Non-relativistic Quantum Mechanics

Let's do some recap on the things we learned in the Quantum Mechanics course last year.

One-dimensional Time Dependent Schrödinger Equation

In QM, a free particle has wave function $\psi = e^{i(kx - \omega t)}$

where $p = \frac{h}{\lambda} \rightarrow k = \frac{p}{\hbar}$ (p is momentum, k is wavenumber)

$E = h\nu \rightarrow \omega = \frac{E}{\hbar}$ (ν is frequency, ω is angular freq.)

The properties of the particle can be obtained by applying operators to this eqn.

$$\hat{E}\psi = i\hbar \frac{\partial \psi}{\partial t}$$

$$\hat{p}\psi = -i\hbar \frac{\partial \psi}{\partial x}$$

The free wave function is an eigenfunction of these operators with E and p being eigenvalues.

For a classical particle in a potential V, due to energy conservation:

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

using operators:

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

where $\hat{H}$ is the hamiltonian operator.

This is the time-dependent Schrödinger equation.

Time independent Schrödinger Equation

In situations where the potential is not dependent on time, the solutions to the SE always have form:

$$\Psi(x,t) = u(x)e^{-iEt/\hbar}$$

The time independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}u(x) + V(x)u(x) = Eu(x)$$

So what does this mean?

In the time independent case, the probability of finding a particle at position x (actually between x and $x+\delta x$) is given by $u^*(x)u(x)\,dx$

Since the particle must be somewhere

$$\int_{-\infty}^{\infty} u^*(x)u(x)\,dx = 1$$

we find expectation values of observable quantities by:

$$\langle x \rangle = \int_{-\infty}^{\infty} u^*(x)\,\hat{x}\,u(x)\,dx = \int_{-\infty}^{\infty} u^*(x)\,x\,u(x)\,dx$$

$$\langle p \rangle = \int_{-\infty}^{\infty} u^*(x)\,\hat{p}\,u(x)\,dx = \int_{-\infty}^{\infty} u^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)u(x)\,dx$$

Proof that Probability is Conserved

If the probability that the particle is in some position decreases then the probability that it is in a different position must increase.

Consider the conservation equation for electric charge:

$$\frac{\partial \rho}{\partial t} + \underline{\nabla} \cdot \underline{J} = 0$$

in 1D:

$$\frac{\partial \rho}{\partial t} + \frac{\partial J^x}{\partial x} = 0 \qquad (*)$$

Now consider the SE. If we do: $-i\psi^*(SE) + (SE)^* i\psi$:

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

$$\Rightarrow \quad \frac{\partial}{\partial t}(\psi^* \psi) + \left(\frac{-i\hbar}{2m}\right) \frac{\partial}{\partial x}\left(\psi^* \frac{\partial}{\partial x}\psi - \psi \frac{\partial}{\partial x}\psi^*\right) = 0$$

This is in the form of $*$ provided $\rho = \psi^* \psi$

so $\psi^* \psi$ is a probability density and we have proved probability is conserved.

Momentum Space Wave Functions

We can set up a wave function $\phi(p)$ such that $\phi^* \phi \, dp$ is the probability of the particle having momentum p to $p + dp$

We require $$\int_{-\infty}^{\infty} \phi^*(p) \, \phi(p) \, dp = 1$$

$$\int_{-\infty}^{\infty} \phi^*(p) \, p \, \phi(p) \, dp = \langle p \rangle$$

$$\int_{-\infty}^{\infty} \phi^*(p) \, i\hbar \frac{\partial}{\partial p} \phi(p) \, dp = \langle x \rangle$$

We can simply use the fourier transform to switch to and from momentum space:

