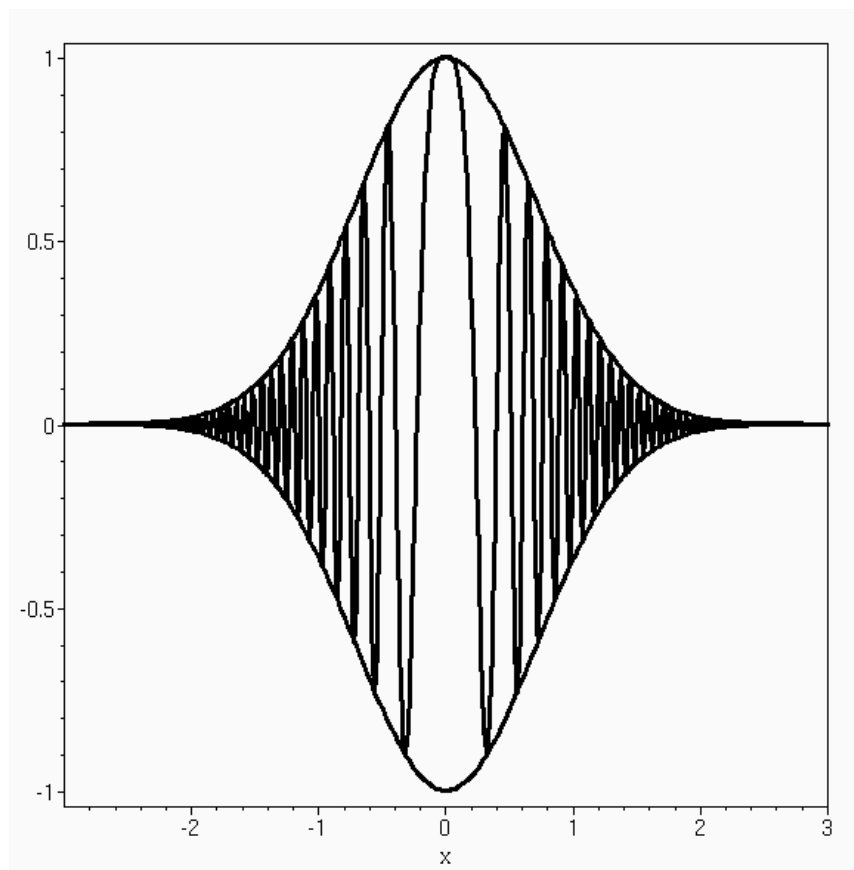
Plot of e^{-x^2} multiplied by $\cos(Ax^2)$. If we integrate, only the value at 0 remains.

Interlude: The Free Particle Propagator in the Momentum (Fourier) Domain

• For a free particle, Schrödinger's equation is

$$i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} \Rightarrow \frac{d\psi}{dt} = \frac{i\hbar}{2m}\frac{d^2\psi}{dx^2}$$

• Switching to the Fourier domain yields

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

• Which is solved by

$$\Psi(u,t) \propto \sqrt{t}\, e^{\frac{ihtu^2}{2m}}\Psi(u,0)$$

• This observation highlights the "convolution nature" of the free particle propagator, and the manner in which it blurs spatially, and sharpens in the frequency (momentum) domain, as time goes on. The convolution kernels are like those in the previous slide.

Interlude: The Density Matrix

• **Expresses the expectation as a linear function of the operator being measured.**

• **Allows to include "usual" uncertainty about the state.**

• **Closely related to Boltzmann distribution and quantum statistical mechanics.**

Let $|u_n\rangle$ be an orthonormal basis. The probability of finding $|\psi(t)\rangle$ in the state $|u_n\rangle$ is $|c_n(t)|^2$, where $|\psi(t)\rangle = \sum_n c_n(t)|u_n\rangle$. If A is an operator, and $A|u_p\rangle = \sum_n A_{np}|u_n\rangle$, then

$$\langle A\rangle_t = \langle\psi(t)|A|\psi(t)\rangle = \sum_{n,p} A_{np} c_n^*(t) c_p(t) = \mathrm{Tr}(\rho(t)A),$$

where $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$ is the density matrix.

Note: $\rho(t)$ is a positive operator, and $\mathrm{Tr}(\rho(t)) = \sum_n c_n(t) c_n^*(t) = 1$. Also, $\rho^2 = \rho$, and $\rho^+ = \rho$ (ρ is Hermitian).

Note: $\rho(t)$ does not have an arbitrary phase factor, hence it captures the physically relevant properties.

From the Schroedinger equation, it follows immediately that

$$\dot{\rho}(t) = \frac{1}{i\hbar}[H, \rho(t)].$$

- **Reminder – what is the probability to obtain a value a_n when measuring A (at time t)?**

Answer: Let P_n be the projection on the subspace of eigenvectors with eigenvalue a_n. It is immediate that the probability to obtain a_n is

$$\langle \psi(t) | P_n | \psi(t) \rangle = \mathrm{Tr}\left(\rho P_n \right).$$

- **Incorporating "classical" uncertainty: suppose the starting conditions of a physical system are not exactly known, and that it has probability p_k to be in state $| \psi_k \rangle$ $(p_k \geq 0, \sum_k p_k = 1)$. Then, the density matrix can be naturally extended by defining**

$$\rho = \sum_k p_k | \psi_k \rangle \langle \psi_k |$$

And linearity immediately proves that the expected value of an operator A is $\mathrm{Tr}(\rho A)$.

- **Some further properties:**

- ρ **is Hermitian.**

- $\mathrm{Tr}(\rho)=1$.

- $\rho^2=\left(\sum_k p_k|\psi_k\rangle\langle\psi_k|\right)^2=\sum_{k,l}p_k p_l\langle\psi_k|\psi_l\rangle|\psi_k\rangle\langle\psi_l|$,

  and since $\{u_n\}$ is an orthonormal basis, $\mathrm{Tr}(\rho^2)=$

  $\sum_n\langle u_n|\rho^2|u_n\rangle=\sum_{n,k,l}p_k p_l\langle\psi_k|\psi_l\rangle\langle u_n|\psi_k\rangle\langle\psi_l|u_n\rangle=$

  $\sum_{k,l}p_k p_l\langle\psi_k|\psi_l\rangle\langle\psi_l|\psi_k\rangle=\sum_{k,l}p_k p_l\left|\langle\psi_k|\psi_l\rangle\right|^2\le$

  $\sum_{k,l}p_k p_l=1$, with equality holding only if all

  of the ψ's are identical (i.e. a "pure state").

- **The meaning of** ρ_{nn} **is the probability to obtain** $|u_n\rangle$ **in a measurement. It is termed "population", while** ρ_{np} **are termed "coherence".**

- **If we're working in the basis of eigenstates of the Hamiltonian** H**, then from the equation for the development of** ρ_{np} **over time, it follows immediately that**

$\rho_{np}(t)=\exp\left(\dfrac{i}{\hbar}(E_p-E_n)t\right)\rho_{np}(0)$.

• **Relation to quantum statistical mechanics: in thermodynamic equilibrium, it turns out that** $\rho = \dfrac{1}{Z}\exp\left(-\dfrac{H}{kT}\right)$, **where k is Boltzmann's constant and T the temperature. Z is chosen so to normalize the trace to 1 (it is the <u>partition function</u>). If $|E_n\rangle$ is the basis of H's eigenstates, then**

$$\rho_{nn} = \frac{1}{Z}\langle u_n|\exp\left(-\frac{H}{kT}\right)|u_n\rangle = \frac{1}{Z}\exp\left(-\frac{E_n}{kT}\right),$$

and $n \neq p \Rightarrow \rho_{np} = 0$

(Boltzmann's distribution).

Path Integrals: Feynman's Formulation of QM

$$U(x,t;x',0) \propto \sum e^{iS[x(t)]/\hbar}$$

Where the summation ranges over all paths connecting $(x',0)$ to (x,t), and S is the classical action (the integral over $x(t)$ of the kinetic minus potential energy).

• What does this mean?

• The classical path is the one with the smallest action. In Feynman's formulation, the propagator is the sum of *all* paths, each weighted by the exponent of i times the action over $\hbar$. What happens for objects with a large mass, for example, is that due to the $\hbar$ in the denominator, the contributions around any path but the classical one are in very different phases and therefore cancel out.

• This formulation is equivalent to the one we had shown, but highlights the connection to classical physics. Also, in some cases (but not usually) it is easier to use it to calculate the propagator.

• Proof of the path integral formulation: look at the propagator with a fixed potential V. Proceeding much like as in the free particle case, this time $|p\rangle$ is an eigenstate with energy $p^2/2m + \mathrm{V}$, so the propagator is

$$U(t) = \int\limits_{-\infty}^{\infty} |p\rangle\langle p| e^{-iE(p)t/\hbar}\, dp =$$

$$\int\limits_{-\infty}^{\infty} |p\rangle\langle p| e^{-i\left(p^2/2m+\mathrm{V}\right)t/\hbar}\, dp =$$

$$e^{-i\mathrm{V}t/\hbar} \int\limits_{-\infty}^{\infty} |p\rangle\langle p| e^{-i\left(p^2/2m\right)t/\hbar}\, dp =$$

$$\left(\frac{m}{2\pi\hbar it}\right)^{\frac{1}{2}} e^{-i\mathrm{V}t/\hbar} e^{im(x-x')^2/2\hbar t}$$

since the integral is exactly the one for the free particle

propagator. Now, if the elapsed time is very small, Δt

(this is the justification for assuming a fixed potential),

and $v(x)$ stands for speed in the interval between x and

x', this equals

$$\left(\frac{m}{2\pi\hbar i(\Delta t)} \right)^{\frac{1}{2}} e^{-iV(x)(\Delta t)/\hbar} e^{imv^2(x)(\Delta t)/2\hbar}$$

Using the postulates in Part I, we compute the amplitude of getting from $(x',0)$ to (x,t) as the sum of the amplitudes of all different paths (think of more and more screens with more and more slits). For every path, the amplitude is the product of amplitudes to go over its sub - paths. In the limit the sub - paths go to zero, and we get the product of the above, following the postulate about the amplitude of events in succession. so the powers in the exponents add to $(i/\hbar)\int_0^t \left(\frac{mv^2(x)}{2} - V(x) \right) dt = (i/\hbar)S[x(t)]$,

which completes the proof *. It turns out that this formulation is equivalent to Schrodinger's.

* up to a scale factor - see following.

• Derivation of the free particle propagator via path integrals:

$$\psi(x,T) = \int_{-\infty}^{\infty} U(x,T;x',0)\psi(x',0)dx' =$$

$$\int_{-\infty}^{\infty}\left[\sum_{\substack{x(0)=x'\\x(T)=x}} e^{\frac{i}{\hbar}S[x(t)]}\right]\psi(x',0)dx' = \int_{-\infty}^{\infty}\left[\sum_{\substack{x(0)=x'\\x(T)=x}} e^{\frac{i}{\hbar}\int_0^T \frac{m}{2}\dot{x}^2(t)dt}\right]\psi(x',0)dx' =$$

$$\int_{-\infty}^{\infty}\left[\sum_{\substack{x(0)=0\\x(T)=0}} e^{\frac{mi}{2\hbar}\int_0^T\left[\dot{x}(t)+\frac{x-x'}{T}\right]^2 dt}\right]\psi(x',0)dx'$$

$$\left(\begin{array}{c}\text{using the fact that the transformation } x(t) \rightarrow x(t) + x' + \dfrac{x-x'}{T}\, t \text{ maps}\\[2mm]\text{the loops starting and ending at 0 to the paths from } x' \text{ to } x\end{array}\right)$$

$$\int_{-\infty}^{\infty}\left[\sum_{\substack{x(0)=0\\x(T)=0}} e^{\frac{mi}{2\hbar}\int_0^T\left[\dot{x}^2(t)+\underbrace{2\left(\frac{x-x'}{T}\right)\dot{x}(t)}_{\substack{\text{integrates}\\\text{to }0,\text{ since}\\x(0)=x(T)}}+\underbrace{\left(\frac{x-x'}{T}\right)^2}_{\substack{\text{independent}\\\text{of }t,\text{ hence}\\\text{integrates to}\\\frac{(x-x')^2}{T}}}\right]dt}\right]\psi(x',0)dx' =$$

$$\underbrace{\left[\sum_{\substack{x(0)=0\\x(T)=0}} e^{\frac{mi}{2\hbar}\int_0^T\dot{x}^2(t)dt}\right]}_{\text{Propagator from 0 to 0}}\underbrace{\int_{-\infty}^{\infty}\left[e^{\frac{mi(x-x')^2}{2\hbar T}}\right]\psi(x',0)dx'}_{\text{Compare to slide 96}}$$

Path Integral Normalization Factor

• The question arises as to how to normalize the summation over all paths.

• Approximate each path by a piecewise linear function:
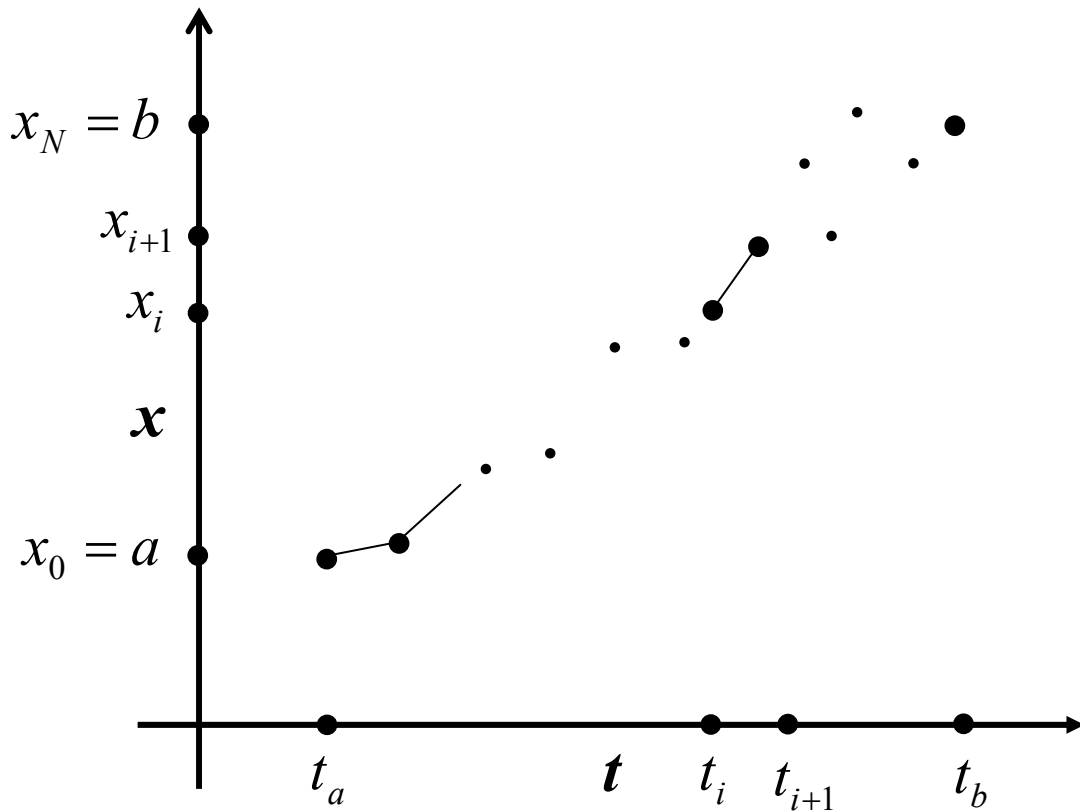
Denote $\varepsilon = t_{i+1} - t_i$, so $N\varepsilon = t_b - t_a \equiv T$.

The free particle propagator is then

(A is a normalizing factor)

$$A \lim_{\varepsilon \to 0} \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}...\int\limits_{-\infty}^{\infty} \exp\left(\frac{i}{\hbar} \sum_{j=1}^{N} \int_{x_{j-1}}^{x_j} \frac{m}{2} \dot{x}^2 dt \right) dx_1...dx_{N-1} \cong$$

$$A \lim_{\varepsilon \to 0} \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}...\int\limits_{-\infty}^{\infty} \exp\left(\frac{mi}{2\varepsilon\hbar} \sum_{j=1}^{N} (x_j - x_{j-1})^2 \right) dx_1...dx_{N-1}$$

which follows immediately by replacing $\dot{x}$ with $\dfrac{x_j - x_{j-1}}{\varepsilon}$.

The Gaussian integral evaluates to

$$AN^{-\frac{1}{2}} \left(\frac{m}{2\hbar\varepsilon i} \right)^{-\frac{N-1}{2}} \pi^{\frac{N-1}{2}} e^{\frac{mi}{2\hbar T}(x_N - x_0)^2}$$

comapring this with the free particle propagator, it must equal

$$\left(\frac{m}{2\pi i \hbar T} \right)^{\frac{1}{2}} e^{\frac{mi}{2\hbar T}(x_N - x_0)^2} . \text{So, } A = \left(\frac{m}{2\pi\hbar i \varepsilon} \right)^{\frac{N}{2}}.$$

It is customary to write the path integral as

$$\lim_{\varepsilon \to 0} \frac{1}{B} \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}...\int\limits_{-\infty}^{\infty} e^{(i/\hbar)S_{cl}[b,a]} \frac{dx_1}{B} \frac{dx_2}{B} ... \frac{dx_{N-1}}{B}, \quad B = \left(\frac{2\pi\hbar i \varepsilon}{m} \right)^{\frac{1}{2}}.$$

Equivalence to Schrödinger's Equation

For an infinitesimal time interval ε, the path integral propagator $U(x,\varepsilon;x',0)$ is approximately

$$\left(\frac{m}{2\pi\hbar i\varepsilon}\right)^{\frac{1}{2}}\exp\left\{i\left[\frac{m(x-x')^2}{2\varepsilon}-\varepsilon V\left(\frac{x+x'}{2},0\right)\right]\middle/\hbar\right\}$$

where the approximations are standard to the first order in ε. Note that there is no external normalizing factor, since there is no midpoint to integrate over. So, $\psi(x,\varepsilon)$ should be

$$\left(\frac{m}{2\pi\hbar i\varepsilon}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty}\exp\left(\frac{im\eta^2}{2\varepsilon\hbar}\right)\exp\left[-\frac{i\varepsilon}{\hbar}V\left(x+\frac{\eta}{2},0\right)\right]\psi(x+\eta,0)d\eta$$

where $\eta = x' - x$. When $\dfrac{im\eta^2}{2\varepsilon\hbar} \geq \pi$, the exponent oscillates very rapidly, so we'll concentrate on the region $|\eta| \leq \left(\dfrac{2\varepsilon\hbar\pi}{m}\right)^{\frac{1}{2}}$.

This means that if we're working to first order in ε, we should work to second order in η.

The integral to compute for $\psi(x,\varepsilon)$ is

$$\int_{-\infty}^{\infty}\exp\left(\frac{im\eta^2}{2\varepsilon\hbar}\right)\exp\left[-\frac{i\varepsilon}{\hbar}V\left(x+\frac{\eta}{2},0\right)\right]\psi(x+\eta,0)d\eta$$

Expanding to first order in ε

$$\psi(x+\eta,0)=\psi(x,0)+\eta\frac{\partial\psi}{\partial x}+\frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2}$$

$$\exp\left[-\frac{i\varepsilon}{\hbar}V\left(x+\frac{\eta}{2},0\right)\right]=1-\frac{i\varepsilon}{\hbar}V(x,0)\text{ (we neglect}$$

terms or order $\eta\varepsilon$, since they're $O(\varepsilon^{3/2})$). The integral

is $\left(\dfrac{m}{2\pi\hbar i\varepsilon}\right)^{\frac{1}{2}}\displaystyle\int_{-\infty}^{\infty}\exp\left(\dfrac{im\eta^2}{2\varepsilon\hbar}\right)\left[\psi(x,0)-\dfrac{i\varepsilon}{\hbar}V(x,0)\psi(x,0)+\right.$

$\left.\eta\dfrac{\partial\psi}{\partial x}+\dfrac{\eta^2}{2}\dfrac{\partial^2\psi}{\partial x^2}\right]d\eta$ (again, $\eta\varepsilon$ etc. terms are dropped).

This is a Gaussian integral in η. Eventually we get

$$\psi(x,\varepsilon)-\psi(x,0)=\frac{-i\varepsilon}{\hbar}\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,0)\right]\psi(x,0)$$

which indeed agrees with Schrodinger's equation
prediction.

Calculating the Path Integral

Usually, it's impossible. For potentials of the form $V = a + bx + cx^2 + d\dot{x} + e\dot{x}x$, the propagator can be computed by expanding around the classical path. Write the path $x(t)$ as $x_{cl}(t) + y(t)$. Since $x(t)$ and $x_{cl}(t)$ agree at the endpoints, $y(0) = y(T) = 0$. So

$$U(x,t;x',0) = \int_0^0 \exp\left\{\frac{i}{\hbar}S[x_{cl}(t) + y(t)]\right\}\mathrm{D}[y(t)]$$

When expanding S, the linear terms vanish, since $x_{cl}(t)$ is an extremum. Also, $\exp\left(\frac{i}{\hbar}S_{cl}\right)$ factors out. So, the

integral equals $\exp\left(\frac{i}{\hbar}S_{cl}\right) \times$

$$\underbrace{\int_0^0 \exp\left[\frac{i}{\hbar}\int_0^T\left(\frac{1}{2}m\dot{y}^2(t) - cy^2(t) - ey(t)\dot{y}(t)\right)dt\right]\mathrm{D}[y(t)]}_{\text{Depends only on } T}$$

Note that the probabilistic information about the wave function can still be extracted, since for a given T we know the function up to a scale factor.

How to compute

$$\int_0^0 \exp\left[\frac{i}{\hbar}\int_0^T\left(\frac{1}{2}m\dot{y}^2(t)-cy^2(t)-ey(t)\dot{y}(t)\right)dt\right]D[y(t)]?$$

For example, for the harmonic oscillator it equals

$$\int_0^0 \exp\left\{\frac{i}{\hbar}\int_0^T\frac{m}{2}\left[\dot{y}^2(t)-\omega^2 y^2(t)\right]dt\right\}D[y(t)] \quad \text{(where } y(0)=y(T)$$

$= 0)$. Represent $y(t)$ as $\displaystyle\sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi t}{T}\right) \equiv \sum_{n=1}^{\infty} a_n y_n$. It is easy to

see that $\displaystyle\int_0^T\left[\dot{y}^2(t)-\omega^2 y^2(t)\right]dt = \sum_{n=1}^{\infty} a_n^2\left[\frac{\pi^2 n^2}{2T}-\frac{\omega^2 T}{2}\right]$. Going to

this representation, and forgetting for the moment about the

Jacobian and other constants, the integral is the infinite

product of the Gaussian integrals $\displaystyle\int_{-\infty}^{\infty}\exp\left(\frac{i}{\hbar}a_n^2\left[\frac{\pi^2 n^2}{2T}-\frac{\omega^2 T}{2}\right]\right)da_n$,

or (forgetting $i, \hbar, \pi...$) $\displaystyle\prod_{n=1}^{\infty}\left[\frac{\pi^2 n^2}{T}-\omega^2 T\right]^{-\frac{1}{2}} =$

$$\prod_{n=1}^{\infty}\left[\left(\frac{\pi^2 n^2}{T}\right)\left(1-\frac{\omega^2 T^2}{\pi^2 n^2}\right)\right]^{-\frac{1}{2}} = K(T)\prod_{n=1}^{\infty}\left(1-\frac{\omega^2 T^2}{\pi^2 n^2}\right)^{-\frac{1}{2}} =$$

$K(T)\left[\dfrac{\sin(\omega T)}{\omega T}\right]^{-\frac{1}{2}}$. Normalization is possible since we know

the limit as $\omega \to 0$ (it's the free particle propagator).

Perturbation Theory and Feynman Diagrams

$$U(x,T;x',0) = \int_{x',0}^{x,T} \exp\left\{\frac{i}{\hbar}\int_0^T \left[\frac{m}{2}\dot{x}^2(t) - V[x(t)]\right]dt\right\}\mathrm{D}x[t]$$

expand the exponent to write the integrand as

$$\exp\left[\frac{i}{\hbar}\int_0^T \frac{m}{2}\dot{x}^2 dt\right] - \frac{i}{\hbar}\exp\left[\frac{i}{\hbar}\int_0^T \frac{m}{2}\dot{x}^2 dt\right]\int_0^T V(x)dt + ...$$

Integrating over all paths, the first summand is just the free particle propagator. To calculate the second summand, look at the discrete approximation (ignoring ε etc.) :

$$\int_{-\infty}^{\infty}...\int_{-\infty}^{\infty}\exp\left\{\frac{mi}{2\hbar}\left[(x_1 - x_0)^2 + ... + (x_N - x_{N-1})^2\right]\right\}\times$$

$$\left[V(x_0) + ... + V(x_N)\right]dx_1...dx_{N-1}$$

To compute the summand with $V(x_j)$, note that in the limit, if we assume bounded variation, then since the time between any two successive x_i goes to zero, $x_{i+1} - x_i \to 0$ as well, and we can drop the terms with $\exp\left\{\frac{mi}{2\hbar}\left[(x_j - x_{j-1})^2 + (x_{j+1} - x_j)^2\right]\right\}$ which goes to 1. We're left with the product of free particle propagators from 0 to t_j and from t_j to T. When this consideration is extended to all summands, we have two variables to integrate over : the time τ and the location at that time, denote it y. So, the integral equals

$$U_1(x,T;x',0) \equiv \int_0^T \int_{-\infty}^{\infty} U_0(x,T;y,\tau)V(y)U_0(y,\tau;x',0)dy\,d\tau$$

where U_0 is the free particle propagator.

The physical meaning is : the particle propagates freely from $(x',0)$ to (y,τ), is then acted upon (scattered) by the potential, and then propagates freely to (x,T). In the same manner, the third summand corresponds to a particle scattered twice by the potential (represented by a quadruple integral), etc. U_1 (U_2) (a "first (second) order perturbation") is represented by the following *Feynman diagram:*
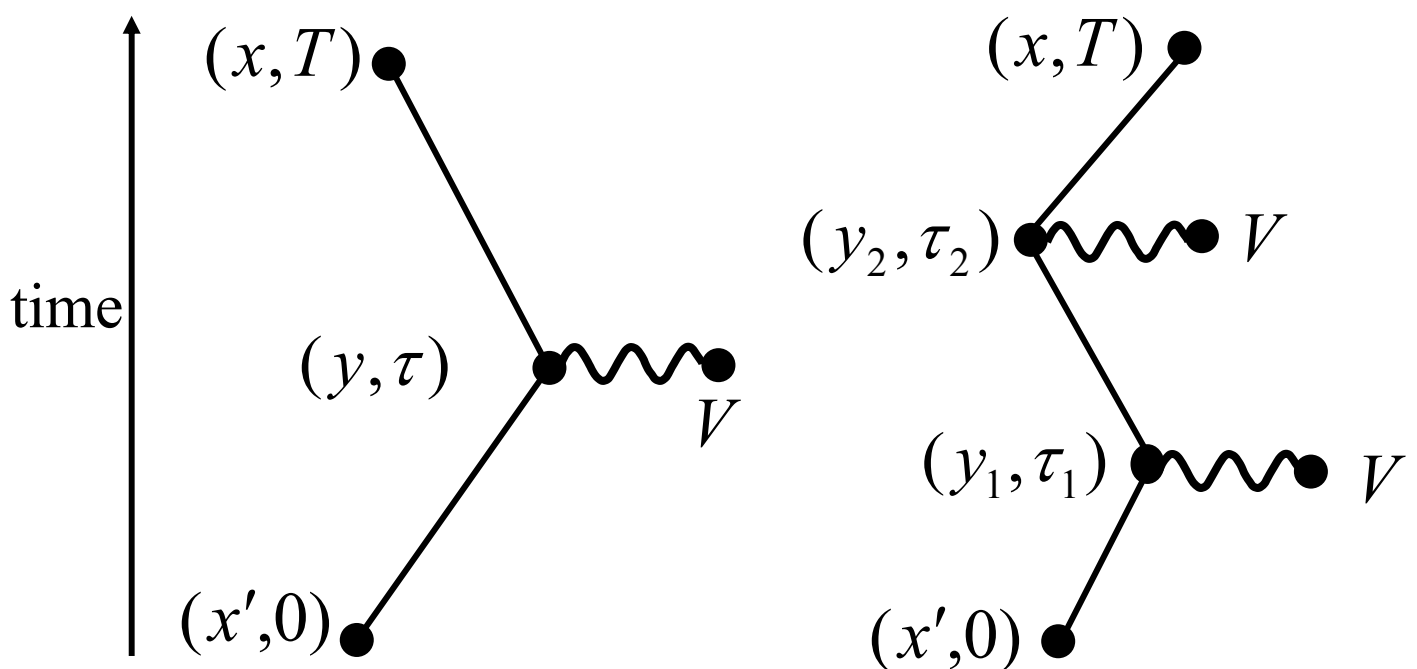
The second order perturbation equals

$$\frac{1}{2!}\left(-\frac{i}{\hbar}\right)^2 \exp\left[\frac{i}{\hbar}\int_0^T \frac{m}{2}\dot{x}^2 dt\right]\left[\int_0^T V[x(s),s]ds\right]\left[\int_0^T V[x(s'),s']ds'\right]$$

which equals

$$\left(-\frac{i}{\hbar}\right)^2 \int_0^T \int_{-\infty}^{\infty}\int_0^{\tau_2}\int_{-\infty}^{\infty} U_0(x,T;y_2,\tau_2)V(y_2)U_0(y_2,\tau_2;y_1,\tau_1)V(y_1)$$

$$U_0(y_1,\tau_1;x',0)dy_1 d\tau_1 dy_2 d\tau_2$$

Note that the $1/2!$ factor (and, in general, the $1/n!$ factor) vanished, because the integral is carried over the set $\tau_1 \le \tau_2$. It is customary to assume that $\tau_2 < \tau_1 \Rightarrow U(?,\tau_2;?,\tau_1) = 0$, which allows to replace τ_2 in the quadruple integral above by T, and the same for higher orders.

In General

$$U_k(x,T;x',0) = \int_0^T \int_{-\infty}^{\infty} U_0(x,T;y,\tau)V(y)U_{k-1}(y,\tau;x',0)dyd\tau$$

and it is easy to deduce from the expansion of the exponent the integral equation : $U(x,T;x',0) = U_0(x,T;x',0) -$

$$\frac{i}{\hbar}\int_0^T \int_{-\infty}^{\infty} U_0(x,T;y,\tau)V(y)U(y,\tau;x',0)dyd\tau$$

A Path Integral Formulation for the Density Matrix

Noting the similarity between the quantum mechanics propagator and the density matrix

$$U(x_2,t_2;x_1,t_1)=\sum_k \exp\left(\frac{-i}{\hbar}E_k(t_2-t_1)\right)\langle x_2|E_k\rangle\langle E_k|x_1\rangle$$

$$\rho(x_2,x_1)=\sum_k \exp\left(-\beta E_k\right)\langle x_2|E_k\rangle\langle E_k|x_1\rangle$$

One sees that the procedure for evaluating a path integral for the propagator can be used to evaluate a path integral expression for the density matrix:

$$\rho(x_2,x_1)=\int \exp\left(-\frac{1}{\hbar}\int_0^{\beta\hbar}\left[\frac{m}{2}\dot{x}^2(u)+V(x(u))\right]du\right)Dx(u)$$

where the integration is over all "paths" such that $x(\beta\hbar)=x_2$, $x(0)=x_1$.

Evolution of a Gaussian Packet

If the initial state is a Gaussian wave function

$$|\psi(x',0)\rangle = \frac{e^{ip_0 x'/\hbar}\, e^{-x^2/2\Delta^2}}{\left(\pi\Delta^2\right)^{1/4}}$$

then a direct integration yields

$$|\psi(x,t)\rangle = \left[\pi^{1/2}\left(\Delta + \frac{i\hbar t}{m\Delta}\right)\right]^{\frac{1}{2}} e^{\left[\frac{-(x-p_0 t/m)^2}{2\Delta^2\left(1+i\hbar t/m\Delta^2\right)}\right]} e^{\left[\frac{ip_0}{\hbar}\left(x - \frac{p_0 t}{2m}\right)\right]}$$

with the probability density

$$\Pr(x,t) = \frac{1}{\sqrt{\pi}\left(\Delta^2 + \hbar^2 t^2/m^2\Delta^2\right)^{1/2}} e^{\frac{-\left[(x-(p_0 t/m)\right]^2}{\Delta^2 + \hbar^2 t^2/m^2\Delta^2}}$$

• The mean position at time t is $p_0 t/m$ (like the classical case).

• The uncertainty in position grows from $\Delta/\sqrt{2}$ at time 0

to $\dfrac{\Delta}{\sqrt{2}}\left(1 + \dfrac{\hbar^2 t^2}{m^2\Delta^4}\right)^{\frac{1}{2}}$ at time t.

Position uncertainty =

$$\frac{\Delta}{\sqrt{2}} \left(1 + \frac{\hbar^2 t^2}{m^2 \Delta^4} \right)^{\frac{1}{2}} \approx \frac{\hbar t}{\sqrt{2} m \Delta} \quad \text{for large } t$$

This can be viewed as t times the initial uncertainty in the velocity.

