3.024 Electrical, Optical, and Magnetic Properties of Materials Spring 2012
Recitation 3 Notes

Outline

1. Schrödinger: Eigenfunction Problems & Operator Properties
2. Piecewise Function/Continuity Review -Scattering from Step Potential

1. Schrödinger: Eigenfunction Problems & Operator Properties

In quantum mechanics, the Hamiltonian is an operator in Schrödinger's equation:

$$\hat{H} \quad = i\hbar\frac{\partial}{\partial t}$$

If $\quad (x,t) = \psi(x)\phi(t)$ which is true of the systems we will currently consider, the equation reduces to simpler time-independent Schrödinger equation using separation of variables:

$$\hat{H}\psi = E\psi$$

In this form, the time-dependent part of the wave function is a simple exponential relationship:

$$\phi(t) = \phi_0 e^{-\frac{iEt}{\hbar}}$$

Going back to the time-independent Schrödinger equation, if we consider $\hat{H}$ as an operator acting upon the function ψ, then it follows that E is an eigenvalue of the operator $\hat{H}$ with eigenfunction ψ. This is analogous to the eigenvalue and eigenvector problems in the vector spaces considered before. In fact, the whole of quantum mechanics can be reformulated from the continuous functional representation of Schrödinger to a Hilbert vector space formulism that Heisenberg first used where the wave functions become infinite dimensional wave vectors and the Hamiltonian an infinite dimensional matrix.

In special cases where there are only a finite possible number of states for a system such as the 2 spin states for a single fermion, then these wave vectors can be represented as a finite vector. Thus the eigenvectors of the Pauli spin matrices discussed previously actually are the basis wave vectors for the spin state of a single fermion.

For now, we will focus on systems using the Schrödinger formulism. To solve eigenvalue problems of this form results in solving differential equations. The general form of the Hamiltonian for 1D systems is:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{x})$$

From classical mechanics, we recognize this as the total energy of the system. However, the hat designation above the momentum and potential energy now implies that these values are quantum operators. Any physical observable in quantum mechanics is described by an operator. The eigenvalues of that observable on its eigenfunctions are then the measurable values of the state of the system with the eigenfunctions containing the probabilities of observing that value. These operators are all Hermitian if they correspond to a physical quantity.

The following are the basic operators of 1D quantum mechanics:

Position

$$\hat{x} = x$$

Momentum

$$\hat{p}_x = -\frac{i\hbar\partial}{\partial x}$$

Using these and taking the classical observable analogs, a quantum operator can be constructed.

e.g. 1: Uniform Electric Field Hamiltonian

Write the classical form of the Hamiltonian for a charged particle with charge q and mass m in a uniform electric field ϵ in the positive x direction. Then convert this to a quantum operator.

The potential energy of the particle is given as

$$V(x) = -q\epsilon x$$

Thus the classical Hamiltonian is simply:

$$H = \frac{p^2}{2m} - q\epsilon x$$

Converting this to a quantum operator:

$$\hat{H} = \frac{\hat{p}^2}{2m} - q\epsilon\hat{x} = \frac{1}{2m}\left(-\frac{i\hbar\partial}{\partial x}\right)^2 - q\epsilon x = \frac{1}{2m}\left(-\frac{i\hbar\partial}{\partial x}\right)^2 - q\epsilon x$$

$$\therefore \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - q\epsilon x$$

e.g. 2: What are the eigenfunctions for $\hat{p}$ if we call its eigenvalues $\hbar k$.

$$\hat{p}\psi = \hbar k\psi$$

$$-\frac{i\hbar\partial\psi}{\partial x} = \hbar k\psi$$

$$\frac{d\psi}{\psi} = ikdx$$

$$\ln\left(\frac{\psi(x)}{\psi_0}\right) = ikx$$

$$\psi(x) = \psi_0 e^{ikx}$$

are the eigenfunctions of $\hat{p}$.

