Massachusetts Institute of Technology

Department of Physics

Physics 8.04 April 6, 1996

Quantum Physics I, Spring 1996

Agenda and **readings** for the week of April 2:

(Note: The abbreviations for the readings are RH = *Resnick and Halliday*, K = *Kroemer*, FT = *French and Taylor*, CN = class notes given out after lecture (also appears on web after lecture).)

- L15 04/09: (1/2) Finite Square Well (with all the rules and lessons and computer demo)
- L16 04/11: (1/2) Finite Square Well, $\delta-$function potential, Transfer Matrix method (if time permits).

Problem Set 7

(Due Friday, April 12 at 5:00 pm sharp.)

Work requested of the students is highlighted by either a question mark (?) or underlining.

1 Computer Assignment # 1

Log into Athena, execute the following commands at the "athena%" prompt, and then follow the instructions given.

athena% add 8.04
athena% solver

2 States, Measurements and Operators

Background: The mathematical theory of wavefunctions and operators which we have built from the de Broglie hypothesis allows us to make very detailed predictions about the results of experiments. This problem takes you through such an example and gives an opportunity to practice applying the operator and wavefunction concepts discussed in lecture.

The *preparation* for our experiments will be to begin with a random collection of systems consisting each of a particle of mass m placed in a box (infinite square well) of width L. The energy of each of systems is measured, those systems which do *not* yield an energy of $E_* = \frac{2\hbar^2\pi^2}{mL^2}$ are immediately *rejected*. Only systems whose energy was measured to be E_* will be used in our experiments. Consider *only* these systems for the questions below.

Assignment:

2.1 Specify the quantum state

What is the wavefunction $\Phi(x)$ for the systems which we use in our experiments?

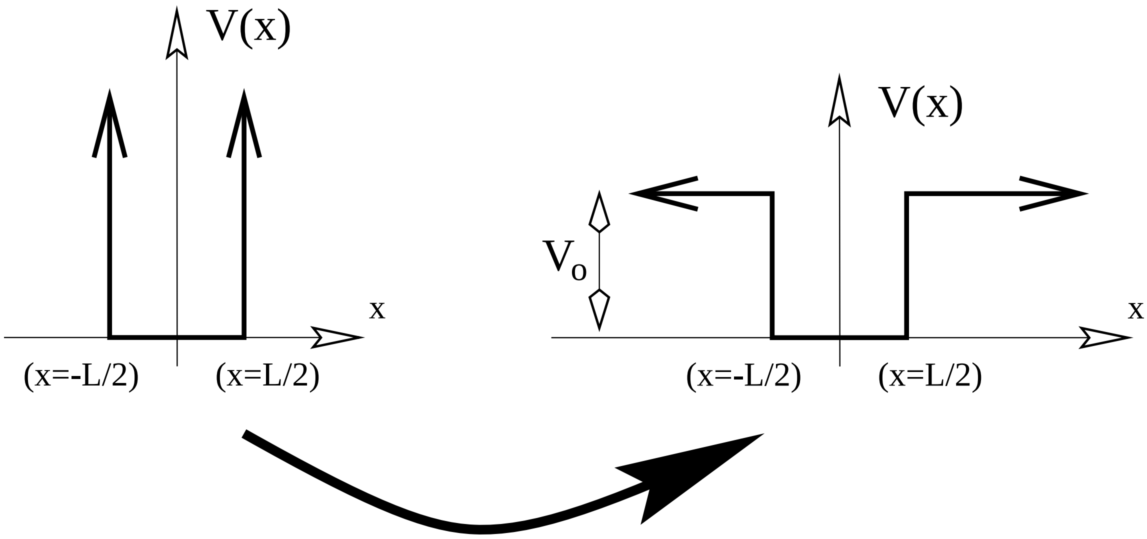

Figure 1: "Box" (Infinite Square Well) partially opening into a Finite Square Well

2.2 Operators and Purity

Compute

$\hat{x}\Phi(x)$, $\hat{p}\Phi(x)$, and $\hat{H}\Phi(x)$. Looking at your results, for which of these observables to you expect measurements on the systems to always yield the same result? In those cases, what value to you expect to always get? Explain.

