6 The time-dependent Schrödinger Equation

$$\imath\hbar\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t) \tag{6.1}$$

where, H is called the Hamiltonian operator. It is the operator in quantum mechanics that corresponds to the energy of the system.

In quantum mechanics, every physically measurable quantity, has a corresponding operator. As we studied in the Stern-Gerlach experiments (and from the subsequent treatment of kets and operators), a measurement "projects" a system onto the eigenstates of the operator.

The operator H can be written as a sum of the kinetic and potential energy:

$$H = K + V = \frac{p^2}{2m} + V \tag{6.2}$$

Now if we substitute the momentum operator in Eq. (4.6), *i.e.* $\hat{p} = -\imath\hbar\frac{\partial}{\partial x}$, we can write down the Hamiltonian operator as

$$H = \frac{p^2}{2m} + V = \frac{1}{2m}\left[-\imath\hbar\frac{\partial}{\partial x}\right]^2 + V = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V \tag{6.3}$$

where $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} = \frac{1}{2m}\left[-\imath\hbar\frac{\partial}{\partial x}\right]^2$ is the kinetic energy operator.

In addition, note that we have used $\psi(x,t)$ in Eq. (6.1) instead of an abstract ket. So we have already chosen a representation, the position (or coordinate) representation.

A general comment: in the coordinate representation, the Schrödinger Equation is a differential equation. (In other representations, it may actually a matrix equation. This is similar to how we noted in the previous class that an operator goes a matrix, while a ket goes to a vector!)

The time-dependent Schrödinger Equation (6.1) can be rationalized from the wave-particle duality. We will proceed to show this below.

1. We have seen earlier in the Stern Gerlach experiments that there is this great analogy between wave-like behavior and particle-like behavior. We noted that the behavior of spin states in the presence of a magnetic field can be exactly reproduced by considering the behavior of plane-polarized light.

2. Hence, can we write $\langle x | \psi \rangle \equiv \psi(x)$ as a collection of waves? Consider the following:

$$h(x) = \int dk f(k) \exp\{\imath kx\} = \int dp f(p) \exp\left\{\imath \frac{p}{\hbar} x\right\} \quad (6.4)$$

   Homework: Why is it true that $\langle x | k \rangle = \exp\{\imath kx\}$? (Hint: Rephrase the question in English.)

3. Note that in Eq. (6.4), $h(x)$ is a linear combination of waves such as those in the Change of basis section.

4. Note further that waves $\exp\{\imath kx\}$ are eigenstates of the momentum operator. (Why is $\exp\{\imath kx\}$ considered to be a wave? Because, $\exp\{\imath kx\} = \cos\{kx\} + \imath \sin\{kx\}$.)

5. Note also that Eq. (6.4) is obtained from resolution of identity in terms of the momentum Eiqenstates. In addition, those of you who have seen Fourier transforms before will note that the function $h(x)$ is now a Fourier transform of the function $f(k)$.

6. **Wavepackets:** Why in Eq. (6.4) do we say that $h(x)$ is a *linear combination of waves* when we write it as an integral? Because:

   (a) $\exp\{\imath kx\}$ forms a continuous representation as noted earlier in Eq. (4.10) (where we have represented the eigenstates of momentum as $|k\rangle$, that is using the abstract *ket* vector).

   (b) As noted in Eq. (4.9) for continuous representations the sum is changed to integral.

   (c) Hence Eq. (6.4) is the *continuous multi-dimensional* analogue of Eq. (A.1).

   (d) Hence we can say that in Eq. (6.4), we have written $h(x)$ as a continuous linear combination of waves. So could we call it a ”packet” of waves then? Indeed!!! In fact, $\psi(x)$ as written on the right hand side of Eq. (6.4) is called a *wavepacket* (as in ”packet-of-waves”).

7. $h(x)$ in Eq. (6.4) does not have a time-dependence. So, lets go ahead and multiply Eq. (6.4) by the quantity $\exp\left\{-\imath\omega t\right\} = \exp\left\{-\imath\frac{E}{\hbar}t\right\}$ so as to maintain the same wave-form as in Eq. (2.6),

$$\psi(x,t) = \int\int dpdE f(p)g(E)\exp\left\{\imath\left[\frac{p}{\hbar}x - \frac{E}{\hbar}t\right]\right\} \tag{6.5}$$

8. Note now the similarities between the integrand in Eq. (6.5) and the plane polarized light seen earlier.

9. Lets go ahead substitute the right hand side of Eq. (6.5) into Eq. (6.1) to see what happens. (Lets forget about V for now.)

10. Differentiating Eq. (6.5) twice with respect to x we obtain:

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\int dpdE f(p)g(E)\exp\left\{\imath\left[\frac{p}{\hbar}x-\frac{E}{\hbar}t\right]\right\} \\ &= -\frac{\hbar^2}{2m}\int\int dpdE f(p)g(E)\left[\imath\frac{p}{\hbar}\right]^2\exp\left\{\imath\left[\frac{p}{\hbar}x-\frac{E}{\hbar}t\right]\right\} \\ &= \frac{1}{2m}\int\int dpdE f(p)g(E)p^2\exp\left\{\imath\left[\frac{p}{\hbar}x-\frac{E}{\hbar}t\right]\right\} \quad (6.6) \end{aligned}$$

11. Note further from Eq. (6.2) that in the absence of V, $E = \frac{p^2}{2m}$. Hence, Eq. (6.6) can be re-written as:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) = \int\int dpdE f(p)g(E)E\exp\left\{\imath\left[\frac{p}{\hbar}x-\frac{E}{\hbar}t\right]\right\} \quad (6.7)$$

12. Differentiating Eq. (6.5) with respect to t we obtain (for the right side of Eq. (6.1) we obtain:

$$\begin{aligned} \imath\hbar\frac{\partial}{\partial t}\psi(x,t) &= \imath\hbar\frac{\partial}{\partial t}\int\int dpdE f(p)g(E)\exp\left\{\imath\left[\frac{p}{\hbar}x - \frac{E}{\hbar}t\right]\right\} \\ &= \imath\hbar\int\int dpdE f(p)g(E)\left[-\imath\frac{E}{\hbar}\right]\exp\left\{\imath\left[\frac{p}{\hbar}x - \frac{E}{\hbar}t\right]\right\} \\ &= \int\int dpdE f(p)g(E)E\exp\left\{\imath\left[\frac{p}{\hbar}x - \frac{E}{\hbar}t\right]\right\} \end{aligned} \tag{6.8}$$

13. Note that the right hand side of Eqs. (6.8) and Eq. (6.7) are identical. Hence the left hand sides of Eqs. (6.8) and (6.7) must be equal to each other which leads to the time-dependent Schrödinger equation.

This provides a good rationalization for the time-dependent Schrödinger Equation (TDSE) in Eq. (6.1) using the wave-particle duality and the analogy to plane-polarized light.

That is, the TDSE holds for all functions that can be written as linear combination of waves.

