Lecture 5:
The Schrödinger equation

We have discussed the properties of a wavefunction, which describes the state of a given quantum system and seen what are the formal properties of operators applied to it. However, we still need to address how a given wavefunction evolves in time. In other word, we need to find an operator A so that:

$$\frac{\partial \psi}{\partial t} = A\psi \tag{1}$$

In order to determine A, let us follow this heuristic reasoning. Let us consider a one-dimensional plane wave:

$$\psi_0 = \text{const.}\, e^{-i(\omega t - kx)} \tag{2}$$

If we take the temporal derivative, we obtain:

$$\frac{\partial \psi_0}{\partial t} = -i\omega\psi_0 = \frac{1}{i\hbar}\hbar\omega\psi_0, \tag{3}$$

where in the last passage we have simply multiplied and divided by $i\hbar$. Apart from this constant value, we have thus obtained the energy E_0 of a monochromatic wave. We can thus rewrite it as:

$$i\hbar\frac{\partial \psi_0}{\partial t} = E_0\psi_0, \tag{4}$$

So, ψ_0 is an eigenfunction of the operator A, with its energy as the eigenvalue. This suggests that the operator A is the Hamiltonian. Moreover, if we take the spatial derivative of the plane wave, we obtain:

$$\frac{\partial \psi_0}{\partial x} = ik\psi_0 = \frac{1}{-i\hbar}\hbar k\psi_0 \tag{5}$$

By remembering De Broglie relation: $p = h/\lambda = k\hbar$ (we have considered that the wavenumber k is defined as $k = 2\pi/\lambda$), we have:

$$-i\hbar\frac{\partial \psi_0}{\partial x} = p\psi_0. \tag{6}$$

This suggests that the operator momentum is equal to $p = -i\hbar\partial/\partial x$ and, in three dimensions: $\vec{p} = -i\hbar\nabla$. This reasoning (that is purely heuristic and it does not represent by any means a rigorous demonstration) suggests then that the operator A substantially is the hamiltonian of the system in which the momentum is defined as $\vec{p} = -i\hbar\nabla$:

$$i\hbar\frac{\partial \psi}{\partial t} = H\psi \tag{7}$$

This is called the Schrödinger equation and it describes the temporal evolution of a quantum system. For a particle in three dimensions:

$$H = \frac{\vec{p}^2}{2m} + V(\vec{r}) = -\frac{\hbar^2 \nabla^2}{2m} + V(\vec{r}) \tag{8}$$

We will now show several properties of this formalism, which suggest its consistency as a generalisation of classical dynamics.

First, it is worthwhile to show that, once a wavefunction is normalised, it remains so if its evolution in time is described by the Schrödinger equation. For simplicity, we will restrict ourselves to a one-dimensional problem. A normalised wavefunction means that:

$$\int_{-\infty}^{+\infty} \psi^* \psi \,\mathrm{d}\, x \equiv \int_{-\infty}^{+\infty} |\psi|^2 \,\mathrm{d}\, x = 1 \tag{9}$$

If we take the temporal derivative:

$$\frac{\mathrm{d}}{\mathrm{d}\, t} \int_{-\infty}^{+\infty} \psi^* \psi \,\mathrm{d}\, x = \int_{-\infty}^{+\infty} \frac{\partial}{\partial t} |\psi|^2 \,\mathrm{d}\, x = \int_{-\infty}^{+\infty} \psi^* \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t} \psi \,\mathrm{d}\, x \tag{10}$$

The Schrödinger equation is:

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar} V(x) \psi \tag{11}$$

and its complex conjugate:

$$\frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar} V(x) \psi^* \tag{12}$$

We thus have:

$$\int_{-\infty}^{+\infty} -\frac{i\hbar}{2m} \frac{\partial^2 \psi^*}{\partial x^2} \psi + \frac{i}{\hbar} V(x) \psi^* \psi + \psi^* \frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} \psi - \frac{i}{\hbar} \psi^* V(x) \psi \,\mathrm{d}\, x \tag{13}$$

The two terms containing the potential $V(x)$ are, generally speaking, different. But, keeping in mind that the potential is an hermitian operator we have:

$$\frac{i}{\hbar} \left[V(x) \psi^* \psi - \psi^* V(x) \psi \right] = \frac{i}{\hbar} \left[V(x) \psi^* \psi - V(x) \psi^* \psi \right] = 0 \tag{14}$$

We are thus left with:

$$\int_{-\infty}^{+\infty} \frac{i\hbar}{2m} \frac{\partial}{\partial x} \left[\psi^* \frac{\partial \psi}{\partial x} \psi - \frac{\partial \psi^*}{\partial x} \psi \right] \mathrm{d}\, x = \frac{i\hbar}{2m} \left[\psi^* \frac{\partial \psi}{\partial x} \psi - \frac{\partial \psi^*}{\partial x} \psi \right]_{-\infty}^{+\infty} \tag{15}$$

Given that the wavefunction must go to zero at $\pm\infty$, Eq. **??** is equal to zero. We have thus demonstrated that the modulus of a wavefunction, over an infinite space, does not change in time. However, the situation might be different if we consider a finite portion of space (a volume Φ), since, intuitively, there might be a stream of particles inward and outaward of this region. In general then, we should write:

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\int_\Phi \psi^*\psi\,\mathrm{d}\,x = \int_\Phi \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left[\psi^*\frac{\partial\psi}{\partial x}\psi - \frac{\partial\psi^*}{\partial x}\psi\right]\mathrm{d}\,x, \tag{16}$$

which, in three dimensions, would read:

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\int_\Phi \psi^*\psi\,\mathrm{d}\,\vec{r} = \int_\Phi \frac{i\hbar}{2m}\nabla\cdot\left[\psi^*\nabla\psi - \nabla\psi^*\psi\right]\mathrm{d}\,\vec{r} = -\int_\Phi \nabla\cdot\vec{J}\,\mathrm{d}\,\vec{r}, \tag{17}$$

where we have introduced the quantity $\vec{J}$ as:

$$\vec{J} = -\frac{i\hbar}{2m}\left[\psi^*\nabla\psi - \nabla\psi^*\psi\right] \tag{18}$$

Eq. **??** must be valid for any volume Φ implying that the integrands must be equal. We have thus obtained a continuity equation:

$$\frac{\mathrm{d}}{\mathrm{d}\,t}|\psi|^2 + \nabla\cdot\vec{J} = 0 \tag{19}$$