2.3 Averages of the distributions

Predict what will be the *average* measured value of the position $< x >$, momentum $< p >$ and energy $< H >$.

2.4 Detailed distributions

Give both expressions and sketches of the probability distribution for measurements of the energy $P(E_n)$, position $\mathcal{P}(x)$, and momentum $\tilde{\mathcal{P}}(k)$.

2.5 Releasing the particles

An new kind of experiment is performed, where now the edges of the box are partially opened, forming the *Finite* Square Well shown in Figure 1, where $V_0 = \frac{\hbar^2\pi^2}{4ML^2}$. In what fraction of such experiments can we expect the particles to remain in the box?

Hints: You may assume that the box is opened so quickly that, during the opening process, the particle does not have time to change its state appreciably. There is only one bound state in this finite square well, and the energy of that state E_0 may be found exactly. Finally, because there is only one bound state, observing the particle remaining in the box is equivalent to measuring its energy as E_0.

2.6 Necessity of wavefunctions in Quantum Mechanics

Construct a state which a) yields the same distribution for the observable x as does $\Phi(x)$ but b) is a different state. Justify you example.

3 The Energy Representation: Eigenstate Expansions

Background: In lecture we explored the representations for quantum state of the system corresponding to the observables of position x and momentum p. We used these representations to derive the forms for operators for position and momentum in both the position and momentum representations. There are more than these two representations for a quantum state. By the quantum principle of superposition, we expect there to be a representation for each physical observable. The observable of energy is no exception to this. In this problem, you will practice the skills developed in lecture for dealing with different representation, but now in a new context.

You will also find that the energy representation is useful for proving many theorems about the time development of quantum states. This is a result of the close relationship between energy and time.

This problem will discuss both general considerations and a specific example. For the general considerations in this problem, we begin by using the principle of superposition to write any quantum state, $\Psi(x)$ or $\Phi(x)$, in terms of the pure states of energy as

$$\Psi(x,t) = \sum_{n=0}^{\infty} c_n \psi_n(x)$$

$$\Phi(x,t) = \sum_{n=0}^{\infty} d_n \psi_n(x).$$

Here, the pure states $\psi_n(x)$ are given by $\hat{H}\psi_n(x) = E_n\psi_n(x)$ and are properly normalized so that $(\psi_n, \psi_m) = \delta_{nm}$.

For the specific considerations, we use use the energy states of the Infinite Square Well of length L, which are given by

$$\theta_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right); \quad n = 1, 2, ...,$$

with energies

$$E_n = \frac{\hbar^2\pi^2}{2mL^2} n^2,$$

where here the Hamiltonian operator is just $\hat{H} = -(\hbar^2/(2m))\partial_x^2$. At times we will also use the (properly normalized) wavefunction

$$\Theta(x) = \sqrt{12/L^3} \begin{cases} x & 0 < x < L/2 \\ 1/2 - x & L/2 < x < L \\ 0 & \text{otherwise} \end{cases}$$

Assignment:

3.1 Orthogonality Condition

3.1.1 General Case

Review how we know $(\psi_n, \psi_m) = 0$ for $n \neq m$.

Hint: Use the defining equation $\hat{H}\psi_n(x) = E_n\psi_n(x)$ for the ψ_n and the Hermiticity of $\hat{H}$.

3.1.2 Specific Case

Verify that the states $\theta_n(x)$ obey $(\theta_n, \theta_m) = \delta_{nm}$.