• Note also that the uncertainty in position grows very slowly – especially for a heavy particle.

• Note that there is a non-zero probability for the particle to "go backwards", that is, be captured at the opposite direction in which it is "generally moving".

• The Gaussian packet has an "average" velocity, associated with the motion of its center. This is the so-called "group velocity".

• Let a (stationary) packet be defined by

$$\psi(x,0) = \int_{-\infty}^{\infty} g(k)e^{ikx}\,dk \equiv \int_{-\infty}^{\infty} |g(k)|e^{i(\alpha(k)+kx)}\,dk$$

where $\alpha(k)$ is the phase of $g(k)$. Assume that $|g(k)|$ has a strong peak at k_0, then the integral can be approximated by

$$\int_{k_0-\Delta k}^{k_0+\Delta k} |g(k)|e^{i(\alpha(k_0)+(k-k_0)\alpha'(k_0)+kx)}\,dk$$

This wave packet has a peak at the location in which the phases of the exponentials change the slowest, since then they interfere the least. This occurs for the x at which the derivative of the phase by k is zero, that is, $x_0 = -\alpha'(k_0)$.

• If the packet is moving, we have

$$\psi(x,t) = \int_{-\infty}^{\infty} |g(k)|e^{i(\alpha(k)+kx-\omega(k)t)}\,dk$$

So the packet's center is at $x_0(t) = -\alpha'(k_0) + \omega'(k_0)t$

and its "group velocity" is $\omega'(k_0)$.

Operator Power Series for the Propagator

- We saw that the propagator for a free particle can be expressed as

$$e^{-iHt/h} = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{iht}{2m}\right)^n \frac{d^{2n}}{dx^{2n}} \Rightarrow |\psi(x,t)\rangle = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{iht}{2m}\right)^n \frac{d^{2n}|\psi(x,0)\rangle}{dx^{2n}}$$

- Sometimes, this can be used to compute $|\psi(x,t)\rangle$.

An apparent counterexample

$$|\psi(x,0)\rangle = \begin{cases} \sin\left(\dfrac{\pi x}{L}\right) & |x| \le \dfrac{L}{2} \\ 0 & \text{otherwise} \end{cases}$$

It appears as if the spread of the wave function is not growing over time, because all the derivative are nonzero only at the interval $|x| \le L/2$. How is this possible?

The operator power series doesn't converge (at the boundaries).

Look more carefully at

$$|\psi(x,t)\rangle = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{iht}{2m}\right)^n \frac{d^{2n}|\psi(x,0)\rangle}{dx^{2n}}$$

You can try and sum a few of the first terms, and obtain a reasonable approximation, if the higher derivative don't diverge and if t is small enough.

• But one has to be cautious: look at a particle moving under the influence of a force f. The Hamiltonian is then (assuming we fix all constants to obtain a simple form):

$$H = \frac{d^2}{dx^2} + fx \Rightarrow H^n|\psi\rangle = \left(\frac{d^2}{dx^2} + fx\right)^n |\psi\rangle$$

The calculation of this operator is tricky because the operators of second derivative and multiplication by x do not commute!

Solving Schrödinger's Equation for a Particle in a Box

• For a particle under the influence of a potential $V(x)$, the states of definite energy satisfy

$$\left(\frac{P^2}{2m} + V(x)\right)|\psi\rangle = E|\psi\rangle \Rightarrow |\psi''\rangle = -\frac{2m(E - V(x))}{\hbar^2}|\psi\rangle$$

• Next, we solve it for a particle bounded by an infinite potential ("walls") on both sides:

$$V(x) = \begin{cases} 0 & |x| \le \dfrac{L}{2} \\ \infty & \text{otherwise} \end{cases}$$
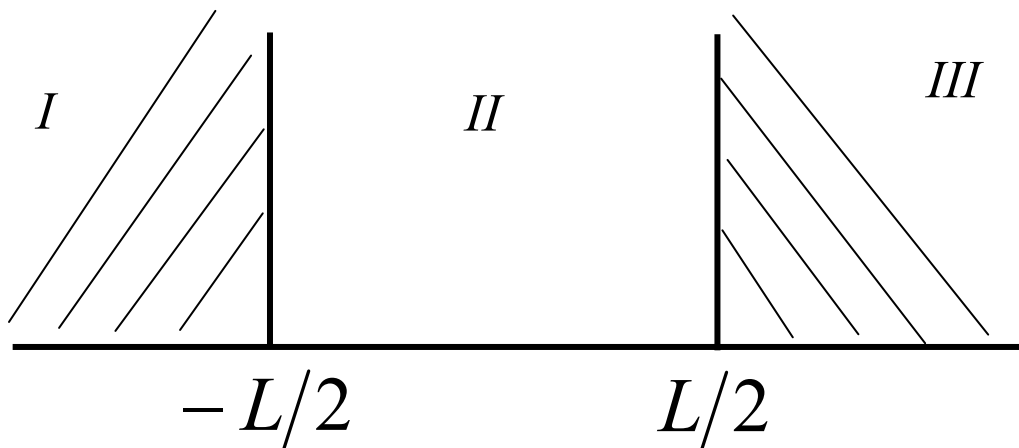
• In regions *I* and *III*,

$$\left|\psi''\right\rangle = -\frac{2m(E-V(x))}{\hbar^2}\left|\psi\right\rangle \Rightarrow \left|\psi''\right\rangle \approx V_0\left|\psi\right\rangle, V_0 \to \infty$$

• So the solutions are

$$\left|\psi\right\rangle = Ae^{\sqrt{V_0}x} + Be^{-\sqrt{V_0}x}$$

• In region *III*, for example, the $Ae^{\sqrt{V_0}x}$ part is not physically allowed, as it diverges to infinity. Only the $Be^{-\sqrt{V_0}x}$ part is allowed, but as $V_0 \to \infty$, the solution is zero. Same holds for region *I*.

• So the solution can be non-zero only in region *II*. The equation there is

$$\left|\psi''\right\rangle = -\frac{2mE}{\hbar^2}\left|\psi\right\rangle \equiv \left|\psi''\right\rangle = -k^2\left|\psi\right\rangle \Rightarrow$$
$$\left|\psi\right\rangle = A\cos(kx) + B\sin(kx)$$

• *Boundary conditions:* $\psi(L/2) = \psi(-L/2) = 0.$

• It immediately follows that the (normalized) solutions are

$$
|\psi_n\rangle = \begin{cases} \left(\dfrac{2}{L}\right)^{\frac{1}{2}} \cos\left(\dfrac{n\pi x}{L}\right) & n = 1,3,5... \\[2em] \left(\dfrac{2}{L}\right)^{\frac{1}{2}} \sin\left(\dfrac{n\pi x}{L}\right) & n = 2,4,6... \end{cases}
$$

• There is no solution corresponding to $n = 0,$ since it equals 0.

• The energy (E) corresponding to $|\psi_n\rangle$ is $E_n = \dfrac{\hbar^2 \pi^2 n^2}{2mL^2}$.
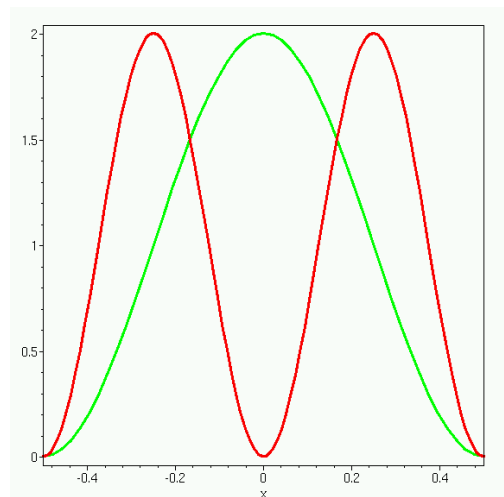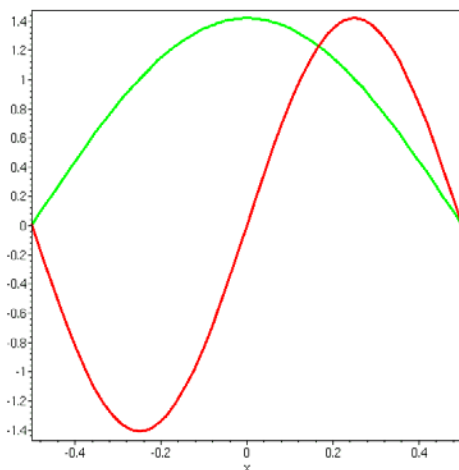
First (green) and second (red) states: left=amplitude, right=probability.

• *There is no state with definite energy 0!*

• A state with energy 0 would violate the uncertainty principle:

• The particle is bound between $-L/2$ and $L/2$, so the position uncertainty is bounded by $L/2$.

$$\Delta X \leq \frac{L}{2}, \Delta X \Delta P \geq \frac{\hbar}{2} \Rightarrow \Delta P \geq \frac{\hbar}{L} \Rightarrow (\Delta P)^2 \geq \frac{\hbar^2}{L^2}$$

• We must have $\langle P \rangle = 0$, else the particle will drift away to infinity, but that's impossible, as it is bound in the box. But

$$(\Delta P)^2 = \langle P - \langle P \rangle \rangle^2 = \langle P \rangle^2 \geq \frac{\hbar^2}{L^2}$$

• What about the average energy? We know that

$$\langle E \rangle^2 = \langle H \rangle^2 = \frac{\langle P \rangle^2}{2m} \geq \frac{\hbar^2}{2mL^2}$$

While the lowest energy level is obtained when $n = 1$ and it equals $\hbar^2 \pi^2 / 2mL^2$ (the *ground state energy*). The uncertainty principle can sometimes be applied to find a rough estimate of the ground state energy.

Example Question (Shankar, 5.2.1):

• A particle is in the ground state in a box of length *L*. Suddenly the box expands to twice its size. What is the probability to find the particle in the ground state of the new box?

• Answer: the two ground state are

$$\left\{ \begin{array}{ll} g_1 = \left(\dfrac{2}{L}\right)^{\frac{1}{2}} \cos\left(\dfrac{\pi x}{L}\right) & \text{small box} \\[4mm] g_2 = \left(\dfrac{1}{L}\right)^{\frac{1}{2}} \cos\left(\dfrac{\pi x}{2L}\right) & \text{big box} \end{array} \right\}$$

And the probability to find g_1 in g_2 is

$$\left(\int_{-L/2}^{L/2} g_1^* g_2 \, dx\right)^2 = \left(\frac{8}{3\pi}\right)^2 \approx 0.72$$

SHOW MAPLE FILE HERE

Development in time of probability amplitude, at $t = 0$ the state is $(\psi_1 + \psi_2)/\sqrt{2}$ (ordering is raster)
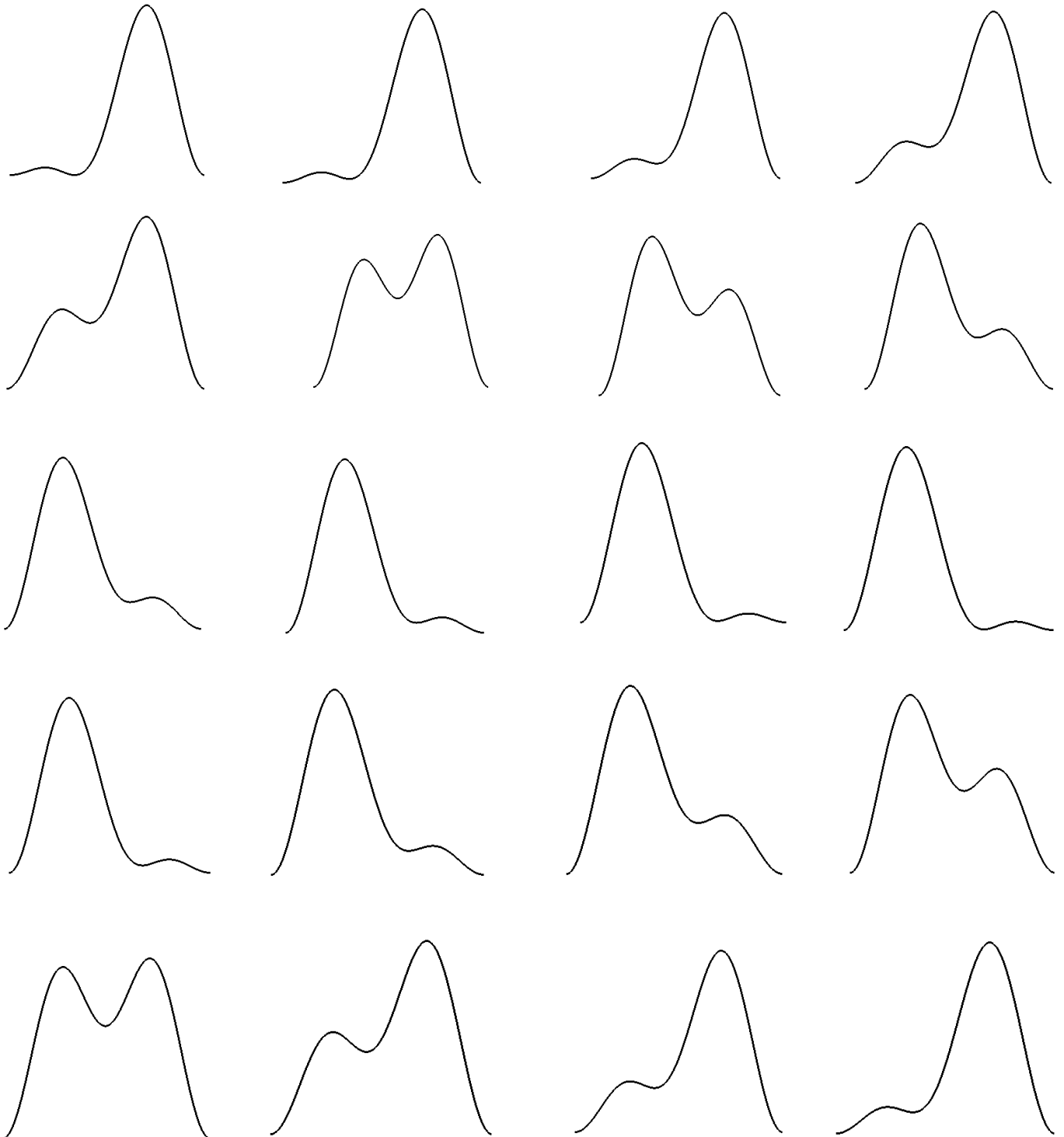
Quantization of Energy

• We saw that the energy levels of the particle in a box are *quantized.*

• A particle which is bound by a potential from escaping to infinity is said to be in a *bound state.*

Formally, $\lim_{x \to \pm\infty} \psi(x) = 0.$

• It turns out that the energy levels of a bound particle are always quantized.

• Why? Look again at Schrödinger's Equation:

$$\left| \psi'' \right\rangle = -\frac{2m(E - V(x))}{\hbar^2} \left| \psi \right\rangle$$

• Assume that $V(x)$ is everywhere bounded. It follows that both ψ and ψ' are continuous. Assume also that there's a bounded region (a "well") in which the particle's energy is larger than the (fixed) potential, but that outside the well the potential is greater than the energy:

$$\left|\psi''\right\rangle = -\frac{2m(E - V(x))}{\hbar^2}\left|\psi\right\rangle$$

I

V > E

$$\left|\psi''\right\rangle = c_I \left|\psi\right\rangle, c_I > 0$$

Solution is sum of rising and decreasing exponentials

II

V < E

$$\left|\psi''\right\rangle = -c_{II}\left|\psi\right\rangle, c_{II} > 0$$

Solution is sum of sines and cosines

III

V > E

$$\left|\psi''\right\rangle = c_{III}\left|\psi\right\rangle, c_{III} > 0$$

Solution is sum of rising and decreasing exponentials
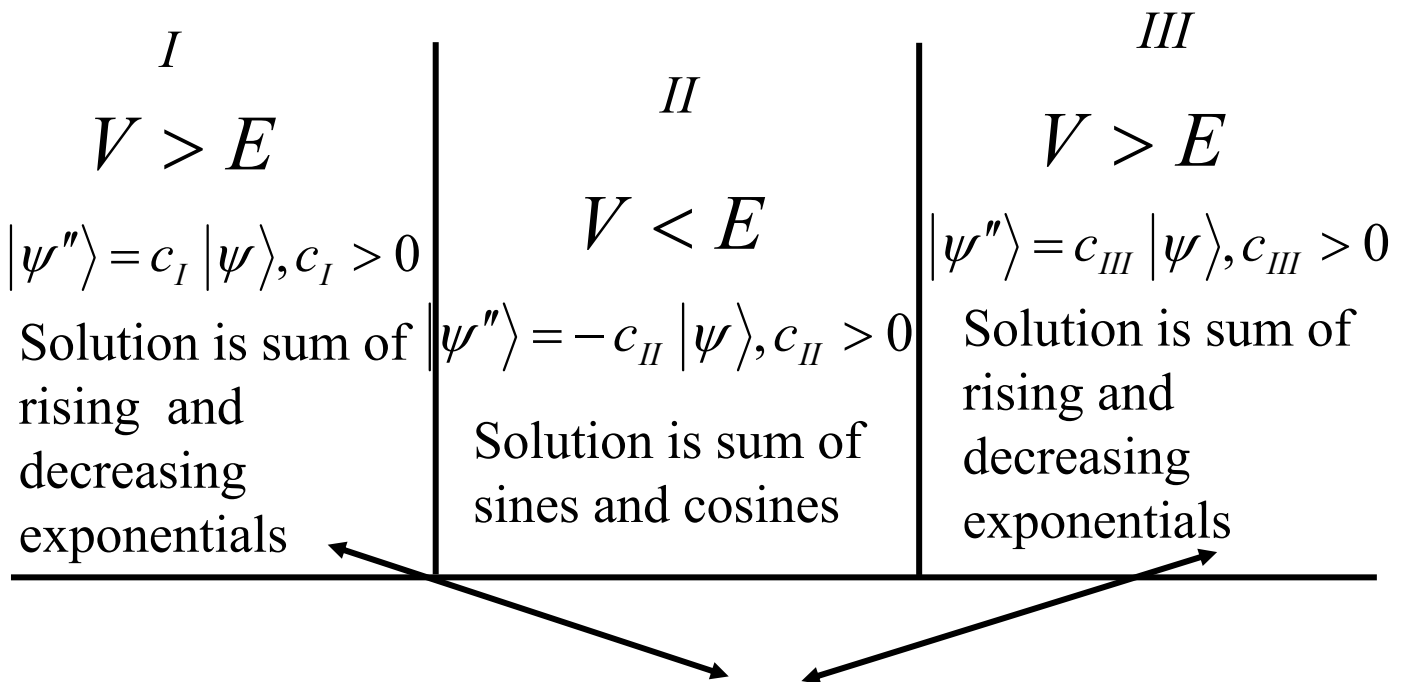
But one of them has to be zero because the rising exponentials go to infinity as $\left|x\right| \rightarrow \infty$.

• So we're left with one parameter (degree of freedom) for each of regions *I* and *III,* and two d.o.f for *II*. We have four constraints – the continuity of the function and its derivatives at each of the borders (just like splines). It appears that we can solve for every *E*; but note that there is a redundancy for multiplying by a scalar, hence we really have 3 d.o.f and four constraints – so there will be a solution only for "special" cases. This is why the energy levels for a bound state are quantized. This argument can be extended to any finite potential. If the potential is infinite (particle in a box) we have to enforce only the continuity of the function, not the derivative.

Finite Potential Well

• Like particle in a box, but the walls are lowered to a finite height: we'll assume the energy to be E_0, which is smaller than V_0.

$x = -a$ $x = a$

$$I \qquad\qquad II \qquad\qquad III$$

$$V_0$$

$$k_2 = \sqrt{\frac{2m(V_0 - E_0)}{\hbar^2}} \qquad\qquad k_2 = \sqrt{\frac{2m(V_0 - E_0)}{\hbar^2}}$$

$$k_1 = \sqrt{\frac{2mE_0}{\hbar^2}}$$
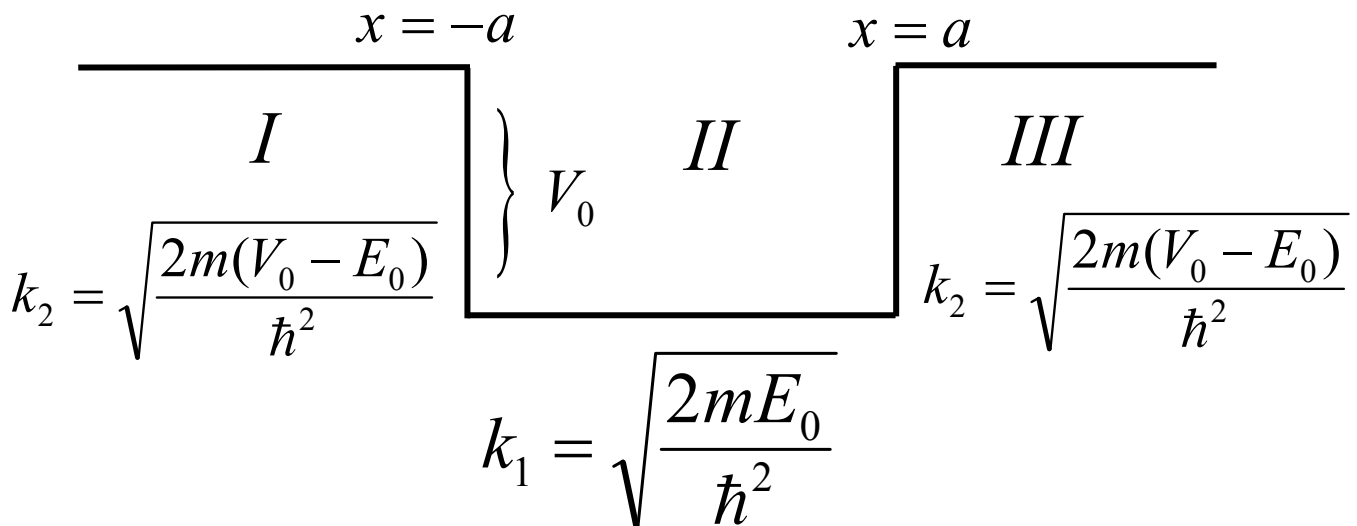
• The solution has the form

$$\begin{cases} \text{region } I: & Ae^{k_2 x} \\ \text{region } II: & Be^{ik_1 x} + Ce^{-ik_1 x} \\ \text{region } III: & De^{-k_2 x} \end{cases}$$

• As noted, enforcing continuity of the function and its derivative yields four equations in A, B, C, D, but these can be solved only up to a scale factor, hence the system is overdetermined and can be solved only for special values of energy. The resulting equations are transcendental and don't have a closed-form solution.

The Probability Current

• For particles, or classical flux, the *current* is the amount of something crossing, say, a unit area during unit time.

• In QM, it makes sense to talk about the *probability current*. If many particles are present, it will be equivalent to the classical definition.

• The probability current is defined for a one-dimensional particle as the amount of probability crossing over: how did the probability to find the particle to the right of x_0 change between time t_0 and $t_0 + \Delta t$?
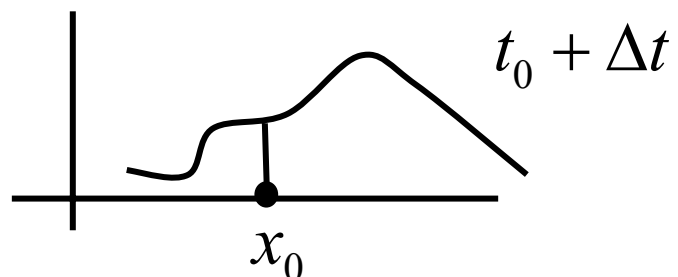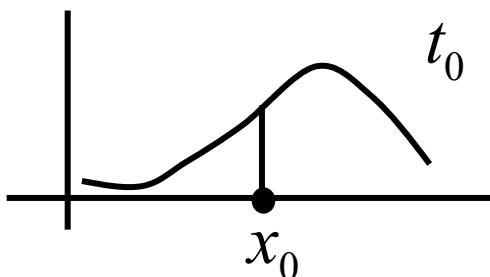
- The probability change is

$$\int_{x_0}^{\infty} \Pr(x, t_0 + \Delta t)dx - \int_{x_0}^{\infty} \Pr(x, t_0)dx =$$

$$\int_{x_0}^{\infty} [\Pr(x, t_0 + \Delta t) - \Pr(x, t_0)]dx \approx \Delta t \left[\int_{x_0}^{\infty} \frac{\partial \Pr(x, t_0)}{\partial t} dx \right]$$

- Assume that there's a function J such that

$$\frac{\partial \Pr}{\partial t} = -\frac{\partial J}{\partial x}$$

Then the probability change is $J\Delta t$, and J is therefore the probability current.

- A straightforward application of Schrödinger's Equation yields

$$J = \frac{\hbar}{2mi} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right)$$
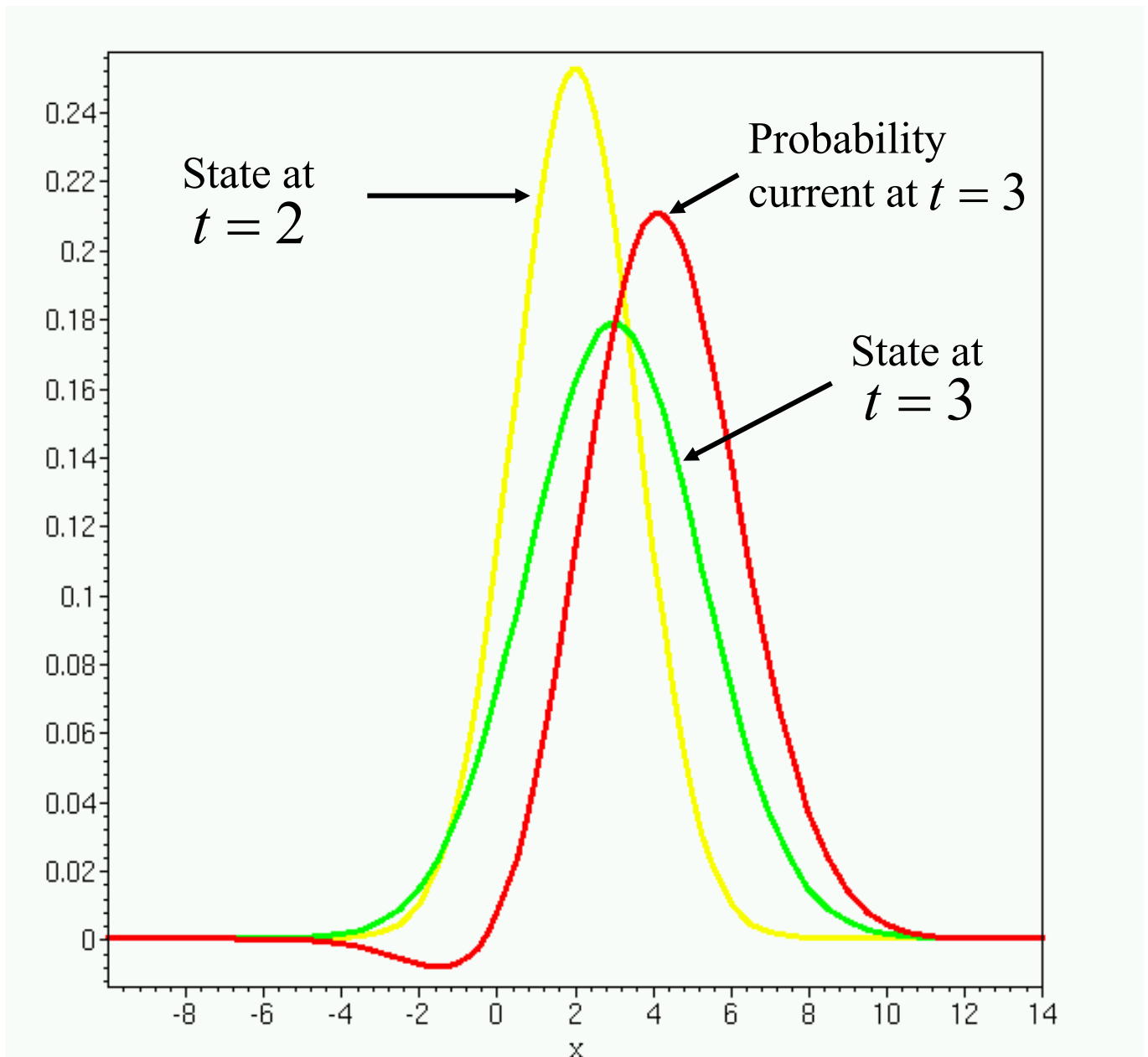
- Initial state: Gaussian packet centered at 0, moving to the right at unit speed.

- Why is the current negative at certain points?

- Because the packet is moving to the right, but is also *expanding!* So there's an area in which the probability to the left of x is increasing.

- For the right moving wave packet

$$Ae^{\frac{i}{\hbar}\left(px - \frac{p^2}{2m}t\right)} = Ae^{\frac{i}{\hbar}(px - Et)}$$

- The probability current is

$$J = |A|^2 \frac{p}{m}$$

- Intuitively, this is true because p/m is the speed of the packet, and the packet is uniform, so the current depends only on the speed.

- It can also be immediately verified that current for two such wave packets moving at the opposite directions is

$$J = \left(|A|^2 - |B|^2\right)\frac{p}{m}$$

Where A,B are the coefficients of the right and left moving packets.

Introduction to Scattering

When a classical particle hits a potential barrier, it either passes it (if its energy is higher than the barrier's energy), or is reflected (if its energy is lower). The situation in QM is rather different.

- Start by considering a **step barrier**

incoming

ψ_I

V_0

$t = 0$

$x = 0$

transmitted

reflected

ψ_T

ψ_R

$t \gg 0$
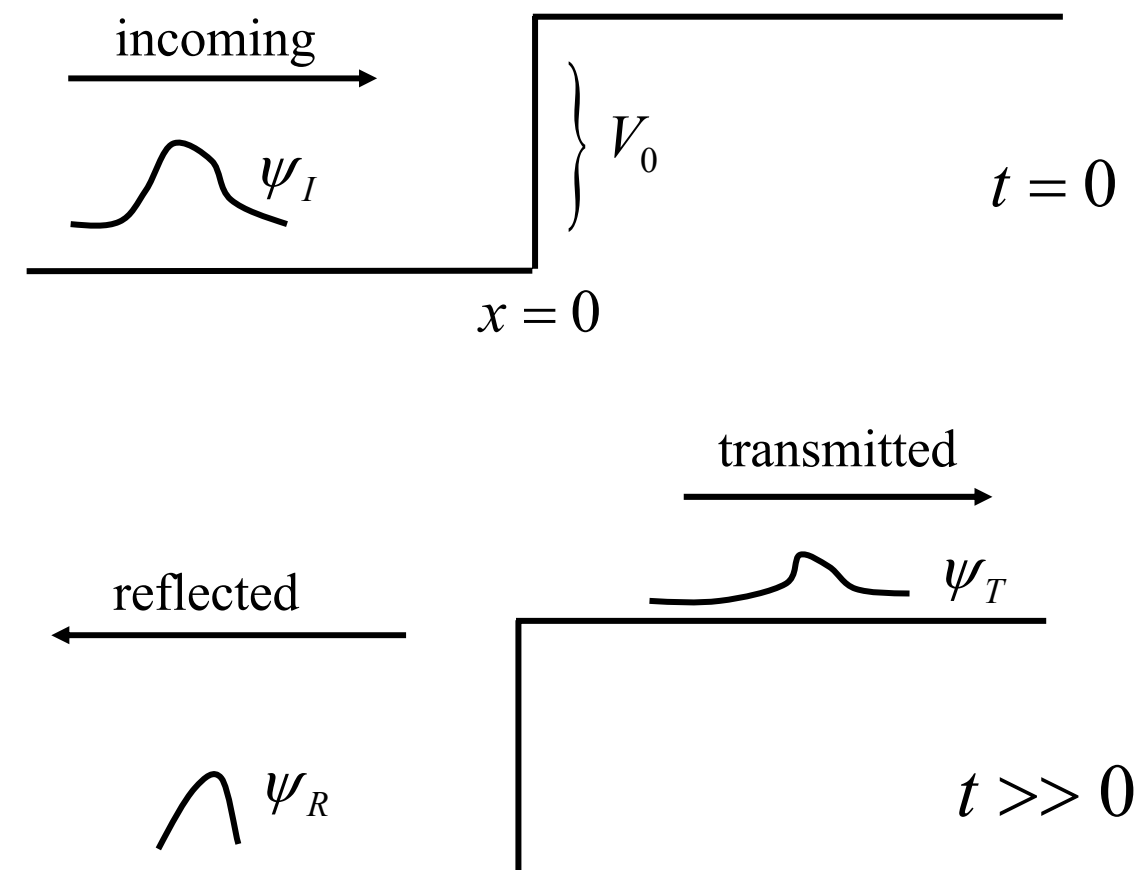
An incoming packet hits the barrier and disintegrates into a left and right going packets.