2. Piecewise Function/Continuity Review

Continuous piecewise functions are defined as follows:

$$f(x) = \begin{cases} f_1(x) & x\epsilon(-\infty, a_1] \\ f_2(x) & x\epsilon[a_1, a_2] \\ \vdots & \vdots \\ f_n(x) & x\epsilon[a_n, \infty) \end{cases}$$

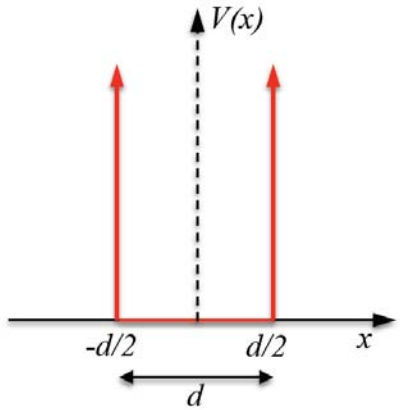
Here we note that the following continuity conditions must be in place for these functions to be piecewise continuous:

$$f_n(a_n) = f_{n+1}(a_n)$$

$$\frac{df_n(a_n)}{dx} = \frac{df_{n+1}(a_n)}{dx}$$

Wave functions must obey the same boundary conditions. Note however that the potential function *V(x)* does not have to be piecewise continuous, just the wave function. There are many problems of interest where $V(x)$ is a piecewise function and not necessarily continuous such as the particle in a 1D box and barrier and potential well problems.

e.g. 3: Particle in a box – symmetric about x-axis



Consider the above system with the piecewise potential energy function $V(x)$ for an electron inside the infinite potential well.

$$V(x) = \begin{cases} \infty & x\epsilon\left(-\infty, -\frac{d}{2}\right) \cup \left(\frac{d}{2}, \infty\right) \\ 0 & x\epsilon\left[-\frac{d}{2}, \frac{d}{2}\right] \end{cases}$$

The wave function is 0 outside the middle region since there is 0 probability of finding the electron in the infinite potential regions.

We write Schrödinger's equation for the middle region.

$$\hat{H}\psi = E\psi$$

$$\frac{\hat{p}^2}{2m}\psi = E\psi \rightarrow \left(\frac{\left(-i\hbar\frac{\partial}{\partial x}\right)^2}{2m}\right)\psi = E\psi$$

$$\therefore \frac{-\hbar^2\frac{\partial^2\psi}{\partial x^2}}{2m} = E\psi$$

The general solution of this equation is:

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

$$\text{with } k^2 = \frac{2mE}{\hbar^2}$$

The boundary conditions (BCs) for this problem are:

$$\psi\left(-\frac{d}{2}\right) = 0 \text{ and } \psi\left(\frac{d}{2}\right) = 0$$

The first BC gives:

$$Ae^{\frac{ikd}{2}} + Be^{-\frac{ikd}{2}} = 0$$

The second BC gives:

$$Ae^{-\frac{ikd}{2}} + Be^{\frac{ikd}{2}} = 0$$

Adding these two equations:

$$A\left(e^{\frac{ikd}{2}} + e^{-\frac{ikd}{2}}\right) + B\left(e^{\frac{ikd}{2}} + e^{-\frac{ikd}{2}}\right) = 0$$

or

$$2A\cos\frac{kd}{2} + 2B\cos\frac{kd}{2} = 0$$

$$2(A+B)\cos\frac{kd}{2} = 0$$

Subtracting the second equation from the first equation:

$$A\left(e^{\frac{ikd}{2}} - e^{-\frac{ikd}{2}}\right) - B\left(e^{\frac{ikd}{2}} - e^{-\frac{ikd}{2}}\right) = 0$$

or

$$2iA\sin\frac{kd}{2} - 2iB\sin\frac{kd}{2} = 0$$

$$2i(A-B)\sin\frac{kd}{2} = 0$$

Thus these equations must simultaneously be true:

$$2(A+B)\cos\frac{kd}{2} = 0$$

$$2(A-B)\sin\frac{kd}{2} = 0$$

If $A = B$:

$$\cos\frac{kd}{2} = 0 \rightarrow kd = n\pi \text{ with } n \text{ odd}$$

If $A = -B$:

$$\sin\frac{kd}{2} = 0 \rightarrow kd = n\pi \text{ with } n \text{ even} > 0$$

Thus the solution to the problem is:

$$\psi_n(x) = \begin{cases} c_{odd}\left(e^{i\frac{n\pi x}{d}} + e^{-i\frac{n\pi x}{d}}\right) \\ c_{even}\left(e^{i\frac{n\pi x}{d}} - e^{-i\frac{n\pi x}{d}}\right) \end{cases} = \begin{matrix} C_{odd}\cos\left(\frac{n\pi x}{d}\right) & n\ odd \\ C_{even}\sin\left(\frac{n\pi x}{d}\right) & n\ even \end{matrix}$$

