

Lecture 7: The Schrödinger equation in one dimension

In this Lecture, we will discuss some fundamental properties of the Schrödinger equation in one dimension. We have seen in the last Lecture that this is not only an idealised problem, since every Hamiltonian with its potential depending on only one spatial variable describes, effectively, a one-dimensional problem. The time-independent Schrödinger equation can thus be written as:

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E\psi(x) \quad (1)$$

For instance, every three-dimensional problem with central symmetry is formally equivalent to Eq. ?? For a free particle ($V(x) = 0$), the Schrödinger equation is:

$$\psi''(x) = -k^2\psi(x) \quad \text{with} \quad k = \sqrt{\frac{2mE}{\hbar^2}} \quad (2)$$

It is trivial to see that the general solution of this equation is:

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad (3)$$

with A, B two complex numbers to be determined via boundary conditions. It is worth noticing here that only positive energies are allowed ($E \geq 0$, which implies $k \in \mathbb{R}$); the wavefunctions whereby $k \in \mathbb{C}$ would in fact be non-normalisable (generally speaking, states in which $E < 0$ correspond to bound states that cannot exist in this case since there is no potential in the Hamiltonian). **If the particle is moving in free space, the spectrum of this equation (i.e., the ensemble of all possible energy eigenvalues) is continuous. On the other hand, if the particle is forced to move in a confined region, the spectrum may become discrete.** For instance, if we assume that the particle is moving in a ring of length L , the wave function must satisfy the periodic condition: $\psi(L + x) = \psi(x)$. The allowed values of k are thus: $k = 2\pi n/L$ with n being any integer number. The energy spectrum is thus:

$$E_n = \frac{(2\pi n)^2 \hbar^2}{2mL^2}, \quad (4)$$

which is discrete. We can now demonstrate the theorem enunciated in the last Lecture: *in a one-dimensional system, every discrete level is non-degenerate.*

In order to demonstrate it, let us proceed by assuming that the contrary is true. If we end up with an obvious contradiction, the enunciate is true. This procedure is quite common in

Mathematics, and it is usually called *demonstration by contradiction*. Let us then suppose that there are two wave functions with the same energy eigenvalue U (this energy eigenvalue is thus degenerate):

$$\psi_1'' = -\frac{2m}{\hbar^2}(E - U)\psi_1 \quad , \quad \psi_2'' = -\frac{2m}{\hbar^2}(E - U)\psi_2 \quad (5)$$

If we multiply the first equation by ψ_2 , the second by ψ_1 , and then subtract the second equation from the first, we obtain:

$$\psi_1''\psi_2 - \psi_2''\psi_1 = 0 \quad (6)$$

We will integrate this equation once, by using integration per parts. This method tells us that, if I have a product between a function (g) and a derivative of a function (f'), its integral is equal to:

$$\int f'gdx = fg - \int fg'dx + \text{const.} \quad (7)$$

for the first part of the equation ($\psi_1''\psi_2$), I have $g = \psi_2$ and $f = \psi_1'$. The integral of it is thus equal to:

$$\int \psi_1''\psi_2dx = \psi_1'\psi_2 - \int \psi_1'\psi_2'dx + \text{const.} \quad (8)$$

Conversely, for the second part of the equation ($\psi_2''\psi_1$), I have $g = \psi_1$ and $f = \psi_2'$. The integral of it is thus equal to:

$$\int \psi_2''\psi_1dx = \psi_2'\psi_1 - \int \psi_2'\psi_1'dx + \text{const.} \quad (9)$$

Putting the two terms together:

$$\psi_1'\psi_2 - \int \psi_1'\psi_2'dx + \text{const.} - \psi_2'\psi_1 + \int \psi_2'\psi_1'dx + \text{const.} = 0 \quad (10)$$

the two remaining integrals cancel out, leaving:

$$\psi_1'\psi_2 - \psi_2'\psi_1 = \text{const.} \quad (11)$$

Integrating again, we obtain:

$$\log \psi_1 = \log \psi_2 + \text{const.} \quad \rightarrow \quad \psi_1 = \text{const.} \psi_2 \quad (12)$$

The two wave functions must then only differ by a multiplying constant: they thus represent the same state. ■

We must remember that the Hamiltonian, being a quantum operator, must be Hermitian. It must then have all real eigenvalues and $V(x)$ and E must be real. The Schrödinger equation thus has only real coefficients, implying that the wavefunction can be chosen to be real. The general behaviour of the wavefunction can thus be deduced from:

$$\psi'' = \frac{2m[V(x) - E]}{\hbar^2} \psi \quad (13)$$

If $E > V(x)$, we are in a classically accessible regime and the wavefunction behaves as:

$$\begin{cases} \psi'' > 0 & \text{if } \psi < 0 \\ \psi'' < 0 & \text{if } \psi > 0 \end{cases} \quad (14)$$

which corresponds to an oscillatory behaviour. On the other hand, if $E < V(x)$ we are in a regime that is classically forbidden and the wavefunction behaves as:

$$\begin{cases} \psi'' > 0 & \text{if } \psi > 0 \\ \psi'' < 0 & \text{if } \psi < 0 \end{cases} \quad (15)$$

which corresponds to an unstable behaviour. Keeping in mind this property, it is not difficult to demonstrate the so-called:

Oscillation Theorem: *the wavefunction of the n^{th} discrete energy level has $n-1$ nodes (zeroes)*

However, for the sake of brevity, we will skip this demonstration.