Straightforward Solution

• Find the basis of the normalized eigenstates of the step potential Hamiltonian.

• Project the initial wave function on that basis.

• Propagate each of the basis functions in time (with the corresponding coefficient).

• As the time tends to infinity, identify the right and left moving components.

It turns out that, under certain assumptions, a much simpler method can be used – which is rooted in classical optics, and in the wave-particle duality.

• The problem can be solved in principle for any packet, but it is impossible to obtain a closed-form expression for the solution.

• Often, one is interested in cases in which the incoming wave is very wide, and therefore has a sharp peak in momentum space.

• In that case, it is possible to derive the ratio of the reflected and transmitted parts with relative ease by essentially reducing it to a *stationary* problem, dependent only on the energy.

• The main trick is to look at *all* the components – incoming, reflected, and transmitted – as coexisting, and to measure the ratio of their probability currents. The justification is: if the incoming wave is very wide, it is impossible to tell when it hits the barrier.

• We'll assume that k_0 is the wave number of the incoming packet, hence its energy and momentum are

$$\text{energy} = E_0 = \hbar k_0^2 / 2m$$

$$\text{momentum} = \hbar k_0$$

And its stationary state behaves like $e^{ik_0 x}$.

- The reflected part has the same wave number (and frequency, of course) as the incoming wave. The transmitted part has a wave number k_1 which must satisfy

$$E_0 - V_0 = \hbar k_1^2 / 2m \Rightarrow k_1 = \sqrt{k_0^2 - \frac{2mV_0}{\hbar^2}}$$

- So, we have the following situation:

$$A e^{ik_0 x}$$

$$B e^{-ik_0 x}$$

$$C e^{ik_1 x}$$

$$x = 0$$
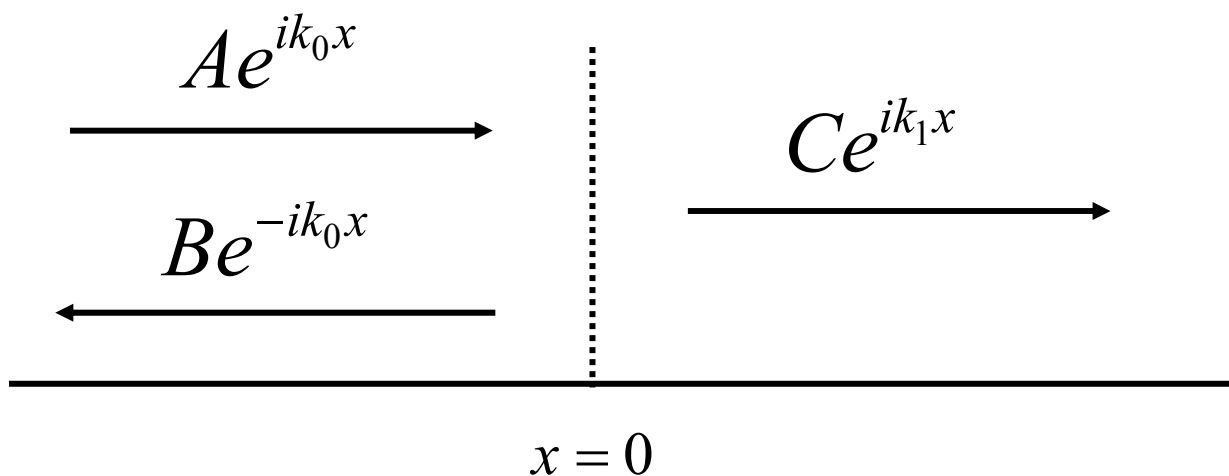
- We can find A,B,C up to a scale factor because the function and its derivatives are continuous at 0:

$$\frac{B}{A} = \frac{k_0 - k_1}{k_0 + k_1}, \quad \frac{C}{A} = \frac{2k_0}{k_0 + k_1}$$

- The currents associated with incoming, reflected, and transmitted are $|A|^2 \hbar k_0 / m, |B|^2 \hbar k_0 / m, |C|^2 \hbar k_1 / m.$

So, the probabilities are:

$$T = \frac{|C|^2 k_1}{|A|^2 k_0} = \frac{|C|^2}{|A|^2} \sqrt{\frac{E_0 - V_0}{E_0}} \qquad R = \frac{|B|^2}{|A|^2} = 1 - T$$

for transmitted   for reflected

Tunneling

- What happens if $V_0 > E_0$?
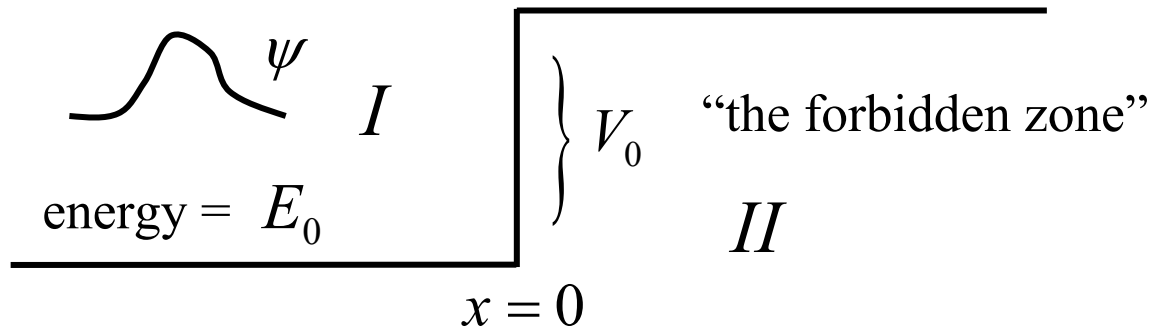
- The solution to Schrödinger's Equation in the forbidden zone is

$$\psi'' + \frac{2m(E_0 - V_0)}{\hbar^2}\psi = 0 \Rightarrow$$

$$\psi \propto e^{-k_2 x}, \, k_2 = \sqrt{\frac{2m(V_0 - E_0)}{\hbar^2}}$$

If $k_1 = \sqrt{2mE_0 / \hbar^2}$, the solutions are
$$\begin{cases} \text{region } I : \; Ae^{ik_1 x} + Be^{-ik_1 x} \\ \text{region } II : \qquad\quad Ce^{-k_2 x} \end{cases}$$

where $\begin{cases} \dfrac{B}{A} = \dfrac{k_1 i + k_2}{k_1 i - k_2} \Rightarrow \left|\dfrac{B}{A}\right|^2 = 1 \\[4mm] \dfrac{C}{A} = \dfrac{2k_1 i}{k_1 i - k_2} \Rightarrow \left|\dfrac{C}{A}\right|^2 = \dfrac{4k_1^2}{k_1^2 + k_2^2} \end{cases}$

• It is immediate to see that the probability current going into the right half is zero; yet – some particles manage to escape into it.

• How can this happen? It seems to violate energy conservation!

• From the uncertainty principle, conservation of energy is violated *only if we can measure this violation.* The position uncertainty for the particle in the forbidden zone is very small (a decreasing exponential), hence the uncertainty in momentum is large enough – and it doesn't allow the measuring process to determine that energy conservation was violated.

• So, a particle can break into the forbidden zone (although it cannot go too far into it). If the potential drops again to zero, the particle can escape through the barrier and then it is free (like some particles escaping from a nucleus).
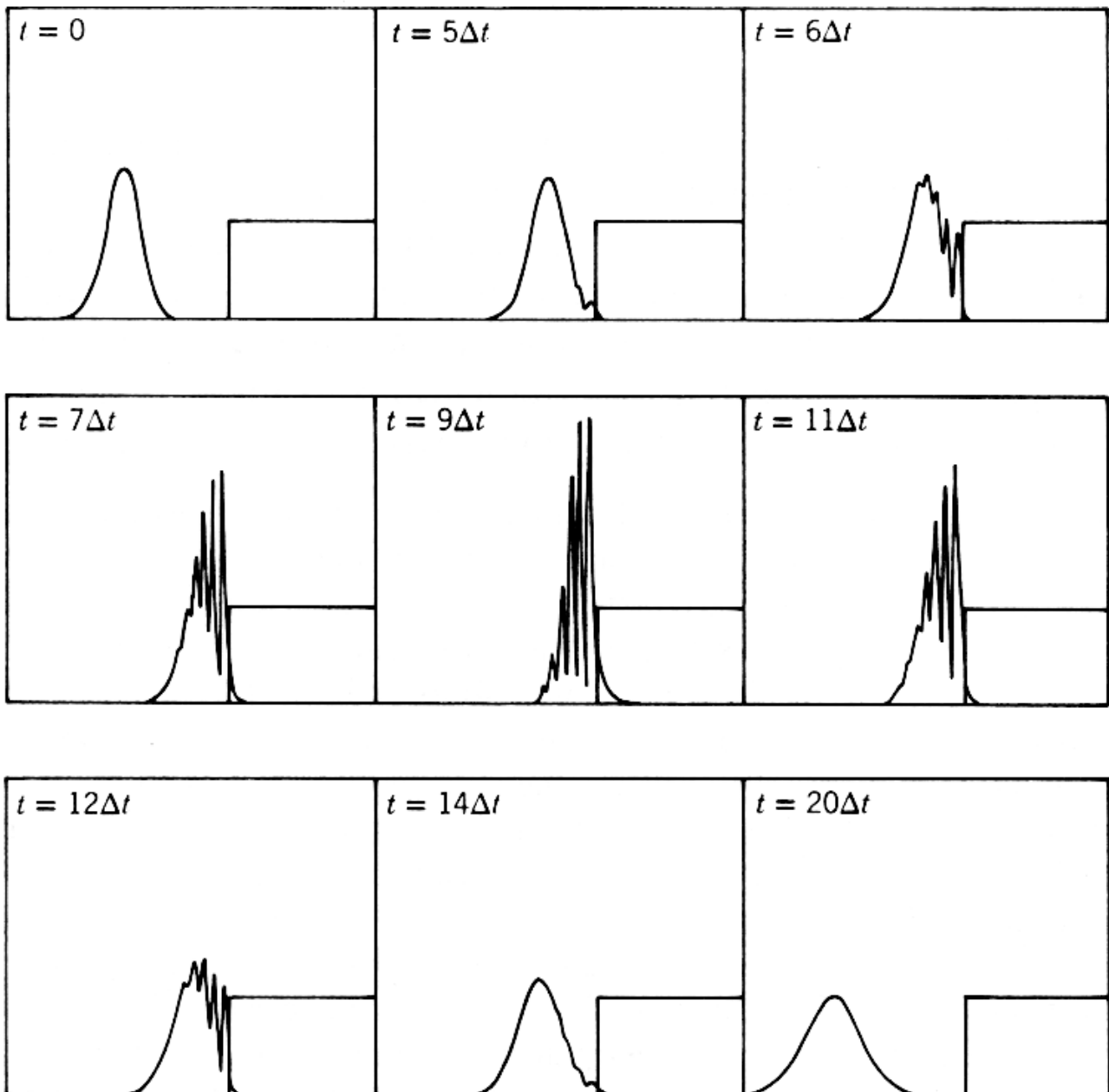
A 1D particle hitting a step with a potential higher than the particle's energy. Note short penetration into the forbidden zone.
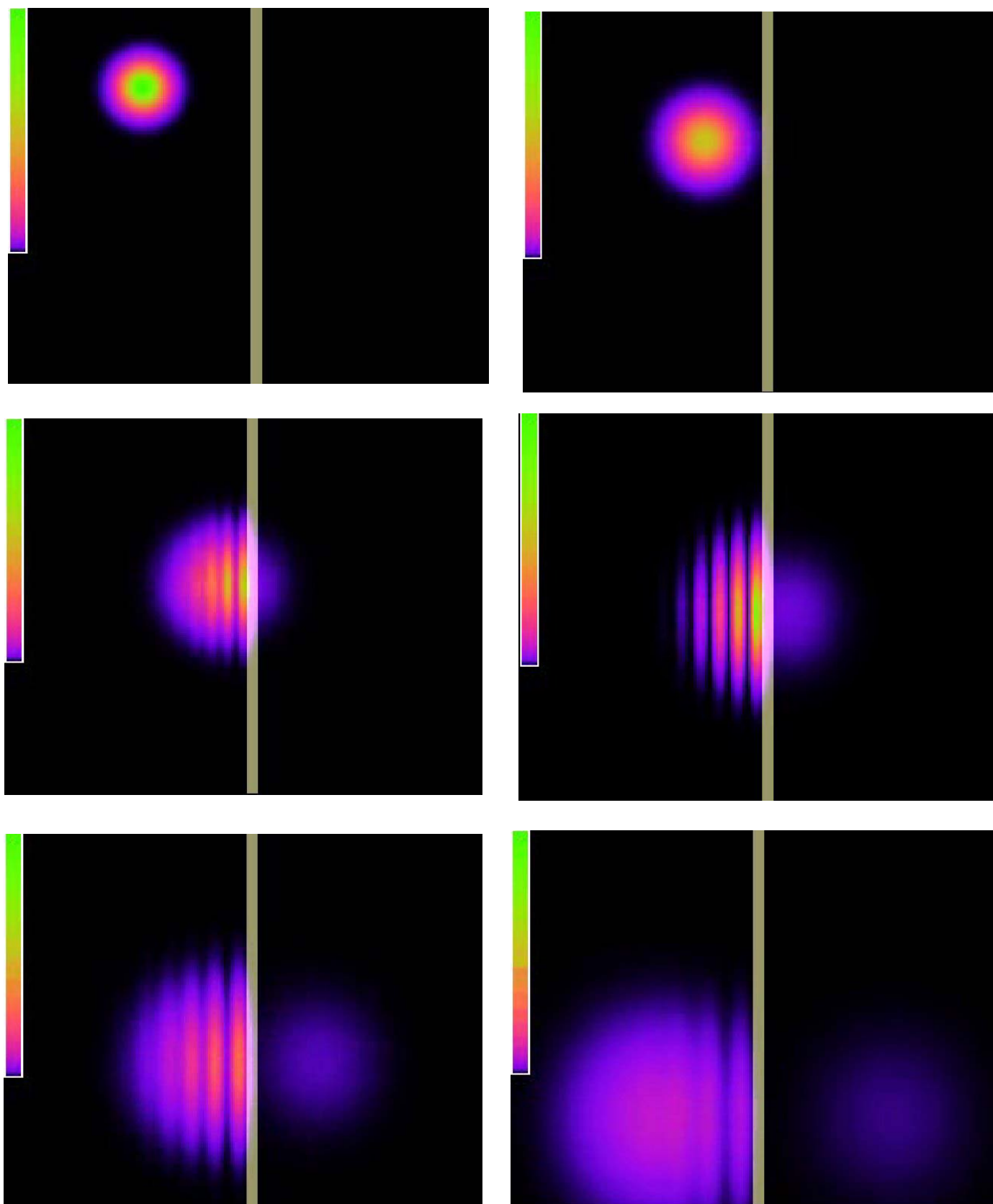
Tunneling: a 2D particle hitting a barrier. The
probability amplitude is depicted.

Potential Barrier

Incoming
(energy $= E_0$)

$V_0 > E_0$

II

I V_0

III

$x = -a$ $x = a$
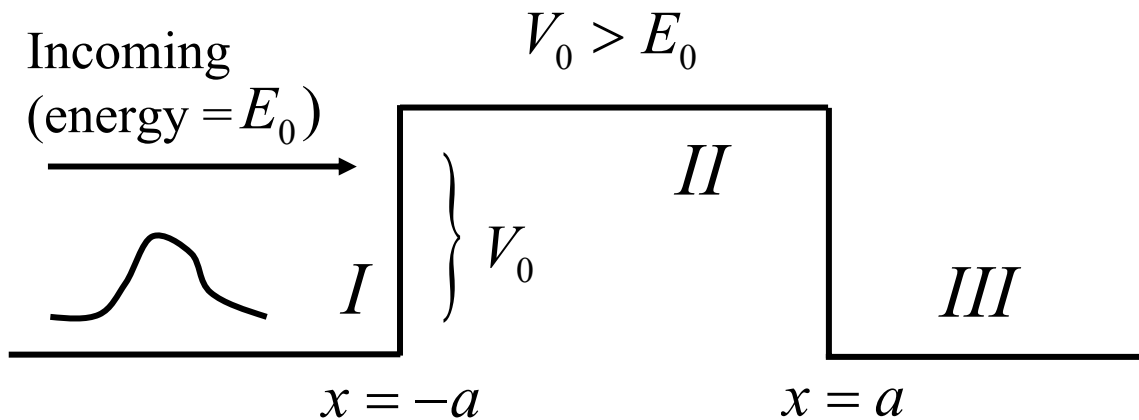
- In *I*, $\psi = Ae^{ik_0x} + Be^{-ik_0x}$, $k_0 = \sqrt{2mE_0/\hbar^2}$

- In *II*, $\psi = Ce^{k_1x} + De^{-k_1x}$, $k_1 = \sqrt{2m(V_0 - E_0)/\hbar^2}$

- In *III*, $\psi = Ee^{ik_0x}$

- As before, enforcing the function and its derivative to be continuous at $x = \pm a$ yields four equations, which can be solved up to a scale factor, and then

$$T = \left|\frac{E}{A}\right|^2 = \frac{1}{\cosh^2(2k_1a) + \alpha^2 \sinh^2(2k_1a)}$$

$$\alpha = \frac{V_0 - 2E_0}{\sqrt{4E_0(V_0 - E_0)}}$$

Scattering off a potential barrier. Horizontal axis is E/V_0, vertical axis is T. Scales are chosen so that

$$2mV_0a^2 = 9\hbar^2$$

(following Eisberg & Resnick, p. 202). Lower is detail of upper; note that T is equal to 1 at certain energies (strange, because we can have *more* transmission at a *lower* energy!).
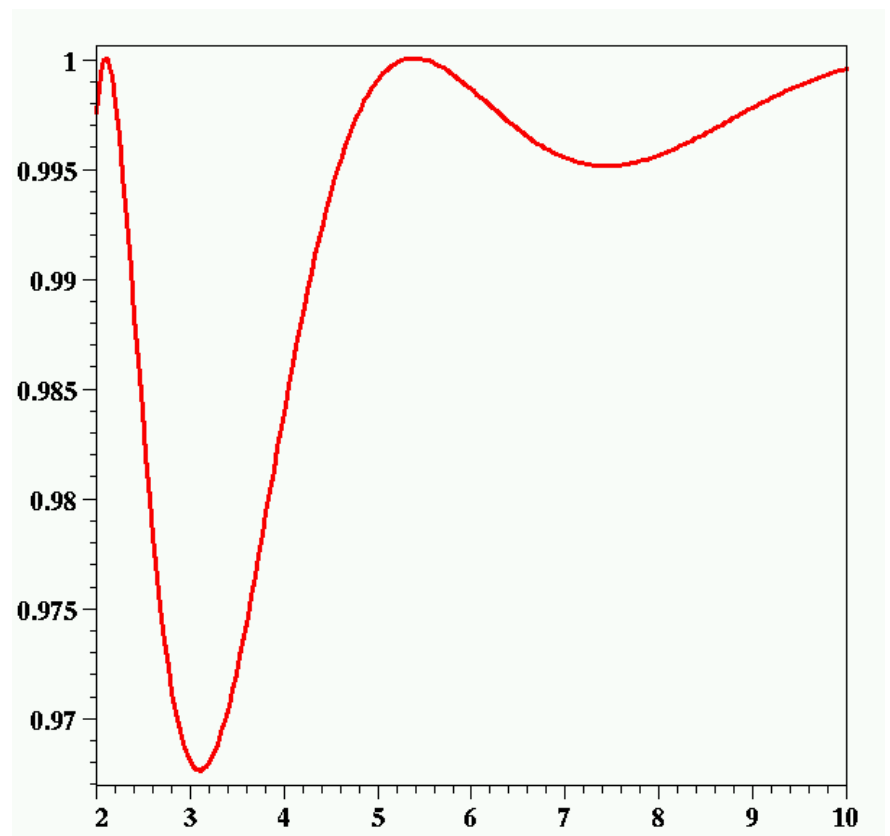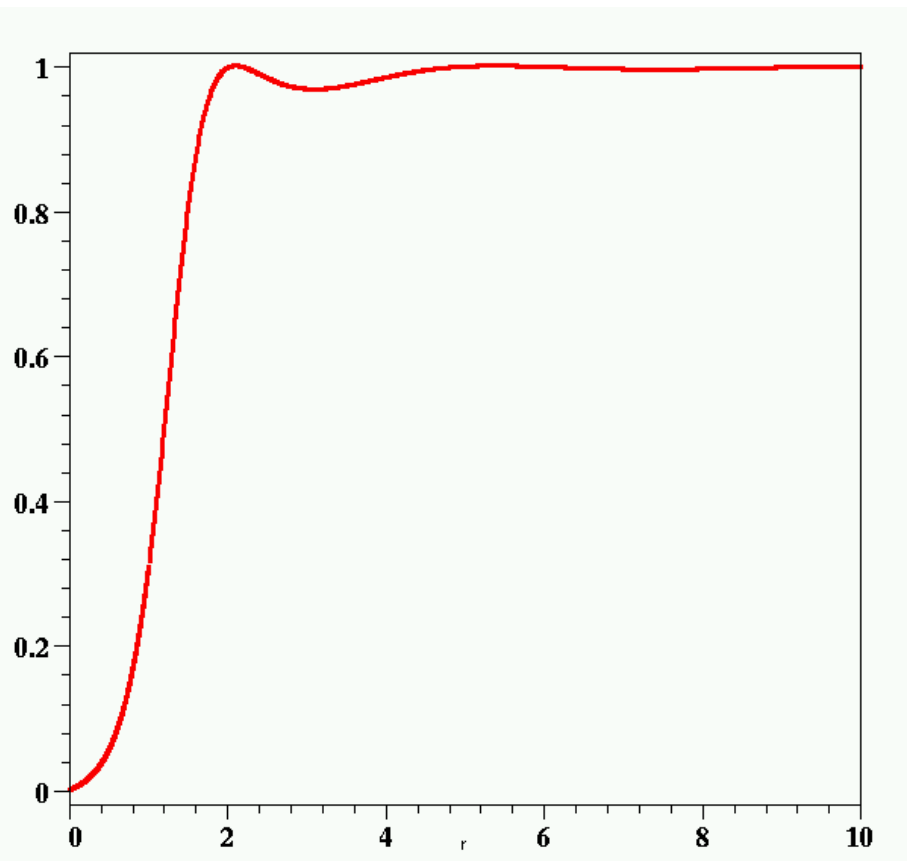
Xmaple code for potential barrier, tunneling

$$V_0 > E$$

```
assume(a,positive); assume(k1,real); assume(k2,real);
psi1:=A*exp(I*k1*x)+B*exp(-I*k1*x); # (-infinity,-a/2) k1=sqrt(2*E*m/h^2)
psi2:=C*exp(k2*x)+DD*exp(-k2*x);  # (-a/2,a/2) k2=sqrt(2*(V0-E)*m/h^2)
psi3:=F*exp(I*k1*x); # (a/2,infinity)

# now force continuity and first derivative continuity

eq1:=subs(x=-a/2,psi1-psi2);
eq2:=subs(x=-a/2,diff(psi1,x)-diff(psi2,x));
eq3:=subs(x=a/2,psi2-psi3);
eq4:=subs(x=a/2,diff(psi2,x)-diff(psi3,x));
sol:=solve({eq1,eq2,eq3,eq4},{F,C,B,DD});
Fsol:=subs(sol,F)/A; numF:=numer(Fsol);
help1:=expand(simplify(numF*conjugate(numF)));
denomF:=denom(Fsol);
help2:=expand(simplify(denomF*conjugate(denomF)));

T:=help1/help2;

T1:=subs({k1=sqrt(2*m*E/h^2),k2=sqrt(2*m*(V0-E)/h^2)},T);
# Following Eisberg & Resnick p. 202
T2:=simplify(subs(h=sqrt(2*m*V0*a^2/9),T1));
T3:=simplify(subs(E=V0*r,T2));

plot1:=plot({T3},r=0..1,thickness=3,axes=boxed,axesfont=[TIMES,BOLD,16],n
umpoints=1000):
```

$V_0 < E$

```
assume(a,positive); assume(k1,real); assume(k2,real);
psi1:=A*exp(I*k1*x)+B*exp(-I*k1*x); # (-infinity,-a/2) k1=sqrt(2*E*m/h^2)
psi2:=C*exp(I*k2*x)+DD*exp(-I*k2*x);  # (-a/2,a/2) k2=sqrt(2*(E-V0)*m/h^2)
psi3:=F*exp(I*k1*x); # (a/2,infinity)

# now force continuity and first derivative continuity

eq1:=subs(x=-a/2,psi1-psi2);
eq2:=subs(x=-a/2,diff(psi1,x)-diff(psi2,x));
eq3:=subs(x=a/2,psi2-psi3);
eq4:=subs(x=a/2,diff(psi2,x)-diff(psi3,x));
sol:=solve({eq1,eq2,eq3,eq4},{F,C,B,DD});
Fsol:=subs(sol,F)/A; numF:=numer(Fsol);
denomF:=denom(Fsol);

T:=simplify(abs(numF/denomF)^2);

T1:=subs({k1=sqrt(2*E*m/h^2),k2=sqrt(2*(E-V0)*m/h^2)},T);
#following Eisenberg&Resnick p. 202
T2:=simplify(subs(h=sqrt(2*m*V0*a^2/9),T1));
T3:=simplify(subs(E=V0*r,T2));

plot2:=plot({T3},r=1..10,thickness=3,axes=boxed,axesfont=[TIMES,BOLD,16],
numpoints=1000):

with(plots):
display({plot1,plot2});
plot(T3,r=2..10,thickness=3,axes=boxed,axesfont=[TIMES,BOLD,16],numpoints
=200);
```

A Delta Function Potential

• Assume the same situation as before, but instead of a step potential we have a "Delta function" potential – that is, a very narrow infinite wall.

$$Ae^{ik_0x}$$

$$\text{Potential} = a\delta(x)$$

$$Be^{-ik_0x}$$

$$Ce^{ik_0x}$$

$$x = 0$$
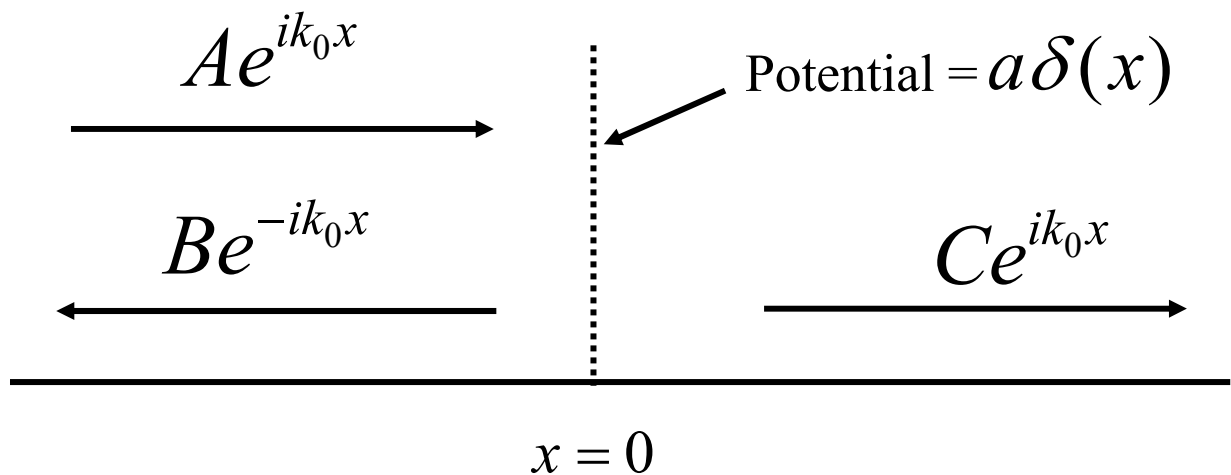
• Note that the wave number on the right of the barrier is the same as on the left, because there is no region in which is loses energy.

• As before, there are two equations: the function has to be continuous at 0 (hence $A+B=C$). The first derivative equation is a bit more tricky, because Schrödinger's Equation is

$$\psi'' = -\frac{2m(E_0 - V_0)}{\hbar^2}\psi = -\frac{2mE_0}{\hbar^2}\psi + \frac{2ma\delta(x)}{\hbar^2}\psi$$

- What happens to ψ' at $x = 0$? Since it is the integral of ψ'', which contains a product of the Delta function, it jumps by $2maC/\hbar^2$ when crossing the barrier from left to right. So, the equation for ψ' is

$$ik(C - A + B) = \frac{2maC}{\hbar^2}$$

- Solving this together with $A+B=C$ yields

$$R = \left|\frac{B}{A}\right|^2 = \frac{m^2 a^2}{m^2 a^2 + k_0^2 \hbar^4}, \quad T = 1 - R$$

- As the particle is heavier, and its wave number smaller, it will tend more to behave classically (that is, reflect).

Arbitrary Barrier
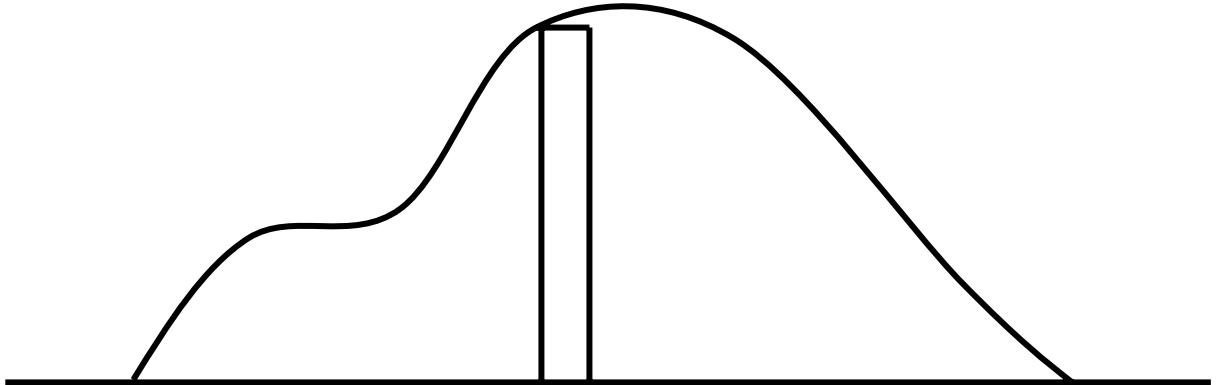
• Express as the limit of rectangular barriers of infinitesimal width, and calculate the limit of the product of the corresponding transmission coefficients.

Some results on Degeneracy

• Recall that an eigenvalue ω is *degenerate* if there are two linearly independent states with eigenvalue ω.

Theorem: there is no degeneracy in one dimensional bounded states.

Proof: assume

$$-\frac{\hbar^2}{2m}\psi_1'' + V\psi_1 = \lambda\psi_1 \, , \, -\frac{\hbar^2}{2m}\psi_2'' + V\psi_2 = \lambda\psi_2$$

Multiply by ψ_2 and ψ_1 and subtract to get

$$\psi_1''\psi_2 - \psi_1\psi_2'' = 0 \Rightarrow \left(\psi_1'\psi_2 - \psi_1\psi_2'\right)' = 0 \Rightarrow$$

$$\psi_1'\psi_2 - \psi_1\psi_2' = const., \text{ take } x \to \infty \text{ to get } const. = 0$$

$$\text{So,} \frac{\psi_1'}{\psi_1} = \frac{\psi_2'}{\psi_2} \Rightarrow \log(\psi_1) = \log(\psi_2) + const. \Rightarrow \psi_1 = e^{const.}\psi_2$$

But a difference in scale factor means that the states represent the same physics. ∎

Theorem: If parity is conserved (that is, the Hamiltonian commutes with the parity operator), then every non-degenerate state of definite energy has definite parity.

Proof: Let Q be the parity operator.

$$H|\psi\rangle = E|\psi\rangle \Rightarrow H\bigl(Q|\psi\rangle\bigr) = Q\bigl(H|\psi\rangle\bigr) =$$

$$Q\bigl(E|\psi\rangle\bigr) = E\bigl(Q|\psi\rangle\bigr) \underset{\text{non-degeneracy}}{\Rightarrow} Q|\psi\rangle = e^{i\delta}|\psi\rangle$$

but $Q^2 = 1 \Rightarrow e^{i\delta} = \pm 1$, so there's definite parity.

There can be degeneracy in two dimensional systems – such as a particle in a 2D box:

• The states of definite energy are products of the 1D states for x and y, and their energy is the sum of energies of the corresponding 1D states.

• So, if we know for example that the energy is $\dfrac{10\hbar^2\pi^2}{2mL^2}$, then the state is not uniquely determined, but instead it can be any normalized linear combination of

$$\left|\psi_{1,3}\right\rangle = \frac{2}{L}\cos\left(\frac{\pi x}{L}\right)\cos\left(\frac{3\pi y}{L}\right), \text{ or}$$

$$\left|\psi_{3,1}\right\rangle = \frac{2}{L}\cos\left(\frac{3\pi x}{L}\right)\cos\left(\frac{\pi y}{L}\right)$$

That is, the state has to be of the form

$$\alpha\left|\psi_{1,3}\right\rangle + \beta\left|\psi_{3,1}\right\rangle, \ |\alpha|^2 + |\beta|^2 = 1$$

The Harmonic Oscillator

• Very important – models the behavior of a system around an equilibrium point, even for many particles (as follows by diagonalizing the Hamiltonian).