Such that:

$$C_{odd} = 2c_{odd} \text{ and } C_{even} = 2ic_{even}$$

The constants C and D are found by the normalization condition for the total probability of finding the particle:

$$1 = \int_{-\frac{d}{2}}^{\frac{d}{2}} \psi_n^*(x)\psi_n(x)\,dx = \begin{cases} \int_{-\frac{d}{2}}^{\frac{d}{2}} C_{odd}^2 \cos^2\left(\frac{n\pi x}{d}\right) dx \rightarrow C_{odd} = \sqrt{\frac{2}{d}} \\ \int_{-\frac{d}{2}}^{\frac{d}{2}} C_{even}^2 \sin^2\left(\frac{n\pi x}{d}\right) dx \rightarrow C_{even} = \sqrt{\frac{2}{d}} \end{cases}$$

Therefore:

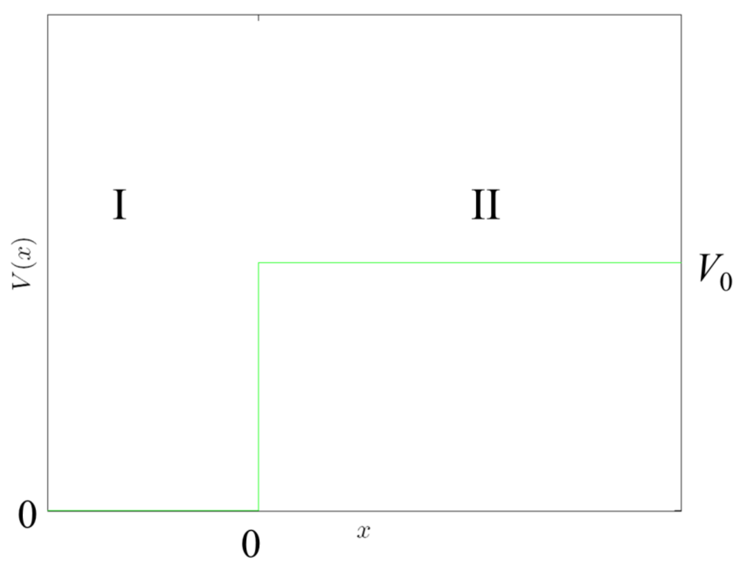
$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{d}}\cos\left(\frac{n\pi x}{d}\right) & n\ odd \\ \sqrt{\frac{2}{d}}\sin\left(\frac{n\pi x}{d}\right) & n\ even \end{cases}$$

The energies of the system are quantized such that:

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2\left(\frac{n\pi}{d}\right)^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2md^2} = \frac{h^2 n^2}{8md^2}$$

e.g. 4: Scattering off a step potential.
Consider the following piecewise potential energy function $V(x)$ for an electron traveling incident from the left side with total energy $E > V_0$.

$$V(x) = \begin{cases} 0 & x\epsilon(-\infty, 0) \\ V_0 & x\epsilon[0, \infty) \end{cases}$$



Find the general form of the wave functions for this potential energy and the transmission and reflections coefficients for the incident electron, *R* and *T*.

First we write Schrödinger's equation in the two regions.

$$\hat{H}\psi = E\psi$$

$$\left(\frac{\hat{p}^2}{2m} + V\right)\psi = E\psi \rightarrow \left(\frac{\left(-i\hbar\frac{\partial}{\partial x}\right)^2}{2m} + V\right)\psi = E\psi$$

In region I:

$V = 0$

$$\therefore \frac{-\hbar^2 \frac{\partial^2 \psi_{\mathrm{I}}}{\partial x^2}}{2m} = E\psi_{\mathrm{I}}$$

In region II:
$V = V_0$

$$\therefore \frac{-\hbar^2 \frac{\partial^2 \psi_{\mathrm{II}}}{\partial x^2}}{2m} + V_0\psi_{\mathrm{II}} = E\psi_{\mathrm{II}}$$

Since the wave function must be piecewise continuous, we have the following boundary conditions (BCs).

