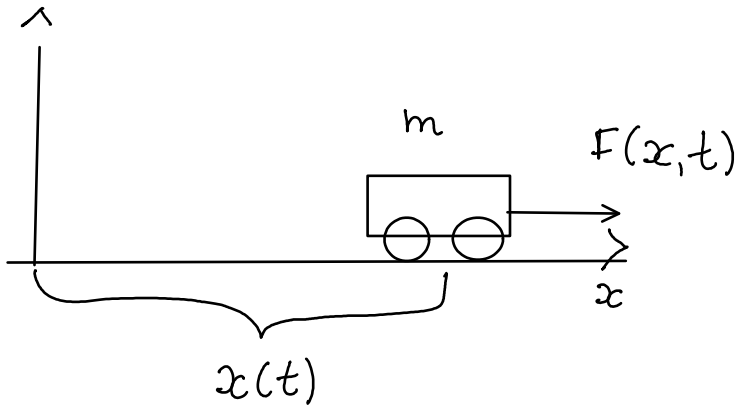# Lectures 3-4

A very brief introduction to quantum mechanics

Classical mechanics (in one dimension):

Particle of mass m, constrained to move along x-axis, subject to some force F(x,t).

Task of classical mechanics: find x(t). If we find x(t), we can find velocity $v = dx/dt$,

momentum p=mv, kinetic energy $T = \frac{1}{2}mv^2$, an so on.

How do we determine x(t)? Use second Newton's law $F_x = ma_x$.

For conservative forces $F_x = -\dfrac{\partial V}{\partial x} \implies$

$$F_x = ma_x \implies m\frac{d^2x}{dt^2} = -\frac{\partial V}{\partial x}$$

+ initial conditions (generally position and velocity at t = 0).

Quantum mechanics (in one dimension)

Task: we want to determine particle's wave function Ψ.

To do so we use Schrödinger equation:

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

+ initial conditions

$\hbar$ is a Plank's constant divided by 2π

$$\hbar = \frac{h}{2\pi} = 1.054572 \times 10^{-34} \text{ Js.}$$

Note: wave function is complex, but $\Psi^*\Psi$ is real and nonnegative. Ψ^* is a complex conjugate of Ψ. So,we can find the wave function.

What is the wave function?

Born's statistical interpretation of the wave function:

$|\Psi(x,t)|^2$ gives the probability of finding the particle at the point x at time t. More precisely,

$$\int_a^b |\Psi(x,t)|^2 dx = \left\{ \begin{array}{l} \text{probability of finding} \\ \text{a and b, at time t} \end{array} \right\}$$

Problem: indeterminacy of the quantum mechanics. Even if you know everything that theory (i.e. quantum mechanics) has to tell you about the particle (i.e. wave function), you can not predict with certainty where this particle is going to be found by the experiment.

Quantum mechanics provides statistical information about possible results.
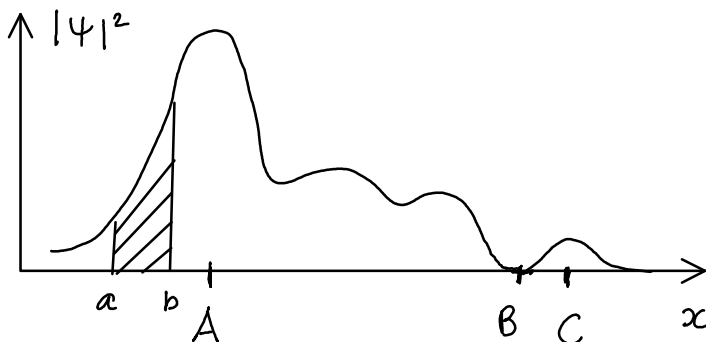
Example: particle is likely to be found in the vicinity of A and is unlikely to be found in the vicinity of B.

Now, suppose we make a measurement and find particle at C.

Question: where was the particle just before the measurement ?

Answer # 1. Realist position.

It was at C. That means quantum mechanics is incomplete theory. Why?
Well, the particle was at C, but quantum mechanics could not predict it.
Therefore, Ψ does not give the whole story and we need additional information
(hidden variables) to provide a complete description of the particle.

Answer #2. The orthodox position.

The particle was not really anywhere. It was an act of measurement that
forced particle to "take a stand". We still have no idea why it "decided" on point C.
Note: there is something very strange about concept of measurement.

Answer #3. The agnostic position.