3.2 Parseval's Theorem

3.2.1 General Case

When we developed the momentum and position representations, we stressed that Parseval's theorem must hold. This is the case for the energy representation, so long as we define as discrete version of the Hermitian inner product as $(c, d) \equiv \sum_n c_n^* d_n$. Prove that with this definition,

$$(c, d) = (\Psi, \Phi).$$

Explain, in terms of probability, why it must be the case that always $(c, c) = (\Psi, \Psi)$.

3.2.2 Specific Case

Show that $\Theta(x)$ may be written as

$$\sum_{\ell=0}^{\infty} (-1)^\ell \sqrt{\frac{96}{\pi^4}} \frac{1}{(2\ell+1)^2} \theta_{2\ell+1}(x),$$

and verify that $\sum_n |c_n|^2$ has the result which you expect.

Hint: You may find the result $1 + 1/3^4 + 1/5^4 + 1/7^4 + \ldots = \pi^4/96$ useful.

3.3 Energy operator

3.3.1 General Case

Using our general procedure for deriving operators, begin with the definition

$$< E >= \sum_n E_n P(E_n),$$

where $P(E_n)$ is the probability of measuring energy E_n, and show that one obtains the same result from

$$< E >= (\Psi, \hat{H}\Psi).$$

This shows that the energy operator is indeed $\hat{H}$.

3.3.2 Specific Case

Verify your result by computing the energy of $\Theta(x)$ both directly from

$$\sum_n E_n P(E_n)$$

and using the operator expression $\int \psi^*(x) \hat{H} \psi(x)\, dx$.

Hints: You may find the result $1 + 1/3^2 + 1/5^2 + 1/7^2 + \ldots = \pi^2/8$ useful. Also, you will find dealing with the discontinuities in $\Theta(x)$ more easy if you first integrate by parts to show $-\int \psi^*(x) \partial_x^2 \psi(x)\, dx = \int |\partial_x \psi(x)|^2\, dx$.

3.4 General Solutions of the Time Dependent Schrödinger Equation (TDSE)

3.4.1 General Case

Show that

$$\Psi(x,t) = \sum_{n=0}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}, \tag{1}$$

satisfies the TDSE.

Background: This expansion is very useful, because it allows us to write down the form of the most general solution to the TDSE, making it simple to prove statements about how quantum states change with time.

3.4.2 Specific Case

If our Infinite Square Well system is initially in state $\Theta(x)$ at time $t_0 = 0$, write down the state of the system (if undisturbed by external influences) at time $t > t_0$.

Hint: You may leave the result as an infinite sum; you need not try to evaluate the sum.

3.5 Conservation of Energy

Use the expansion Eq. (1) to show that the average energy $< E >$ associated with a wavefunction $\Psi(x,t)$ does not vary with time.

4 Solutions of the Time Independent Schrödinger Equation (TISE)

Background: While, as in Problem 3, many general facts may be derived from the eigenstate expansion, to answer specific questions we need the solutions to the TISE. This problem develops that skill.

This problem will center on the solutions to various limits of the potential sketched in Figure 2.

4.1 Wavefunctions of the Even States

Show that to be consistent with the boundary conditions at $\pm\infty$ and the additional constraint that the wavefunction is an even function of x, that the *most general* acceptable solution of the TISE must be of the form,

$$\psi(x) = \begin{cases} Ae^{\kappa_1(x+2a)} & \text{if } x < -2a, \text{ Region I} \\ B\cos(k(x+a)) + B'\sin(k(x+a)) & \text{if } -2a < x < -a, \text{ Region II} \\ C\cosh(\kappa_2 x)) & \text{if } -a < x < a, \text{ Region III} \\ B\cos(k(x-a)) - B'\sin(k(x-a)) & \text{if } a < x < 2a, \text{ Region IV} \\ Ae^{-\kappa_1(x-2a)} & \text{if } 2a < x, \text{ Region V} \end{cases} . \tag{2}$$

Be sure to verify that this form satisfies the TISE in each region and that is is the *only one* consistent with the boundary conditions and symmetry. Give the appropriate values for κ_1, κ_2 and k in terms of V_0, V_1, $\hbar$, m and E.