BC are $\psi_{\mathrm{I}}(0) = \psi_{\mathrm{II}}(0)$ and $\frac{\partial \psi_{\mathrm{I}}}{\partial x}(0) = \frac{\partial \psi_{\mathrm{II}}}{\partial x}(0)$

Now, to solve these we write the general solutions for the wave function in each region and apply boundary conditions.

Let $k^2 \equiv \frac{2mE}{\hbar^2}$ and $\rho^2 \equiv \frac{2m(E-V_0)}{\hbar^2}$
In region I:
$k^2\psi_{\mathrm{I}} + \frac{\partial^2 \psi_{\mathrm{I}}}{\partial x^2} = 0$ which has solutions of the form $\psi_{\mathrm{I}}(x) = Ae^{ikx} + Be^{-ikx}$
In region II:

$$\rho^2\psi_{\mathrm{II}} + \frac{\partial^2 \psi_{\mathrm{II}}}{\partial x^2} = 0 \text{ which has solutions of the form } \psi_{\mathrm{II}}(x) = Ce^{-i\rho x} + De^{i\rho x}$$

Since the electron is incident from the left, there can never be a rightward propagating wave from the right side.

$$C = 0 \rightarrow \psi_{\mathrm{II}}(x) = De^{i\rho x}$$

The coefficients *R* and *T* are simply related to the coefficients *A*, *B*, and *D* such that *A* corresponds to the incident electron, *B* the reflected electron, and *D* any transmission electron.
The exact correspondence comes from the conservation of the flux of electrons from the left equaling the flux of the electrons on the right.
The probability current/flux is simply the probability amplitudes times the velocity of the electron.

$$v = \frac{p}{m} = \frac{\hbar k}{m}$$

$$F = A^2 v$$

We have 3 probability currents/fluxes, incident, reflected, and transmitted.

$$I + R = T$$

$$A^*A\frac{\hbar k}{m} + B^*B\frac{\hbar k}{m} = D^*D\frac{\hbar \rho}{m}$$

Assuming $I = 1$, we can normalize this current/flux equation by A^*Ak and obtain the following relations for R and T.

We can thus write $R = \frac{B^*B}{A^*A}$ and $T = \frac{D^*D}{A^*A}\frac{\rho}{k}$.

Now, using the boundary conditions:

$$\psi_{\mathrm{I}}(0) = \psi_{\mathrm{II}}(0) \rightarrow Ae^{ik0} + Be^{-ik0} = De^{i\rho 0} \rightarrow A + B = D$$

$$\frac{\partial \psi_{\mathrm{I}}}{\partial x}(0) = \frac{\partial \psi_{\mathrm{II}}}{\partial x}(0) \rightarrow ik(Ae^{ik0} - Be^{-ik0}) = i\rho De^{i\rho 0} \rightarrow A - B = \frac{i\rho}{ik}D$$

Subtracting the second equation from the 1st times $\frac{ik}{i\rho}$ we can find R:

$$\left(1 - \frac{ik}{i\rho}\right)A + \left(1 + \frac{ik}{i\rho}\right)B = 0$$

$$\frac{B}{A} = -\frac{\left(1 - \frac{ik}{i\rho}\right)}{\left(1 + \frac{ik}{i\rho}\right)} = \frac{i\rho - ik}{i\rho + ik} = \frac{\rho - k}{\rho + k}$$

$$R = \frac{B^*B}{A^*A} = \left(\frac{\rho - k}{\rho + k}\right)^2$$

$$R = \left(\frac{\rho - k}{\rho + k}\right)^2$$

$$R = \frac{\frac{2m(E - V_0)}{\hbar^2} - 2\frac{2m\sqrt{E(E - V_0)}}{\hbar^2} + \frac{2mE}{\hbar^2}}{\frac{2m(E - V_0)}{\hbar^2} + 2\frac{2m\sqrt{E(E - V_0)}}{\hbar^2} + \frac{2mE}{\hbar^2}}$$

$$\therefore R = \frac{(E - V_0) - \sqrt{E(E - V_0)} + E}{(E - V_0) + \sqrt{E(E - V_0)} + E}$$