Refuse to answer. Since the only way to know if you were right is to make a
measurement, you no longer get "before the measurement". Therefore,
it can not be tested.

In 1964, Bell shown that it makes an observable difference if the particle
has a precise (but unknown) position before measurement, which rules out
answer #3.

What if we make a second measurement after the first?

Repeated measurement returns the same value.

$$C$$
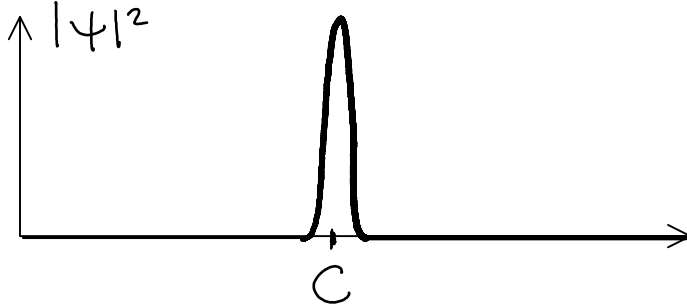
The first measurement alters the wave function and it collapses to a spike at C.
After that, it will start evolving according to Schrödinger equation.

Note: $$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, dx = 1$$ "particle must be somewhere".

Bosons and fermions

If the particle one is in state $\psi_a(\vec{r})$ and particle two is in state $\psi_b(\vec{r})$, then the total state can be written as the simple product (we will ignore spin for now):

$$\psi(\vec{r}_1, \vec{r}_2) = \psi_a(\vec{r}_1)\, \psi_b(\vec{r}_2). \qquad Eq.(1)$$

Note of caution: by no means assume that all two-particle states can be separated into simple product states. All entangled states can not be separated into product states. Here is example of the entangled state.

Suppose each of two particles can be in spin state up ↑ or down ↓, then the following state can not be separated into product states:

$$\psi_{12} = \frac{1}{\sqrt{2}} \left(\uparrow\downarrow - \downarrow\uparrow \right)$$

#1   #2   #1   #2

This state means that if the spin of one particle is up, then the spin of the other particle must be down. Such state can not be separated into the product state as neither particle is in definite state of being spin up or spin down.

Equation (1) above assumes that we can tell which particle is particle one and which particle is particle two. In classical mechanics, you can always identify which particle is which. In quantum mechanics, you simply can't say which electron is which as you can not put any labels on them to tell them apart.

There are two possible ways to deal with indistinguishable particles, i.e. to construct two-particle wave function that is non committal to which particle is in which state:

$$\psi_+(\vec{r}_1, \vec{r}_2) = A\left[\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) + \psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\right]$$

$$\psi_-(\vec{r}_1, \vec{r}_2) = A\left[\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) - \psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\right].$$

Therefore, quantum mechanics allows for two kinds of identical particles: **bosons** (for the "+" sign) and **fermions** (for the "-" sign). In our non-relativistic quantum mechanics we accept the following statement as an axiom:

**All particles with integer spin are bosons,
all particles with half integer spin are fermions.**

From the above, two identical fermions can not occupy the same state:

$$\Psi_-(\vec{r}_1, \vec{r}_2) = A[\psi_a(\vec{r}_1)\psi_a(\vec{r}_2) - \psi_a(\vec{r}_2)\psi_a(\vec{r}_1)] = 0.$$

$$\underbrace{\phantom{\psi_a(\vec{r}_1)\psi_a(\vec{r}_2)}}_{\text{same state}}$$

It is called **Pauli exclusion principle**.

We introduce operator P that interchanges two particles (exchange operator)

$$P f(\vec{r}_1, \vec{r}_2) = f(\vec{r}_2, \vec{r}_1). \qquad\qquad P^2 = 1$$

If particles are identical $\quad [P, H] = 0 \qquad (PH - HP = 0).$

Then, we can find solutions to Schrödinger equation that are either symmetric or antisymmetric:

$$\boxed{\psi(\vec{r}_1, \vec{r}_2) = \pm \psi(\vec{r}_2, \vec{r}_1).} \qquad (2)$$

Wave function is required to satisfy (2) for identical particles.

