MASSACHUSETTS INSTITUTE OF TECHNOLOGY

5.73 Quantum Mechanics I
Fall, 2002

Professor Robert W. Field

Problem Set #3

DUE: At the start of Lecture on Friday, September 27.

Reading: Merzbacher, pages 113-134

Note: We are going to return to some of these problems once we learn how to use perturbation theory.

Problems:

1. Airy Functions, piecewise linear potentials

For the following 5 potentials, find the energies of the 5 lowest energy eigenstates.

Let $\left(\frac{\hbar^2 C^2}{2m}\right)^{1/3} = 2\times10^{-6}$ erg. for all potentials. You are free to choose specific values, as needed to make computer programs work, for all unspecified constants (m, L).

A. "Vee-box."

$$V(x) = C|x| \qquad C > 0$$

(*optional*) B. "Vee-box plus δ-function" (a symmetric double minimum potential)

$$V(x) = C|x| + a\delta(x) \qquad a = 10C,\ C > 0$$

C. "Vee-bottom box".

$$V(x) = \infty \qquad |x| > L/2$$

$$V(x) = Cx - \frac{CL}{4} \qquad 0 < x \le L/2$$

$$V(x) = -Cx - \frac{CL}{4} \qquad -L/2 \le x < 0$$

Warning: This is tricky. You will need to use *both* A*i* and B*i*.

D. "Inverted Vee-bottom infinite box."

$$V(x) = \infty \qquad |x| > L/2$$
$$V(x) = -Cx + \frac{CL}{4} \qquad 0 < x \le L/2$$
$$V(x) = Cx + \frac{CL}{4} \qquad -L/2 \le x < 0$$

E. "Slant-bottom infinite box. "

$$V(x) = \infty \qquad |x| > L/2$$
$$V(x) = Cx \qquad |x| \le L/2$$

(*optional*) F. Compare the energies from parts A and B and discuss in terms of "tunneling".

G. Compare the energies from parts C, D, and E to the energies of an ordinary infinite box, $V(x) = \infty$ for $|x| > L/2$, $V(x) = 0$ for $|x| \le L/2$. All three boxes have the same average depth. If the energies are not identical, explain. If they are identical, perhaps the WKB quantization condition (even though it is inapplicable here for several reasons), applied at $E = CL/2$, will provide an explanation.
[**HINT**: Box D is a symmetric double minimum potential, unlike boxes E and F.]

(*optional*) H. Return to the potential of part B and choose $a < 0$. Consider only the lowest energy level. Is there any value of a for which the energy of the lowest energy level *does not* fall below $E = 0$? Is there any value of a for which more than one level has $E < 0$? [The second part requires no calculation, only words.]

2. Consider the two-δ-function potential:

$$V(x) = \infty \qquad |x| > L/2$$
$$V(x) = -a[\delta(x - L/6) + \delta(x + L/6)].$$

A. List all of the $(-L/2, L/2)$ infinite box eigenstates that have nodes at $x = \pm L/6$. Give the general expression for the energies of these special states in the two-δ-function potential.

B. The states that do not have nodes at $x = \pm L/6$ will come in two flavors, those with $\psi(-L/6) = \psi(L/6) \neq 0$ and those with $\psi(-L/6) = -\psi(L/6) \neq 0$. It is possible that one of these

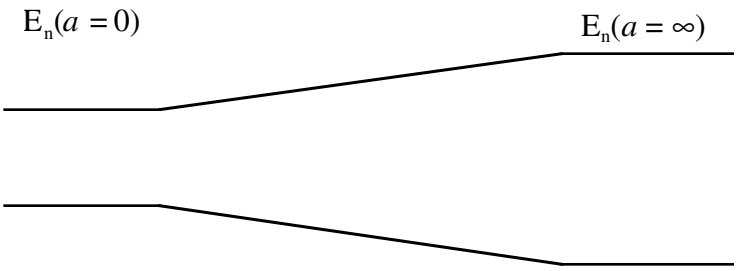
flavors will have to be treated as two separate sub-flavors, $\psi(|x| = L/6) > 0$ and $\psi(|x| = L/6) < 0$. *Without doing any calculations at all*, predict whether each of the flavors of states is shifted to higher or lower energy than the ordinary infinite box states. Also, are the energy shifts of the two sub-flavors of $\psi(-L/6) = \psi(L/6)$ states identical?

