Lecture 6:
Properties of the Schrödinger equation

In the last lecture, we have introduced the Schrödinger equation and discussed one of its most fundamental properties: a normalised wavefunction over an infinite portion of space remains so if its temporal evolution is described by the Schrödinger equation. In a limited region of space, this is generally not true, since a stream of particles can flow within and without the region under interest. In general, this relation holds:

$$\frac{\mathrm{d}}{\mathrm{d}\,t}|\psi|^2 + \nabla \cdot \vec{J} = 0, \tag{1}$$

where:

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

is the current density. We will now proceed to demonstrate another series of interesting properties of the Schrödinger equation. First of all, it is worth mentioning that the Schrödinger equation allows us to write an important relation for the temporal evolution of the mean value of an operator:

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\langle O\rangle_\psi = \langle\psi|\left(\frac{\partial}{\partial \mathrm{t}}O + \frac{1}{i\hbar}\left[O, H\right]\right)|\psi\rangle \tag{3}$$

To demonstrate this important relation, let us expand the right hand-side of it, remembering that $[O, H] = OH - HO$ and that $\langle O\rangle_\psi = \langle\psi|O|\psi\rangle$:

$$\langle\psi|\left(\frac{\partial}{\partial \mathrm{t}}O + \frac{1}{i\hbar}\left[O, H\right]\right)|\psi\rangle = \langle\psi|\frac{\partial}{\partial \mathrm{t}}O|\psi\rangle + \frac{1}{i\hbar}\langle\psi|OH|\psi\rangle - \frac{1}{i\hbar}\langle\psi|HO|\psi\rangle \tag{4}$$

The last two terms, written in the integral formulation, read:

$$\frac{1}{i\hbar}\int \psi^* OH\psi\,\mathrm{d}\,r - \frac{1}{i\hbar}\int \psi^* HO\psi\,\mathrm{d}\,r \tag{5}$$

Substituting Schrödinger equation ($i\hbar\frac{\mathrm{d}}{\mathrm{d}\,t}\psi = H\psi$), we obtain:

$$\int \psi^* O\frac{\mathrm{d}}{\mathrm{d}\,t}\psi\,\mathrm{d}\,r + \int \frac{\mathrm{d}}{\mathrm{d}\,t}\psi^* O\psi\,\mathrm{d}\,r \tag{6}$$

The relation now reads:

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\langle O\rangle_\psi = \langle\psi|\frac{\partial}{\partial \mathrm{t}}O|\psi\rangle + \int \psi^* O\frac{\mathrm{d}}{\mathrm{d}\,t}\psi\,\mathrm{d}\,r + \int \frac{\mathrm{d}}{\mathrm{d}\,t}\psi^* O\psi\,\mathrm{d}\,r \tag{7}$$

which is the definition of the total derivative of a mean value of an operator. ■

This is an important relation, that strongly relies on the temporal evolution of a wavefunction being described by the Schröndinger equation. An important consequence of this relation is that, if an operator is time-indipedent and commutes with the Hamiltonian, then its mean value is constant in time:

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\langle O\rangle_\psi = 0 \tag{8}$$

For the interested student, this formulation is formally identical to the one obtainable in classical mechanics, provided that the commutator is replaced with the Poisson's parentheses.

Another important consequence is that the mean values of position, momentum and potential obey classical relations:

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\langle m\vec{r}\rangle = \langle\vec{p}\rangle \tag{9}$$

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\langle\vec{p}\rangle = -\langle\nabla V\rangle \tag{10}$$

This is known as the *Ehrenfest Theorem* and the demonstration is straightforward, once the relation **??** is taken into account. For the operator position ($O = \vec{r}$):

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\langle m\vec{r}\rangle = \langle\psi|\left(\frac{\partial}{\partial \mathrm{t}}O + \frac{1}{i\hbar}[m\vec{r}, H]\right)|\psi\rangle = \langle\psi|\frac{1}{i\hbar}[m\vec{r}, H]|\psi\rangle \tag{11}$$

The last equality holds since the operator position is not explicitly dependent on time. We are thus left to calculate the commutator $[m\vec{r}, H]$:

$$[m\vec{r}, H] = [m\vec{r}, \frac{\vec{p}^2}{2m} + V(\vec{r})] = [m\vec{r}, \frac{\vec{p}^2}{2m}] = \frac{1}{2}[\vec{r}, \vec{p}^2] \tag{12}$$

where we have used the fact that the position commutes with the potential (and, in fact, with any arbitrary function of the sole position). We are thus left to calculate the commutator $[\vec{r}, \vec{p}^2]$. An elegant way to know the result of this commutator, without explicitly calculating it, is to recall that $[L, M^2] = 2M$ if $[L, M] = 1$, with l and M being any operator (see Exercise 4.2 in Lecture 4). Generalising this property, it is straightforward to demonstrate that $[L, M^2] = 2\alpha M$ if $[L, M] = \alpha$, being α any complex number (including zero). Since $[\vec{r}, \vec{p}] = i\hbar$ (see Lecture 3), we have $[\vec{r}, \vec{p}^2] = 2i\hbar\vec{p}$. Substituting this result into Eq. **??** we have:

$$[m\vec{r}, H] = i\hbar\vec{p} \tag{13}$$

Substituting this last relation into Eq. **??** demonstrates the Ehrenfest theorem. ■

This theorem has the fundamental physical consequence that a wave packet obeys Newton's equation, justifying the classical concept of particle. This last statement must not be taken literally though; a wave function is not a physical object as such, but it only represents a distribution of probability. However, the mean values of its position and momentum are relatable to those of a classical particle.

It is worth mentioning that, for a time-independent wavefunction, the Schrĭondinger equation reads:

$$H\psi = E\psi \tag{14}$$

where E represent an eigenvalue of the energy. Improperly, Eq. **??** is commonly referred to as the Schrödinger equation. We conclude this Lecture by enunciating an important theorem: *in a one-dimensional system, every discrete level is non-degenerate*.

This is equivalent to say that for any discrete eigenvalue of the energy E_n there is only one eigenfunction ψ_n or, in other words, that the energy of the system univocally determines the wave function of the system for a given Hamiltonian. The demonstration of this theorem will be given in the next Lecture.

This might seem as a purely theoretical result only: the world is clearly not uni-dimensional. However, it is possible to demonstrate that, if the potential is dependent on only one spatial variable (see for instance gravity), then the physical system under interest is equivalent to a one-dimensional problem.