Hint: You may find a sketch of the wavefunctions to be useful in your thinking.

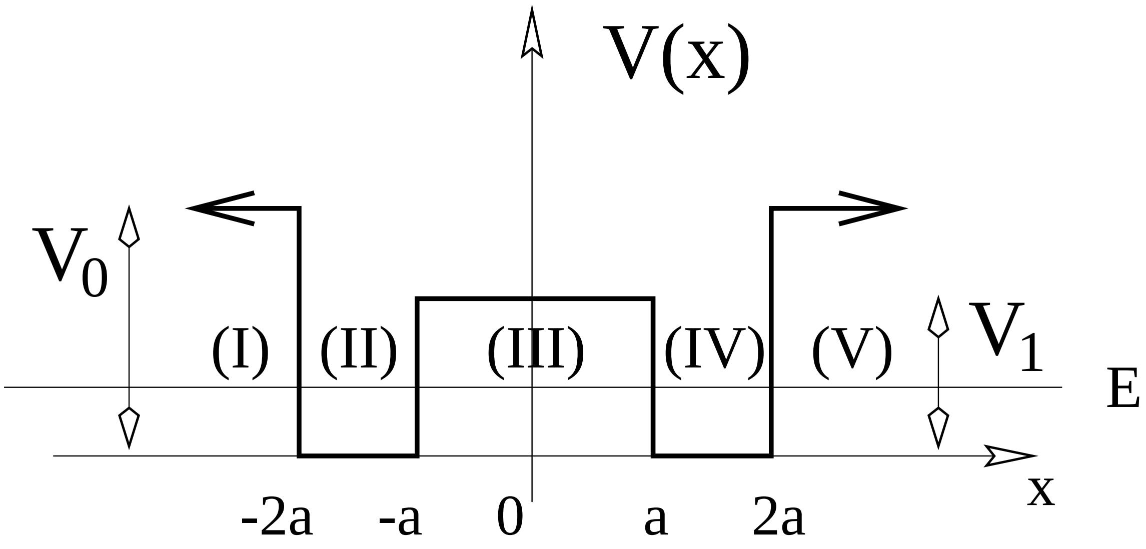

Figure 2: "Bumpy" Finite Square Well Potential

4.2 Eigenenergies of the Even States

Use the matching boundary conditions at $x = -2a, -a, a, 2a$ to derive the transcendental equation which the eigenenergies E must satisfy in terms of only the parameters given in the figure and $\hbar$. You may use intermediate variables such as κ_1 to reduce your writing as long as you express them in terms of the allowed variables.

Warning: Do not attempt to solve this equation, not even graphically!

4.3 Limit of an infinite "bump"

What does your condition on E become in the limit $V_1 \to \infty$? Show that your result is the same as for the *odd states* of a finite square well of width $2a$ and depth V_0.

4.4 States with zero curvature

For a given value of V_0, how large can the bump V_1 be and still allow states with $E < V_1$.

Hint: Find the value of V_1 where $E_0 = V_1$. After making a sketch of this wavefunction, you should be able to write down a transcendental equation which you can solve graphically.

4.5 Limit of infinite walls

First, reproduce the wavefunction and condition for eigenenergies as in Eq. (2), but for the case where $E > V_1$. (**Hint:** If you are good with complex trigonometry, you can save yourself some effort by noting what happens when you define $k_2 = i\kappa_2$.)

Now, what does your condition on E become in the limit $V_0 \to \infty$? Show that as the quantum number $n \to \infty$, the energies you find are higher than the corresponding infinite square well energies by $V_1/2$.

Hint: You may find a graphical solution useful.

4.6 Odd states

Produce the condition on the eigenenergies for *odd solutions* of the well, in both cases, where $E > V_1$ and where $E < V_1$.