PH101: Physics 1

Module 3: Introduction to Quantum Mechanics

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Observables, Linear Operators, Commutation Relations

Let A and B are two linear operators (why do we talk about linear operators in Q.Mech.?)

The Commutator of A and B, $$C = [A, B]$$

Show that C is also a linear operator

Suppose A and B share a common eigenvalue ϕ. Show that $C\phi = 0$

Initial conditions in classical physics

The Newton's second law in classical physics viz.

$$m\,\frac{d^2x(t)}{dt^2} = F(x(t), t)$$

is a second order differential equation. This means two derivatives with respect to time are involved. In order to obtain the trajectory we have to solve this equation by some form of integration to get rid of the two derivatives. Each time an integration is performed an integration constant appears that has to be specified before the solution can be thought of specific to a given problem. Since the above equation has two derivatives with respect to time, we may expect that upon integrating twice (not directly but in some clever way so as to get x(t)) we end up with two integration constants whose values have to be fixed.

One way to fix this is to specify x(0) and v(0) - the initial position and initial speed (where v(t) = $\frac{dx(t)}{dt}$) so that these two integration constant go away and the solution becomes unique.

Initial and boundary conditions in quantum physics

In quantum physics, as we know very well by now, there is nothing like a trajectory - so that it is not Newton's Second Law that we should be integrating, but Schrodinger's matter wave equation. This as we know may be written as,

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right)\psi(x,t) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

This is an equation with two x derivatives and one t derivative. This is called a partial differential equation. Fixing the boundary conditions on this somewhat more technical so let us focus on the simpler case of stationary states. In case of stationary states $V(x)$ is independent of time so that,

$$\psi(x,t) = e^{-\frac{i}{\hbar}Et}\,\varphi(x)$$

Substituting into (1) gives us the so-called time independent Schrodinger equation -

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\varphi(x) = E\,\varphi(x)$$

contd…

Now this is somewhat like our Newton's second law which has two derivatives with respect to one independent variable. As before, integrating this twice will give us $\varphi(x)$. But each time an integration is performed, we have to introduce an integration constant. To get rid of the two integration constants and write down a unique solution, we have to **specify $\boldsymbol{\varphi(x_0)}$ *and* $\boldsymbol{\varphi'(x_0)}$. This is known as specifying boundary conditions** (if time is the independent variable, it is called initial condition). This is fully analogous to the case in Newtonian mechanics where we have to specify $\mathrm{x}(t_0)$ and $\mathrm{x}'(t_0) \equiv \mathrm{v}(t_0)$.

Also, keep in mind that Schrodinger's equation is a homogeneous equation – this means that if $\psi(x,t)$ is a solution then $\lambda\, \psi(x,t)$ is also a solution where λ is any complex constant. This also applies to the time independent equation – if $\varphi(x)$ is a solution then $\lambda\, \varphi(x)$ is also a solution where λ is any complex constant. This ambiguity is removed by imposing **the normalization condition,** i.e. by applying the condition that the total probability of finding the particle somewhere in space is one.

Normalization condition: $\int_{-\infty}^{\infty} dx\, |\varphi(x)|^2 = 1$

The time independent Schrodinger equation may also be rewritten as

$$\varphi''(x) = -\frac{2m}{\hbar^2}(E - V(x))\,\varphi(x)$$

Think of some region surrounding $x = x_0$. Let us assume that $\varphi(x)$ is continuous in the neighborhood of $x = x_0$. This means the continuity or otherwise of the second derivative will depend on the nature of the potential function $V(x)$ in this region.

Case a) $V(x)$ is finite in the neighborhood of $x = x_0$. Then $\varphi''(x)$ is also finite which means $\varphi'(x)$ is continuous. We have already assumed that $\varphi(x)$ is continuous. Therefore in regions where the potential function is finite, both the wave function and its first derivative are continuous.

