6.728 Applied Quantum and Statistical Physics

Department of Electrical Engineering and Computer Science Massachusetts Institute of Technology

PROBLEM SET 4

<u>Issued:</u> 9-26-02

Due: 10-02-02, in-class

Problem 4.1 Heisenberg Uncertainty

This problem explores the use of the Heisenberg Uncertainty Relation to make estimates of the ground state behavior of two quantum mechanical systems. In the parts below, assume that the Heisenberg Relation is actually an equality:

$$\Delta x \, \Delta p \equiv \frac{\hbar}{2}$$

We expect that in most systems it will not turn out to be an equality; however, it is useful as an estimate of ground state behavior. Later, when we study the closed form solutions of these potentials, we can compare the full solution with what we obtain from Heisenberg.

(a) Assume a quadratic potential energy V(x) for a particle of mass m:

$$V(x) = \frac{1}{2}Kx^2$$

First write out the expression for the total energy of the particle.

- i) Describe the lowest energy state as available to the particle in classical mechanics. Describe the lowest energy state in quantum mechanics.
- ii) Given that the particle has position uncertainty, Δx , and momentum uncertainty, Δp , find the value of Δx that corresponds to the ground state (lowest energy state).
- iii) What is the value of the ground state energy?

(b) Repeat for a potential of the form:

$$V(x) = \frac{1}{6}\widetilde{K}x^4$$

Problem 4.2 Potential Well

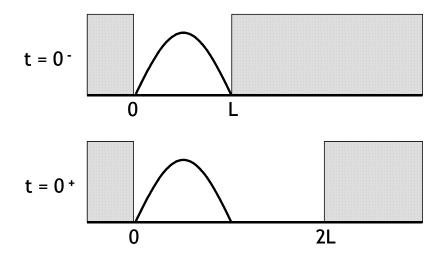
An electron is initially in the ground state of a square well potential of width L as shown in the figure below. The ground state wavefunction in this case is

$$\psi(x,0) = \begin{cases} 0 & \text{for } x < 0\\ \sqrt{\frac{2}{L}} \sin(\pi x / L) & \text{for } 0 \le x \le L\\ 0 & \text{for } x > L \end{cases}$$

The initial energy of the particle is

$$E = \frac{\hbar^2 \pi^2}{2mL^2}$$

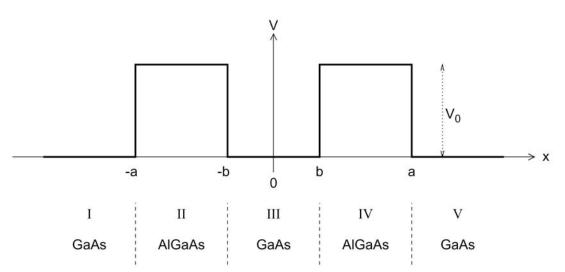
At $t = 0^+$, the right wall of the square is suddenly (and instantaneously) moved to x = 2L. During this event the wavefunction does not have time to change (see the figure).



- (a) What are the eigenfunctions and bound state energies of the new well configuration?
- (b) Is the energy $\langle \hat{H} \rangle$ conserved during this time (from $t = 0^-$ to $t = 0^+$)?
- (c) Construct a solution for t > 0 in terms of the eigenfunctions of the new well configuration. Specify the expansion coefficients in terms of integrals that are well defined, but you need not evaluate integrals in this step.
- (d) What is the probability that the particle is in the ground state of the new well configuration? Determine the answer in terms of a number.
- (e) What would you expect for the result of a sequence of measurements performed to determine the particle energy, with identical replications of the state preparation as above?

Problem 4.3 Resonant Tunneling Through a Double Barrier

A multi-layer structure of GaAs | AlGaAs | GaAs | GaAs | GaAs is grown with thicknesses 1000Å | 40Å | 100Å | 40Å | 1000Å. We model this layered structure with linear piece-wise potentials as shown in the figure below, with V₀ = 0.3 eV, b = 50Å, and a = 90Å.



