Massachusetts Institute of Technology
Department of Electrical Engineering and Computer Science
Department of Mechanical Engineering

6.050J/2.110J **Information and Entropy** **Spring 2006**

Issued: April 25, 2006

Problem Set 10

Due: April 28, 2006

Note: This problem set is substantially the same as ones used in earlier years. There are so few geometries for which the Schrödinger equation can be solved that it is impossible to create a new problem every year. Please do not refer to the solutions from previous years because if you do you will not learn anything from this problem set.

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

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \qquad (10\text{–}1)$$

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 $x = -L/2$ and $x = L/2$ 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.

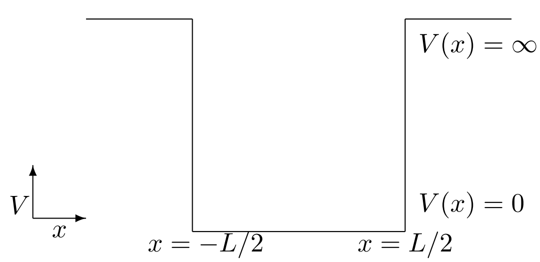

Figure 10–1: Infinite square well

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 $\psi(-L/2,t) = 0$ and $\psi(L/2,t) = 0$. These two equations will serve as boundary conditions for the wave functions you will calculate.

Next, consider the region inside the well, i.e., for $-L/2 \leq x \leq L/2$.

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

$$i\hbar\phi(x)\left(\frac{df(t)}{dt}\right) = -\left(\frac{\hbar^2}{2m}\right)f(t)\left(\frac{d^2\phi(x)}{dx^2}\right) \tag{10–2}$$

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

$$f(t) = e^{-iEt/\hbar} \tag{10–3}$$

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

$$\phi(-L/2) = \phi(L/2) = 0 \tag{10–4}$$

The general solution to this equation is the sum of terms like[5]

$$\phi(x) = a\sin(kx) + b\cos(kx) \tag{10–5}$$

where the constants a, b, and k may be complex. Consider one such term.

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 values of k for which a or b could be nonzero. Hint: $\cos(z) = 0$ only for $z = (\pi/2)(2j+1)$ and $\sin(z) = 0$ only for $z = (\pi/2)(2j)$ for integers j, so it is convenient to associate each of the possible values of k with an integer j.

[5] It may not be obvious why solutions have this form. The reason is that sin and cos are the functions that resemble their second derivatives.

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 positive integers 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 15 nanometers (15×10^{-9} meters) in Joules.

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

Problem 2: As time goes by... (Extra Credit)

Schrödinger's equation tells us about the dynamics of a particle. The particle is represented by a complex function of time and space, $\psi(x,t)$, the famous wave function. The name of wave function is due to the resemblance that Schrödinger pointed out between the equation that bears his name and the wave equation. In the probabilistic interpretation of quantum mechanics wave functions act as "pre-probabilities", because squaring them yields a probability distribution $p(x,t)$ of where to find the particle at a given time[6]. That is $\psi(x,t)^*\psi(x,t) = p(x,t)$. In this problem you will derive the form of the dependence of the wave functions with time, in the case of a stationary solution (how come a stationary solution depends on time?,... well, stationary does not mean static, but wait and see for yourself).

Consider the probability distribution $p(x,t)$ as a starting point

a. Assume that time and space are independent random variables, and recall the form their joint probability distribution $p(x,t)$ takes under this assumption from Chapter 5.

   Really we are interested in stationary solutions so we expect that $p(x,t) = p(x)$. This means that after squaring, the dependence with time of the wave function $\psi(x,t)$ will become 1.

b. Rewrite the joint probability distribution in terms of wave functions $f(t)$ and $\phi(t)$. Also, express the condition $f(t)$ must meet to force the solution to be stationary.*(HINT: you should get something that allows you to separate $\psi(x,t) = f(t)\phi(x)$. Remember that $f(t)$ and $\phi(t)$ are complex functions)*

In equation 10–2 we already introduced the idea of considering a form of solution to Schrödinger's equation that would be the product of a function of time and a function of position. We can rearrange equation 10–2 by putting all the functions depending on time to the left and the functions depending on space to the right, we will get

$$i\hbar \frac{1}{f(t)} \left(\frac{df(t)}{dt} \right) = - \left(\frac{\hbar^2}{2m} \right) \frac{1}{\phi(x)} \left(\frac{d^2\phi(x)}{dx^2} \right) \tag{10–1}$$

[6]despite the notation similarity interpreting $p(x,t)$ as a joint probability distribution requires some subtle clarifications about the meaning of a probability distribution over time

What we just did is a common strategy to solve some partial differential equations, it is referred to as "separation of variables"; in our case we justified using this strategy when we said we were going to search for stationary solutions. The result is a function of time on the left hand side, and a function of space on the right hand side. In general the only way that two such functions can be equal is if they are both constant.[7]

c. Take the left hand side of equation 10–1, and equal it to a constant, let us call it C for the moment. Using the replacement $y = \ln(f(t))$, simplify the equation.[8] *(HINT: you should get $dy/dt = -iC/\hbar$)*

d. The result of the previous part can be integrated easily, the result is $y = -iCt/\hbar$. Undo the replacement of $y = lnf(t)$ and get an expression for $f(t)$.

e. What are the units of C? Compare your result with equation 10–3

f. To be mathematically rigorous. You should verify one more thing, that the function $f(t)$ you obtained allows you to reach equation 10–1. Why? What would you do to verify it? (we do not actually ask you to do the verification, just to tell us what needs to be verified)

g. So, how come a stationary solution depends on time?

The procedure you just followed may seem cumbersome at first, but is worth taking the time to understand it because you will see it appear in a rich variety of different contexts.

Turning in Your Solutions

You may turn in this problem set by e-mailing your written solutions, M-files, and diary to 6.050-submit@mit.edu. 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. Alternatively, you may turn in your solutions on paper in room 38-344. The deadline for submission is the same no matter which option you choose.

Your solutions are due 5:00 PM on Friday, April 28, 2006. Later that day, solutions will be posted on the course website.

[7] This is a subtle point. Think of a function that depends only on time ($f(t)$), how could it be equal to another function that depends only on space ($g(x)$)? Well, right now $f(now)$ takes one and only one definite value, if $f(now)$ ought to be equal to all of $g(x)$, $g(x)$ better take the same value for all x. But even if they are the same now, one instant from now the value of $f(now + 1\, instant)$ will presumably differ from $f(now)$, yet $g(x)$ will remain the same, so they will not be the same anymore! Unless, of course, f does not change either.

[8] remember that the derivative of the natural logarithm is $\frac{dln(\theta)}{d\theta} = \frac{1}{\theta}$