Adding the two equations we can find T:

$$2A = \left(1 + \frac{i\rho}{ik}\right)D$$

$$\frac{D}{A} = \frac{2}{\left(1 + \frac{i\rho}{ik}\right)} = \frac{2ik}{(ik + i\rho)} = \frac{2k}{k + \rho}$$

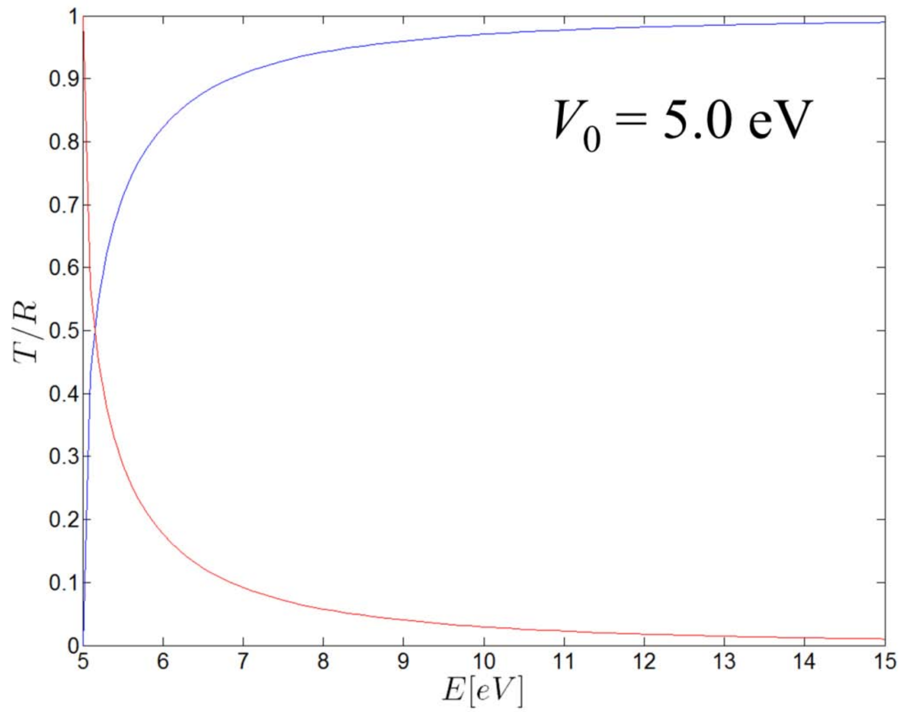
$$T = \frac{D^*D}{A^*A}\frac{\rho}{k} = \left(\frac{2k}{k + \rho}\right)^2\frac{\rho}{k} = \left(\frac{4\rho k}{(k + \rho)^2}\right)$$

$$T = \left(\frac{4\frac{2m\sqrt{E(E - V_0)}}{\hbar^2}}{\frac{2m(E - V_0)}{\hbar^2} + 2\frac{2m\sqrt{E(E - V_0)}}{\hbar^2} + \frac{2mE}{\hbar^2}}\right)$$

$$\therefore T = \frac{4\sqrt{E(E - V_0)}}{(E - V_0) + \sqrt{E(E - V_0)} + E}$$

Note that classically a particle would always reflect, but here there is a finite probability of transmission.

Plotting R (red) and T (blue) versus E.



For the case $E < V_0$, $i\rho$ becomes real, so let $i\rho = \alpha$.

$$\frac{B}{A} = \frac{\alpha - ik}{\alpha + ik}$$

$$R = \frac{B^*B}{A^*A} = \left(\frac{\alpha + ik}{\alpha - ik}\right)\left(\frac{\alpha - ik}{\alpha + ik}\right) = \frac{\alpha^2 + k^2}{\alpha^2 + k^2} = 1$$

For this case, the entire wave is reflected, analogous to the classical case. The wave function in region II is a decaying exponential, which is not classical. This implies even though electrons are reflected if their energy is lower than the barrier potential, they have a finite probability of penetrating the step barrier before being reflected.

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