

Lecture 9 - Time-independent Schrödinger equation

What's important:

- time-independent Schrödinger equation
- eigenfunctions and eigenvalues
- particle in a 1D box

Text: Gasiorowicz, Chap. 4

Time-independent Schrödinger equation

Let's apply the ideas of eigenfunctions to the *time-dependent* Schrödinger equation to extract the *time-independent* Schrödinger equation. In this, and the next several lectures, we continue to work in one dimension. Recall the explicit representation of the Schrödinger equation:

$$\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t), \quad (1)$$

where we have made the potential energy a function only of position. If an equation can be segregated into parts which depend on only one variable, then a fruitful approach to solving it is the so-called separation of variables approach. As implemented here, that means we should try to write the wavefunction $\psi(x,t)$ as a product of two functions, one containing all the position dependence and one containing all the time dependence:

$$\psi(x,t) = T(t) \cdot u(x). \quad (2)$$

Aside: not everyone uses this notation; frequently one sees $\Psi(x,t)$ for the complete wavefunction, and $\psi(x)$ for the position dependent part.

Substituting (2) into (1), and shuffling some functions to show what derivatives need attention

$$\hbar u(x) \frac{dT(t)}{dt} = -\frac{\hbar^2}{2m} T(t) \frac{d^2 u(x)}{dx^2} + T(t) V(x) u(x).$$

Note how ∂ has become d . Dividing by $T(t) \cdot u(x)$ yields

$$\hbar \frac{dT(t)/dt}{T(t)} = \frac{-(\hbar^2/2m)(d^2 u(x)/dx^2) + V(x)u(x)}{u(x)} \quad (3)$$

Now, the time dependence is completely isolated on the left hand side, and the position dependence is on the right hand side. Since the LHS cannot depend on x , and the RHS cannot depend on t , then NEITHER side can depend on x or t . That is, both sides must be equal to a constant, which we define with some foreshadowing as E . Treating the LHS first, we can now write

$$i\hbar \frac{dT(t)}{dt} = E T(t) \quad (4)$$

This has the obvious solution

$$T(t) = Ce^{-iEt/\hbar} \quad (5)$$

The RHS cannot be explicitly solved until we know the functional form of $V(x)$. However, it can be explicitly written out as

$$-\frac{\hbar^2}{2m} \frac{d^2u(x)}{dx^2} + V(x)u(x) = E u(x) \quad (6)$$

Eq. (6) is the *time-independent Schrödinger equation* and it is now obvious why we chose to call the constant E , the energy. Eq. (6) is an eigenvalue equation.

Eigenfunctions and eigenvalues

Eq. (4) is an example of an eigenvalue equation. It states that if we operate on the function $T(t)$ with the operator $i\hbar d/dt$, we regain the function multiplied by a constant, namely the energy E . Here, E is the eigenvalue and $T(t)$ is the eigenfunction. Gasiorowicz reviews a number of properties of eigenvalues *etc.* which the student is encouraged to review. The eigenvalue equation selects both the eigenvalue and the eigenfunction from all of the values and functions available.

Hopefully, most of this material has been seen in MATH 232, and there is no need to establish them again. An analogy emphasized by Gasiorowicz is the rotation of a vector in three dimensions. Calling the vector \mathbf{A} and the rotation matrix $R(\theta)$ for a rotation by θ around the z-axis, in general the operation

$$R(\theta)\mathbf{A}$$

carries \mathbf{A} to a new vector \mathbf{B} having the same length as \mathbf{A} but pointing in a different direction. An eigenvalue equation like

$$R(\theta)\mathbf{A} = c\mathbf{A}$$

for $\theta = 0, \pi/2, \dots$ would lead to

$$c = +1$$

\mathbf{A} pointing along the rotation axis.

In other words, both c and \mathbf{A} are selected by the equation. If we choose the special values for θ (like $\theta = \pi/2$), a more general set of vectors \mathbf{A} might be selected.

Particle in a 1D box

We referred to this problem in Lec. 1, in describing a particle travelling in one dimension between hard walls; the standing wave condition on the de Broglie wavelength lead to a set of solutions satisfying

$$L = n \lambda / 2 = nh / 2p \quad n = 1, 2, 3...$$

or

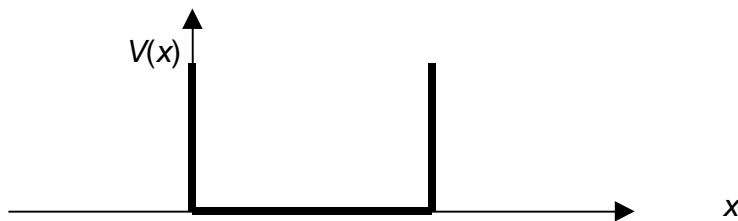
$$p = n \hbar / L. \quad (7)$$

We now revisit this problem with the time-independent Schrödinger equation (6)

$$-\frac{\hbar^2}{2m} \frac{d^2 u(x)}{dx^2} + V(x)u(x) = E u(x)$$

for the potential

$$\begin{aligned} V &= 0 & 0 < x < a \\ V &= + & x < 0 \text{ and } x > a. \end{aligned}$$



