Part I: The Time-Dependent Schrödinger Equation

Many books only present the time-independent form of the Schrödinger equation. This is misleading, because even for cases where you can use the time-independent formulation, there is STILL A TIME DEPENDENT term needed in the full expression for the wave function. In these problems, we will work from the time-dependent Schrödinger equation and see how, for many cases, we can solve for the time-dependence and the position-dependence of the wave function separately.

Here is the time dependent Schrödinger's equation (TDSE):

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + U(x,t)\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) \tag{1a}$$

where $\hbar$ is the reduced Planck's constant, m is the mass of a particle, $\Psi(x,t)$ is the wavefunction of the particle, and $U(x,t)$ is the potential energy of the system as a function of position and time. For our purposes, we will assume U varies only with position, not time.

(a) Show that, if you re-express the total wave function $\Psi(x,t)$ as a function of position – lower case $\psi(x)$ – times a function of time – lower case $\phi(t)$:

$$\Psi(x,t) = \psi(x)\phi(t) \tag{1a}$$

you can rewrite the TDSE as:

$$-\frac{\hbar^2}{2m}\phi(t)\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x)\phi(t) = i\hbar\psi(x)\frac{d\phi(t)}{dt} \tag{2}$$

(b) Show that equation (2) can be rearranged so that all of the terms involving position are on one side and all of the terms involving time are on the other side (This is called *separation of variables*: we are separating *x* and *t*):

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} + U(x) = i\hbar\frac{1}{\phi(t)}\frac{d\phi(t)}{dt} \tag{3}$$

1. Explain why you could not separate the variables in this way if the potential energy function was changing with time.

2. Explain why the only possible solution for this equation is for both sides to be equal to a constant (we'll call it C). That is:

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} + U(x) = i\hbar\frac{1}{\phi(t)}\frac{d\phi(t)}{dt} = C \tag{4}$$

such that we end up with 2 expressions:

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} + U(x) = C \qquad \text{and} \qquad i\hbar\frac{1}{\phi(t)}\frac{d\phi(t)}{dt} = C \tag{5}$$

Part II: Solving the Time Equation

To find $\phi(t)$, we must now solve the time equation:

$$i\hbar \frac{1}{\phi(t)} \frac{d\phi(t)}{dt} = C \tag{6}$$

1. Show that the equation can be written as $\dfrac{d\phi(t)}{dt} = -\dfrac{iC}{\hbar}\phi(t).$

2. Show that $\phi(t) = e^{-iCt/\hbar}$ is a solution to the equation.

3. Express this solution also in terms of sines and cosines.

4. What are the angular frequency (ω) and the frequency (f) of this solution?

5. Given that the relationship between energy and frequency is the same for matter particles and for photons, what is the relationship between C and the energy (E) of the electron (or matter particle) in this case? What is $\phi(t)$ in terms of E?

✓ **STOP HERE** and check your results with your instructor before proceeding to the next section!

Part III, A: Solving boundary conditions

In solving ODEs and PDEs, you inevitably come to a point where you have a trial function with some undetermined coefficients, and a "boundary condition" that helps you pick (or constrain) those coefficients. Let's consider two common examples.

Your trial function is $f(x) = Ae^{kx} + Be^{-kx}$. You do not yet know A, B, or k (but I am assuming that k is real). The boundary conditions are $f(0) = 0$, and $f(L) = 0$, where L is a known length

1. What does $f(0) = 0$ tell you about A, B, and/or k?
   (Hint: it might tell you about *some* but not *all* of them.)

2. Given the above, what additional information does $f(L) = 0$ give you?

3. Summarize: what does $f(x)$ look like? Is it unique, or are there many possibilities?

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Part III, B: Solving boundary conditions

Your trial function is $f(x) = C\sin(kx) + D\cos(kx)$. You do not yet know C, D, or k (k is real). The boundary conditions are $f(0) = 0$, and $f(L) = 0$, where L is a known length

1. Which of these conditions do you think will be most useful to start with? Why? Start with it — what does it tell you?

2. What additional information does the other boundary condition yield?

3. Summarize: what does $f(x)$ look like? Is it unique, or are there many possibilities? Discuss!

4. If $f(x)$ is meant to represent a wavefunction $\psi(x)$, describe how you could figure out your remaining constant.

✓ **Check** your results with your instructor!