[**HINT**: What do you know about the energy of $e^{i\phi}\psi_j$, where ψ_j is an eigenstate of **H**?]

C. As a increases from zero, first there will be one eigenstate with $E < 0$ and then there will be two. To which flavor of state does the unique $E < 0$ eigenstate belong at small a? When there are two $E < 0$ eigenstates, to which flavor(s) do they belong? Does the lowest energy state always belong to the same flavor of state for all values of a? Can there ever be more than two $E < 0$ eigenstates at very large a?

[**HINT**: All of these questions can be answered without doing any numerical calculation.]

(*optional*) D. Solve for the energies of the ten states with 0 through 9 internal nodes. Construct a "correlation diagram" that shows how the energies of these states evolve from $a = 0$ to $a = \infty$.



(*optional*) E. Speculate about the form of the level diagram for $a \to -\infty$? Would it be reasonable to take the $0 \le a < \infty$ correlation diagram and extend it by naïve extrapolation to a two-sided correlation diagram:

$$E(a = -\infty) \qquad E(a = 0) \qquad E(a = +\infty).$$

3. WKB Quantization

Consider the Lennard-Jones potential:

$$V(x) = \varepsilon + 4\varepsilon\left[\left(\frac{\sigma}{x}\right)^{12} - \left(\frac{\sigma}{x}\right)^{6}\right]$$

Let $\varepsilon = 100$, m = 100, $\sigma = 1$, $\hbar = 1$, and $h = 2\pi$.

A. What is the value of V(x) at the minimum of the potential (when $\frac{dV}{dx}$=0)?

B. What is the difference in energy between $V(x_{min})$ and $V(\infty)$? This is called the dissociation energy, D_e.

C. Use WKB quantization to determine the total number of levels bound in $V(x)$. This (not necessarily integer) number is v_D. [Hint: $E_D = V(\infty)$, solve for $x_-(E_D)$.]

D. The classical period of oscillation is $h\frac{dn}{dE}$. Use the d/dE form of the WKB quantization condition to determine dn/dE. Compute the oscillation period for the 3 integer values of v_D just below the (noninteger) v_D. [It may be necessary to resort to numerical rather than analytic integration.]

E. Estimate the locations of the *first interior node* just to the right of $x_-(E)$ and just to the left of $x_+(E)$ for the three vibrational levels in part D. [Hint: WKB wavefunctions start with phase $\pi/4$ at turning point and the phase increases as one moves away from the turning point into the classical region. The first node occurs at an accumulated phase of $3\pi/4$.]

F. Calculate, using classical mechanics, the time it takes for a classical particle to move from $x_\pm(E)$ to the first internal node. Recall that Force $= -\frac{dV}{dx}$. It is a good approximation here to treat $V(x)$ as linear with slope equal to the slope at $x_\pm(E)$. Do this calculation for the inner and outer turning point regions for each of the three levels you considered in part D.

G. What fraction of the oscillation period does the system spend in the outermost lobe of the vibrational wavefunction? [More correct language would be: "What is the probability of finding the system within the specified range of x?"] In the innermost lobe? What is the ratio of times [or more correctly, probabilities] in these two lobes for the three highest vibrational levels? You are supposed to be surprised by the result you obtain.

H. Suggest an explanation, based entirely on your answer to part G, for why the long-range expression

$$D\left(v_D - v\right)^3 = E_{v_D} - E_v ,$$

where D is a constant, can be determined entirely by the x^{-6} dependence of the attractive limb of the potential and be totally insensitive to the nature of the x^{-12} dependent repulsive limb. Does the value you obtain for D satisfy Le Roy's long range theory for a C_6R^{-6} long-range potential?