Case b) $V(x)$ is infinite at $x = x_0$. $V(x_0) = \pm\infty$. In this case, $\varphi''(x_0) = \pm\infty$. This means $\varphi'(x)$ is discontinuous at $x = x_0$. In such cases we have to rewrite Schrodinger's equation for point very near $x = x_0$ as follows –

$$\varphi''(x) \approx \frac{2m}{\hbar^2} V(x)\,\varphi(x_0)$$

Or the discontinuity in the first derivative may be expressed as,

$$\varphi'(x_0 + \epsilon) - \varphi'(x_0 - \epsilon) \approx \frac{2m}{\hbar^2}\left(\int_{x_0-\epsilon}^{x_0+\epsilon} dx\ V(x)\right)\varphi(x_0)$$

Particle in a box (infinite square well)

$$V(x) = \begin{cases} 0, & \text{if } 0 \le x \le a, \\ \infty, & \text{otherwise} \end{cases}$$

V = 0 (particle is completely free)

Particle doesn't exist at all in the region

x > *a* and *x* < *0*

So, the time independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi,$$

or $$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar}.$$

The equation is similar to **simple harmonic oscillator**. The solution is thus of the form

$$\psi(x) = A \sin kx + B \cos kx$$

where *A* and *B* are arbitrary constants fixed by the **boundary conditions** of the problem.

Boundary conditions is that the wave function is continuous, i.e.,

$$\psi(0) = \psi(a) = 0$$

$$\psi(0) = A \sin 0 + B \cos 0 = B = 0$$

and hence $\psi(x) = A \sin kx.$

$$\psi(a) = A \sin ka = 0$$

either $A = 0$ or $\sin ka = 0$ **(*A* = 0, trivial solution)**

$ka = 0, \pm\pi, \pm 2\pi, \pm 3\pi, \ \ldots$ **(*k* = 0, trivial solution)**

contd…

$$k_n = \frac{n\pi}{a}, \quad \text{with } n = 1, 2, 3, \ldots$$

So, the **energy** of such a particle in the box is given by

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}.$$

To find A, we *normalize* ψ

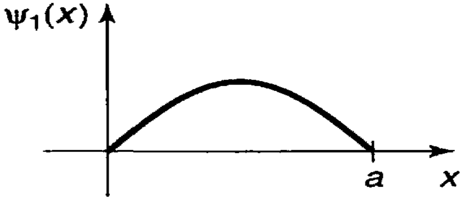
$$\int_0^a |A|^2 \sin^2(kx)\,dx = |A|^2\frac{a}{2} = 1, \quad \text{so} \quad |A|^2 = \frac{2}{a}.$$

Inside the well, the solutions are (the phase of *A* carries no physical significance, hence is taken as positive)

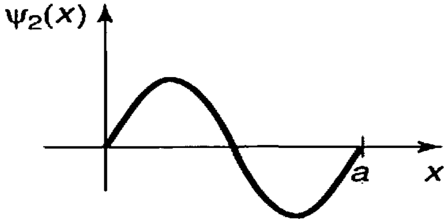
$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right).$$

The time-independent Schrodinger equation has an infinite set of solutions (one for each positive integer n).

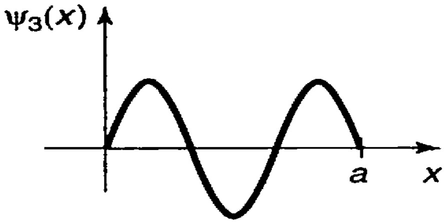
Plot the ground state, first and second excited states



Ground state



First excited state



Second excited state

Important properties of the wave function:

1. They are alternately even and odd, with respect to the center of the well: ψ_1 is even, ψ_2 is odd, ψ_3 is even, and so on.

2. As you go up in energy, each successive state has one more node (zero-crossing): ψ_1 has none (the end points don't count), ψ_2 has one, ψ_3 has two, and so on.

3. They are mutually orthogonal, in the sense tha $\int \psi_m(x)^* \psi_n(x)\, dx = 0$, whenever $m \neq n$.

To understand why this idea corresponds to orthogonality we have to understand the geometry of Hilbert space.