6.007 – Electromagnetic Energy: From Motors to Lasers
Spring 2011

Tutorial 10: Quantum Mechanics in 1-D Potentials

Quantum mechanical model of the universe, allows us describe atomic scale behavior with great accuracy—but in a way much divorced from our perception of everyday reality. Are photons, electrons, atoms best described as particles or waves? Simultaneous wave-particle description might be the most accurate interpretation, which leads us to develop a mathematical abstraction.

1 Rules for 1-D Quantum Mechanics

Our mathematical abstraction of choice is the wave function, sometimes denoted as ψ, and it allows us to predict the statistical outcomes of experiments (i.e., the outcomes of our measurements) according to a few rules

1. At any given time, the state of a physical system is represented by a wave function $\psi(x)$, which—for our purposes—is a complex, scalar function dependent on position. The quantity $\rho(x) = \psi^*(x)\psi(x)$ is a probability density function. Furthermore, ψ is complete, and tells us everything there is to know about the particle.

2. Every measurable attribute of a physical system is represented by an operator that acts on the wave function. In 6.007, we're largely interested in position ($\hat{x}$) and momentum ($\hat{p}$) which have operator representations in the x-dimension

$$\hat{x} \to x \qquad \hat{p} \to \frac{\hbar}{i}\frac{\partial}{\partial x}. \tag{1}$$

Outcomes of measurements are described by the expectation values of the operator

$$\langle \hat{x} \rangle = \int dx\, \psi^* x \psi \qquad \langle \hat{p} \rangle = \int dx\, \psi^* \frac{\hbar}{i}\frac{\partial \psi}{\partial x}. \tag{2}$$

In general, any dynamical variable Q can be expressed as a function of x and p, and we can find the expectation value of

$$\langle Q(x,p) \rangle = \int dx\, \psi^* Q\left(x, \frac{h}{i}\frac{\partial}{\partial x}\right)\psi. \tag{3}$$

3. The time evolution of the wave function is described by the Schrodinger wave equation, a partial differential equation that is fundamentally a statement of energy conservation:

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

$$= -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(\hat{x})\psi. \tag{4}$$

The operator acting on ψ on the right is called the Hamiltonian. Fixed energy solutions—eigenstates—of this equation are called stationary states (because they don't evolve in time), and are found by solving the "time-independent" Schrodinger wave equation:

$$E\psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(\hat{x})\psi. \tag{5}$$

2   Heisenberg Uncertainty and Photons

In lecture, our characterization of measurement uncertainty dealt with the observation of electrons with photons of definite energy and momentum

$$E = \hbar\omega \qquad p = \hbar k = \frac{2\pi\hbar}{\lambda}. \tag{6}$$

The Heisenberg microscope shows that it's difficult to *simultaneously* know the position and momentum of observed electrons with great precision:

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \tag{7}$$

From basic probability theory, it can be shown that the uncertainty in x is given by,

$$\langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 = \int dx \psi^* x^2 \psi - (\int dx \psi^* x \psi)^2. \tag{8}$$

2.1   Infinite Square-Well

Using the tools of quantum mechanics we can numerically solve for energy levels of an electron trapped in a potential well of any arbitrary shape. However, if instead of using numerical methods and a computer, we want to calculate the solutions to the Schrodinger equation analytically, we will find that very few potential shapes are exactly-analytically-solvable in quantum mechanics. One of the exactly-solvable problems is that of an infinitely tall square potential for which we can calculate energy eigenstates of an electron trapped within such well. Here are the solutions you will find:

1. Solutions to 1-D Schrodinger equation are eigenstates given by wavefinctions

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin(k_n x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right) \tag{9}$$

   with associated energies

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mL^2}. \tag{10}$$

   Note that these are called energy eigenstates because they were states of definite energy, meaning that $\Delta E = 0$.

2. The eigenstates are alternately even and odd with respect to the center of the well.

3. The eigenstates are mutually orthogonal, meaning that

$$\int \psi_m^* (x) \, \psi_n (x) = \delta_{mn}, \tag{11}$$

where δ_{mn} is 0 if $m \neq n$, and 1 if $m = n$. For calculating expectation values for the infinite square well where $m = n$, the following identity will be useful:

$$\sin^2 (\theta) = \frac{1}{2} \left[1 - \cos (2\theta) \right]. \tag{12}$$

3   Qualitative Properties of Wave Functions

When we are only interested in qualitative behavior of the wave function then we can sketch expected wave functions for different energy levels following some simple rules:

1. Outside of the potential well we expect the wave function to decay smoothly to zero. The larger the difference between the potential V and the particle energy E, the faster we expect the wave function to decay. If the potential V at the boundary is infinite, then the wave function will go to zero right at the boundary.

2. Inside the potential well, we expect the wave function to behave roughly like a sine or cosine function.

3. We expect any symmetry in the potential well to be reflected in the wave function. If we identify a point of symmetry in the potential, then the wave function should be either an even or odd function about that point.

4. The number of nodes in the wave function for a state should be the state number (n) minus 1 ($n = 1$ for ground state, 2 for first excited state, and so on).

5. The curvature of the wave function is related to the kinetic energy of the state. If the well has a potential that varies with position, then in regions with higher kinetic energy the wave function should have a shorter "wavelength".

6. If the well has a potential that varies with position, the particle will spend less time in regions where it has higher potential energy so the wave function will be (relatively) smaller in those regions.

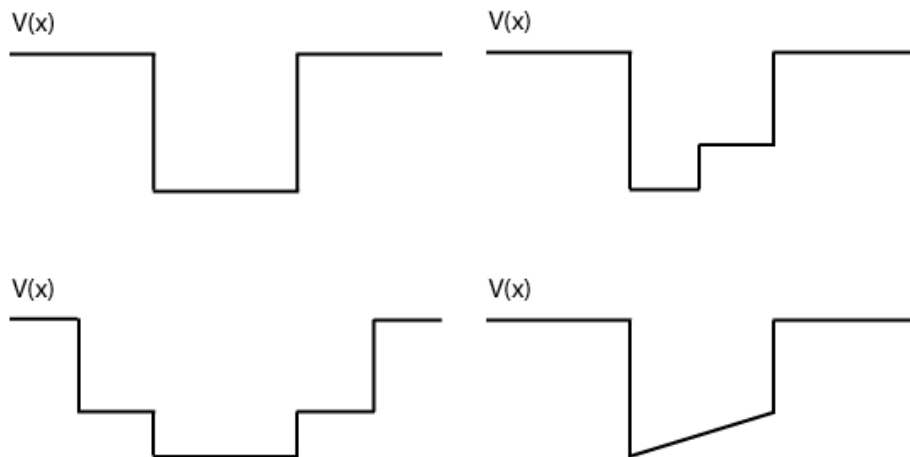**Example** 1: **Mystery Wave Function**

Consider the wave function

$$\psi(x,t) = Ae^{-\lambda|x|}e^{-i\omega t}, \tag{13}$$

where A, λ, and ω are positive, real constants.

1. Normalize ψ.

2. Determine the expectation values of x and x^2.

3. Find the standard deviation of x. Sketch the graph of $|\psi|^2$, as a function of x, and mark the points $\langle x \rangle + \sigma$ and $\langle x \rangle - \sigma$ to illustrate the sense in which σ represents the 'spread' in x. What is the probability that the particle would be found outside this range?

Example 2: **Qualitative Wave Functions**

Using the rules from "Qualitative Properties of Wave Functions", sketch the wave function for the first several energy states for the following potential wells.

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