MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Department of Electrical Engineering and Computer Science
Department of Mechanical Engineering

| 6.050J/2.110J | **Information and Entropy** | Spring 2003 |

Issued: April 11, 2003   **Problem Set 9**   Due: April 18, 2003

Note: The **quiz** will be held Thursday, April 24, 2003, 12:00 noon - 1:00 PM. The quiz will be **closed book** except that you may bring one sheet of 8 1/2 x 11 inch paper with notes on both sides. Calculators will not be necessary but you may bring one if you wish. Material through the end of Problem Set 8 may be covered on the quiz.

Problem 1: Well, Well, Well

Generally it is impossible to express in closed form a wave function that obeys the Schrödinger equation. However, in a few very simple cases this can be done. One such case is the infinitely deep potential well (an area of space where the potential is low compared with the surrounding region). In this problem you will find the energy levels and stationary states of an object in a one-dimensional potential well.

In Chapter 11 of the notes, the wave function of an object was assumed to depend on three spacial dimensions as well as time. For simplicity here, we will consider the case where it only depends on only one spacial variable, x. Thus $\psi = \psi(x, t)$. The Schrödinger equation obeyed by this wave function is then

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \qquad (9\text{--}1)$$

where i is the (imaginary) square root of -1, m is the mass of this object, $V(x)$ is the potential energy function, whose spacial gradient is the negative of the force on the object, and $\hbar = h/2\pi = 1.054 \times 10^{-34}$ Joule-seconds.

You will solve this equation for a particular potential function $V(x)$, namely one that is 0 Joules between $x = -L$ and $x = 0$ meters, and infinitely high outside this range. The well has walls that prevent the object from penetrating the region outside the well. You can think of them as physical walls in a gravitational field, or non-conducting walls in the case of charged particles.
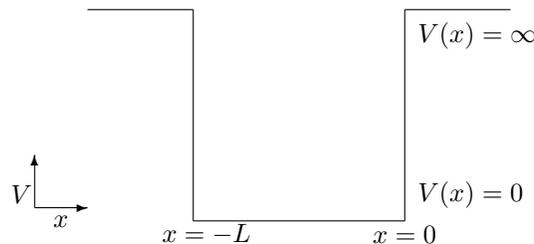

Figure 9–1: Infinite square well

If you are uncomfortable with the notion of infinity, you can think of this potential well as being of a finite but large depth, where the depth is much larger than any of the other energies encountered in the problem.

If you think of an everyday object in such a well, there is no reason it cannot simply sit still on the bottom of the well. On the other hand, it might continually bounce back and forth between the walls, in which case it would have some kinetic energy. In fact, any (nonnegative) amount of energy would lead to a possible situation.

Things are different in the quantum world. There is a minimum amount of energy, not zero, implied by the Schrödinger equation (this is known as the "ground state energy"). Also, only for discrete values of energy is a wave function possible.

First, consider the region outside the well. Since $V(x)$ is infinite there, the only way the Schrödinger equation can be obeyed is if $\psi(x,t) = 0$ there. Since $\psi(x,t)$ is a continuous function of x, it must therefore be zero at the edges of the well. Thus $\psi(-L,t) = 0$ and $\psi(0,t) = 0$. These two equation will serve as boundary conditions for the wave functions you will calculate.

Next, consider the region inside the well, i.e., for $-L \le x \le 0$.

a. Write the one-dimensional Schrödinger equation in the well.

Next, to calculate the stationary states, assume that the wave function is a product of a function of time $f(t)$ and another function of space $\phi(x)$. Then the Schrödinger equation becomes

$$i\hbar\phi(x)\left(\frac{df(t)}{dt}\right) = -\left(\frac{\hbar^2}{2m}\right)f(t)\left(\frac{d^2\phi(x)}{dx^2}\right) \qquad (9\text{--}2)$$

where the partial derivatives have become normal derivatives.

Consider first the time function $f(t)$. This does not depend on x. For any value of x this equation is a first-order linear differential equation and the most general solution is an exponential, e raised to the power of some constant times time t. For convenience we will say this constant is $-iE/\hbar$ (because of this definition E has the dimensions of energy, and we will interpret it as the energy of the state calculated). Thus

$$f(t) = \exp\left(\frac{-iEt}{\hbar}\right) \qquad (9\text{--}3)$$

b. The constant E can be real, imaginary, or complex and still be consistent with the Schrödinger equation. However, we will consider only real values. Why? What problem is caused if E is not real? Hint: what happens as t approaches infinity?

c. Substitute $f(t)$ in the Schrödinger equation and eliminate $f(t)$. Write the resulting second-order differential equation for the space function $\phi(x)$.

The next step is to solve this equation for $\phi(x)$ subject to the boundary conditions

$$\phi(-L) = \phi(0) = 0 \qquad (9\text{--}4)$$

The general solution to this equation has the form

$$\phi(x) = a\sin(kx) + b\cos(kx) \qquad (9\text{--}5)$$

where the constants a, b, and k may be complex.

d. Substitute this form into the equation for $\phi(x)$ and deduce the relationship between k and E.

e. What can you determine from the boundary conditions about a and b?

f. Use the boundary conditions to determine possible values for k. Hint: $\sin(j\pi) = 0$ for integers j.

Each of the possible values of k and the associated value for E corresponds to one of the stationary states. For $j = 0$ the wave function is zero so it does not represent an object. The wave functions for positive and negative j have the same shape so only one need be considered. Therefore the stationary states can be indexed by j starting with $j = 1$.

g. Using j as an index over the stationary states, find the energy of that state (call it e_j).

h. Find the stationary state wave function $\phi_j(x)$ of that state (do not worry about normalizing the wave function).

i. The stationary state with the lowest energy is known as the "ground state." What is its energy as a function of $\hbar$, m, and L?

j. The stationary state with the second lowest energy is known as the "first excited state." What is its energy as a function of $\hbar$, m, and L?

k. Find the value of the ground-state energy of an object with the mass of an electron (9.109×10^{-31} kilograms) confined in a one-dimensional potential well of width 20 nanometers (2×10^{-8} meters) in Joules.

l. Express this ground-state energy in electron-volts (1 eV= 1.602×10^{-19} Joules).

Turning in Your Solutions

You may turn in this problem set by e-mailing your written solutions, M-files, and diary. Do this either by attaching them to the e-mail as *text* files, or by pasting their content directly into the body of the e-mail (if you do the latter, please indicate clearly where each file begins and ends). If you have figures or diagrams you may include them as graphics files (GIF, JPG or PDF preferred) attached to your email.
The deadline for submission is the same no matter which option you choose.

Your solutions are due 5:00 PM on Friday, April 18, 2003. Later that day, solutions will be posted on the course website.

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