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} \, dx$$

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p) e^{ipx/\hbar} \, dp$$

Let's try $\int_{-\infty}^{\infty} \phi^* \phi \, dp = 1$:

$$\int_{-\infty}^{\infty} \phi^*(p)\, \phi(p)\, dp = \frac{1}{2\pi\hbar} \int dp \left[\int dx' e^{ipx'/\hbar} \psi^*(x')\right] \times \left[\int dx'' e^{-ipx''/\hbar} \psi^*(x'')\right]$$

$$= \int dx' \int dx'' \frac{1}{2\pi\hbar} \psi^*(x') \psi(x'') \underbrace{\int dp\, e^{-ip(x''-x')/\hbar}}$$

but $\delta(x - x_0) = \frac{1}{2\pi} \int e^{-ik(x-x_0)} dk$ so this is $\delta(x''-x')$

$$\Rightarrow \int_{-\infty}^{\infty} \phi^* \phi \, dp = \int dx' \int dx'' \, \delta(x''-x')\, \psi^*(x')\, \psi(x'')$$

$$= \int dx' \, \psi^*(x')\, \psi(x) = \underline{\underline{1}}$$ as required.

Now let's try $\int_{-\infty}^{\infty} \phi^* (i\hbar \frac{\partial}{\partial p}) \phi \, dp = \langle x \rangle$:

$$\int_{-\infty}^{\infty} \phi^*(p) (i\hbar \tfrac{\partial}{\partial p}) \phi(p)\, dp = \frac{1}{2\pi\hbar} \int dp \left[\int dx' e^{ipx'/\hbar} \psi^*(x')\right]\left(i\hbar\left(-\frac{ix''}{\hbar}\right)\right) \times \left[\int dx'' e^{-ipx''/\hbar} \psi(x'')\right]$$

$$= \int dx' \int dx'' \frac{1}{2\pi\hbar} \psi^*(x')\, x''\, \psi(x'') \int dp\, e^{-ip(x''-x')/\hbar}$$

$$= \int dx' \int dx'' \, \delta(x''-x')\, \psi^*(x')\, x''\, \psi(x'') = \int dx \, \psi^*(x')\, x'\, \psi(x')$$

$$= \underline{\underline{\langle x \rangle}}$$ as required

Finally let's try $\int \phi^*(p)\, p\, \phi(p) = \langle p \rangle$:

$$\int_{-\infty}^{\infty} \phi^*(p)\, p\, \phi(p)\, dp = \frac{1}{2\pi\hbar} \int dp \left[\int dx' e^{ipx'/\hbar} \psi^*(x') \right] \times \left[\int dx'' e^{-ipx''/\hbar} \left(-i\hbar \frac{\partial}{\partial x''} \psi(x'') \right) \right]$$

$$= \int dx' \int dx'' \, \delta(x'' - x')\, \psi^*(x') \left(-i\hbar \frac{\partial}{\partial x''} \right) \psi(x'')$$

$$= \int dx'\, \psi^*(x') \left(-i\hbar \frac{\partial}{\partial x} \right) \psi(x')$$

$$= \underline{\underline{\langle p \rangle}}$$ as required.

So this definition of momentum space wave function $\phi(p)$ is valid!

Heisenberg Uncertainty Principle

From the definitions of $\phi(p)$ and $\psi(x)$ as fourier transforms, we see that if we localise a particle in x, its range of momentum widens and similarly vice versa.

This is Heisenberg's uncertainty principle:

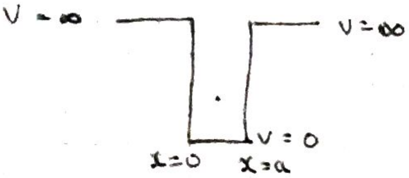
$$\Delta x \, \Delta p \geq \frac{\hbar}{2}$$

Similarly, for energy-time uncertainty:

$$\Delta E \, \Delta t \geq \frac{\hbar}{2}$$

Square Well Example

consider an infinite square well potential with a particle inside:



The particle can only move inside the well so;
$\psi = 0$ for $x \leq 0$ $x \geq a$

The potential is time independent so the solution has form

$$\Psi(x,t) = u(x)\, e^{-iEt/\hbar}$$

which must solve

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}u(x) + V(x)\,u(x) = E\,u(x)$$

$V = 0$ in the region of interest.