• The Hamiltonian is the same one as in classical mechanics, with the usual substitution $p \rightarrow P, x \rightarrow X$:

$$H = \frac{P^2}{2m} + \frac{m\omega^2 X^2}{2}$$

• Since X and P are Hermitian, it follows that H cannot have negative eigenvalues.

• To find the definite energy states, we must solve

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{m\omega^2 x^2}{2}\right)\psi = 0$$

- Define constants and a variable change

$$b = \left(\frac{\hbar}{mw}\right)^{\frac{1}{2}}, \; \varepsilon = \frac{E}{\hbar\omega}, \; x = by$$

- To obtain $\psi'' + (2\varepsilon - y^2)\psi = 0$

- To solve it, look at the asymptotic behaviors:

$$y \to \infty \Rightarrow \psi'' - y^2\psi \approx 0 \Rightarrow \psi \approx Ay^m e^{\pm\frac{y^2}{2}}$$

- But $\; Ay^m e^{\frac{y^2}{2}} \;$ is ruled out from physical considerations.

- At the other end

$$y \to 0 \Rightarrow \psi'' + 2\varepsilon\psi \approx 0 \Rightarrow$$
$$\psi \approx A\cos(\sqrt{2\varepsilon}\,y) + B\sin(\sqrt{2\varepsilon}\,y) =$$
$$A + cy + O(y^2), \; c = B\sqrt{2\varepsilon}$$

- Next, guess a solution $\psi(y) = u(y)e^{-\frac{y^2}{2}}$

Where

$$u(y) \xrightarrow[y\to 0]{} A + cy + \text{(higher powers)}$$

$$u(y) \xrightarrow[y\to\infty]{} y^m + \text{(lower powers)}$$

$$u'' - 2yu' + (2\varepsilon - 1)u = 0$$

- Guess further $u(y) = \sum_{n=0}^{\infty} C_n y^n$

- And obtain $C_{k+2} = \dfrac{2k+1-2\varepsilon}{(k+2)(k+1)} C_k \xrightarrow[k\to\infty]{} \dfrac{2}{k} C_k$

- This in itself would not be very bad, but it's trivial to verify that $u(y)$ behaves like e^{y^2} when $y \to \infty$, which implies that

$$\psi(y) \underset{y\to\infty}{\approx} e^{\frac{y^2}{2}},$$ but that is physically untenable.

- Fortunately, there's a way out: look at the recursion

$$C_{k+2} = \frac{2k+1-2\varepsilon}{(k+2)(k+1)}C_k$$

This has to stop somewhere in order to prevent the solution from diverging, so we must have

$$\boxed{\varepsilon = \frac{2k+1}{2}, \quad k = 0,1,2...}$$

- So, energy quantization somehow came (again) into the picture. The solution for energy E is

$$\psi_E(x) = \left(\frac{m\omega}{\pi\hbar 2^{2n}(n!)^2}\right)^{\frac{1}{4}} H_n\left[\left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} x\right] e^{-\frac{m\omega}{2\hbar}x^2}$$

Where $E = \left(n + \frac{1}{2}\right)\hbar\omega$

Hermite, not Hamiltonian!

- The *H*'s are the *Hermite polynomials*. The first are

$$H_0(y) = 1 \quad H_1(y) = 2y \quad H_2(y) = -2(1 - 2y^2)$$

$$H_3(y) = -12\left(y - \frac{2}{3}y^3\right) \quad H_4(y) = 12\left(1 - 4y^2 + \frac{4}{3}y^4\right)$$

A few examples. The upright arrows mark the classical turning point for an oscillator with the given energy; note that, much like as with the potential barrier, the oscillator enters the classically forbidden zone with non-zero probability. Note also that as the energy increases, the behavior starts to resemble the classical behavior.
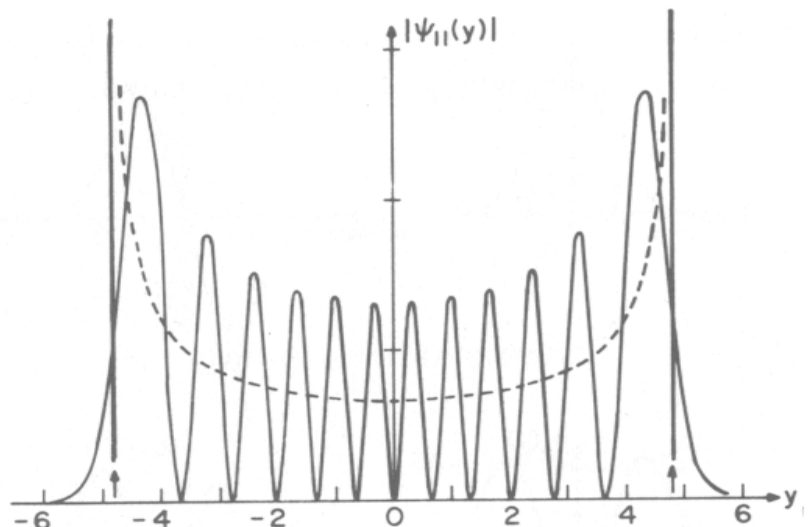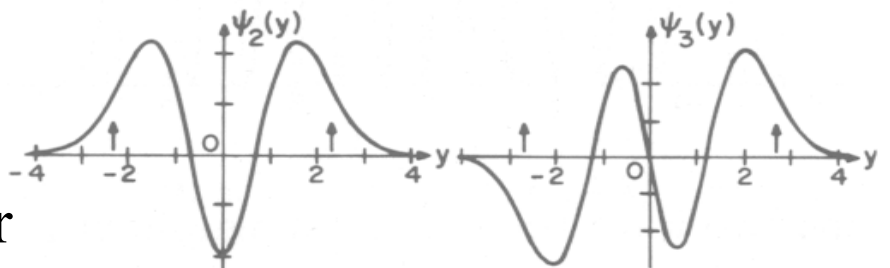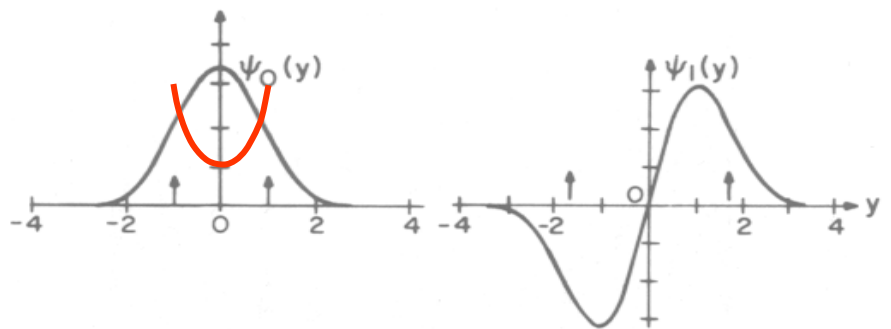
Interlude: Finding the Oscillator's Ground State from the Uncertainty Principle

$$H = \frac{P^2}{2m} + \frac{m\omega^2 X^2}{2}$$

• Let's search for the minimal energy state, that is, the normalize $|\psi\rangle$ which minimizes $\langle\psi|H|\psi\rangle$:

$$\langle\psi|H|\psi\rangle = \frac{1}{2m}\langle\psi|P^2|\psi\rangle + \frac{1}{2}m\omega^2\langle\psi|X^2|\psi\rangle$$

Recall that $\langle\psi|X^2|\psi\rangle = (\Delta X)^2 + \langle X\rangle^2$ (just as with ordinary average and variance), and the same for P. Since we want a minimum, take $\langle X\rangle = \langle P\rangle = 0$, and then

$$\langle\psi|H|\psi\rangle = \frac{1}{2m}(\Delta P)^2 + \frac{1}{2}m\omega^2(\Delta X)^2$$

We know that

$$(\Delta P)^2(\Delta X)^2 \geq \frac{\hbar^2}{4} \Rightarrow (\Delta P)^2 \geq \frac{\hbar^2}{4(\Delta X)^2}$$

And therefore

$$\langle\psi|H|\psi\rangle \geq \frac{\hbar^2}{8m(\Delta X)^2} + \frac{1}{2}m\omega^2(\Delta X)^2$$

The minimum is obtained when

$$(\Delta X)^2 = \frac{h}{2m\omega}, \text{ for which } \langle H\rangle = \frac{h\omega}{2}$$

• We proved that the minimum is obtained for a Gaussian; since $\Delta X = \Delta P = 0$, the Gaussian is centered at 0 and has no phase (momentum) shift, which after normalizing equals

$$\psi_{\min}(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}}$$

• Due to the non-degeneracy of one dimensional bounded states, $\psi_{\min}$ must indeed be the ground state (there's only one state with the minimal energy equal to its eigenvalue). Thus, to quote Shankar, we have found the ground state by "systematically hunting in Hilbert space".

• Example question: a potential barrier is added, so that the potential for $x \geq 0$ is ∞. What is the ground state energy?

• Answer: no even solutions are possible, since they are non-zero at $x = 0$. So the ground state energy is $(3/2)\hbar\omega$.

Analysis of the Oscillator with the "Raising" and "Lowering" Operators

• An important and particularly attractive technique due to Dirac for solving the oscillator in the energy basis.

• In order to solve

$$H|E\rangle = \left(\frac{P^2}{2m} + \frac{m\omega^2 X^2}{2} \right)|E\rangle = E|E\rangle$$

• Define the two operators

$$a = \left(\frac{m\omega}{2\hbar} \right)^{\frac{1}{2}} X + i\left(\frac{1}{2m\omega\hbar} \right)^{\frac{1}{2}} P$$

$$a^+ = \left(\frac{m\omega}{2\hbar} \right)^{\frac{1}{2}} X - i\left(\frac{1}{2m\omega\hbar} \right)^{\frac{1}{2}} P$$

- It readily follows that their commutator is

$$[a, a^+] = aa^+ - a^+ a = 1$$

- And they "nearly factor" H ("nearly" because X, P do not commute):

$$H = (a^+ a + 1/2)\hbar\omega, \text{ so define } \hat{H} = \frac{H}{\hbar\omega} = a^+ a + \frac{1}{2}$$

- Let's try and solve $\hat{H}|\varepsilon\rangle = \varepsilon|\varepsilon\rangle$

- The action of a^+ and a on the eigenvectors of $\hat{H}$ is very simple, because

$$[a, \hat{H}] = a, [a^+, \hat{H}] = -a^+$$

$$\hat{H}|\varepsilon\rangle = \varepsilon|\varepsilon\rangle, \hat{H}a|\varepsilon\rangle = (a\hat{H} - [a, \hat{H}])|\varepsilon\rangle =$$

$$(a\hat{H} - a)|\varepsilon\rangle = (\varepsilon - 1)(a|\varepsilon\rangle).$$

$$\text{Similarly, } \hat{H}a^+|\varepsilon\rangle = (\varepsilon + 1)(a^+|\varepsilon\rangle)$$

- So, operating with a, a^+ lowers and raises the eigenvalues of $\hat{H}$. But since H (and therefore $\hat{H}$) are positive definite, the operation by a has to stop somewhere:

$$\exists_{\varepsilon_0} \ a|\varepsilon_0\rangle = 0 \Rightarrow a^+ a|\varepsilon_0\rangle = 0 \Rightarrow$$

$$\left(\hat{H} - 1/2\right)|\varepsilon_0\rangle = 0 \Rightarrow \hat{H}|\varepsilon_0\rangle = \tfrac{1}{2}|\varepsilon_0\rangle$$

- Due to the non-degeneracy of one dimensional bounded states, every such "decreasing sequence" has to end with the same $|\varepsilon_0\rangle$, denote it $|0\rangle$.

- Label the successive operations of a^+ on $|\varepsilon_0\rangle$ by $|n\rangle$.

It follows that $a|n\rangle = \sqrt{n}\,|n-1\rangle, a^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$, because : $|n\rangle$ is $\left(a^+\right)^n|0\rangle$

normalized. Since $\hat{H}|0\rangle = (1/2)|0\rangle$ and every a^+ raises by 1, we have

$\hat{H}|n\rangle = (n+1/2)|n\rangle$. Now, $\hat{H}a|n\rangle = \left(a\hat{H} - a\right)|n\rangle = (n-1/2)\left(a|n\rangle\right)$ and since $\hat{H}$ is

non - degenerate and $\hat{H}|n-1\rangle = (n-1/2)|n-1\rangle$ there's a constant C such that

$a|n\rangle = C|n-1\rangle$. Take adjoints to obtain $\langle n|a^+ = \langle n-1|C^*$, and multiply to get

$\langle n|a^+a|n\rangle = |C|^2$. But $\langle n|a^+a|n\rangle = \langle n|H - 1/2|n\rangle = (n+1/2)-1/2 = n$.

$$\text{So: } |n\rangle = \frac{\left(a^+\right)^n}{(n!)^{1/2}}|0\rangle$$

- So, the representations of a, a^+, H in the $|n\rangle$ basis are very simple, and so are those of X and P:

$$X = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\left(a + a^+\right), P = i\left(\frac{m\omega\hbar}{2}\right)^{\frac{1}{2}}\left(a^+ - a\right)$$

Example question:

• What are $\langle X \rangle, \langle X^2 \rangle$ in the state $|n\rangle$?

• Up to a constant $c = (\hbar/2m\omega)^{\frac{1}{2}}$, $X = a + a^+$.
Ignoring c for the moment,

$$\langle X \rangle = \langle n|a + a^+|n\rangle = \langle n|a|n\rangle + \langle n|a^+|n\rangle = 0 + 0 = 0$$

Since a, a^+ lower and raise $|n\rangle$ and since $\langle n|m\rangle = \delta_{m,n}$

$$\langle X^2 \rangle = \langle n|(a + a^+)^2|n\rangle = \langle n|a^2|n\rangle + \langle n|(a^+)^2|n\rangle +$$
$$\langle n|a^+a|n\rangle + \langle n|aa^+|n\rangle = 0 + 0 + \langle n|a^+a|n\rangle + \langle n|aa^+|n\rangle$$

Now, use the identities

$$a|n\rangle = \sqrt{n}\,|n-1\rangle, \; a^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

To obtain (after multiplying by c^2)

$$\langle X^2 \rangle = \left(n + \frac{1}{2}\right)\frac{\hbar}{m\omega}$$

Passage from the Energy Basis to <u>the Coordinate Basis</u>

$$a = \left(\frac{m\omega}{2\hbar}\right)^{\frac{1}{2}} X + i\left(\frac{1}{2m\omega\hbar}\right)^{\frac{1}{2}} P \Leftrightarrow$$

$$\left(\frac{m\omega}{2\hbar}\right)^{\frac{1}{2}} x + \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} \frac{d}{dx} \quad \text{denote } y = (m\omega/\hbar)^{1/2} x$$

$$\text{so } a = 2^{-\frac{1}{2}}\left(y + \frac{d}{dy}\right), a^+ = 2^{-\frac{1}{2}}\left(y - \frac{d}{dy}\right)$$

• To find the ground state in the coordinate basis:

$$a|\psi_0\rangle = 0 \Rightarrow \left(y + \frac{d}{dy}\right)|\psi_0\rangle = 0 \Rightarrow \text{the ground state is}$$

$$|\psi_0\rangle = A_0 e^{-\frac{y^2}{2}} = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}} \text{ (after normalization)}$$

And the other eigenstates can be derived (up to a normalizing factor) by

$$|\psi_n\rangle = \frac{(a^+)^n}{(n!)^{1/2}}|\psi_0\rangle = \frac{2^{-\frac{n}{2}}}{(n!)^{1/2}}\left(y - \frac{d}{dy}\right)^n|\psi_0\rangle$$

Coherent States

• Seek the "classical limit" of the oscillator, i.e. states with a relatively small uncertainty in energy etc.

• Time development of classical oscillator:

$$\dot{x}(t) = (1/m)p(t), \; \dot{p}(t) = -m\omega^2 x(t)$$

Define $\hat{x}(t) = \beta x(t), \; \hat{p}(t) = (1/\hbar\beta)p(t)$

$$\left(\beta = \sqrt{m\omega/\hbar}\right)$$

$$\dot{\hat{x}}(t) = \omega\hat{p}(t), \; \dot{\hat{p}}(t) = -\omega\hat{x}(t).$$

Define $\alpha(t) = \left(1/\sqrt{2}\right)\left[\hat{x}(t) + i\hat{p}(t)\right]$

$$\dot{\alpha}(t) = -i\omega\alpha(t) \Rightarrow \alpha(t) = \alpha(0)e^{-i\omega t}$$

$$\hat{x}(t) = \left(1/\sqrt{2}\right)\left[\alpha_0 e^{-i\omega t} + \alpha_0^* e^{i\omega t}\right]$$

$$\hat{p}(t) = \left(-i/\sqrt{2}\right)\left[\alpha_0 e^{-i\omega t} - \alpha_0^* e^{i\omega t}\right]$$

The energy (for all t) $= \hbar\omega|\alpha_0|^2$

• There is a lot of similarity between these relations and the average behavior of the quantum oscillator:

$$\hat{X} = \beta X = \left(1/\sqrt{2}\right)\left(a + a^+\right)$$

$$\hat{P} = \left(1/\hbar\beta\right)P = \left(-i/\sqrt{2}\right)\left(a - a^+\right)$$

$$H = \hbar\omega\left(a^+ a + 1/2\right)$$

$$\hat{X}(t) = \left(1/\sqrt{2}\right)\left[\langle\alpha\rangle(0)e^{-i\omega t} + \langle\alpha\rangle^*(0)e^{i\omega t}\right]$$

$$\hat{P}(t) = \left(-i/\sqrt{2}\right)\left[\langle\alpha\rangle(0)e^{-i\omega t} - \langle\alpha\rangle^*(0)e^{i\omega t}\right]$$

This is almost identical to the classical oscillator equations, with $\langle\alpha\rangle_0$ playing the role of α_0. We therefore ask that $\langle\psi(0)|a|\psi(0)\rangle = \alpha_0$. For the energy to behave similarly, we should have $\langle H\rangle = \hbar\omega\langle a^+ a\rangle(0) = \hbar\omega|\alpha_0|^2$ -- but $\langle H\rangle = \hbar\omega\left[1/2 + |\alpha_0|^2\right]$. Assume then that $|\alpha_0|^2 \gg 1/2$.

- This analysis suggests to require

$$\langle\psi(0)|a|\psi(0)\rangle=\alpha_0, \ \langle\psi(0)|a^+a|\psi(0)\rangle=|\alpha_0|^2$$

The simplest way to enforce this is to require $a|\psi(0)\rangle=\alpha_0|\psi(0)\rangle$.

How do the eigenvectors of a look like?
Let $a|\alpha\rangle=\alpha|\alpha\rangle$, denote $|\alpha\rangle=\sum_n c_n(\alpha)|n\rangle$.

So $a|\alpha\rangle=\sum_n c_n(\alpha)a|n\rangle=\sum_n c_n(\alpha)\sqrt{n}|n-1\rangle=$

$$\alpha\sum_n c_n(\alpha)|n\rangle\Rightarrow c_n(\alpha)=\frac{\alpha c_{n-1}(\alpha)}{\sqrt{n}}\Rightarrow$$

$$c_n(\alpha)=\frac{\alpha^n}{\sqrt{n!}}c_0(\alpha)$$

And after normalization:

$$|\alpha\rangle=e^{-|\alpha|^2/2}\sum_n\frac{\alpha^n}{\sqrt{n!}}|n\rangle.$$

- It follows that:

$$\langle H \rangle_{\alpha} = \hbar \omega \left[|\alpha|^2 + \frac{1}{2} \right], \langle H^2 \rangle_{\alpha} = \hbar^2 \omega^2 \left[|\alpha|^4 + 2|\alpha|^2 + \frac{1}{4} \right]$$

And so $\Delta H_{\alpha} = \hbar \omega |\alpha| \Rightarrow \dfrac{\Delta H_{\alpha}}{\langle H \rangle_{\alpha}} \ll 1$.

Since X, P are expressible in terms of α, α^+, it is straightforward to derive:

$$\langle X \rangle_{\alpha} = \sqrt{\frac{2\hbar}{m\omega}} \operatorname{Re}(\alpha), \langle P \rangle_{\alpha} = \sqrt{2m\omega\hbar} \operatorname{Im}(\alpha)$$

$$\Delta X_{\alpha} = \sqrt{\frac{\hbar}{2m\omega}}, \Delta P_{\alpha} = \sqrt{\frac{m\omega\hbar}{2}} \Rightarrow \Delta X_{\alpha} \Delta P_{\alpha} = \frac{\hbar}{2}$$

Time evolution:

$$e^{-|\alpha_0|^2/2} \sum_n \frac{\alpha_0^n}{\sqrt{n!}} e^{-iE_n t/\hbar} |n\rangle =$$

$$e^{-i\omega t/2} e^{-|\alpha_0|^2/2} \sum_n \frac{\left(\alpha_0 e^{-i\omega t} \right)^n}{\sqrt{n!}} e^{-iE_n t/\hbar} |n\rangle = e^{-i\omega t/2} \left| \alpha_0 e^{-i\omega t} \right\rangle$$

So, the state remains an eigenvector of a. This also means that $\Delta X_{\alpha}, \Delta P_{\alpha}$ don't change. The wave function is a "small" Gaussian which moves back and forth.

The Operator $D(\alpha)$ and the Wave Function $\psi_\alpha(x)$

Define $D(\alpha)=e^{\alpha a^+ - \alpha^* a}$, $D(\alpha)$ is unitary. Since $\left[\alpha a^+, \alpha^* a\right]=-|\alpha|^2$, it follows from Galuber's formula for two operators which commute with their commutator that $D(\alpha)=e^{-|\alpha|^2} e^{\alpha a^+} e^{-\alpha^* a}$.

$e^{-\alpha^* a}|0\rangle=|0\rangle$, and $e^{\alpha a^+}|0\rangle=\sum \frac{\alpha^n}{\sqrt{n!}}|n\rangle$, so

$D(\alpha)|0\rangle=e^{-|\alpha|^2} \sum \frac{\alpha^n}{\sqrt{n!}}|n\rangle=|\alpha\rangle$, which allows to calculate the wave function $\psi_\alpha(x)=\langle x|\alpha\rangle=\langle x|D(\alpha)|0\rangle$. The result is

$$\psi_\alpha(x)=e^{i\theta_\alpha}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\left[\frac{x-\langle X\rangle_\alpha}{2\Delta X_\alpha}\right]^2+i\langle P\rangle_\alpha\frac{x}{\hbar}\right)$$

Field Quantization

- **For two coupled oscillators, new variables can be defined which decouple them. This can also be done for an infinite chain of oscillators, a continuous string, and the electromagnetic field.**

- **The Hamiltonian for a pair of coupled oscillators equals**

$$\frac{p_1^2}{2m}+\frac{p_2^2}{2m}+\frac{1}{2}m\omega^2\left(x_1-a\right)^2+\frac{1}{2}m\omega^2\left(x_2+a\right)^2+\lambda m\omega^2\left(x_1-x_2\right)^2$$

  where λ controls the strength of the coupling.

- **Defining new variables and new masses**

$$x_G(t)=\frac{x_1(t)+x_2(t)}{2},x_R(t)=\frac{x_1(t)-x_2(t)}{2},\mu_G=2m,\mu_R=\frac{m}{2}$$

  decouples the resulting differential equations, and the Hamiltonian can be written as

$$\frac{p_G^2}{2\mu_G}+\frac{p_R^2}{2\mu_R}+\frac{1}{2}\mu_G\omega_G^2 x_G^2+\frac{1}{2}\mu_R\omega_R^2\left(x_R-\frac{2a}{1+4\lambda}\right)^2+m\omega^2 a^2\frac{4\lambda}{1+4\lambda}$$

  where $p_G(t)=p_1(t)+p_2(t),p_R(t)=\dfrac{p_1(t)-p_2(t)}{2},\omega_G=\omega,$

  $\omega_R=\omega\sqrt{1+4\lambda}$

- **The quantum mechanics case proceeds similarly: new observables are defined by**

$$X_G = \frac{X_1 + X_2}{2}, P_G = P_1 + P_2, X_R = X_1 - X_2, P_R = \frac{P_1 - P_2}{2}$$

- **From the commutation relations of the original observables**

$$[X_1, P_1] = [X_2, P_2] = i\hbar \text{ (and the other commutators} = 0)$$

It follows that the same relations hold for the new observables. It also follows that the Hamiltonian

$$\frac{P_1^2}{2m} + \frac{P_2^2}{2m} + \frac{1}{2}m\omega^2(X_1 - a)^2 + \frac{1}{2}m\omega^2(X_2 + a)^2 + \lambda m\omega^2(X_1 - X_2)^2$$

equals

$$\underbrace{\frac{P_G^2}{2\mu_G} + \frac{1}{2}\mu_G\omega_G^2 X_G^2}_{H_G} + \underbrace{\frac{P_R^2}{2\mu_R} + \frac{1}{2}\mu_R\omega_R^2\left(X_R - \frac{2a}{1+4\lambda}\right)^2}_{H_R} + m\omega^2 a^2\frac{4\lambda}{1+4\lambda}$$

Note that this is true only because of the commutation relations between the new observables.

A basis for the system's wave functions is given by the tensor product of the corresponding eigenvectors of H_G and H_R, which are given by the respective raising and lowering operators:

$$a_G^+ = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{\mu_G \omega_G}{\hbar}}X_G - \frac{i}{\sqrt{\mu_G \omega_G \hbar}}P_G\right]$$

$$a_R^+ = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{\mu_R \omega_R}{\hbar}}X_R' - \frac{i}{\sqrt{\mu_R \omega_R \hbar}}P_R\right], X_R' = X_R - \frac{2a}{1+4\lambda}$$

the eigenvectors of H_G are given by

$$\left|\psi_n^G\right\rangle = \frac{1}{\sqrt{n!}}\left(a_G^+\right)^n\left|\psi_0^G\right\rangle \text{ ,with an eigenvalue of}$$

$$\left(n+\frac{1}{2}\right)\hbar\omega_G \text{, and similarly for } \left|\psi_n^R\right\rangle.$$

The eigenvectors of the system are given by

$$\left|\psi_{n,p}\right\rangle = \frac{1}{\sqrt{n!p!}}\left(a_G^+\right)^n\left(a_R^+\right)^p\left|\psi_{0,0}\right\rangle \text{ ,with an energy of}$$

$$\left(n+\frac{1}{2}\right)\hbar\omega_G + \left(p+\frac{1}{2}\right)\hbar\omega_R + m\omega^2 a^2\frac{4\lambda}{1+4\lambda}$$

• In the (0,0) state, both the average and the distance between the two masses are Gaussians around zero.

• In the (1,0) state, the average's distribution has two peaks away from zero, and the distance is a Gaussian around zero.

• In the (0,1) state, the average's distribution is a Gaussian around zero, and the distance's distribution has two peaks away from zero.

• In the (1,1) state, the distributions of both the average and the distance have two peaks away from zero.
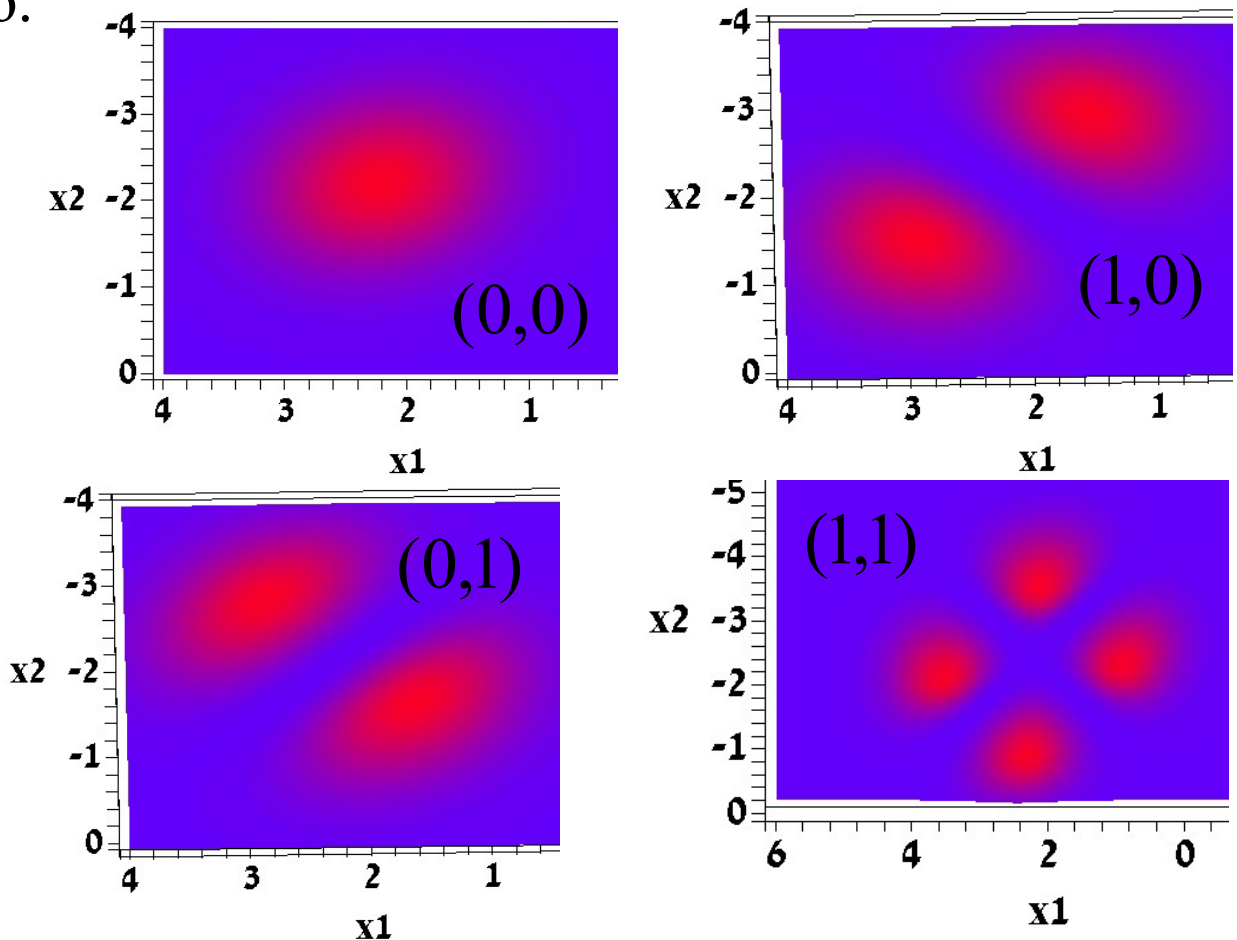
Continuous String
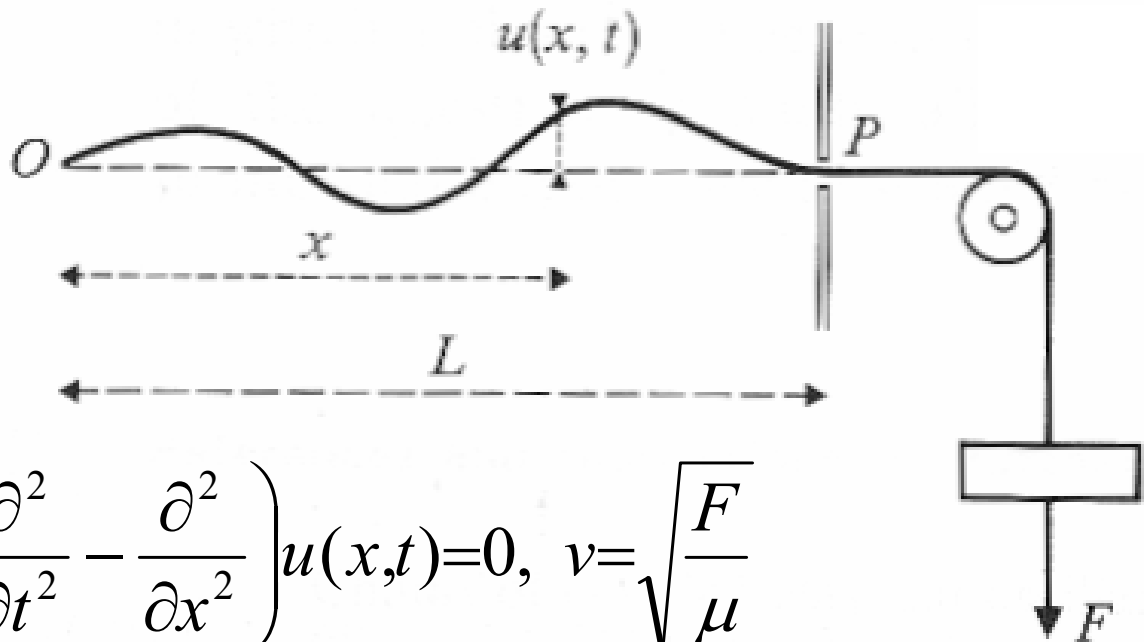
$$\left(\frac{1}{v^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} \right)u(x,t)=0, \quad v=\sqrt{\frac{F}{\mu}}$$

$$\text{Potential energy} = \frac{F}{2}\int_0^L \left(\frac{\partial u(x,t)}{\partial x} \right)^2 dx$$

$$\text{Kinetic energy} = \frac{\mu}{2}\int_0^L \left(\frac{\partial u(x,t)}{\partial t} \right)^2 dx$$

Fourier expansion with $f_k(x)=\sqrt{\frac{2}{L}}\sin\left(k\frac{\pi x}{L} \right)$:

$$u(x,t)=\sum_{k=1}^{\infty}q_k(t)f_k(x) \Rightarrow q_k(t),\dot{q}_k(t) \text{ determine}$$

the state of the string at time t.