Formalism of quantum mechanics

In quantum mechanics, the state of the system is described by its wave function and the observables are represented by operators. Wave functions satisfy requirements for vectors and operators act on the wave functions as linear transformations. Therefore, it is natural to use language of linear algebra.
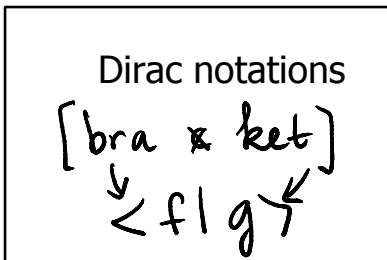
Only normalizable wave functions represent physical states. The set of all square-integrable functions, on a specified interval,

$$f(x) \quad \text{such that} \quad \int_a^b |f(x)|^2 \, dx < \infty$$

constitutes a Hilbert space. Wave functions live in Hilbert space.

The inner product of two functions f and g is defined as

$$\langle f | g \rangle \equiv \int_a^b f^*(x) \, g(x) \, dx.$$

Dirac notations

$$[\text{bra} \quad \& \quad \text{ket}]$$
$$\langle f | g \rangle$$

$$|g\rangle : \text{ket} \qquad \qquad \langle f| : \text{bra}$$

$$\langle f | = \int f^* [\ldots] \, dx$$

In a finite-dimensional vector space, where the vectors expressed as columns,

$$|\alpha\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

the corresponding bra is a row vector

$$\langle \alpha | = \begin{pmatrix} a_1^* & a_2^* & \ldots & a_n^* \end{pmatrix}.$$

A function is said to be **normalized** if its inner product with itself is one.

$$\langle f | f \rangle = \int_a^b |f(x)|^2 \, dx$$

Two wave functions are **orthogonal** if their inner product is zero.

$$\langle f | g \rangle = 0$$

A set of functions is **orthonormal** if they are normalized and mutually orthogonal.

$$\langle f_m | f_n \rangle = \delta_{mn}$$

Observables in quantum mechanics are represented by **hermitian operators**, i.e. such as

$$\langle f | \hat{Q} f \rangle = \langle \hat{Q} f | f \rangle \quad \text{for all } f(x)$$

The **expectation value** of an observable Q (x, p) can be written as

$$\langle Q \rangle = \int \Psi^* \hat{Q} \Psi \, dx = \langle \Psi | \hat{Q} \Psi \rangle$$

Determinate states : such states that every measurement of Q is certain to return the same value q. **Determinate states are eigenfunctions of Q and q is the corresponding eigenvalue.**

$$\boxed{\hat{Q} \Psi = q \Psi}$$

Generalized statistical interpretation:

If your measure observable Q on a particle in a state $\Psi(x,t)$ you will get one of the eigenvalues of the hermitian operator $\hat{Q}$. If the spectrum of $\hat{Q}$ is discrete, the probability of getting the eigenvalue q_n associated with orthonormalized eigenfunction $f_n(x)$ is

$$|c_n|^2, \quad \text{where} \quad c_n = \langle f_n | \Psi \rangle.$$

It the spectrum is continuous, with real eigenvalues $q(z)$ and associated Dirac-orthonormalized eigenfunctions $f_z(x)$, the probability of getting a result in the range dz is

$$|c(z)|^2 \, dz, \quad \text{where} \quad c(z) = \langle f_z | \Psi \rangle$$

The wave function "collapses" to the corresponding eigenstate upon measurement.

$$\boxed{\sum_n |c_n|^2 = 1 \quad \text{and} \quad \langle Q \rangle = \sum_n q_n |c_n|^2 \quad \begin{array}{l} \text{Discrete} \\ \text{Spectrum} \end{array}}$$

Summary: Postulates of quantum mechanics (1-3)

Postulate 1

The state of a system at any instant of time may be represented by a wave function Ψ which is continuous and differentiable. Specifically, if a system is in the state $\Psi(\bar{r}, t)$, the average of any physical observable C relevant he this system in time t is

$$\langle C \rangle = \int \Psi^* \hat{C} \, \psi \, d^3r$$

Postulate 2

To any self-consistently and well-defined observable Q , such as linear momentum, energy, angular momentum, or a number of particles, there correspond an operator $\hat{Q}$ such that measurement of Q yields values (call these measured values q) which are eigenvalues of Q. That is, the values q are those for which the equation

$$\hat{Q}\psi = q\psi \quad \Leftarrow \text{eigenvalue equation}$$

has a solution ψ. The function ψ is called the eigenfunction of $\hat{Q}$ corresponding to the eigenvalue q.

Postulate 3

Measurement of the observable Q that yields the value q leaves the system in the state ψ_q , where ψ_q is the eigenfunction of Q that corresponds to the eigenvalue q.