The solution takes form $u(x) = A\sin kx + B\cos kx$

using boundary conditions, $u(x) = 0$ at $x = 0$ and $x = a$

$$\Rightarrow \quad u_n(x) = A\sin\frac{n\pi x}{a}$$

Note, if you are having trouble understanding any of this, go and recap the Quantum physics module from last year.

substituting this into the SE, we find:

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2$$

we need to finally find a normalisation constant for ψ

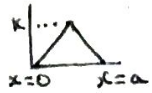
$$\int_{-\infty}^{\infty} \psi^* \psi \, dx = 1 \Rightarrow \int_0^a A^2 \sin^2\frac{n\pi x}{a}\, dx = A^2\frac{a}{2} = 1$$

$$\Rightarrow \quad A = \sqrt{\frac{2}{a}}$$

$$\therefore \quad \Psi_n(x,t) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{n\pi x}{a}\right) e^{-iE_n t/\hbar}$$

Completeness

The fourier nature of wave functions we saw earlier gives us some interesting properties. Particularly, that our initial wave functions can be written as fourier series. For example, if our wave function at $t=0$ is a triangular wave:



$$\psi(x, t=0) = \sum_{n=1}^{\infty} c_n u_n(x) \quad \text{where} \quad c_n = \frac{8K}{n^2\pi^2}\sqrt{\frac{a}{2}}\,\sin\left(\frac{n\pi}{2}\right)$$

the fourier coefficient

The time evolution is provided by the term $e^{-iE_nt/\hbar}$

so $$\psi(x,t) = \sum_{n=1}^{\infty} c_n u_n(x)\, e^{-iE_nt/\hbar}$$

in Quantum Mechanics, completeness means any wave function can be expanded as a series of the eigenfunction solutions of the SE relevant to that problem.
So we saw for a triangle wave, it can be expanded with u_n being the eigenfunction solutions of the SE.

So in any problem, we can write

$$\phi(x) = \sum_n c_n u_n(x)$$

where $Hu_n = E_n u_n$

Orthogonality

It is important in these problems that there is only one way of writing $\Psi(x, t=0) = \sum_n c_n u_n(x)$ because otherwise, given an initial condition there may be more than one expansion and this would not make sense physically.

each $u_n(x)$ thus contains unique information and we require:

$$\int_{-\infty}^{\infty} u_n^*(x)\, u_m(x)\, dx = \delta_{nm}$$

$\uparrow$ kronecker delta $= \begin{cases} =1 & \text{if } n=m \\ =0 & \text{otherwise} \end{cases}$

we can prove this:

consider $\quad H u_n(x) = E u_n(x)$

$$\therefore \int u_i^* H u_j\, dx = \int u_i^* E_j u_j\, dx = E_j \int u_i^* u_j\, dx$$

$$\hookrightarrow = \int E_i u_i^* u_j\, dx = E_i \int u_i^* u_j\, dx$$

This is because the H operator can act left or right

$$\Rightarrow E_i \int u_i^* u_j\, dx = E_j \int u_i^* u_j\, dx$$

This can only be true if:

$i = j$

or both sides are 0

So we require $\underline{\int u_i^* u_j\, dx = \delta_{ij}}$

3D Schrödinger Equation

We can extend the equation to 3D by extending the necessary operators to 3D.

in 1D: $\hat{p} = -i\hbar \frac{\partial}{\partial x}$

in 3D: $\hat{p} = -i\hbar \underline{\nabla}$

so the SE becomes:

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

where the probability of the particle being in some volume dV is:

$$\int_{-\infty}^{\infty} \psi^* \psi \, dV$$

Wave Function Collapse

We can think of a quantum of the particle's energy being "smeared" across the wave function. When we make a measurement, all of the energy is released at the point of measurement, making it look like the particle is at that point only. This is "Wave Function Collapse"

But this would mean that all of the information of the particle's energy is instantaneously (faster than light) "known" at the point of measurement. We have different competing theories that try to explain this:

Copenhagen Interpretation - too complicated to explain here

Hidden Variables - there is a insofar unknown deterministic description of QM

Many Worlds - all outcomes happen in parallel universes.