- In Fourier domain, the equations are decoupled: $\ddot{q}_k(t) + \omega_k^2 q_k(t) = 0$, $\omega_k \equiv \dfrac{k\pi v}{L}$

- It's straightforward to see that the Lagrangian equals $L = \dfrac{\mu}{2} \sum_{k=1} \left[\dot{q}_k^2 - \omega_k^2 q_k^2 \right]$

- The momentum conjugate to q_k is

$$p_k = \frac{\partial L}{\partial \dot{q}_k} = \mu \dot{q}_k$$

- The Hamiltonian is $H = \dfrac{\mu}{2} \sum_{k=1} \left[\dfrac{p_k^2}{2\mu} + \dfrac{\mu}{2} \omega_k^2 q_k^2 \right]$

Denoting $\hat{q}_k \equiv \beta_k q_k$, $\hat{p}_k = \dfrac{1}{\beta_k \hbar} p_k$ $\left(\beta_k \equiv \sqrt{\dfrac{\mu \omega_k}{\hbar}} \right)$

yields $H = \sum \dfrac{1}{2} \hbar \omega_k \left[\hat{q}_k^2 + \hat{p}_k^2 \right]$

A schematic proof that $q_k, p_k = \dot{q}_k$ are canonical (most constants ignored, $L = 2\pi$):

Lagrangian $= L = \int_0^{2\pi} \left[\left(\partial u(x,t)/\partial t \right)^2 - \left(\partial u(x,t)/\partial x \right)^2 \right] dx$,

and the momentum conjugate to $u(x)$ is $\partial L/\partial \dot{u} \approx \dot{u}$. Fourier expansion with $f_k(x) = \sin(kx)$:

$$u(x,t) = \sum_{k=1}^{\infty} q_k(t) f_k(x) \Rightarrow \dot{u}(x,t) = \sum_{k=1}^{\infty} \dot{q}_k(t) f_k(x), \text{ so}$$

$$q_k \approx \int_0^{2\pi} u(x,t) f_k(x) dx, \quad p_k \approx \int_0^{2\pi} \dot{u}(x,t) f_k(x) dx.$$

Commutation relations: $\{q_k, q_l\} =$

$$\int_0^{2\pi} \left[\underbrace{\frac{\partial q_k}{\partial u(x)} \frac{\partial q_l}{\partial \dot{u}(x)}}_{0} - \underbrace{\frac{\partial q_k}{\partial \dot{u}(x)} \frac{\partial q_l}{\partial u(x)}}_{0} \right] dx = 0, \text{ same for } \{p_k, p_l\}.$$

$$\{q_k, p_l\} = \int_0^{2\pi} \left[\frac{\partial q_k}{\partial u(x)} \frac{\partial p_l}{\partial \dot{u}(x)} - \frac{\partial q_k}{\partial \dot{u}(x)} \underbrace{\frac{\partial p_l}{\partial u(x)}}_{0} \underbrace{}_{0} \right] dx =$$

$$\int_0^{2\pi} f_k(x) f_l(x) dx = \delta_{kl}.$$

- Now, quantize by promoting $\hat{q}_k, \hat{p}_k$ to

Operators $\hat{Q}_k, \hat{P}_k$ satisfying $[\hat{Q}_{k_1}, \hat{P}_{k_2}] = i\delta_{k_1 k_2}$.

(note: as for one particle, the classic variables $\dot{q}_k, q_k$ are time-dependent, but the operators are not).

- Denote $H_k = \frac{1}{2}\hbar\omega_k\left(\hat{Q}_k^2 + \hat{P}_k^2\right)$. It has

eigenstates and eigenvalues

$$H_k |n_k\rangle = \left(n_k + \frac{1}{2}\right)\hbar\omega_k.$$

- Since the H_k commute, a general state can be defined by $|n_1\rangle|n_2\rangle...|n_k\rangle$, with energy $\sum_k n_k \hbar\omega_k$ above the ground state.

As before, define creation and annihilation operators: $a_k = \left(1/\sqrt{2}\right)\left(\hat{Q}_k + i\hat{P}_k\right)$,

$a_k^+ = \left(1/\sqrt{2}\right)\left(\hat{Q}_k - i\hat{P}_k\right)$.

$$a_k |n_1 ... n_k ...\rangle = \sqrt{n_k} |n_1 ... n_k - 1 ...\rangle$$

$$a_k^+ |n_1 ... n_k ...\rangle = \sqrt{n_k + 1} |n_1 ... n_k + 1 ...\rangle$$

$$|n_1 ... n_k ...\rangle = \frac{\left(a_1^+\right)^{n_1}}{\sqrt{n_1!}} \ ... \ \frac{\left(a_k^+\right)^{n_k}}{\sqrt{n_k!}} \ ... \ |0\rangle$$

The observable $u(x,t)$ is promoted to an operator $U(x) = \sum\limits_k f_k(x) Q_k =$

$$\frac{1}{\sqrt{2}} \sum_k \frac{1}{\beta_k} f_k(x)\left(a_k + a_k^+\right) \quad \left(\beta_k \approx \sqrt{k}\right)$$

And it is not hard to show that $\langle U(x)\rangle(t)$ satisfies the classical equation.

• What is the ground state $|0\rangle$? Its *k*'th Fourier coefficient is an oscillator with frequency proportional to *k*, at its ground state – i.e. a Gaussian with variance $\approx 1/k$. So a sample of the ground state is a function with slowly decreasing Fourier coefficients. This decrease reflects the coupling in the spatial domain, and the samples are not random noise, but have some measure of smoothness associated with them.

• The ground state is a *fractal* of dimension 2.

• An excited state is the superposition of sinusoids with the ground state.

Quantization of the EM Field

Maxwell's Equations :

$$\nabla \cdot E = 4\pi\rho \quad \nabla \cdot B = 0 \quad \nabla \cdot J = -\frac{\partial \rho}{\partial t}$$

$$\nabla \times E = -\frac{1}{c}\frac{\partial B}{\partial t} \quad \nabla \times B = \frac{4\pi}{c}J + \frac{1}{c}\frac{\partial E}{\partial t}$$

Potentials : $\nabla \times A = B,\ E = -\nabla\phi - \frac{1}{c}\frac{\partial A}{\partial t}$

Gauge transform: $A' = A - \nabla\Lambda,\ \phi' = \phi + \frac{1}{c}\frac{\partial \Lambda}{\partial t}$

Coulomb gauge: $\nabla \cdot A = 0,\ (\phi = 0$ if $\rho = 0, J = 0)$

Lorentz gauge: $\nabla \cdot A = -\frac{1}{c}\frac{\partial \phi}{\partial t} \Rightarrow$

$$\Box^2\phi = -4\pi\rho \qquad \Box^2 A = -\frac{4\pi J}{c}$$

$$\Box^2 \equiv \nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}$$

Force on a charged particle: $q\left(E + \dfrac{v}{c} \times B\right)$

Energy of the EM field: $\dfrac{1}{8\pi} \iiint \left[E^2 + B^2\right] d^3\mathrm{r}$

- Experimental motivation for quantizing the EM field: spontaneous decay of hydrogen atoms when no field is present.

- Recipe for quantization: find canonical coordinates A_i and momenta Π_j such that $\Pi_i = \partial L / \partial \dot{A}_i$, $\{A_i, \Pi_j\} = \delta_{ij}$, and promote them to operators with similar commtation relations.

- **The EM Lagrangian is**

$$L = \frac{1}{8\pi} \iiint \left[E^2 - B^2 \right] d^3\mathrm{r} =$$

$$\frac{1}{8\pi} \iiint \left[\left\| -\frac{1}{c} \frac{\partial \mathrm{A}}{\partial t} - \nabla \phi \right\|^2 - \left\| \nabla \times \mathrm{A} \right\|^2 \right] d^3\mathrm{r}$$

and indeed it yields Maxwell's equations when varied with respect to the potentials.

- **But since** $\dot{\phi}$ **does not appear in** *L,* ϕ **has no conjugate momentum.**

- **Since we're working in free space (no charges/currents), this problem can be alleviated by working in Coulomb gauge with** $\phi=0.$

- **The Lagrangian is then simpler, but it doesn't yield the equation** $\nabla \cdot \mathrm{E} = 0$ **any more. This condition now has to be enforced.**

- **This will result in one less degree of freedom for the vector potential A.**

- **The coordinates are** $A_i(\mathbf{r})$ **, and the**

conjugate momenta are $\Pi_i(r) = \dfrac{-E_i(\mathbf{r})}{4\pi c}$.

- **Alas, they are not canonical. We'd like to have**

$$\{A_i(\mathbf{r}), \Pi_j(\mathbf{r}')\} = \delta_{ij}\delta(\mathbf{r} - \mathbf{r}')$$

but taking the divergence with respect to r **yields zero on the left-hand side, but not the right-hand side.**

- **The way out of this is to parameterize A by independent variables, so that** $\nabla \cdot A = 0$ **will hold. As in some cases in classical mechanics, this is easier to do in the Fourier domain, in which the condition is algebraic and not differential, and in which the coordinates can be decoupled.**

• Since $A(r)$ and $\Pi(r)$ are real, there is a complex vector function a(k) satisfying:

$$A(r)=\int\left[a(k)e^{i\mathbf{k}\cdot\mathbf{r}}+a*(k)e^{-i\mathbf{k}\cdot\mathbf{r}}\right]d^3k$$

$$\Pi(r)=\frac{1}{4\pi ic}\int k\left[a(k)e^{i\mathbf{k}\cdot\mathbf{r}}-a*(k)e^{-i\mathbf{k}\cdot\mathbf{r}}\right]d^3k$$

• The existence of a(k) is guaranteed by the redundancy in the Fourier transforms of the real functions **A** and Π : for a real f, $F(-k)=F^{*}(k)$.

• The choice of a(k) is guided by the following identities for the oscillator:

$$X=\left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(a+a^{+}\right),\ P=i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\left(a^{+}-a\right)$$

• The conditions $\nabla \cdot A = \nabla \cdot \Pi = 0$ are expressed in the Fourier domain by

$$k \cdot [a(k) + a*(-k)] = k \cdot [a(k) - a*(-k)] = 0 \Rightarrow k \cdot a(k) = 0$$

which suggests to expand a(k) in a basis orthogonal to k.

• Define for every k an orthonormal basis $\varepsilon(k1), \varepsilon(k2), \varepsilon(k3)$, such that $\varepsilon(k3) \| k$.

• For every k expand a(k) as follows:

$$a(k) = \sum_{\lambda=1}^{3} \left(c^2 / 4\pi^2 \omega \right)^{1/2} a(k\lambda) \varepsilon(k\lambda) \quad (\omega = kc)$$

This yields

$$A(r) = \sum_{\lambda} \int \left(\frac{c^2}{4\pi^2 \omega} \right)^{1/2} \left[a(k\lambda)\varepsilon(k\lambda)e^{ik\cdot r} + a*(k\lambda)\varepsilon(k\lambda)e^{-ik\cdot r} \right] d^3k$$

$$\Pi(r) = \sum_{\lambda} \int \frac{1}{i} \left(\frac{\omega}{64\pi^4} \right)^{1/2} \left[a(k\lambda)\varepsilon(k\lambda)e^{ik\cdot r} - a*(k\lambda)\varepsilon(k\lambda)e^{-ik\cdot r} \right] d^3k$$

• Before imposing transversality

$$\left\{A_i(r), A_j(r')\right\} = \left\{\Pi_i(r), \Pi_j(r')\right\} = 0,$$

$$\left\{A_i(r), \Pi_j(r')\right\} = \delta_{ij}\delta(r-r')$$

And it follows that

$$\left\{a(k\lambda), a(k'\lambda')\right\} = \left\{a*(k\lambda), a*(k'\lambda')\right\} = 0,$$

$$\left\{a(k\lambda), a*(k'\lambda')\right\} = -i\delta_{\lambda\lambda'}\delta^3(k-k')$$

Outline of proof : ignoring all constants,

$$a(k\lambda) = \left[i\int A(r)e^{-ik\cdot r}d^3r + \int \Pi(r)e^{-ik\cdot r}d^3r\right]\cdot \varepsilon(k\lambda)$$

$$a*(k\lambda) = \left[-i\int A(r)e^{ik\cdot r}d^3r + \int \Pi(r)e^{ik\cdot r}d^3r\right]\cdot \varepsilon(k\lambda)$$

Now continue as usual, with the derivatives by

$A_j(r_0), \Pi_j(r_0)$ given by $e^{-ik\cdot r_0}\varepsilon_j(k\lambda)$, etc.

- Next, discard $a(k3)$ which must be zero due to the transversality.

- The EM Hamiltonian is

$$H = \frac{1}{8\pi} \iiint \left[E^2 + B^2 \right] d^3\text{r}$$

and it equals

$$\sum_{\lambda=1}^{2} \int \omega a*(k\lambda) a(k\lambda) d^3\text{k}$$

• Guided by the oscillator equations, define

$$q(k\lambda) = \frac{1}{(2\omega)^{1/2}} \left[a(k\lambda) + a*(k\lambda) \right]$$

$$p(k\lambda) = -i \left(\frac{\omega}{2} \right)^{1/2} \left[a(k\lambda) - a*(k\lambda) \right]$$

it can be verified that they satisfy the canonical Poisson bracket relations.

• It immediately follows that

$$H = \frac{1}{2}\sum_{\lambda}\int \left[p^2(k\lambda) + \omega^2 q^2(k\lambda) \right] d^3k$$

so the field is a sum of a continuous family of oscillators, two at each frequency.

• Next, promote $p(k\lambda), q(k\lambda)$ to operators $P(k\lambda), Q(k\lambda)$ satisfying the canonical commutation relations

$$\left[P(k\lambda), Q(k'\lambda') \right] = i\hbar \delta_{\lambda\lambda'} \delta^3(k - k')$$

and define raising and lowering operators

$$a(k\lambda) = \left(\frac{\omega}{2\hbar} \right)^{1/2} Q(k\lambda) + i\left(\frac{1}{2\omega\hbar} \right)^{1/2} P(k\lambda)$$

$$a^+(k\lambda) = \left(\frac{\omega}{2\hbar} \right)^{1/2} Q(k\lambda) - i\left(\frac{1}{2\omega\hbar} \right)^{1/2} P(k\lambda)$$

which satisfy

$$\left[a(k\lambda), a^+(k'\lambda') \right] = \delta_{\lambda\lambda'} \delta^3(k - k')$$

A and Π are also promoted to operators:

$$A(r) = \sum_\lambda \int \left(\frac{\hbar c^2}{4\pi^2 \omega} \right)^{1/2} \left[a(k\lambda)\varepsilon(k\lambda)e^{ik\cdot r} + a^+(k\lambda)\varepsilon(k\lambda)e^{-ik\cdot r} \right] d^3k$$

$$\Pi(r) = \sum_\lambda \int \frac{1}{i} \left(\frac{\hbar\omega}{64\pi^4} \right)^{1/2} \left[a(k\lambda)\varepsilon(k\lambda)e^{ik\cdot r} - a^+(k\lambda)\varepsilon(k\lambda)e^{-ik\cdot r} \right] d^3k$$

To find the Hamiltonian, symmetrize $a * a$

by $(1/2)(aa * + a * a)$ to obtain

$$H = \sum_\lambda \int \left[a^+(k\lambda)a(k\lambda) + \frac{1}{2} \right] \hbar\omega \, d^3k$$

- In the ground state, ALL the oscillators are in their ground state, so for all k, λ

$$a(k\lambda)|0\rangle = 0.$$

- Formally, the energy of the ground state

("vacuum") is $E_0 \equiv \sum_\lambda \int (1/2)\hbar\omega \, d^3k = ??$

• It can be verified from the definition of H and from the commutation relations that

$$H\left(a^+(k\lambda)|0\rangle\right) = \hbar\omega a^+(k\lambda)|0\rangle = (\hbar k c)a^+(k\lambda)|0\rangle$$

(this is computed "above" E_0).

• The momentum operator of the field can be computed by promoting the classical EM momentum $\dfrac{1}{4\pi c}\int(\mathbf{E}\times\mathbf{B})d^3\mathbf{r}$ to

$$P = \sum_\lambda \int \left[a^+(k\lambda)a(k\lambda)\right]\hbar\mathbf{k}d^3\mathbf{k}$$

And it can be verified that the momentum of $a^+(k\lambda)|0\rangle \equiv |k\lambda\rangle$ is $\hbar\mathbf{k}$. Since $E^2 = p^2c^2 + m^2c^4$ it follows that $|k\lambda\rangle$ is a massless particle – the *photon*. Its wave function is

$$|k\lambda\rangle \rightarrow \frac{\varepsilon(k\lambda)e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{3/2}}$$

• The state of the field is given by the number of photons at each $k, \lambda,$ that is, by successive application of creation operators (**Fock state**):

$$\left(\frac{a^+(k_1\lambda_1)^{n_1}}{\sqrt{n_1!}} \frac{a^+(k_2\lambda_2)^{n_2}}{\sqrt{n_2!}} \dots \right) \left| 0 \right\rangle =$$

n_i photons with wave number k_i and polarization λ_i, and linear combinations of such states.

• Expected value and variance of vacuum electric field in location r:

$$\left\langle 0 \left| E(\mathrm{r}) \right| 0 \right\rangle = 0, \text{ but } \left\langle 0 \left| E^2(\mathrm{r}) \right| 0 \right\rangle = \infty$$

• Why? It's enough to prove for $\Pi(\mathrm{r}):$

- For simplicity's sake, write

$$\Pi(r) \approx \int k^{1/2} \left[a(\mathrm{k}) e^{i\mathrm{k}\cdot\mathrm{r}} - a^+(\mathrm{k}) e^{-i\mathrm{k}\cdot\mathrm{r}} \right] d^3\mathrm{k}$$

So $\langle 0|\Pi(r)|0\rangle =$

$$\langle 0| \int k^{1/2} \left[a(\mathrm{k}) e^{i\mathrm{k}\cdot\mathrm{r}} - a^+(\mathrm{k}) e^{-i\mathrm{k}\cdot\mathrm{r}} \right] d^3\mathrm{k} |0\rangle$$

but for all k: $a(\mathrm{k})|0\rangle = 0, \langle 0|a^+(\mathrm{k}) = 0$.

Now to the variance:

$$\langle 0| \iint k_1^{1/2} k_2^{1/2} \left[\left(a(\mathrm{k}_1) e^{i\mathrm{k}_1\cdot\mathrm{r}} - a^+(\mathrm{k}_1) e^{-i\mathrm{k}_1\cdot\mathrm{r}} \right) \right.$$

$$\left. \left(a(\mathrm{k}_2) e^{i\mathrm{k}_2\cdot\mathrm{r}} - a^+(\mathrm{k}_2) e^{-i\mathrm{k}_2\cdot\mathrm{r}} \right) \right] d^3\mathrm{k}_1 d^3\mathrm{k}_2 |0\rangle =$$

$$\langle 0| \iint k_1^{1/2} k_2^{1/2} e^{i(\mathrm{k}_1-\mathrm{k}_2)\cdot\mathrm{r}} a(\mathrm{k}_1) a^+(\mathrm{k}_2) d^3\mathrm{k}_1 d^3\mathrm{k}_2 |0\rangle =$$

$$\langle 0| \iint k_1^{1/2} k_2^{1/2} e^{i(\mathrm{k}_1-\mathrm{k}_2)\cdot\mathrm{r}} \left[a^+(\mathrm{k}_2) a(\mathrm{k}_1) + \delta^3(\mathrm{k}_1 - \mathrm{k}_2) \right]$$

$$d^3\mathrm{k}_1 d^3\mathrm{k}_2 |0\rangle =$$

$\langle 0| \int k_1 d^3\mathrm{k}_1 |0\rangle = O\left(k_0^4\right)$ for a frequency cutoff k_0.

The Classical Limit

• We should hope that, as mass and energy scales increase to "everyday scale", QM laws should converge to Newtonian mechanics laws. Look for example at the harmonic oscillator when the energy increases – it resembles the behavior of a "Newtonian" oscillator.

• It makes sense, in this regard, to look at the average, or expectation, of position and momentum. Therefore let us look at how the average changes over time: let Ω be a function of X and P. Then

$$\frac{d}{dt}\langle\Omega\rangle = \frac{d}{dt}\langle\psi|\Omega|\psi\rangle =$$
$$\langle\dot{\psi}|\Omega|\psi\rangle + \langle\psi|\dot{\Omega}|\psi\rangle + \langle\psi|\Omega|\dot{\psi}\rangle$$

• Assuming Ω has no explicit time dependence, $\dot{\Omega} = 0$. We then obtain, using Schrödinger's Equation

$$\frac{d}{dt}\langle\Omega\rangle = \left(\frac{-i}{\hbar}\right)\langle[\Omega,H]\rangle \left(\frac{d\omega}{dt} = \{\omega,H\}\right)$$

Ehrenfest's theorem   Remember!

- For example

$$\frac{d}{dt}\langle X \rangle = \left(\frac{-i}{\hbar}\right)\langle [X,H] \rangle = \frac{\langle P \rangle}{m} = \left\langle \frac{\partial H}{\partial P} \right\rangle$$

$$\left(\text{assuming } H = \frac{P^2}{2m} + V(X) \right)$$

- and $\dfrac{d}{dt}\langle P \rangle = -\left\langle \dfrac{dV(x)}{dx} \right\rangle = -\left\langle \dfrac{\partial H}{\partial X} \right\rangle$

- which look just like Hamilton's equations. Alas, we cannot argue that the latter hold for average quantities, since in general

$$\left\langle \frac{\partial H}{\partial P} \right\rangle \neq \frac{\partial \langle H \rangle}{\partial \langle P \rangle}, \quad \text{etc.}$$

- However, it's still a good approximation.

Rotational Invariance and Angular Momentum

Motivation: Central Potential (Atoms)
2D Translations

- Translations in 2D are given by

$$P_x \rightarrow -i\hbar \frac{\partial}{\partial x}, P_y \rightarrow -i\hbar \frac{\partial}{\partial y}$$

and linear combinations of these. Much like in the 1D case, translation by a vector **a** is given by

$$T(\text{a}) = e^{-i\text{a} \cdot \text{P}/\hbar}, \text{P} = P_x \text{i} + P_y \text{j}$$

$$\text{In 1D}: \quad P|\psi\rangle = -i\hbar \frac{d\psi}{dx}, \quad \frac{d}{dx} = \frac{i}{\hbar}P,$$

$$U_a(\psi(x)) = \psi(x-a) =$$

$$\psi(x) - a\psi'(x) + \frac{a^2}{2}\psi''(x) - \ldots =$$

$$\left[I - a\frac{d}{dx} + \frac{a^2}{2!}\frac{d^2}{dx^2} - \ldots \right]\psi =$$

$$e^{-a\frac{d}{dx}} = e^{\frac{-iaP}{\hbar}}.$$

One can also see this via infinitesimal translations :

$$\left(\frac{dU_a}{da}\right)\psi = \lim_{\varepsilon \to 0} \frac{U_{a+\varepsilon}(\psi) - U_a(\psi)}{\varepsilon} =$$

$$\lim_{\varepsilon \to 0} \frac{\psi(x-a-\varepsilon) - \psi(x-a)}{\varepsilon} = -\frac{d\psi(x-a)}{dx} = \left(-\frac{d}{dx}U_a\right)\psi$$

$$\text{so,} \quad \frac{d}{da}U_a = -\frac{d}{dx}U_a \Rightarrow U_a = e^{a\left(-\frac{d}{dx}\right)} = e^{\frac{-iaP}{\hbar}}$$

- Let a 2D rotation be described by

$$\begin{pmatrix} x \\ y \end{pmatrix} \rightarrow \begin{pmatrix} \cos(\phi_0) & -\sin(\phi_0) \\ \sin(\phi_0) & \cos(\phi_0) \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

- The operator that rotates the 2D vectors is denoted by $R(\phi_0 \mathrm{k})$, and the corresponding Hilbert space operator is denoted $U\big[R(\phi_0 \mathrm{k})\big]$.

For an infinitesimal rotation,

$$U\big[R(\varepsilon_z \mathrm{k})\big] = I - \frac{i\varepsilon_z L_z}{\hbar}, \quad U\big[R(\phi_0 \mathrm{k})\big] = e^{-i\phi_0 L_z/\hbar}$$

$$L_z = XP_y - YP_x \underset{\substack{\text{in polar} \\ \text{coordinate}}}{=} -i\hbar \frac{\partial}{\partial \phi}$$

- Physical interpretation: if $\big[L_z, H\big] = 0$, H is rotationally invariant, and experiments will yield the same results in the coordinates are rotated. Also, there is a common basis for H and L_z .

L_z's Eigenvalues

$$L_z \left| l_z \right\rangle = l_z \left| l_z \right\rangle \Rightarrow -i\hbar \frac{\partial \psi_{l_z}(\rho,\phi)}{\partial \phi} = l_z \psi_{l_z}(\rho,\phi) \Rightarrow$$

$$\psi_{l_z}(\rho,\phi) = R(\rho)e^{il_z\phi/\hbar} \quad (R \text{ has to be normalizable w.r.t } \int_0^\infty \rho d\rho)$$

Imposing Hermiticity, $\left\langle \psi_1 \left| L_z \right| \psi_2 \right\rangle = \left\langle \psi_2 \left| L_z \right| \psi_1 \right\rangle^*$, implies

$$\psi(\rho,0) = \psi(\rho,2\pi) \Rightarrow e^{2\pi i l_z/\hbar} = 1 \Rightarrow l_z = m\hbar, \, m = 0,\pm1,\pm2...$$

m is called the <u>magnetic quantum number</u>. Why can we impose Hermicity? It's a postulate.

- There are still an infinite number of degrees of freedom for choosing $R(\rho)$. This is solved by demanding that the eigenvectors of L_z are also the eigenvectors of, say, a rotationally invariant Hamiltonian. Physically, this means that the state is determined not only by its angular momentum, but also by its energy.

Define $\Phi_m(\phi) = (2\pi)^{-1/2} e^{im\phi} \left(\int_0^{2\pi} \Phi_m(\phi) \Phi_{m'}(\phi) d\phi = \delta_{mm'} \right)$

Examples (Shankar p. 315):

• A particle's wave function is

$$\psi(\rho,\phi) = Ae^{-\rho^2/2\Delta^2}\cos^2(\phi).$$

Prove that

$$P(l_z = 0) = \frac{2}{3}, P(l_z = 2\hbar) = P(l_z = -2\hbar) = \frac{1}{6}.$$

Solution : to calculate $P(l_z = m\hbar)$, the ρ part is only a normalizing factor. So, up to normalization,

$$P(l_z = m\hbar) = \left|\int_0^{2\pi}\psi^*(\rho,\phi)\Phi_m(\phi)d\phi\right|^2 = \begin{cases} \pi^2 & m = 0 \\ \pi^2/4 & m = \pm 2 \\ 0 & \text{otherwise} \end{cases}$$

• A particle's wave function is

$$\psi(\rho,\phi) = Ae^{-\rho^2/2\Delta^2}\left(\frac{\rho}{\Delta}\cos(\phi) + \sin(\phi)\right).$$

Prove that $P(l_z = \hbar) = P(l_z = -\hbar) = \frac{1}{2}.$

Solution: the same as above – note that

$$\left|\int_0^{2\pi}(A\cos(\phi) + \sin(\phi))\Phi_m(\phi)d\phi\right|^2 = \begin{cases} const. & m = \pm 1 \\ 0 & \text{otherwise} \end{cases}$$

Rotationally Invariant Problems

Assume that $V(\rho, \phi) = V(\rho)$. Then the eigenvalue
equation for H is (μ denotes the mass):

$$\left[\frac{-\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \right) + V(\rho) \right] \psi_E(\rho, \phi) = E \psi_E(\rho, \phi)$$

• Note that in this case H commutes with L_z,
since L_z is represented by $\partial / \partial \phi$, and we must
have

$$V\left(\frac{\partial \psi}{\partial \phi} \right) = \frac{\partial}{\partial \phi} (V\psi)$$

which will hold if V is a function of ρ only.

• We seek common eigenvectors of H and L_z of
the form (separation of variables):

$$\psi_{Em} = R_{Em}(\rho) \Phi_m(\phi) \Rightarrow \text{The radial equation:}$$

$$\left[\frac{-\hbar^2}{2\mu} \left(\frac{d^2}{d\rho^2} + \frac{1}{\rho} \frac{d}{d\rho} - \frac{m^2}{\rho^2} \right) + V(\rho) \right] R_{Em}(\rho) = E R_{Em}(\rho)$$

Angular Momentum in 3D

Three (Hermitian) generators : $L_x = YP_z - ZP_y$,

$L_y = ZP_x - XP_z$, $L_z = XP_y - YP_x$, which satisfy :

$\left[L_x, L_y\right] = i\hbar L_z$, $\left[L_y, L_z\right] = i\hbar L_x$, $\left[L_z, L_x\right] = i\hbar L_x$

or $L \times L = i\hbar L$ or

$$\left[L_i, L_j\right] = i\hbar \sum_{k=1}^{3} \varepsilon_{ijk} L_k \ , \ \varepsilon_{ijk} = \text{antisymmetric tensor.}$$

- The *total angular momentum operator (squared) is defined by*

$$L^2 = L_x^2 + L_y^2 + L_z^2 \Rightarrow \left[L^2, L_x\right] = \left[L^2, L_y\right] = \left[L^2, L_z\right] = 0$$

The square root of L^2 is regarded as the total angular momentum of the system. The goal is to characterize a "pure" state by its (definite) total angular momentum, energy, and magnetic quantum number (the last being the angular momentum around the z-axis).

Finite Rotations in 3D

• Rotations are represented by

$$\theta = \theta\hat{\theta}, \theta = \text{rotation angle,}$$

$$\hat{\theta} = \text{rotation axis (unit vector)}$$

• Turns out that $U[R(\theta)] = e^{-i\theta\hat{\theta}\cdot L/\hbar} = e^{-i\theta\cdot L/\hbar}$

Proof: when a vector **r** is rotated by an infinitesimal angle $\delta\theta$, it moves to $r + \delta\theta \times r$ (because the addition to the vector is perpendicular both to the vector and the rotation axis). So, the infinitesimal change induced by $U[R(\delta\theta)]$ is

$$\psi(r) \rightarrow \psi(r + \delta\theta \times r) = \psi(r) + (\delta\theta \times r) \cdot \nabla\psi$$

Putting aside $\hbar, i$ for the moment, we should show that this change in $\psi(r)$ is also induced by $I + (\delta\theta)(L \cdot \hat{\theta}).$ the vector product term is

$$\delta\theta \begin{vmatrix} \hat{\theta}_x & \hat{\theta}_y & \hat{\theta}_z \\ r_x & r_y & r_z \\ \psi_x & \psi_y & \psi_z \end{vmatrix}$$

and the change induced by $I + (\delta\theta)(L \cdot \hat{\theta})$ is $(\delta\theta)(\hat{\theta}_x L_x + \hat{\theta}_y L_y + \hat{\theta}_z L_z)\psi$ To prove that the two changes are equal, compare e.g. the coefficients of $\hat{\theta}_z$ (and remember that $L_z = XP_y - YP_x$).

If H is invariant under rotation ($U[R]H = HU[R]$),
then, since L_x, L_y, L_z are represented by infinitesimal
rotations, $[H, L_i] = 0$, and so $[H, L^2] = 0$. Hence, all
the three components of L, and the total angular
momentum, are conserved.
However, one cannot find a base which diagnolaizes
H, L_x, L_y, L_z, since the L_i don't commute. But $[L^2, L_i] = 0$,
so one usually tries to simultaneously diagonalize H, L^2, L_z.

Common Eigenvalues for L^2 and L_z

Following the paradigm used for the oscillator to
common eigenvectors $L^2|\alpha\beta\rangle = \alpha|\alpha\beta\rangle, L_z|\alpha\beta\rangle = \beta|\alpha\beta\rangle$
Here, too, there are lowering and raising operators :
$L_\pm = L_x \pm iL_y \Rightarrow [L_z, L_\pm] = \pm\hbar L_\pm$. Note $[L_\pm, L^2] = 0$.
$L_z(L_+|\alpha\beta\rangle) = (L_+L_z + \hbar L_+)|\alpha\beta\rangle = (\beta + \hbar)(L_+|\alpha\beta\rangle)$.
$L^2(L_+|\alpha\beta\rangle) = \alpha(L_+|\alpha\beta\rangle). L_+|\alpha\beta\rangle = C_+(\alpha,\beta)|\alpha,\beta+\hbar\rangle$
And similarly $L_-|\alpha\beta\rangle = C_-(\alpha,\beta)|\alpha,\beta-\hbar\rangle$
So, given $|\alpha\beta\rangle$, the action of $L_\pm$ on it creates $|\alpha, \beta \pm k\hbar\rangle$
This has to end somewhere, since for a given total angular momentum
(α), the angular momentum around z (β) has to be bounded.