The wave function is piecewise continuous, with

$$\psi_1 = e^{ik_1x} + Be^{-ik_1x}$$

$$\psi_2 = Ce^{ik_2x} + De^{-ik_2x}$$

$$\psi_3 = Fe^{ik_1x} + Ge^{-ik_1x}$$

$$\psi_4 = He^{ik_2x} + Ie^{-ik_2x}$$

$$\psi_5 = Je^{ik_1x}$$

where

$$k1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$k2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

(a) Match the boundary conditions and show that

$$\overline{\overline{M}} \ \overline{C} = \overline{A}$$

where

$$\overline{C} = \begin{pmatrix} B \\ C \\ D \\ F \\ G \\ H \\ I \\ J \end{pmatrix} \qquad \overline{A} = \begin{pmatrix} e^{-ik_{1}a} \\ k_{1}ae^{-k_{1}a} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\overline{\overline{M}} = \begin{pmatrix} -e^{ik_1a} & e^{-ik_2a} & e^{ik_2a} & 0 & 0 & 0 & 0 & 0 \\ k_1ae^{ik_1a} & k_2ae^{-ik_2a} & -k_2ae^{ik_2a} & 0 & 0 & 0 & 0 \\ 0 & -e^{-ik_2b} & -e^{ik_2b} & e^{-ik_1b} & e^{ik_1b} & 0 & 0 & 0 \\ 0 & -k_2be^{-ik_2b} & k_2be^{ik_2b} & k_1be^{-ik_1b} & -k_1be^{ik_1b} & 0 & 0 & 0 \\ 0 & 0 & 0 & -e^{ik_1b} & -e^{-ik_1b} & e^{ik_2b} & e^{-ik_2b} & 0 \\ 0 & 0 & 0 & -k_1be^{ik_1b} & k_1be^{-ik_1b} & k_2be^{ik_2b} & -k_2be^{-ik_2b} & 0 \\ 0 & 0 & 0 & 0 & -e^{ik_2a} & -e^{-ik_2a} & e^{ik_1a} \\ 0 & 0 & 0 & 0 & 0 & 0 & -k_2ae^{ik_2a} & k_2ae^{-ik_2a} & k_1ae^{ik_1a} \end{pmatrix}$$

(b) This problem can be solved for the coefficient vector \overline{C} by

$$\overline{C} = \overline{\overline{M}}^{-1} \ \overline{A}$$

The transmission coefficient is then

$$T = \left|\overline{C}(8)\right|^2 = \left|J\right|^2$$

Copy the files rtplot.m and rtwell.m from

/web.mit.edu/6.728/www/script/locker/ to plot this. This program takes a few minutes to run because of the small incremental spacing in energy that is needed. (Note: You are also welcome to write your own simulation in a different simulation package).

- (c) Run the program rtplot.m using the fact that the effective mass of the electron in GaAs and GaAlAs is $0.07 m_e$, where m_e is the mass of the electron. Find the energies below 0.3 eV where T = 1. (Hint: use the "ginput" command in Matlab.) For these energies, what would T be if the electron tunneled through just one barrier?
- (d) Show that these energies are roughly equal to the particle-in-a-box energies with box width = 2b. (As you can see, this approximation only holds strictly for a very deep box, but is often cited in the literature.)

Problem 4.4 Design a Notch Filter and a Resonant Tunnel Diode

For the purpose of this problem, assume that you are given a job of a semiconductor device designer and are asked to specify semiconductor structures that can be used for various applications. Just the same as in problem 4.3 you are told to design your structures using GaAs and AlGaAs materials and to again assume $V_0 = 0.3$ eV and electron mass = 0.07 m_e .

- (a) Design a quantum well structure that can be used as a notch filter for CO_2 laser radiation at 10.6 μ m. (Using the figure in problem 4.3, you can choose to make dimension *a* very big. You then need to choose dimension *b* so that spacing between the lowest two quantum well states corresponds to the CO_2 laser radiation.)
- (b) Design a resonant tunnel diode structure (such as that drawn in problem 4.3 figure) that passes electrons with energy of 0.15 eV 100 times more efficiently than thermal electrons.