Eq. (6) tells us that the wavefunction $u(x)$ must vanish at $x = 0$ and a where the potential becomes infinite. In the intervening range of x , the wavefunction must satisfy

$$d^2 u / dx^2 = - (2mE / \hbar^2) u. \quad (8)$$

Now, if we define

$$k^2 = 2mE / \hbar^2 \quad (9)$$

then Eq. (8) has the particularly simple form

$$d^2 u / dx^2 = -k^2 u. \quad (10)$$

This equation has the usual sine and cosine functions as a solution. The cosine set $\cos(kx)$, where the argument has been made dimensionless as appropriate, does not satisfy the boundary condition $u(0) = 0$. Hence, only the sine functions are admissible:

$$u(x) = A \sin(kx)$$

where A is a normalization constant. The second boundary condition $u(a) = 0$ places a constraint on k via

$$ka = n \quad n = 1, 2, 3, \dots \quad (11)$$

and the normalization condition to make $u(x)$ a probability density

$$\int_0^a u^*(x) u(x) dx = 1$$

leads to

$$\begin{aligned} 1 &= A^2 \int_0^a \sin^2(n x/a) dx \\ &= A^2 (a/n) \int_0^n \sin^2\theta d\theta \\ &= A^2 (a/n) n (\frac{1}{2}) \quad (\frac{1}{2} \text{ from the usual } \int_0^n \sin^2 = \frac{1}{2}n) \\ &= A^2 a/2. \end{aligned}$$

Thus

$$A = (2/a)^{1/2}. \tag{12}$$

Gasiorowicz further establishes that the wavefunctions are orthogonal (see p. 59)

$$\int_0^a u_n^*(x) u_m(x) dx = 0 \quad n \neq m$$

by evaluating the integral with the trig identity

$$\sin a \sin b = \frac{1}{2} [\cos(a-b) - \cos(a+b)].$$

In summary, the solutions

$$u_n = (2/a)^{1/2} \sin(n x/a)$$

form an **orthonormal** set of functions - they are both normalized and mutually orthogonal:

$$\int_0^a u_n^*(x) u_m(x) dx = \delta_{nm}. \tag{13}$$

Note that in general, even if a set of solutions contains some functions with the same energy (called **degenerate** solutions), they are nevertheless orthogonal.

What about the energy and momentum of these solutions? Now that k is known from Eq. (11), the energy in Eq. (9) becomes

$$\begin{aligned} E_n &= \hbar^2 k^2 / 2m \\ &= \frac{\hbar^2}{2m} n^2 \pi^2 / a^2, \end{aligned} \tag{14}$$

which is the same as we found from the de Broglie condition. This still doesn't tell us p^2 , which must be found from the expectation

$$\begin{aligned} \langle p^2 \rangle &= \int_0^a u^*(x) p^2 u(x) dx = -\hbar^2 (2/a) \int_0^a \sin(kx) (d/dx)^2 \sin(kx) dx \\ &= -\hbar^2 (2/a) (-k^2) \int_0^a \sin(kx) \sin(kx) dx \\ &= (\hbar k)^2. \end{aligned}$$

Again, we regain the de Broglie expression.

A couple of miscellaneous issues:

1. The expression for the kinetic energy can be rearranged as follows:

$$\begin{aligned} K &= \langle p^2 \rangle / 2m = -(\hbar^2 / 2m) \int u^*(x) (d/dx)^2 u(x) dx \\ &= -\frac{\hbar^2}{2m} \int \frac{d}{dx} u^* \frac{du}{dx} - \frac{du^*}{dx} \frac{du}{dx} dx \end{aligned}$$

As usual, both u and its derivative vanish at infinity, so the first term, after performing the $(d/dx) dx$ must vanish. This leaves

$$K = (\hbar^2 / 2m) \int |du/dx|^2 dx, \quad (15)$$

showing that the kinetic energy is proportional to the complex square of the curvature of the wavefunction.

2. We showed in an earlier lecture how a periodic function could be expressed as a Fourier series - a sum over a set of functions $\sin(kx)$ just like the u 's here. In other words, a general wavefunction for this problem could have the form

$$\psi(x) = \sum_n A_n u_n(x). \quad (16)$$

Gasiorowicz shows that $|A_n|^2$ is the probability that the system will be found to have an energy E_n during a measurement.