$\langle \alpha\beta | L^2 - L_z^2 | \alpha\beta \rangle = \langle \alpha\beta | L_x^2 + L_y^2 | \alpha\beta \rangle$, but $L_x^2 + L_y^2$ is positive definite (since L_x, L_y are Hermitian), so we must have $\alpha \geq \beta^2$. So there's an $|\alpha\beta_{\max}\rangle$ that cannot be raised: $L_+ |\alpha\beta_{\max}\rangle = 0$. Applying L_- to both sides and using $L_- L_+ = L^2 - L_z^2 - \hbar L_z$, we get $\underline{\alpha = \beta_{\max}(\beta_{\max} + \hbar)}$, similarly $\underline{\alpha = \beta_{\min}(\beta_{\min} + \hbar)}$ It follows that $\beta_{\min} = -\beta_{\max}$. Since we got from $|\alpha\beta_{\min}\rangle$ to $|\alpha\beta_{\max}\rangle$ in k steps of size $\hbar$, we must have

$$\beta_{\max} = \frac{\hbar k}{2}, \ k = 0,1,2..., \ \alpha = \hbar^2 \left(\frac{k}{2}\right)\left(\frac{k}{2}+1\right).$$

$\frac{k}{2} = \frac{\beta_{\max}}{\hbar}$ is called the angular momentum of the state. Unlike in classical mechanics, it's smaller than the total angular momentum.

Angular Momentum $\left(\dfrac{k}{2}\right)$	$\beta_{\max}$	α	$\lvert\alpha\beta\rangle$
0	0	0	$\lvert 0,0\rangle$
1/2	$\hbar/2$	$\left(\dfrac{1}{2}\right)\left(\dfrac{3}{2}\right)\hbar^2$	$\left\lvert\left(\dfrac{3}{4}\right)\hbar^2,\dfrac{\hbar}{2}\right\rangle$ $\left\lvert\left(\dfrac{3}{4}\right)\hbar^2,-\dfrac{\hbar}{2}\right\rangle$
1	$\hbar$	$(1)(2)\hbar^2$	$\lvert 2\hbar^2,\hbar\rangle$ $\lvert 2\hbar^2,0\rangle$ $\lvert 2\hbar^2,-\hbar\rangle$
3/2	..	..	..
:	:	:	:

But we proved that l_z can only have integer multiplies of $\hbar$??

$$\underline{L\times L = i\hbar L}$$

• Answer: here we only used the $\underbrace{\text{commutation rules}}$, not the operators' specific shapes.

• There are particles whose wave function is more complicated (non-scalar). For these particles, there are rotation-like operators **J** which satisfy the commutation rules

$$\boxed{\mathbf{J} \times \mathbf{J} = i\hbar\mathbf{J}}$$

• For example:

$$\psi(x, y, z) = \psi_x(x, y, z)\mathbf{i} + \psi_y(x, y, z)\mathbf{j} + \psi_z(x, y, z)\mathbf{k}$$

• Rotations of such a function involve rotating both the *components* and the *coordinates*: under an infinitesimal rotation $\varepsilon_z \mathbf{k}$,

$$\psi_x \rightarrow \psi_x(x + y\varepsilon_z, y - x\varepsilon_z) - \varepsilon_z \psi_y(x + y\varepsilon_z, y - x\varepsilon_z) = \psi_x'$$

$$\psi_y \rightarrow \varepsilon_z \psi_x(x + y\varepsilon_z, y - x\varepsilon_z) + \psi_y(x + y\varepsilon_z, y - x\varepsilon_z) = \psi_y'$$

$$\begin{bmatrix} \psi_x' \\ \psi_y' \end{bmatrix} = \left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{i\varepsilon_z}{\hbar} \begin{bmatrix} L_z & 0 \\ 0 & L_z \end{bmatrix} - \frac{i\varepsilon_z}{\hbar} \begin{bmatrix} 0 & -i\hbar \\ i\hbar & 0 \end{bmatrix} \right) \begin{bmatrix} \psi_x \\ \psi_y \end{bmatrix}$$

$$J_z = L_z^{(1)} \otimes I^{(2)} + I^{(1)} \otimes S_z^{(2)} = L_z + S_z \,.\, S_z = \text{e.g. spin.}$$

$I^{(2)} = 2 \times 2$ identity matrix w.r.t the vector components,

$I^{(1)} = $ identity operator w.r.t x, y.

- Just as before:

$$J^2 \left| jm \right\rangle = j(j+1)\hbar^2 \left| jm \right\rangle, \quad j = 0, \frac{1}{2}, 1, \frac{3}{2} \ldots$$

$$J_z \left| jm \right\rangle = m\hbar \left| jm \right\rangle, \quad m = j, j-1, \ldots 0, \ldots -j$$

As before, $J_\pm \left| jm \right\rangle = C_\pm(j,m) \left| j, m \pm 1 \right\rangle$

$$\left(J_\pm \equiv J_x \pm iJ_y \right)$$

$$J_+ \left| jm \right\rangle = C_+(j,m) \left| j, m+1 \right\rangle \underbrace{\Rightarrow}_{\text{adjoint}}$$

$$\left\langle jm \right| J_- = C_+^*(j,m) \left\langle j, m+1 \right| \Rightarrow$$

$$\left| C_+(j,m) \right|^2 = \left\langle jm \right| J_- J_+ \left| jm \right\rangle = \left\langle jm \right| J^2 - J_z^2 - \hbar J_z \left| jm \right\rangle =$$

$$j(j+1)\hbar^2 - m^2 \hbar^2 - m\hbar^2$$

so $J_\pm \left| jm \right\rangle = \hbar \left[(j \mp m)(j \pm m + 1) \right]^{\frac{1}{2}} \left| j, m \pm 1 \right\rangle$

Since $J_x = \dfrac{J_+ + J_-}{2}, J_y = \dfrac{J_+ - J_-}{2i}$, it is straightforward

to write their matrices in the $\left| jm \right\rangle$ basis as well. These

matrices are block diagonal in the fixed j blocks. This

makes the calculation of $e^{-i\theta \cdot \mathbf{J}/\hbar}$ more feasible :

Finite Rotations

- In order to compute the transformation induced by finite (as opposed to infinitesimal) rotations, one has to calculate

$$U\left[R(\theta)\right] = e^{\frac{-i\theta\hat{\theta}\cdot J}{\hbar}} = e^{\frac{-i\theta\cdot J}{\hbar}}.$$

- The calculation is facilitated by the fact that the matrices for J_x, J_y, J_z are all block diagonal in the constant j blocks.

- Also, since the eigenvalues of $\hat{\theta} \cdot J$ (in the constant-j block) are

$$-j, -j+1, \dots j, \text{ then } \left(J \cdot \hat{\theta} + jI\right) \dots \left(J \cdot \hat{\theta} - jI\right) = 0$$

(since obviously its action on any vector is 0).

- This allows to express $\left(\hat{\theta} \cdot J\right)^{2j+1}$ as a linear combination of $I, \left(\hat{\theta} \cdot J\right), \left(\hat{\theta} \cdot J\right)^2 \dots \left(\hat{\theta} \cdot J\right)^{2j}$, so the powers in the exponential usually have a simple periodic behavior which allows to write it down as simple functions of θ (see also discussion here on Stern-Gerlach apparatuses).

The Matrices of Angular Momentum Operators

Spin half   Spin one

J^2	$j'm'$ \ jm	$(0,0)$	$\left(\frac{1}{2},\frac{1}{2}\right)$	$\left(\frac{1}{2},-\frac{1}{2}\right)$	$(1,1)$	$(1,0)$	$(1,-1)$
	$(0,0)$	0	0	0	0	0	0
	$\left(\frac{1}{2},\frac{1}{2}\right)$	0	$(3/4)\hbar^2$	0	0	0	0
	$\left(\frac{1}{2},-\frac{1}{2}\right)$	0	0	$(3/4)\hbar^2$	0	0	0
	$(1,1)$	0	0	0	$2\hbar^2$	0	0
	$(1,0)$	0	0	0	0	$2\hbar^2$	0
	$(1,-1)$	0	0	0	0	0	$2\hbar^2$

J_z	$j'm'$ \ jm	$(0,0)$	$\left(\frac{1}{2},\frac{1}{2}\right)$	$\left(\frac{1}{2},-\frac{1}{2}\right)$	$(1,1)$	$(1,0)$	$(1,-1)$
	$(0,0)$	0	0	0	0	0	0
	$\left(\frac{1}{2},\frac{1}{2}\right)$	0	$(1/2)\hbar$	0	0	0	0
	$\left(\frac{1}{2},-\frac{1}{2}\right)$	0	0	$-(1/2)\hbar$	0	0	0
	$(1,1)$	0	0	0	$\hbar$	0	0
	$(1,0)$	0	0	0	0	0	0
	$(1,-1)$	0	0	0	0	0	$-\hbar$

Spin half **Spin one**

J_x

$j'm'$ \ jm	$(0,0)$	$\left(\frac{1}{2},\frac{1}{2}\right)$	$\left(\frac{1}{2},-\frac{1}{2}\right)$	$(1,1)$	$(1,0)$	$(1,-1)$
$(0,0)$	0	0	0	0	0	0
$\left(\frac{1}{2},\frac{1}{2}\right)$	0	0	$\hbar/2$	0	0	0
$\left(\frac{1}{2},-\frac{1}{2}\right)$	0	$\hbar/2$	0	0	0	0
$(1,1)$	0	0	0	0	$\hbar/\sqrt{2}$	0
$(1,0)$	0	0	0	$\hbar/\sqrt{2}$	0	$\hbar/\sqrt{2}$
$(1,-1)$	0	0	0	0	$\hbar/\sqrt{2}$	0

J_y

$j'm'$ \ jm	$(0,0)$	$\left(\frac{1}{2},\frac{1}{2}\right)$	$\left(\frac{1}{2},-\frac{1}{2}\right)$	$(1,1)$	$(1,0)$	$(1,-1)$
$(0,0)$	0	0	0	0	0	0
$\left(\frac{1}{2},\frac{1}{2}\right)$	0	0	$-i\hbar/2$	0	0	0
$\left(\frac{1}{2},-\frac{1}{2}\right)$	0	$i\hbar/2$	0	0	0	0
$(1,1)$	0	0	0	0	$-i\hbar/\sqrt{2}$	0
$(1,0)$	0	0	0	$i\hbar/\sqrt{2}$	0	$-i\hbar/\sqrt{2}$
$(1,-1)$	0	0	0	0	$i\hbar/\sqrt{2}$	0

Angular Momentum Functions in the Coordinate Basis

Start with the "topmost" state $|ll\rangle$, satisfying $L_+|ll\rangle = 0$.

In the coordinate basis, $L_\pm = \pm\hbar e^{\pm i\phi}\left(\dfrac{\partial}{\partial\theta} \pm i\cot(\theta)\dfrac{\partial}{\partial\phi}\right)$

(note that the r part is left out, and the ϕ part is taken care of by multiplying with $\exp(il\phi)$).

This allows to find $|ll\rangle$, and the others can be found by successive operations with L_-. As before, we separate the r part, and search for eigenfunctions with definite total angular and $z-$momentum, $Y_l^m(\theta,\phi)$ (spherical harmonics). They are orthonormal under the inner product

$$\int d\Omega = \int_{-1}^{1}\int_0^{2\pi} d(\cos(\theta))d\phi.$$

If $\psi(r,\theta,\phi) = \displaystyle\sum_{l=0}^{\infty}\sum_{m=-l}^{l} C_l^m(r)Y_l^m(\theta,\phi)$, where

$C_l^m(r) = \int\left(Y_l^m(\theta,\phi)\right)^*\psi(r,\theta,\phi)d\Omega$, then

$$\Pr(L^2 = l(l+1)\hbar^2, L_z = m\hbar) = \int_0^{\infty}\left|C_l^m(r)\right|^2 r^2 dr$$

That is, $C_l^m(r)$ is the amplitude to find the particle at radius r and with momentum(s) l, m.

$$Y_0^0 = (4\pi)^{-1/2}$$

$$Y_1^{\pm 1} = \mp(3/8\pi)^{1/2}\sin(\theta)e^{\pm i\phi}$$

$$Y_1^0 = (3/4\pi)^{1/2}\cos(\theta)$$

$$Y_2^{\pm 2} = (15/32\pi)^{1/2}\sin^2(\theta)e^{\pm 2i\phi}$$

$$Y_2^{\pm 1} = \mp(15/8\pi)^{1/2}\sin(\theta)\cos(\theta)e^{\pm i\phi}$$

$$Y_2^0 = (5/16\pi)^{1/2}\left(3\cos^2(\theta) - 1\right)$$

$$Y_l^m(\theta,\phi) = (-1)^m\left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\right]^{\frac{1}{2}}e^{im\phi}P_l^m(\cos(\theta))$$

$$P_l^m(x) = \frac{1}{2^l l!}(1-x^2)^{\frac{m}{2}}\frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l$$

• Example question (Shankar, 12.5.13): a particle's state is proportional to $(x+y+2z)e^{-ar}$. Prove that $\Pr(l_z = 0) = 2/3, \Pr(l_z = \hbar) = \Pr(l_z = -\hbar) = 1/6$.

• Answer: It's immediate to see that

$$z = 2r\sqrt{\frac{\pi}{3}}Y_1^0, \ x = r\sqrt{\frac{4\pi}{6}}\left(Y_1^{-1} - Y_1^1\right), \ y = ri\sqrt{\frac{4\pi}{6}}\left(Y_1^{-1} + Y_1^1\right)$$

So all that's left is to compare the coefficients of Y_1^0, Y_1^{-1}, Y_1^1 in $x + y + 2z$.
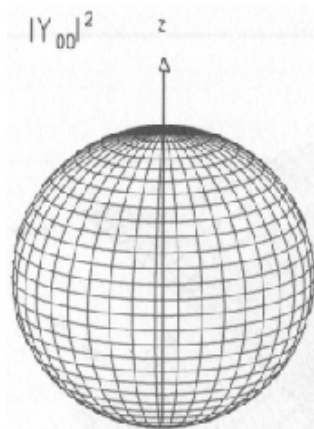
Note that as *m* grows, there is more of the momentum in the *z* direction, and the probability to have large *z* values decreases.
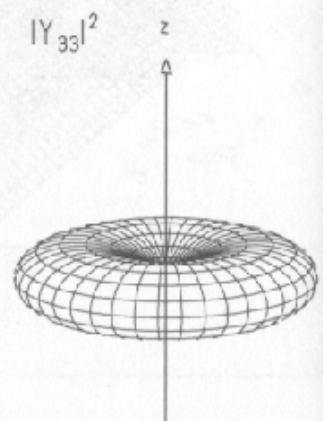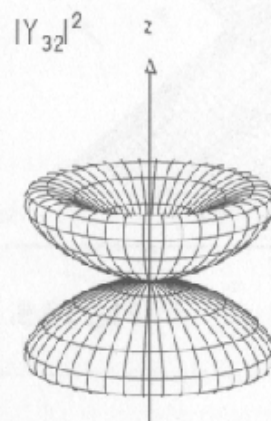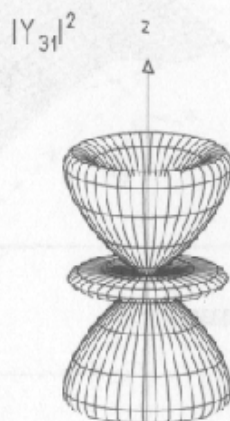
Solution of Rotationally Invariant Problems

Note: μ **is mass (to avoid confusion with** *m***).**

If $V(r,\theta,\phi)=V(r)$, the Schrödinger equation becomes

$$\left[\frac{-\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\sin(\theta)\frac{\partial}{\partial\theta}+\right.\right.$$

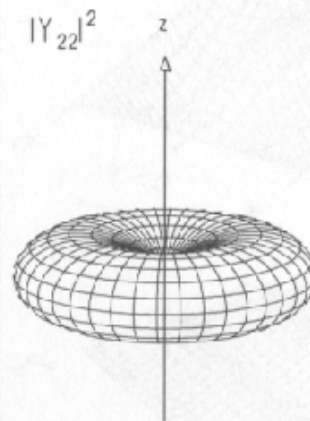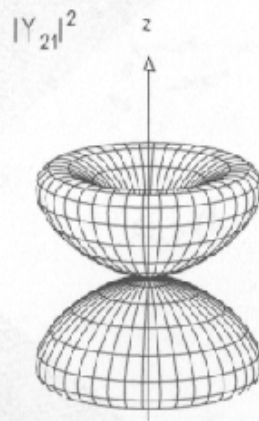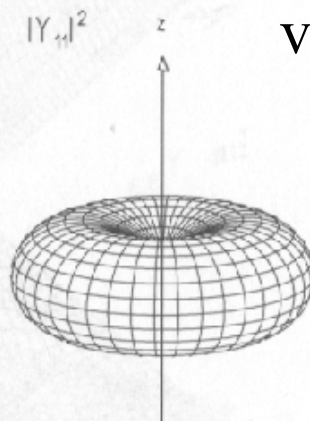$$\left.\left.\frac{1}{r^2\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right)+V(r)\right]\psi_E(r,\theta,\phi)=E\psi_E(r,\theta,\phi)$$

Since in this case $[H,L]=0$, seek simultaneous eigenkets
of $H,L^2,L_z:\psi_{Elm}(r,\theta,\phi)=R_{Elm}(r)Y_l^m(\theta,\phi)$. As in 2D,
get a radial equation:

$$\left\{\frac{-\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}-\frac{l(l+1)}{r^2}\right]+V(r)\right\}R_{El}=ER_{El}\text{ (no }m\text{)}.$$

$$R_{El}=\frac{U_{El}}{r}\Rightarrow\left\{\frac{d^2}{dr^2}+\frac{2\mu}{\hbar^2}\left[E-V(r)-\frac{l(l+1)\hbar^2}{2\mu r^2}\right]\right\}U_{El}=0$$

which is equivalent to

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]U_{El}\equiv D_l(r)U_{El}=EU_{El}$$

Imposing Hermiticity of D_l with regard to

$$U_{El}, \int_0^\infty U_1^* \left(D_l U_2 \right) dr = \left[\int_0^\infty U_2^* \left(D_l U_1 \right) dr \right]^* \Rightarrow$$

$$\int_0^\infty \left(U_1^* U_2'' - \left(U_1^* \right)'' U_2 \right) dr = 0 \Rightarrow \begin{array}{c} \text{integration} \\ \text{by parts} \end{array}$$

$$\left(U_1^* \frac{dU_2}{dr} - U_2 \frac{dU_1^*}{dr} \right) \Bigg|_0^\infty = 0$$

Next, address the normalization of U_{El}, R_{El} : to integrate R_{El}

one must take $\int_0^\infty r^2 R_{El} \, dr = \int_0^\infty U_{El} \, dr$. For this to be normalizable,

we must have either $U_{El} \xrightarrow[r \to \infty]{} 0$ (bound state) or $U_{El} \xrightarrow[r \to \infty]{} e^{ikr}$

(unbound state). In both cases, the upper limit in

$$\left(U_1^* \frac{dU_2}{dr} - U_2 \frac{dU_1^*}{dr} \right) \Bigg|_0^\infty \quad \text{vanishes and the Hermiticity depends on}$$

whether $\left(U_1^* \frac{dU_2}{dr} - U_2 \frac{dU_1^*}{dr} \right)(0) = 0$. This is satisfied if

$U_{El} \xrightarrow[r \to 0]{} c = const$. If c is not zero, $R \propto \dfrac{U}{r} \propto \dfrac{c}{r}$

Diverges at the origin, which is impossible since $\frac{c}{r}$ does not satisfy Schrödinger's equation at the origin, as $\nabla^2(1/r) = -4\pi\delta^3(r)$. So, we must have $U_{El} \xrightarrow[r\to 0]{} 0$.

General Properties of U_{El}

• The goal is to further study the asymptotic behavior of U_{El} as r tends to zero or infinity, depending on the potential.

As $r \to 0$, and assuming that $V(r)$ is less singular than r^{-2}, then the equation is dominated by the so-called centrifugal barrier : $U_l'' \cong \frac{l(l+1)}{r^2}U_l$ (E becomes inconsequential in the limit).

Guessing a solution $U_l \cong r^\alpha$ yields

$$U_l \cong \begin{cases} r^{l+1} \text{ (regular)} \\ r^{-l} \text{ (irregular, ruled out following previous analysis)} \end{cases}$$

• Intuitively – as before, as the angular momentum increases, the particle avoids the origin more and more.

• Next, let us study the behavior at infinity. Assume that the potential does not dominate the behavior at infinity; a condition which will be justified later is

$$rV(r) \xrightarrow[r \to \infty]{} 0$$

For large r, the equation becomes $\dfrac{d^2 U_E}{dr^2} = -\dfrac{2\mu E}{\hbar^2} U_E$

(l does not influence the behavior at infinity).

There are then two cases :

$E > 0$: Particle may escape to infinity, we expect U_E to oscillate at infinity.

$E < 0$: The region $r \to \infty$ is classicaly forbidden, we expect U_E to exponentially decrease as $r \to \infty$.

Assume $E > 0$. The solutions are

$$U_E = Ae^{ikr} + Be^{-ikr}, k = \left(2\mu E / \hbar^2\right)^{1/2}$$

Let us now write $U_E = f(r)e^{\pm ikr}$, and check whether $f \to const.$ as $r \to \infty$. To do that, plug the above form into

$$\left\{ \frac{d^2}{dr^2} + \frac{2\mu}{\hbar^2} \left[E - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2} \right] \right\} U_{El} = 0$$

To obtain at infinity

$$f'' \pm (2ik)f' - \frac{2\mu V(r)}{\hbar^2} f = 0$$

Assuming the second derivative is small :

$$\frac{df}{f} = \mp \frac{i}{k} \frac{\mu}{\hbar^2} V(r) dr$$

$$f(r) = f(r_0) \exp \left[\mp \left(\frac{i\mu}{k\hbar^2} \right) \int_{r_0}^{r} V(r') dr' \right]$$

If $rV(r) \xrightarrow[r \to \infty]{} 0$, the integral tends to

a constant as $r \to \infty$. But if e.g. $V(r) = -\dfrac{e^2}{r}$,

as in the Coulomb potential , then

$$f(r) = f(r_0) \exp\left[\pm\left(\frac{i\mu e^2}{k\hbar^2}\right)\ln\left(\frac{r}{r_0}\right)\right]$$

$$U_E(r) \propto \exp\left[\pm i\left(kr + \frac{\mu e^2}{k\hbar^2}\ln(r)\right)\right]$$

So, the potential influences the particle no matter how far it is from the origin.

For the case $E < 0$, the results carry over with the change $k \rightarrow i\kappa$, $\kappa = \left(2\mu|E|/\hbar^2\right)^{1/2}$,

$U_E \xrightarrow[r \rightarrow \infty]{} Ae^{-\kappa r} + Be^{\kappa r}$, and $B = 0$ as usual.

As before, this is true only if $rV(r) \rightarrow 0$.

In the coulomb case (Hydrogen atom) we expect as before

$$U_E \propto \exp\left(\pm \frac{\mu e^2}{\kappa\hbar^2}\ln(r)\right)e^{\mp kr} = r^{\pm\left(\mu e^2/\kappa\hbar^2\right)}e^{\mp kr}$$

For $E < 0$, the energy eigenkets are normalizable to unity. The operator $D_l(r)$ is non-degenerate (see proof in the discussion on degeracy), hence $U_{El}\vee$ are orthogonal for different E, and so $R_{El}(r)Y_l^m(\theta,\phi)$ are orthogonal for different $\{E, l, m\}$. This means that the energy, the total angular momentum, and the z-axis angular momentum fully determine a state.

The Free Particle in Spherical Coordinates

As before: start with $\psi_{Elm} = R_{El}(r) Y_l^m(\theta, \phi)$

Define U_{El} as before, and since $V = 0$ we get

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} \right] U_{El} = 0, \quad k^2 = \frac{2\mu E}{\hbar^2}$$

$$\rho = kr \Rightarrow \left[-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2} \right] U_l = U_l$$

This resembles the harmonic oscillator, so define lowering and raising operators

$$d_l = \frac{d}{d\rho} + \frac{l+1}{\rho}, d_l^+ = -\frac{d}{d\rho} + \frac{l+1}{\rho}, \left(d_l d_l^+ \right) U_l = U_l$$

$$d_l^+ \left(d_l d_l^+ \right) U_l = d_l^+ U_l, d_l^+ d_l = d_{l+1} d_{l+1}^+ \Rightarrow$$

$$d_{l+1} d_{l+1}^+ (d_l^+ U_l) = d_l^+ U_l \Rightarrow d_l^+ U_l = c_l U_{l+1}$$

So d_l^+ is a raising operator. We need to start with U_0: $U_0^A(\rho) = \sin(\rho)$ or $U_0^B(\rho) = \cos(\rho)$.

Taking c_l to be unity, and re-introducing R_l, it's easy to prove that

$$R_l = (-\rho)^l \left(\frac{1}{\rho} \frac{\partial}{\partial \rho} \right)^l R_0 \text{ , which generates solutions}$$

$$R_l^A \equiv j_l = (-\rho)^l \left(\frac{1}{\rho} \frac{\partial}{\partial \rho} \right)^l \left(\frac{\sin(\rho)}{\rho} \right) \text{(spherical Bessel)}$$

$$R_l^B \equiv j_l = (-\rho)^l \left(\frac{1}{\rho} \frac{\partial}{\partial \rho} \right)^l \left(\frac{-\cos(\rho)}{\rho} \right) \text{(Neumann)}$$

So, free particle solutions which are regular in the entire space are given by

$$\psi_{Elm}(r, \theta, \phi) = j_l(kr) Y_l^m(\theta, \phi), E = \frac{\hbar^2 k^2}{2\mu}$$

• Example (Shankar 12.6.8): Find the energy levels of a particle in a sphere of radius r_0 , given $l=0$.

• Solution: for $l=0$, we must have $\sin(\rho) = 0$ at the boundary, hence

$$kr_0 = n\pi \Rightarrow E_n = \frac{n^2 \pi^2 \hbar^2}{2\mu r_0^2} \left(\text{since } k^2 = \frac{2\mu E}{\hbar^2} \right)$$

(note that the quantization is finer as the radius increases)

Relation to Cartesian Coordinates Solution

In Cartesian coordinates, $\psi_E(x,y,z) = \dfrac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$,

$E = \dfrac{p^2}{2\mu} = \dfrac{\hbar^2 k^2}{2\mu}$. If the particle is going up the z−axis with

momentum p, $\psi_E(r,\theta,\phi) = \dfrac{1}{(2\pi\hbar)^{3/2}} e^{ikr\cos(\theta)}$, so it must be

possible to express it as a sum of the eigenstates computed in

spherical coordinates :

$e^{ikr\cos(\theta)} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} C_l^m \, j_l(kr) Y_l^m(\theta,\phi)$. But only $\phi = 0$ is relevant,

as the left-hand side doesn't depend on ϕ (physically, a

particle going up the z−axis has no angular momentum in

that direction). Since $Y_l^0(\theta) = \left(\dfrac{2l+1}{4\pi}\right)^{1/2} P_l(\cos(\theta))$, then

$e^{ikr\cos(\theta)} = \sum_{l=0}^{\infty} C_l \, j_l(kr) P_l(\cos(\theta))$, $C_l = C_l^0 \left(\dfrac{2l+1}{4\pi}\right)^{1/2}$. It can be

shown that $C_l = i^l (2l+1)$, so that

$e^{ikr\cos(\theta)} = \sum_{l=0}^{\infty} i^l (2l+1) \, j_l(kr) P_l(\cos(\theta))$

The Isotropic Oscillator

$$H = \frac{P_x^2 + P_y^2 + P_z^2}{2\mu} + \frac{1}{2}\mu\omega^2\left(X^2 + Y^2 + Z^2\right)$$

$$\psi_{Elm} = \frac{U_{El}}{r} Y_l^m(\theta,\phi) \Rightarrow$$

$$\left\{\frac{d^2}{dr^2} + \frac{2\mu}{\hbar^2}\left[E - \frac{1}{2}\mu\omega^2 r^2 - \frac{l(l+1)}{2\mu r^2}\right]\right\}U_{El} = 0$$

$$r \to \infty \Rightarrow U \approx e^{-y^2/2}, \, y = \left(\frac{\mu\omega}{\hbar}\right)^{\frac{1}{2}} r$$

So assume $U(y) = v(y)e^{-y^2/2} \Rightarrow$

$$v'' - 2yv' + \left[2\lambda - 1 - \frac{l(l+1)}{y^2}\right]v = 0, \, \lambda = \frac{E}{\hbar\omega}$$

Incorporating the previous analysis about the behavior near the origin, guess that

$$v(y) = y^{l+1}\sum_{n=0}^{\infty} C_n y^n$$

Substituting this into the equation yields a recursion relation between C_n and C_{n-2}, which implies that $\lambda = n + l - \dfrac{1}{2}$. However, it's easy to verify that the coefficient of y^l is C_1, which has to be zero (since all is zero), hence there are only even powers in the expansion. The case $n=0$ is ruled out because we start with C_2, and therefore the quantized energy levels are

$$n = 2(k+1) \Rightarrow E = \left(2k + l + \frac{3}{2} \right) \hbar \omega, k = 0,1,2...$$

(one could guess that the ground state energy is $(3/2)\hbar\omega$ by separation of variables, and since GSE for a 1D oscillator is $(1/2)\hbar\omega$. But this solution ties the state directly to the angular momentum).

The principle quantum number is defined by $n=2k+l$, and it determines the energy, $E=(n+3/2)\hbar\omega$. At each n, the allowed l values are $l=n-2k=n,n-2,n-4...1$ or 0. The first eigenstates are

$n=0$ $l=0$ $m=0$

$n=1$ $l=1$ $m=\pm1,0$

$n=2$ $l=0(k=1),2(k=0)$ $m=\underbrace{0}_{l=0};\underbrace{\pm2,\pm1,0}_{l=2}$

$n=3$ $l=1(k=1),3(k=0)$ $m=\underbrace{\pm1,0}_{l=1};\underbrace{\pm3,\pm2,\pm1,0}_{l=3}$

The degeneracy in l will be explained later. It is a result of symmetries in the Hamiltonian.

The Hydrogen Atom

• Assume in the meanwhile that the proton's mass is infinitely larger than the electron's, so only the electron's wave function is sought. The potential is induced by the attraction between the proton and electron, and the equation has the form

$$\left\{ \frac{d^2}{dr^2} + \frac{2m}{\hbar^2} \left[E + \frac{e^2}{r} - \frac{l(l+1)}{2mr^2} \right] \right\} U_{El} = 0, \text{ and as usual}$$

$$\psi_{Elm}(r,\theta,\phi) = R_{El}(r) Y_l^m(\theta,\phi) = \frac{U_{El}(r)}{r} Y_l^m(\theta,\phi)$$

It was proved before that under such a potential, then up to a polynomial factor, at infinity we have $U_{El}(r) \approx e^{\left[-\left(2mW/\hbar^2 \right) r \right]}$, where $W = -E$ is the binding energy (which it would take to liberate the electron), and as $r \to 0$ we have $U_{El}(r) \approx r^{l+1}$.

Define $\rho = \left(2mW/\hbar^2 \right)^{1/2} r, U_{El}(r) = e^{-\rho} v_{El}$. Considering

the behavior at 0, assume $v_{El} = \rho^{l+1} \sum_{k=0}^{\infty} C_k \rho^k$. This yields

(as opposed to the other cases), a <u>successive</u> recursion

relation for the equation $\dfrac{d^2v}{d\rho^2} - 2\dfrac{dv}{d\rho} +$

$$\left[\dfrac{e^2\lambda}{\rho} - \dfrac{l(l+1)}{\rho^2}\right]v = 0, \quad \lambda = \left(2m/\hbar^2 W\right)^{1/2} :$$

$$\dfrac{C_{k+1}}{C_k} = \dfrac{-e^2\lambda + 2(k+l+1)}{(k+l+2)(k+l+1) - l(l+1)},$$

as usual the series has to terminate and we get
the energy quantization levels defined by

$$E = -W = \dfrac{-me^4}{2\hbar^2(k+l+1)^2}, \quad k = 0,1,2..,\ l = 0,1,2..$$

In terms of the principle quantum number,
$n = k + l + 1$, the allowed energies are

$$E_n = \dfrac{-me^4}{2\hbar^2 n^2}.$$ At each n the allowed l values are

$n-1, n-2...0,$ and for each of those there are the
appropriate $2l+1$ $z-$axis angular momentum values.
So, for a given n which specifies an energy level, the

total degeneracy is $2(n-1) + 1 + 2(n-2) + 1 + ... = \underline{n^2}$

The series terminates at $k = n - l - 2$, and there's a ρ^{l+1} factor outside. So the solutions are polynomials of degree $n - 1 : R_{nl}(\rho) \approx e^{-\rho} L_{n-l-1}^{2l+1}(2\rho)$, where the latter are the associated Laguerre polynomials :

$$L_p^0 = e^x \left(d^p / dx^p \right)\left(e^{-x} x^p \right), L_p^k = (-1)^k \left(d^k / dx^k \right) L_{p+k}^0$$

When $r \to \infty, R_{nl} \approx r^{n-1} e^{-cr}$.

