

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

5.73 Quantum Mechanics I
Fall, 2018

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Problem Set #3

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 $\left(\frac{\hbar^2 C^2}{2m}\right)^{1/3} = 2 \times 10^{-6}$ 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.”

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

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

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

C. “Vee-bottom box”.

$$\begin{array}{llll} V(x) = \infty & |x| > L/2 & V(x) = \infty & |x| > L/2 \\ V(x) = Cx - \frac{CL}{4} & 0 < x \leq L/2 & V(x) = Cx - \frac{CL}{4} & 0 < x \leq L/2 \\ V(x) = -Cx - \frac{CL}{4} & -L/2 \leq x < 0 & V(x) = -Cx - \frac{CL}{4} & -L/2 \leq x < 0 \end{array}$$

Warning: This is tricky. You will need to use *both* A_i (for $x > 0$) and B_i (for $x < 0$).

D. “Inverted Vee-bottom infinite box.”

$$\begin{aligned}
 V(x) &= \infty & |x| > L/2 \\
 V(x) &= -Cx + \frac{CL}{4} & 0 < x \leq L/2 \\
 V(x) &= Cx + \frac{CL}{4} & -L/2 \leq x < 0
 \end{aligned}$$

E. “Slant-bottom infinite box.”

$$\begin{aligned}
 V(x) &= \infty & |x| > L/2 \\
 V(x) &= Cx & |x| \leq L/2
 \end{aligned}$$

(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 $|x| \leq L/2$. 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 C and E.]

(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. 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 ν_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 ν just below the (noninteger) ν_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 the 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. For the three vibrational levels from part D, 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 the 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

$$A(\nu_D - \nu)^3 = E_{\nu_D} - E_{\nu},$$

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

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