Define $a_0 = \hbar^2 / me^2$.

$$\psi_{1,0,0} = \left(\frac{1}{\pi a_0^3} \right)^{\frac{1}{2}} e^{-r/a_0}$$

$$\psi_{2,0,0} = \left(\frac{1}{32\pi a_0^3} \right)^{\frac{1}{2}} \left(2 - \frac{r}{a_0} \right) e^{-r/2a_0}$$

$$\psi_{2,1,0} = \left(\frac{1}{32\pi a_0^3} \right)^{\frac{1}{2}} \frac{r}{a_0} e^{-r/2a_0} \cos(\theta)$$

$$\psi_{2,1,\pm 1} = \left(\frac{1}{32\pi a_0^3} \right)^{\frac{1}{2}} \frac{r}{a_0} e^{-r/2a_0} \sin(\theta) e^{\pm i\theta}$$

For $l = n-1, \psi_{n,n-1,m} \propto e^{-r/na_0} r^{n-1} Y_{n-1}^{m}(\theta, \phi)$

Therefore, the probability to be in a spherical shell of radius r and thickness dr is $\propto e^{-2r/na_0} r^{2n}$.

This is a maximum when $r = n^2 a_0$, hence a_0 is the average distance of the electron from the nucleus in the ground state.

In general, $\langle r \rangle = \dfrac{a_0}{2}\left[3n^2 - l(l+1)\right]$

Java Applet Window

Complex Orbitals (phys.)

n = 1

l = 0 (s)

m = 0

No Slicing

☐ Stopped

☐ Alternate Rendering

Simulation Speed

Brightness

Image Resolution

Scale

http://www.falstad.com

Screen width = 234 pm

Java Applet Window

Complex Orbitals (phys.)

n = 2

l = 0 (s)

m = 0

No Slicing

☐ Stopped

☐ Alternate Rendering

Simulation Speed

Brightness

Image Resolution

Scale

http://www.falstad.com

Screen width = 976 pm

Screen width = 819 pm

Complex Orbitals (phys.)

n = 2
l = 1 (p)
m = 0
No Slicing
☐ Stopped
☐ Alternate Rendering
Simulation Speed
Brightness
Image Resolution
Scale
http://www.falstad.com

Screen width = 819 pm

Complex Orbitals (phys.)

n = 2
l = 1 (p)
m = 1
No Slicing
☐ Stopped
☐ Alternate Rendering
Simulation Speed
Brightness
Image Resolution
Scale
http://www.falstad.com

Java Applet Window

Complex Orbitals (phys.)

n = 3
l = 0 (s)
m = 0
No Slicing

☐ Stopped
☐ Alternate Rendering

Simulation Speed

Brightness

Image Resolution

Scale

http://www.falstad.com

Screen width = 2186 pm

Java Applet Window

Complex Orbitals (phys.)

n = 3
l = 1 (p)
m = 0
No Slicing

☐ Stopped
☐ Alternate Rendering

Simulation Speed

Brightness

Image Resolution

Scale

http://www.falstad.com

Screen width = 2069 pm

Java Applet Window

Complex Orbitals (phys.)

n = 3

l = 1 (p)

m = 1

No Slicing

☐ Stopped

☐ Alternate Rendering

Simulation Speed

Brightness

Image Resolution

Scale

http://www.falstad.com

Screen width = 2069 pm

z

x

Java Applet Window

Complex Orbitals (phys.)

n = 3

l = 2 (d)

m = 0

No Slicing

☐ Stopped

☐ Alternate Rendering

Simulation Speed

Brightness

Image Resolution

Scale

http://www.falstad.com

Screen width = 1718 pm

z

x

Java Applet Window

Complex Orbitals (phys.)

n = 3
l = 2 (d)
m = 1

No Slicing

☐ Stopped
☐ Alternate Rendering

Simulation Speed

Brightness

Image Resolution

Scale

http://www.falstad.com

z

x

Screen width = 1718 pm

Java Applet Window

Complex Orbitals (phys.)

n = 3
l = 2 (d)
m = 2

No Slicing

☐ Stopped
☐ Alternate Rendering

Simulation Speed

Brightness

Image Resolution

Scale

http://www.falstad.com

z

x

Screen width = 1718 pm

Java Applet Window

Complex Orbitals (phys.)

n = 10

l = 0 (s)

m = 0

No Slicing

☐ Stopped

☐ Alternate Rendering

Simulation Speed

Brightness

Image Resolution

Scale

http://www.falstad.com

Screen width = 25122 pm

Java Applet Window

Complex Orbitals (phys.)

n = 10

l = 8

m = 0

No Slicing

☐ Stopped

☐ Alternate Rendering

Simulation Speed

Brightness

Image Resolution

Scale

http://www.falstad.com

Screen width = 19181 pm
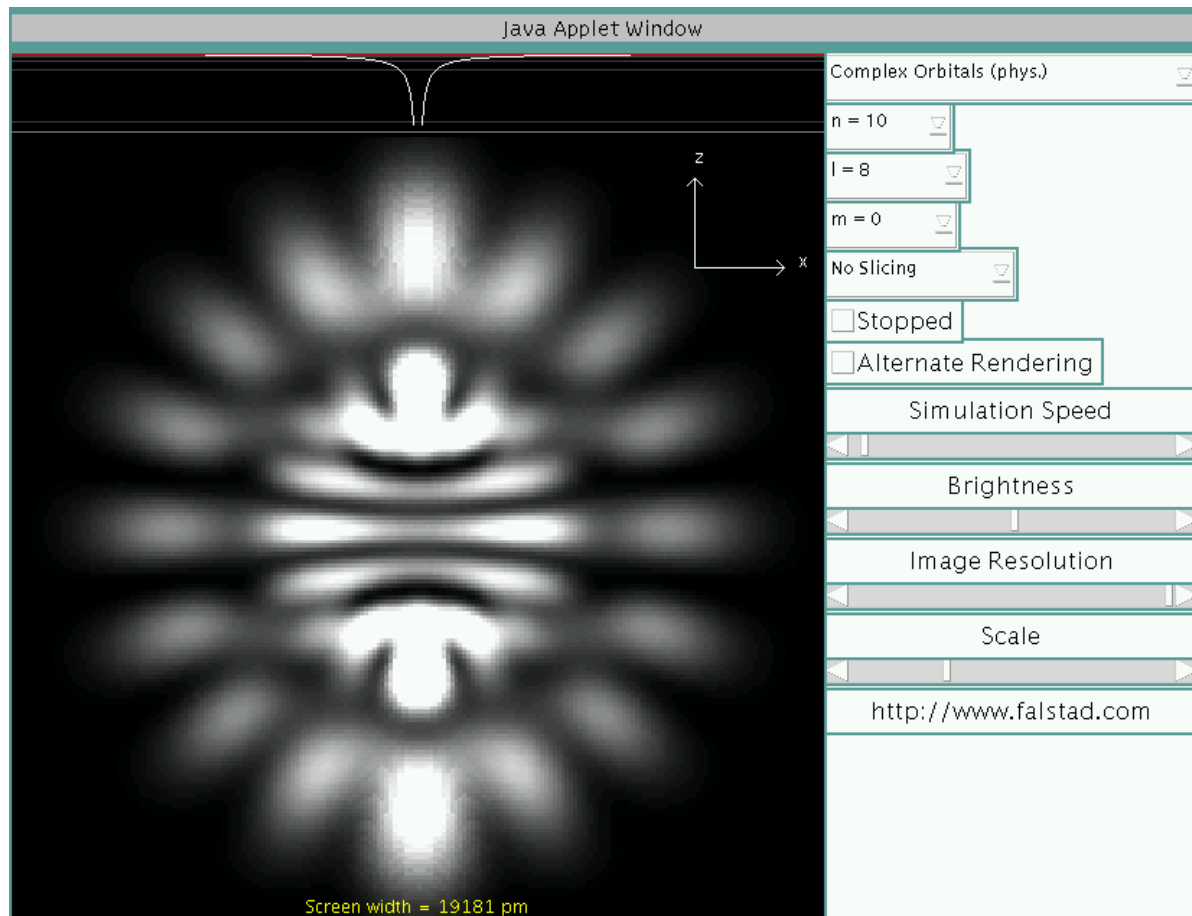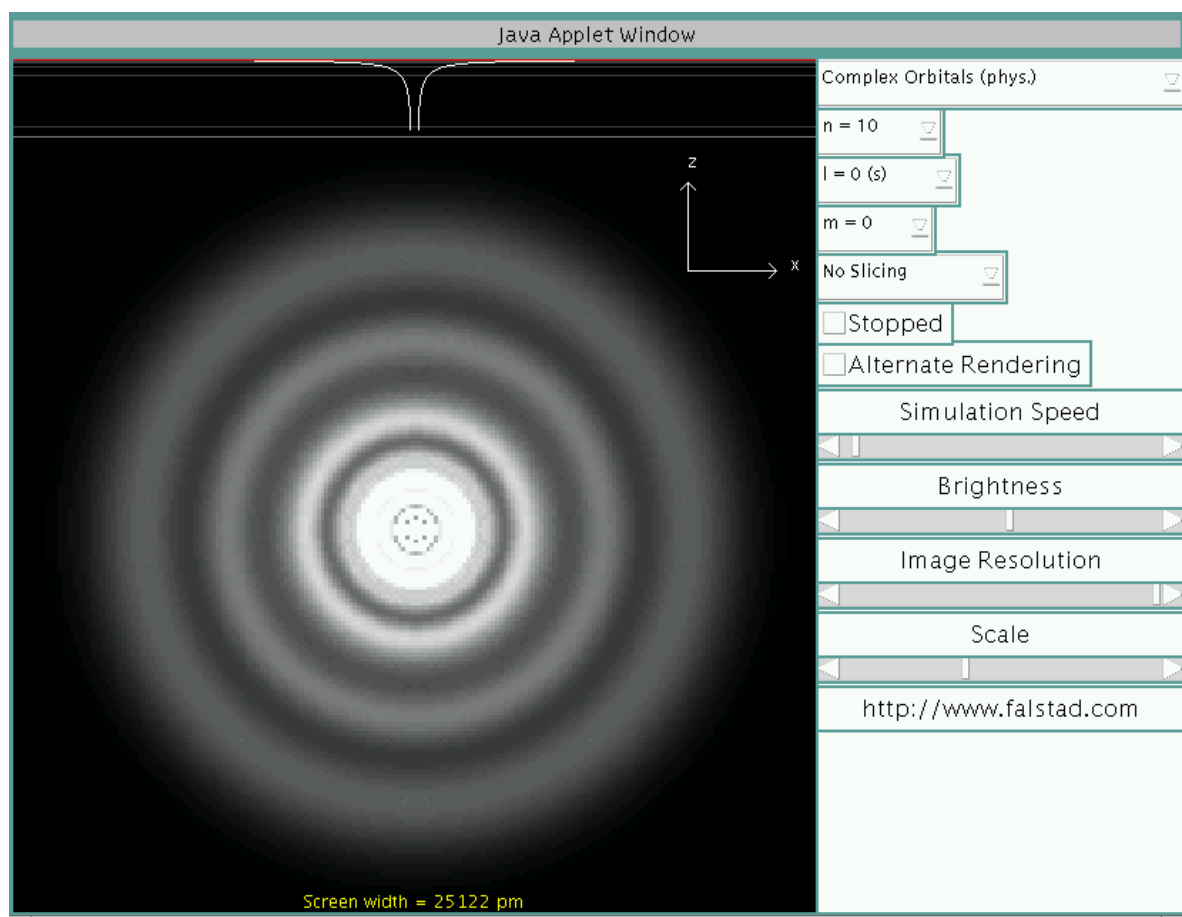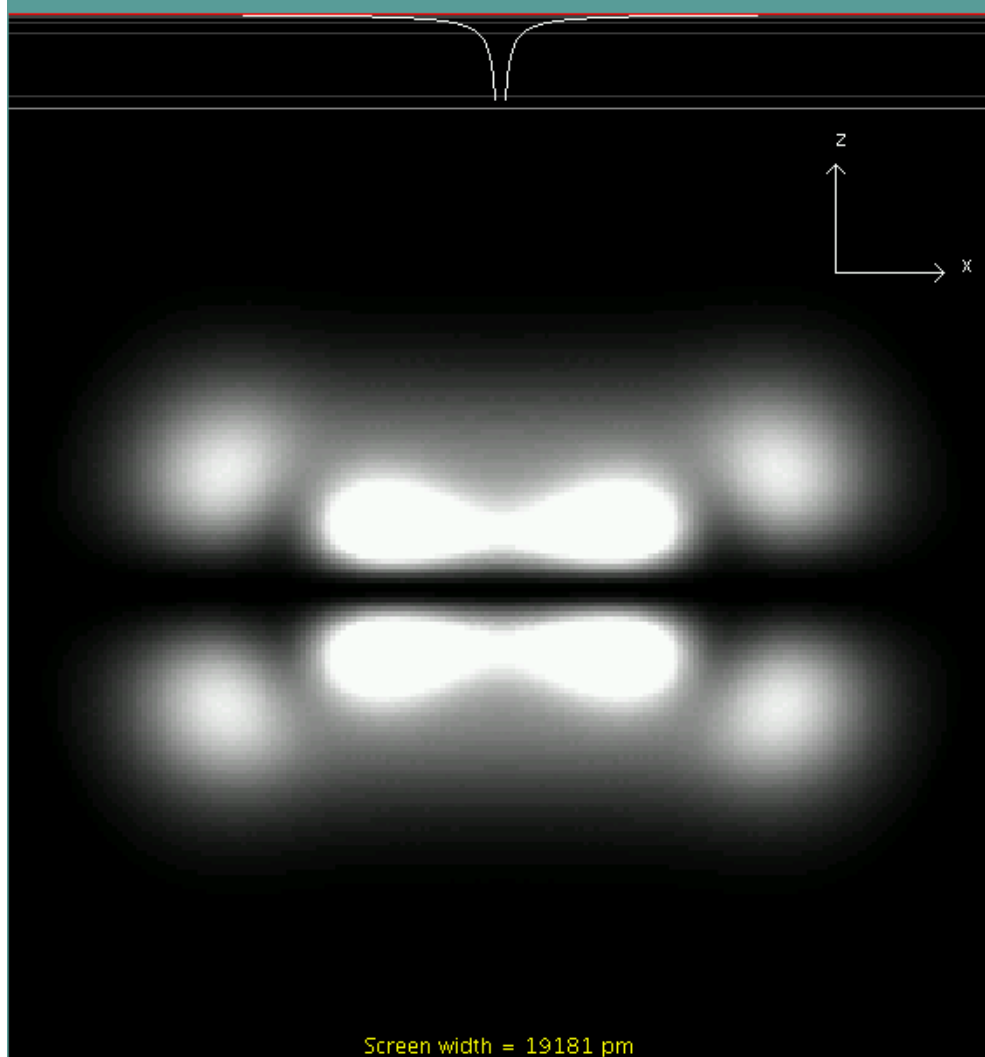
Java Applet Window

Complex Orbitals (phys.)

n = 10

l = 8

m = -7

No Slicing

☐ Stopped

☐ Alternate Rendering

Simulation Speed

Brightness

Image Resolution

Scale

http://www.falstad.com

Screen width = 19181 pm

z

x

Multi-Electron Atoms

• Due to the Pauli exclusion principle, two electrons cannot occupy the same state if their parameters (energy + angular momentum + z-axis momentum + spin) are identical.

• Hence, first the lowest energy level, $n = 1$, is filled: Hydrogen and Helium. There are two $n = 1$, electrons there (two spins). Then, for $n = 2$, the degeneracy is 4, multiplied by two spins given 8, and this accounts for the following 8 elements (Lithium to Neon). For $n = 3$, first the $l = 0$ are filled (two electrons: there's a $2l + 1 = 1$ degeneracy, multiplied by two spins). Same for $l=1$, for which there are six electrons (3 "l levels" multiplied by two spins). By then we are at 2+8+8=18 (Argon). However, the next electron (in Potassium) does *not* choose *n=3&l=2,* but *n=4&l=0.* **WHY?**

• The answer lies in the interaction of the electron's charges with each other (which we have neglected). The $n=4 \& l=0$ is farther away from the nucleus then the $n=3 \& l=2$ electron (see equation for average distance). So, it is partially screened from the Coulomb potential by the charge of the other electrons.

<u>Spin</u>

• Spin has no analogue in classical physics.

• An electron is prepared in a state of zero linear momentum (i.e. space-independent) state. Since all the angular momentum operators involve derivatives w.r.t *x,y,z*, we expect that its angular momentum(s) will all be zero. However, upon measurement along, say, the *z*-axis, the results of measuring L_z are $\pm \hbar/2$.

• So, the electron has some kind of "intrinsic" angular momentum. Same holds for other particles.

• The wave function of a particle with spin has a few components, and the spin operators linearly mix these *components* – as opposed to the orbital momentum operators, which mix the *coordinates*.

• The number of components is determined by the number of values which the "intrinsic" angular momentum can attain. The wave function is then just a direct product unifying the "ordinary" wave function with these different "intrinsic" values.

The generalized rotation operator is then $J = L + S$, where L is orbital angular momentum and S the spin operator. Under an infinitesimal rotation around the $z-$axis, the wave function changes according to

$$\begin{bmatrix} \psi_1' \\ \cdot \\ \cdot \\ \cdot \\ \psi_n' \end{bmatrix} = \left(I - \frac{i\varepsilon}{\hbar} \begin{bmatrix} -i\hbar \, \partial/\partial\theta & \cdots & 0 \\ & \cdot & & \cdot \\ & & \cdot & & \cdot \\ & & & \cdot \\ 0 & \cdots & -i\hbar \, \partial/\partial\theta \end{bmatrix} - \frac{i\varepsilon}{\hbar} S_z \right) \begin{bmatrix} \psi_1 \\ \cdot \\ \cdot \\ \cdot \\ \psi_n \end{bmatrix}$$

where S_z is also an $n \times n$ matrix.

$$|\psi'\rangle = \left[I - \frac{i\varepsilon}{\hbar} J_z \right] |\psi\rangle, \ \ J_z = L_z + S_z$$

Now the number of components has to be recovered, as well as the form of the operators S_x, S_y, S_z. Since the number of possible results for measurement of S_z is 2, we assume the dimension is 2. We also assume that J satisfies the commutation relations $\left[J_i, J_j \right] = i\hbar \sum_k \varepsilon_{ijk} J_k$, and since L and S commute, these relations are also satisfied for S_x, S_y, S_z.

The commutation rules determine the S operators, just as they did in the general analysis in the general discussion on angular momentum:

$$S_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \ S_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \ S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

So the electron is described by a two-component wave function:

$$|\psi\rangle = \begin{bmatrix} |\psi_+(x,y,z)\rangle \\ |\psi_-(x,y,z)\rangle \end{bmatrix} = |\psi_+(x,y,z)\rangle \begin{bmatrix} 1 \\ 0 \end{bmatrix} + |\psi_-(x,y,z)\rangle \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

This is called a spinor. It has two complex components. For the case of zero momentum, since the momentum operator P yields zero, we can deduce that $|\psi_+\rangle, |\psi_-\rangle$ are independent of x,y,z.

The total spin is given by $S^2 = S_x^2 + S_y^2 + S_z^2 = \frac{3}{4}\hbar^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

and so it yields a value of $(3/4)\hbar^2$ on any state. Unlike the total orbital angular momentum, the total spin cannot be changed and it is intrinsic to the particle. The electron spin is defined as 1/2.

Hereafter the notation $|\psi_{\pm}(x,y,z)\rangle$ will combine the spin and position amplitudes, and the normalization condition is therefore

$$\iiint \left(|\psi_{+}|^2 + |\psi_{-}|^2 \right) dx\,dy\,dz = 1.$$

Assume for the moment that the orbital wave function evolves independently from the spin. We can then limit the discussion to a 2D Hilbert space, whose kets are $|s, s_z\rangle = |s, m\hbar\rangle \equiv |s, m\rangle$, where s is the total spin (1/2 in our case), and m the spin along the $z-$axis. A basis is given by

$$|s,m\rangle = \left|\frac{1}{2}, \frac{1}{2}\right\rangle \underset{S_z \text{ basis}}{\rightarrow} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Remember that we're assuming that

$$\psi(x,y,z,s_z,t) = \psi(x,y,z,t)\chi(t)$$

where $\chi(t)$ is a two component spinor independent of the position.

$$|s,m\rangle = \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \underset{S_z \text{ basis}}{\rightarrow} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

and a general state by

$$|\chi\rangle = \alpha \left|\frac{1}{2}, \frac{1}{2}\right\rangle + \beta \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \underset{S_z \text{ basis}}{\rightarrow} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}, \quad |\alpha|^2 + |\beta|^2 = 1$$

Define $S=\left(S_x, S_y, S_z\right)=S_x\mathbf{i}+S_y\mathbf{j}+S_z\mathbf{k}$
If $|\hat{n},\pm\rangle$ are the eigenstates of $\hat{n}\cdot S$, for a unit vector $\hat{n}$, $\langle\hat{n},\pm|S|\hat{n},\pm\rangle=\pm(\hbar/2)\hat{n}$ (can be proved by direct computation) and these states are said to have spin up/down the $\hat{n}$ direction. Denote $\left(\hat{n}_x, \hat{n}_y, \hat{n}_z\right)=$
$\left(\sin(\theta)\cos(\phi),\sin(\theta)\sin(\phi),\cos(\theta)\right)$, then
$\hat{n}\cdot S=n_x S_x+n_y S_y+n_z S_z=$

$$\frac{\hbar}{2}\begin{bmatrix} \cos(\theta) & e^{-i\phi/2}\sin(\theta) \\ e^{i\phi/2}\sin(\theta) & -\cos(\theta) \end{bmatrix},\text{with}$$

eigenvectors (and eigenvalues $\pm\hbar/2$):

$$|\hat{n}\ \text{up}\rangle\equiv|\hat{n}+\rangle=\begin{bmatrix} e^{-i\phi/2}\cos(\theta/2) \\ e^{i\phi/2}\sin(\theta/2) \end{bmatrix}$$

$$|\hat{n}\ \text{down}\rangle\equiv|\hat{n}-\rangle=\begin{bmatrix} -e^{-i\phi/2}\sin(\theta/2) \\ e^{i\phi/2}\cos(\theta/2) \end{bmatrix}$$

• Note that knowing $\langle S \rangle$ determines the state. Actually, instead of specifying a state by α and β, we can specify a unit vector $\hat{n}$ such that the state is an eigenstate of $\hat{n} \cdot S$ with eigenvalue $\hbar/2$.

• The most direct way to see this is the following: let there be two complex numbers α, β such that $|\alpha|^2 + |\beta|^2 = 1$. We can multiply by a phase factor (physically meaningless) and assume that their angles are opposite: $\alpha = \rho_1 e^{-i\phi}$, $\beta = \rho_2 e^{i\phi}$. Since $\rho_1^2 + \rho_2^2 = 1$, we can take $\rho_1 = \cos(\theta), \rho_2 = \sin(\theta)$, and (up to the division by a factor of 2) this is the general form of the eigenvectors of $\hat{n} \cdot S$.

Note: this indicates that any state can be prepared by a Stern-Gerlach appartus, with its axis at the corresponding polar angle. This is because we're measuring the angular momentum at that direction.

The form of the spin operators leads to the definition of the Pauli matrices σ, $S = (\hbar/2)\sigma$:

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

- They anti-commute with each other.
- They satisfy $\sigma_x \sigma_y = i\sigma_z$, and cyclic permutations which can be immediately derived: $[\sigma_i, \sigma_j] = (2i)\sum_k \varepsilon_{ijk}\sigma_k$, $[\sigma_i, \sigma_j]_+ = 2I\delta_{ij}$
- They are traceless.
- Their squares equal the identity, and more generally $(\hat{n}\cdot\sigma)^2 = I$: since each such matrix $\hat{n}\cdot S$ has eigenvalues $\pm(\hbar/2)$, it follows that

$$\left(\hat{n}\cdot S + \frac{\hbar I}{2}\right)\left(\hat{n}\cdot S - \frac{\hbar I}{2}\right) = 0$$

> The eigenvectors span the space, and if the operator is zero on them then it's zero on all the space.

so $(\hat{n}\cdot S)^2 = (\hbar^2/4)I \Rightarrow (\hat{n}\cdot\sigma)^2 = I$.

- If we add the identity I, we get an orthonormal basis under the inner product $(1/2)\mathrm{Tr}(AB)$.

Since $\left(\hat{n}\cdot S\right)^2 = I$, it's relatively easy to calculate the powers of $\hat{n}\cdot S$, which helps in calculating the propagator and the rotation operator. For the latter, recall that

$$U[R(\theta)] = e^{-i\theta\cdot S/\hbar} = e^{-i\theta\cdot\sigma/2} =$$

$$\exp\left[-i\left(\frac{\theta}{2}\right)\hat{\theta}\cdot\sigma\right] = \cos\left(\frac{\theta}{2}\right)I - i\sin\left(\frac{\theta}{2}\right)\hat{\theta}\cdot\sigma$$

(follows immediately by equating coefficients).

Spin Dynamics (How Spin Behaves in a Magnetic Field)
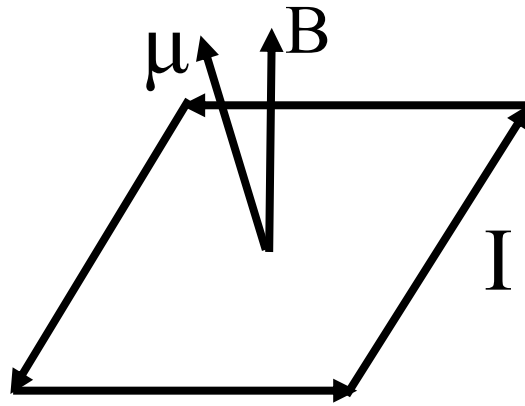
• The torque induced by the magnetic field **B** on the current carrying loop is to align its normal with the field. The torque is given by $T = \mu \times B$,

Where $\mu = \dfrac{I \cdot A}{c} e_\perp$ is the *magnetic moment*, A the loop area, and $e_\perp$ a unit vector perpendicular to the loop's plane. See slides 27-8 in electrodynamics file.

• The interaction energy between the loop and **B** is given by $-\mu \cdot B$ (so that the gradient of this expression is the force acting on the loop).

Carry the preceding analysis with the loop replaced by a particle of mass m and charge q, moving at speed v in a circle of radius r. The "current" is then

$I = \dfrac{qv}{2\pi r}$, and the magnetic moment has a magnitude which is the product of the current and the area :

$$\mu = \frac{qv}{2\pi r} \cdot \frac{\pi r^2}{c} = \underbrace{\left(\frac{q}{2mc}\right)}_{\substack{\text{gyromagnetic} \\ \text{ratio } \gamma}} l, \; l = mvr = \text{the magnitude of}$$

angular momentum. Since μ and l are parallel, $\mu = \gamma \cdot l$.

The effect of T here is not to align μ with B; instead, it results in a <u>precession</u> of μ around B.

The equation of motion is $T = \dfrac{dl}{dt} =$

$\mu \times B = \gamma(l \times B)$

$\Rightarrow \Delta l = \gamma(l \times B)\Delta t$

$\Rightarrow \Delta l = \gamma l B \sin(\theta)\Delta t$

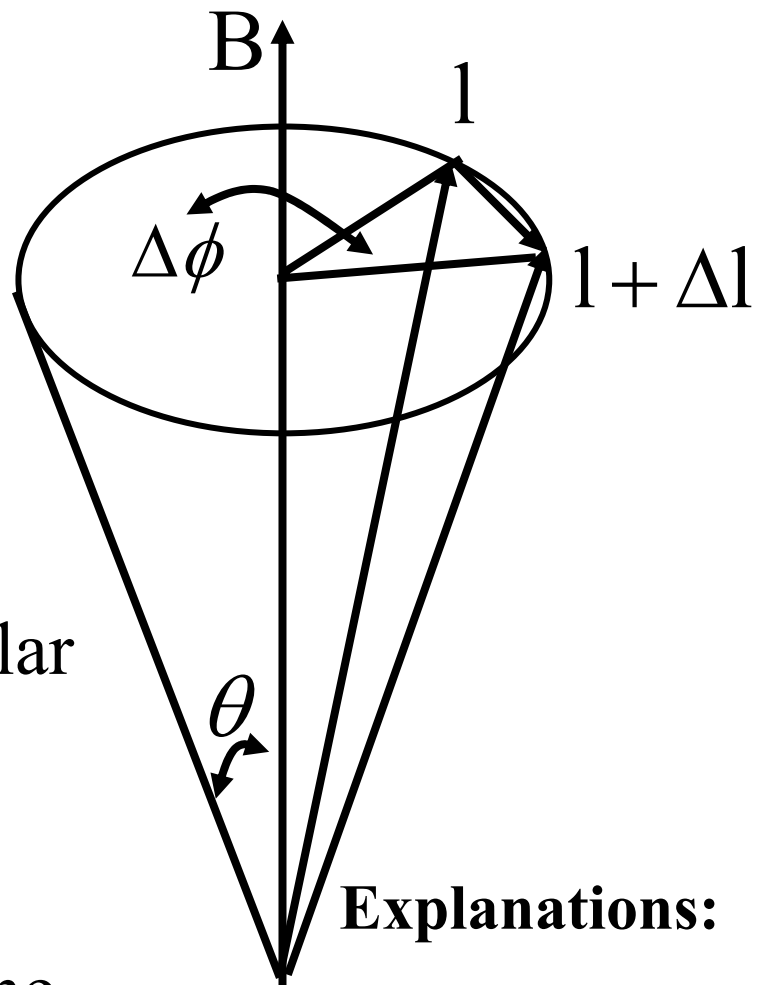But Δl is perpendicular to l and B (it's proportional to their vector product), so the tip of the vector l moves by an angle (relative to B) of

$$\Delta \phi = \left(\dfrac{-\Delta l}{l \sin(\theta)} \right) = (-\gamma B)\Delta t,$$

so it precesses at a frequency

$\omega_0 = -\gamma B$.

Explanations:

1. **The particle rotates around l**

2. **T is torque (two slides earlier).**

The "real" reason this happens is the colinearity of the magnetic and angular moments.

• What is the equivalent of these ideas in QM?

• The Hamiltonian of a particle of mass m and charge q in a magnetic field is

$$H = \frac{(\mathrm{P}-q\mathrm{A}/c)^2}{2m} = \frac{|\mathrm{P}|^2}{2m} \underbrace{- \frac{q}{2mc}(\mathrm{P}\cdot\mathrm{A}+\mathrm{A}\cdot\mathrm{P}) + \frac{q^2|\mathrm{A}|^2}{2mc^2}}_{\text{interaction Hamiltonian}}$$

where A is the vector potential satisfying $\nabla\times\mathrm{A}=\mathrm{B}$. Taking $\mathrm{A}=(B/2)(-y\mathrm{i}+x\mathrm{j}) \Rightarrow$ $\nabla\times\mathrm{A}=\mathrm{B}=B\mathrm{k}$. Dropping the quadratic term in H, the interaction part turns out to be

$H_{\text{int}} = -\dfrac{q}{2mc}\mathrm{L}\cdot\mathrm{B} \equiv -\mu\cdot\mathrm{B}$, where μ is a conjectured magnetic moment operator, and the analogy is adopted from the classical case in which the interaction Hamiltonian is given by the same expression.

So we take $\mu \equiv \dfrac{q}{2mc}\mathrm{L}$.

• The spin magnetic moment is assumed to be of the same shape:

$$H_{\text{int}} = -\mu \cdot B \propto \sigma \cdot B$$

The related constant turns out to satisfy (as justified both by experiment and theory):

$$H = -\gamma S \cdot B, \ \gamma = -(e/mc)$$

which is <u>twice the orbital case.</u>

The evolution of the electron state $|\psi(0)\rangle$ is given as usual by $|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle =$

$e^{i\gamma t(S \cdot B)/\hbar}|\psi(0)\rangle$, but the $e^{-i\theta \cdot S/\hbar}$ operator rotates by θ – just like we proved for J, which shares the same properties as S (slides207-8)– so the effect on the electron is to rotate the state by an angle $\theta(t) = -\gamma t B$. So, $\langle S \rangle$ precesses around B at a frequency $\omega_0 = -\gamma B$.

For example, consider B to be along the z−axis, B=Bk. So $U(t)=e^{i\gamma t S_z B/\hbar}=e^{i\omega_0 t \sigma_z/2}$,

and since σ_z is diagonal the exponent equals

$$U(t)=\begin{bmatrix} e^{i\omega_0 t/2} & 0 \\ 0 & e^{-i\omega_0 t/2} \end{bmatrix}.$$ If an electron

starts in $|\psi(0)\rangle = |\hat{n},+\rangle \rightarrow \begin{bmatrix} \cos(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{i\phi/2} \end{bmatrix}$

then $|\psi(t)\rangle = \begin{bmatrix} \cos(\theta/2)e^{-i(\phi-\omega_0 t)/2} \\ \sin(\theta/2)e^{i(\phi-\omega_0 t)/2} \end{bmatrix}$

For example, if it starts with spin along the x−axis, it will change to spin along y, etc:

$$\underbrace{(\theta=\pi/2, \phi=0)}_{\text{eigenstate of } S_x} \rightarrow \underbrace{(\theta=\pi/2, \phi=\pi/2)}_{\text{eigenstate of } S_y} \rightarrow ...$$

Which is precession around the z-axis.

Energy Levels of an Electron in a Magnetic Field

• As noted before, if the Hamiltonian separates into a spin and orbital parts, we have twice the number of orbital states – each one will now have a $\pm(1/2)$ spin.

• Now assume there's a magnetic field $\mathbf{B}=B\mathbf{k}$ present. For the hydrogen atom, the coupling of the proton to $\mathbf{B}$ can be ignored because its mass to charge ratio is much higher than the electron's. For the electron, the combined Hamiltonian is

$$H = H_{\text{Coulomb}} - \left(\frac{-eB}{2mc}\right)L_z - \left(\frac{-eB}{mc}\right)S_z$$

(remember that the coupling coefficient of the spin is twice as large). Since H commutes with $H_{\text{Coulomb}}, L_z, L^2$, and S_z, it is diagonalized by the same states as before : $\left| nlmm_s \right\rangle$ (m_s is the spin). However, the eigenvalues are different :

$$H\left| nlmm_s \right\rangle = \left[\frac{-R_y}{n^2} + \frac{eB\hbar}{2mc}(m + 2m_s)\right]\left| nlmm_s \right\rangle$$

$$H|nlmm_s\rangle = \left[\frac{-R_y}{n^2} + \frac{eB\hbar}{2mc}(m + 2m_s) \right] |nlmm_s\rangle$$

This results in the reduction of the $2n^2$ degenracy. For example, the first level $(n = 1)$, which had a degenracy level of 2, now has two levels; $m = 0$, but $m_s = \pm(1/2)$, and therefore the energy levels are now $E_{n=1} = -R_y \pm \dfrac{eB\hbar}{2mc}$ (so no degeneracy). The $n = 2$ level, which was eightfold degenerate, now splits into five levels : the only degeneracy remains in states in which $m + 2m_s$ are equal :

$$E_{n=2} = -R_y \pm c_1 \cdot \begin{bmatrix} 2\ (m = 1, m_s = 1/2) \\ 1\ (m = 0, m_s = 1/2, l = 0,1) \\ 0\ (m = 1, m_s = -1/2 \text{ or } m = -1, m_s = 1/2) \\ -1\ (m = 0, m_s = -1/2, l = 0,1) \\ -2\ (m = -1, m_s = -1/2) \end{bmatrix}$$

$$\left(c_1 = \frac{eB\hbar}{2mc} \right)$$

This splitting is named the Zeeman effect.

The Stern-Gerlach Experiment Revisited

• As in classical electrodynamics, an inhomogenous magnetic field creates a force on a dipole, which is given by $\mu_z \dfrac{\partial B_z}{\partial z}$ **k** (assuming the field is in the z-direction). So particles with positive spin will go upwards, and those with negative spin downwards. By blocking one of the paths, we can ensure that the particle leaving the apparatus will have a definite and known spin in the z-direction (i.e. we know that it is an eigenstate of S_z, and we know the eigenvalue). This results in a space quantization of the emerging particles (they're not continuously scattered, but emerge only at distinct points corresponding to the different spins; spin half will concentrate at two points etc). Note, especially, that not only the total spin is quantized, but the spin at every axis as well.

- Suppose we have a sequence of SG apparatuses. We may ask what percentage of those leaving apparatus *i* will leave apparatus *i+1* (see slides 48-51). We can now solve this problem rigorously, since the equations for the behavior of spin under rotation of the axis have been derived.
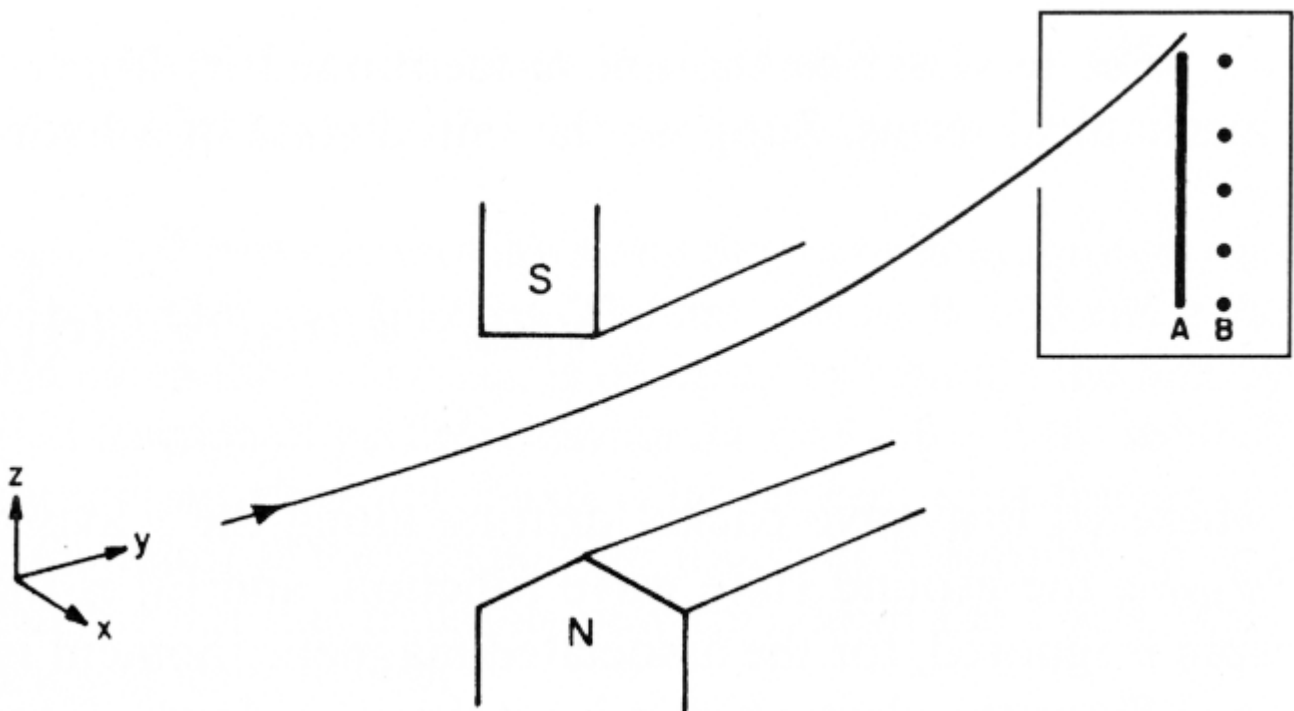
- The electron is in a mixed spin state $\left(\alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right)$.

Due to the heavy proton, the behavior is semi-classical, so the spin up part induces an upwards moving wave-packet, and similarly for the spin down part. So the wave packet has really two components – upwards and downwards. The blocking is like a measurement, and it forces the spin into a single state; if the lower beam is blocked, we get "pure" spin up.

Examples

• Spin half particles are moving along the *y*-axis (see drawing) enter two collinear SGAs, the first with its field along the *z*-axis and the second's field is along the *x*-axis (i.e. it is the first, rotated by $\pi/2$). What portion of those leaving the first will exit the second, if the lower beams in the two SGAs are blocked?

• Answer: we can think of the particles leaving the first being rotated by $\pi/2$ and then entering an SGA identical to the first. The equation for rotation of spin half particles was developed before (slide 210):

$$U[R(\theta)] = e^{-i\theta \cdot S/\hbar} = e^{-i\theta \cdot \sigma/2} =$$

$$\exp\left[-i\left(\frac{\theta}{2}\right)\hat{\theta}\cdot\sigma\right] = \cos\left(\frac{\theta}{2}\right)I_2 - i\sin\left(\frac{\theta}{2}\right)\hat{\theta}\cdot\sigma$$

In our case

$$\hat{\theta} = (0,1,0), \theta = \pi/2 \Rightarrow U[R(\theta)] =$$

$$\frac{1}{\sqrt{2}}\left(I_2 - i\sigma_y\right) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

Note: all calculations are carried out in the S_z basis

• Since the lower path of the first SGA is blocked,

those emerging from it are in a state $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, and after

$U[R(\theta)]$ acts on them they become $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

The probability for them to exit the second SGA (which after the rotation also has its field pointing up the z-axis), equals their probability to yield 1 when their z-spin is measured, i.e. the square of the projection of the state vector on the eigenvector of S_z with eigenvalue 1, but this eigenvector is $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, so the probability is clearly $1/2$.

• Now, assume that another SGA is placed after the second, which transmits only spin down along the z-axis. How many of those entering it will exit? We know that those leaving the second have a spin up along x, so their state vector is the eigenvector of S_x with eigenvalue 1, which equals $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

The probability of this particle going through a *z*-spin down SGA is clearly $1/2$, and so $1/4$ of those leaving the first will exit the third.

• Note that if the middle SGA has both beams unblocked (i.e. all those entering it leave it), then <u>no</u> particle which leaves the first will exit the third (they leave the first with spin up and all are therefore blocked by the third). So, the blocking in the middle one <u>increases</u> the percentage of those leaving the third.

• Other way to compute: to see what happens with the particle after it leaves the first (and is in a $(1,0)^t$ state in the *z*-basis) upon entering the rotated SGA: simplest way to understand it is to rotate the entire system by $-\pi/2$, since then we're back with an SGA with its field along *z*, calculate there, and rotate back by $\pi/2$.

SGA's Acting on Spin One Particles

• The computation proceeds very much like for spin half. Suppose that the first SGA passes only *z*-spin up particles, and the second one is rotated around the *y*-axis by an angle θ. What percentage of those exiting the first will leave the second?

• Answer: as before, we compute what such a rotation does to the particle's state. Just like for spin half, the rotation operator is defined by

$$U[R(\theta)] = e^{-i\theta \cdot S/\hbar}$$

To compute the exponents of spin one operators, note that, since the eigenvalues are $0, \pm\hbar$ then

$$(\hat{n} \cdot S + \hbar I)(\hat{n} \cdot S)(\hat{n} \cdot S - \hbar I) = 0 \Rightarrow (\hat{n} \cdot S)^3 = (\hat{n} \cdot S)$$

The Pauli matrices are defined just like for spin half, but here we shall denote $S = \hbar\sigma$ (not $\hbar/2$). for example,

$$\sigma_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

See slides 207-8

So in our case, $\theta = (0, \theta, 0)$, and $U[R(\theta)] =$

$$e^{-i\theta \cdot S/\hbar} = e^{-i\theta\sigma_y} = I_3 - i\theta\sigma_y - \frac{1}{2!}\theta^2\sigma_y^2 +$$

$$i\frac{1}{3!}\theta^3\sigma_y + \frac{1}{4!}\theta^4\sigma_y^2 ... \text{(remember}: \sigma_y^3 = \sigma_y)$$

Collecting terms : $I_3 + [\cos(\theta) - 1]\sigma_y^2 - i\sin(\theta)\sigma_y =$

$$\begin{pmatrix} \dfrac{1+\cos(\theta)}{2} & -\dfrac{\sin(\theta)}{\sqrt{2}} & \dfrac{1-\cos(\theta)}{2} \\ \dfrac{\sin(\theta)}{\sqrt{2}} & \cos(\theta) & -\dfrac{\sin(\theta)}{\sqrt{2}} \\ \dfrac{1-\cos(\theta)}{2} & \dfrac{\sin(\theta)}{\sqrt{2}} & \dfrac{1+\cos(\theta)}{2} \end{pmatrix}$$

So, since we started with a particle with z − spin

up, $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, it transforms to $\left(\dfrac{1+\cos(\theta)}{2}, \dfrac{\sin(\theta)}{\sqrt{2}}, \dfrac{1-\cos(\theta)}{2} \right)$

and its probability to be in z − spin up is

$\left(\dfrac{1+\cos(\theta)}{2} \right)^2$, and that portion will exit the second

SGA.

Addition of Angular Momenta

• Question: how does a system with two spin half particles appear (in terms of spin) when viewed as a single object?

• Such systems are naturally described in QM by the direct (tensor) product. For example, the system with two spin half particles is the vector space of dimension 4 spanned by $|++\rangle, |+-\rangle, |-+\rangle, |--\rangle$

S_{1z} acts as usual on the first component and is equal to the identity on the second component, etc.

Define $S_z = S_{1z} + S_{2z}$. Then the matrix of S_z in this product basis is

and the matrix of $S^2 = (S_1 + S_2) \cdot (S_1 + S_2) = S_1^2 + S_2^2 + \underbrace{2S_1 S_2}$ is

$$
\begin{array}{cccc}
++ & +- & -+ & --
\end{array}
$$

$$
\hbar \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}
$$

$$
\begin{array}{cccc}
++ & +- & -+ & --
\end{array}
$$

$$
\hbar^2 \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}
$$

$$
\boxed{\begin{aligned} S_{1x}S_{2x} + \\ S_{1y}S_{2y} + \\ S_{1z}S_{2z} \end{aligned}}
$$

As can be verified by directly computing the tensor product.

However, the following basis diagonalizes

$$S^2, S_z, S_1^2 (= S_{1x}^2 + S_{1y}^2 + S_{1z}^2), S_2^2 :$$

$$|s = 1, m = 1\rangle : \quad |++\rangle$$

$$|s = 1, m = 0\rangle : \quad 2^{-1/2}\big(|+-\rangle + |-+\rangle\big)$$

$$|s = 1, m = -1\rangle : \quad |--\rangle$$

$$|s = 0, m = 0\rangle : \quad 2^{-1/2}\big(|+-\rangle - |-+\rangle\big)$$

Note that s, m stand for the total spin and total spin in the $z-$ axis. Thus, $s = 1$ in $|++\rangle$ because when S^2 operates on it, it multiplies the state by $2\hbar^2$. But according to the formalism developed for general angular momentum operators, the total momentum operator has eigenstates with eigenvalue of $l(l+1)\hbar^2$, so here clearly the total spin is 1.

So the system of two spin half states is spanned by :

$$\left| s = 1, m = 1 \right\rangle, \left| s = 1, m = 0 \right\rangle, \left| s = 1, m = -1 \right\rangle, \left| s = 0, m = 0 \right\rangle.$$

- This means that the tensor product of two spin-half particles behaves like the direct sum of a spin one and spin zero particle – since each state can be viewed as a linear combination of the three spin one states (*l=1,m=1,0,-1*) and the spin zero state (*l=m=0*) (careful – the spin one particles requires three, not one, scalars to describe its state!).

- Formally, we write
$$\boxed{\frac{1}{2} \otimes \frac{1}{2} = 1 \oplus 0}$$

- And in general, for two particles of spin j_1 and j_2 :

$$j_1 \otimes j_2 = \left(j_1 + j_2 \right) \oplus \left(j_1 + j_2 - 1 \right) \oplus ... \oplus \left(j_1 - j_2 \right)$$

As follows by counting arguments and from considering the upper and lower bounds for the total spin. It remains to calculate the coefficients of the basis transformation. All this carries over to systems with more than two particles, e.g.

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = \frac{3}{2} \oplus \frac{1}{2} \oplus \frac{1}{2}$$

The Hyperfine Interaction in Hydrogen

• In addition to the Coulomb interaction, there's an interaction Hamiltonian of the form $H_{hf} = A S_1 S_2$ between the proton and electron, due to their magnetic moment. It splits the ground state to two

levels: $E_+ = -R_y + A\hbar^2/4, \; -R_y - 3A\hbar^2/4$

Proof : compute the matrix of

$S_1 \cdot S_2 = S_{1x} \cdot S_{2x} + S_{1y} \cdot S_{2y} + S_{1z} \cdot S_{2z}$

So up to constants it is

$$\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z = \begin{matrix} |++\rangle & |+-\rangle & |-+\rangle & |--\rangle \end{matrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

which has eigenvalues and eigenvectors

$$1, \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} \quad 1, \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad 1, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad -3, \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$$

$$\underbrace{|+-\rangle + |+-\rangle \quad |++\rangle \quad |--\rangle}_{\text{Triplets}} \quad \underbrace{|+-\rangle - |+-\rangle}_{\text{Singlet}}$$

A Very Short Introduction to Scattering

• Assume that a plane wave $\exp(ikz)$ hits a potential centered around the origin, and which decreases faster than $1/r$ (so the potential has no effect at infinity).

• Asymptotically $(r \to \infty)$ the scattered wave will behave like a free particle. The solutions are known to be of the form

$$\sum_{l,m} \left(\frac{A_l \sin(kr - l\pi/2)}{kr} + \frac{B_l \cos(kr - l\pi/2)}{kr} \right) Y_l^m(\theta, \phi)$$

for the wave to be purely outgoing, this must equal $\dfrac{\exp(ikr)}{r} f(\theta, \phi)$, and the total wave is therefore $\exp(ikz) + \dfrac{\exp(ikr)}{r} f(\theta, \phi)$, that is, the sum of the incident and reflected parts. This expression can be guessed from physical considerations.

• The stationary states satisfy (up to a choice of constants) $\left[\Delta + k^2 - U(\mathrm{r}) \right] \psi(\mathrm{r}) = 0$ (k^2 is proportional to the energy).

• The *cross-section* (amount of particles scattered per angle) is proportional to $\left| f(\theta, \phi) \right|^2$. It also turns out that, asymptotically, the scattered current is only radial.

The Integral Scattering Equation and Green's Function

$$\left[\Delta + k^2 - U(\mathrm{r})\right]\psi(\mathrm{r}) = 0 \Rightarrow \left[\Delta + k^2\right]\psi(\mathrm{r}) = U(\mathrm{r})\psi(\mathrm{r})$$

• Try to solve with a *Green function* for the operator:
$\left[\Delta + k^2\right]G(\mathrm{r}) = \delta(\mathrm{r})$. The idea : given an operator A
and equation $A\psi(\mathrm{r}) = U(\mathrm{r})\psi(\mathrm{r})$, find $G(\mathrm{r})$ such that
$AG(\mathrm{r}) = \delta(\mathrm{r})$, and then a solution also satisfies
$\psi(\mathrm{r}) = \psi_0(\mathrm{r}) + G(\mathrm{r}) * U(\mathrm{r})\psi(\mathrm{r})$, where $\psi_0(\mathrm{r})$ is a solution
to the homogenous equation, $A\psi_0(\mathrm{r}) = 0$:
$A\psi(\mathrm{r}) = A\left[\psi_0(\mathrm{r}) + G(\mathrm{r}) * U(\mathrm{r})\psi(\mathrm{r})\right] = A\left(G(\mathrm{r}) * U(\mathrm{r})\psi(\mathrm{r})\right) =$
$\delta(\mathrm{r}) * U(\mathrm{r})\psi(\mathrm{r}) = U(\mathrm{r})\psi(\mathrm{r})$. The integral equation allows an
iterative solution in powers of $U(\mathrm{r})$. Meaningful solutions
for the scattering problem are $\psi_0 = \exp(ikz)$ and
$G_\pm(\mathrm{r})$ (up to a constant) - $\exp(\pm ikr)/r)$, $G_+(\mathrm{r})$ is the outgoing
wave in which we're interested here.
The equation is therefore

$$\psi(\mathrm{r}) = \exp(ikz) - \int \frac{\exp(ik\|\mathrm{r} - \mathrm{r}'\|)}{\|\mathrm{r} - \mathrm{r}'\|} U(\mathrm{r}')\psi(\mathrm{r}')d^3\mathrm{r}'$$

Since the potential is spatially limited, and we're interested in
the behavior when $r \to \infty$, we can assume that in the
meaningful range of the integrand, $r \gg r'$. It is easy to see that
then $\|\mathrm{r} - \mathrm{r}'\| \approx r - (u, \mathrm{r}')$, where u is a unit vector in the direction
of r; in the denominator we can replace $\|\mathrm{r} - \mathrm{r}'\|$ with r, which

yields the asymptotic approximation

$$\psi(\mathbf{r}) \approx \exp(ikz) - \frac{\exp(ikr)}{r} \int \exp(-ik\mathbf{u}\mathbf{r}')U(\mathbf{r}')\psi(\mathbf{r}')d^3\mathbf{r}'$$

which is indeed in the form $\exp(ikz) + \dfrac{\exp(ikr)}{r} f(\theta,\phi)$,

since r depends only on θ, ϕ.

• It is customary to use the following notations: The *incident wave vecto r*, $\mathbf{k}_i$, is the vector of modulus k which is directed along the the axis of the beam, so $\exp(ikz) = \exp(i\mathbf{k}_i \cdot \mathbf{r})$. Similarly, the *scattered wave vector* in the direction θ, ϕ is defined by $\mathbf{k}_d = k\mathbf{u}$. The *scattering (or transferr ed) wave v ector* in the direction θ, ϕ is $\mathbf{K} = \mathbf{k}_d - \mathbf{k}_i$.

The Born Approximation

$\psi = \exp(i\mathbf{k}_i \mathbf{r}) + \int G_+(\mathbf{r} - \mathbf{r}')U(\mathbf{r}')\psi(\mathbf{r}')d^3\mathbf{r}' =$

$\exp(i\mathbf{k}_i \mathbf{r}) + \int G_+(\mathbf{r} - \mathbf{r}')U(\mathbf{r}')\exp(i\mathbf{k}_i \cdot \mathbf{r}')d^3\mathbf{r}' +$

$\iint G_+(\mathbf{r} - \mathbf{r}')G_+(\mathbf{r}' - \mathbf{r}'')U(\mathbf{r}')U(\mathbf{r}'')\psi(\mathbf{r}'')d^3\mathbf{r}'d^3\mathbf{r}'' + ...$

This is the <u>Born expansion</u>, which is useful if the potential is small. Plugging $\psi = \exp(i\mathbf{k}_i \cdot \mathbf{r}) + \dfrac{\exp(ikr)}{r}f(\theta,\phi)$ into the first order Born expansion

and using $\int G_+(\mathbf{r} - \mathbf{r}')U(\mathbf{r}')\exp(i\mathbf{k}_i \cdot \mathbf{r}')d^3\mathbf{r}' \approx$

$-\dfrac{\exp(ikr)}{r}\int \exp(-ik\mathbf{u}\cdot\mathbf{r}')U(\mathbf{r}')\exp(i\mathbf{k}_i \cdot \mathbf{r}')d^3\mathbf{r}' =$

$-\dfrac{\exp(ikr)}{r}\int \exp(-i\mathbf{k}_d \cdot \mathbf{r}')U(\mathbf{r}')\exp(i\mathbf{k}_i \cdot \mathbf{r}')d^3\mathbf{r}' \Rightarrow$

$f(\theta,\phi) = -\int \exp(-i\mathbf{K}\cdot \mathbf{r}')U(\mathbf{r}')d^3\mathbf{r}'$, which is the Born approximation. It relates the Fourier transform of the potential to the scattering amplitude. Higher order expansion relate to "secondary scatterings" scattered again from the potential, etc.

Some examples of the Born approximation (left – the potential, right – dependence of $f(\theta)$ on θ. This is 2D, the incoming wave is at the *x*-direction).
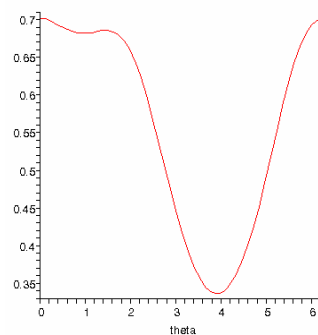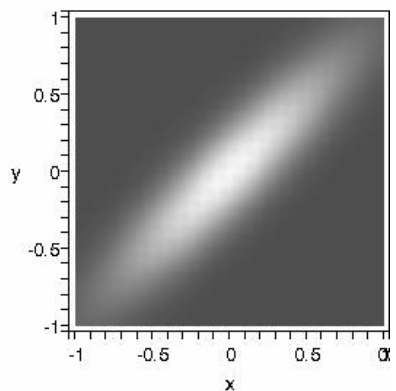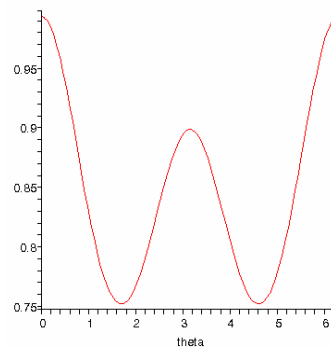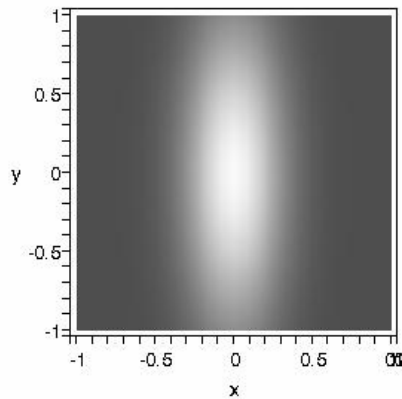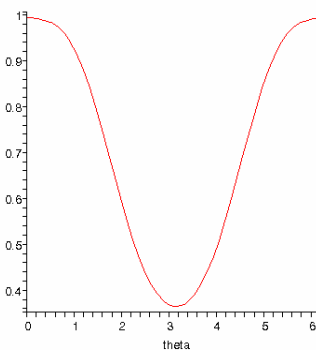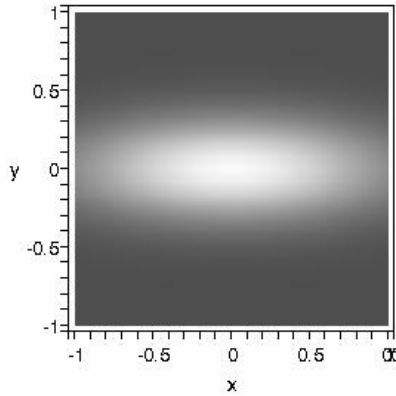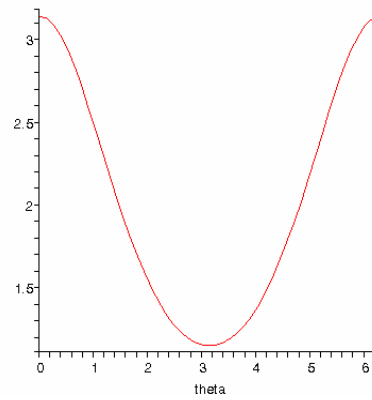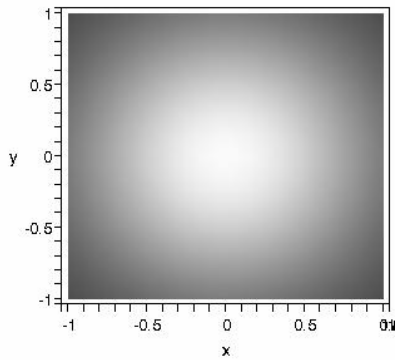
Partial Waves

• If the potential is rotationally symmetric (central), the scattered wave can be studied by separately analyzing its components which have fixed angular momentum.

$$\exp(ikz) = \sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)}\, j_l(kr) Y_l^0(\theta) \text{ (no } \phi \text{ dependence)}.$$

Similarly, we can write $f(\theta,k) = \sum_{l=0}^{\infty}(2l+1)a_l(k)P_l(\cos(\theta))$

$$\left(P_l(\cos(\theta)) = \left(\frac{4\pi}{2l+1}\right)^{\frac{1}{2}} Y_l^0(\theta) \right). \; a_l(k) \text{ are called the } lth \; partial$$

wave amplitude. Since $j_l(kr) \xrightarrow[r\to\infty]{} \dfrac{\sin(kr - l\pi/2)}{kr}$, we get for the

free particle (no potential) $\exp(ikz) \xrightarrow[r\to\infty]{}$

$$\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\frac{\exp(ikr) - \exp(i(kr - l\pi))}{r}P_l(\cos(\theta));$$ thus for each l

there are incoming and outgoing waves of the same amplitude, with a phase difference due to the centrifugal barrier. The two waves induce opposite probability currents which cancel out (since there should be no probability flow in the steady state). If a potential is present, then at infinity the only difference relative to the free particle can be in the phase; so denote

$$\psi_k(r) \xrightarrow[r\to\infty]{} \sum_{l=0}^{\infty} A_l \frac{\exp(i(kr - l\pi/2 + \delta_l)) - \exp(i(kr - l\pi/2 + \delta_l))}{r} P_l(\cos(\theta))$$

Comparing with the free particle, the incoming wave must be the same, so $A_l = \dfrac{2l+1}{2ik}\exp(i(l\pi/2+\delta_l))$, and

$$\psi_k(\mathrm{r}) \underset{r\to\infty}{\to} \frac{1}{2ikr}\sum_{l=0}^{\infty}(2l+1)\left[\exp(ikr)\exp(2i\delta_l)-\exp(-i(kr-l\pi))\right]\times$$

$$P_l(\cos(\theta))=\exp(ikz)+\left[\sum_{l=0}^{\infty}(2l+1)\frac{\exp(2i\delta_l)-1}{2ik}P_l(\cos(\theta))\right]\times$$

$\dfrac{\exp(ikr)}{r}$. Recalling how $f(\theta,\phi)$ was defined,

$a_l(k)=\dfrac{\exp(2i\delta_l)-1}{2ik}$. The effect of the potential is therefore to attach a phase shift $\exp(2i\delta_l)$ to the outgoing wave. The cross section can be simply expressed as a function of the δ_l:

$$\sigma=\left(4\pi/k^2\right)\sum_{l=0}^{\infty}(2l+1)\sin^2(\delta_l)$$

To find the phase shift, one imposes continuity between the solution at infinity and the solution of the steady state at the vicinity of the origin.

The main motivation to use partial waves is when l,k, and the range of the potential are such that only a small number of $a_l(k)$ need to be considered, since for $l>l_{max}$ the particle doesn't come closer to the origin more than l_{max}/k, and if this is larger than the extent of the potential such l's don't scatter (since the momentum is $\approx k$ and therefore the angular momentum is roughly kr_0, where r_0 is the particle's distance from the origin).

Example: scattering of *l*=1 from a hard sphere

The potential is $V(r)=0$ for $r>r_0$, $V(r)=\infty$ for $r<r_0$.
The general method of solution is as follows: look at the outgoing wave as $r \to \infty$. It is of the form $\exp(ikz)$ (the homogenous part) plus the solution of the radial equation in $u(r)=rR_{k,l}$ (see slides of "Solution of Rotationally Invariant Problems"). The equation is

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{l(l+1)\hbar^2}{2\mu r^2}+V(r)\right]u_{k,l}(r)=\frac{\hbar^2 k^2}{2\mu}u_{k,l}(r).$$

Since $u_{k,l}(r)$ includes already the divison by r (see previous slides on scattering), one only has to compute the phase shift in $u_{k,l}(r)$ relative to the free particle shift, $l\pi/2$:

$$u_{k,l}(r)\underset{r\to\infty}{\approx} C\sin(kr-l\pi/2+\delta_l).\ \delta_l \text{ is the desired shift.}$$

Let's compute the phase shift for the hard sphere and l=1. Inside the sphere, the wave function is zero (since the potential is infinite). In the outside, the radial equation

reduces to $\left[-\dfrac{d^2u}{dr^2}+\dfrac{2}{r^2}\right]u=k^2u \Rightarrow$

$u(r)=C\left[\dfrac{\sin(kr)}{kr}-\cos(kr)+a\left(\dfrac{\cos(kr)}{kr}+\sin(kr)\right)\right]$ which,

as $r\to\infty$, should equal (up to a constant factor) $\sin(kr-\pi/2+\delta_1)=-\cos(\delta_1)\cos(kr)+\sin(\delta_1)\sin(kr)$, so $a=\tan(\delta_1)$. Now it remains to enforce continuity at $r=r_0$:

The wave function has to be zero there, so we must have

$$\frac{\sin(kr_0)}{kr_0}-\cos(kr_0)+a\left(\frac{\cos(kr_0)}{kr_0}+\sin(kr_0)\right)=0\Rightarrow$$

$$a=-\frac{\dfrac{\sin(kr_0)}{kr_0}-\cos(kr_0)}{\dfrac{\cos(kr_0)}{kr_0}+\sin(kr_0)},\text{ which in very low energies }(k\rightarrow0)$$

is of the order $(r_0k)^3$. Since for small angles $\theta\approx\tan(\theta)$, this is also the order of $\delta_1(k)$. Using asymptotic properties of the spherical Bessel and Neumann functions (see slide 222) it turns out that for every l, $\delta_l(k)\approx(r_0k)^{2l+1}$.