Oct. 8, 2007

Chem. 1410

Problem Set 5, due Oct. 15, 2007

Do the following problems; these are *not* to be handed in for grading; solutions will be distributed via .pdf.

Engel Chapter 8: P8.3, P8.4, P8.11, P8.14, P8.20

and

0) **Particle in a Finite Depth Box: Odd Parity States.**

Repeat the analysis done in class for a particle, mass m, in a finite-depth 1D box specified by the potential energy function:

$$V(x) = \{ \begin{matrix} 0, x < |a/2| \\ V_0, x > |a/2| \end{matrix}$$

for the case of *odd* parity states. In particular,

a) Show that the energy eigenfunctions for odd parity states have the form:

$$\psi_I(x) = -Ae^{\kappa x}$$

$$\psi_{II}(x) = \sin(kx)$$

$$\psi_{III}(x) = Ae^{-\kappa x}$$

with $k(E) \equiv \sqrt{2mE}/\hbar$ and $\kappa(E) \equiv \sqrt{2m(V_0 - E)}/\hbar$. [Note: as for the even parity case discussed in class, regions *I,II,III* cover *x<-a/2*, *-a/2<x<a/2*, *x>a/2*, respectively.]

b) The allowed values of *E* (and the corresponding values of *A*) are determined by matching $\psi(x)$ and $d\psi(x)/dx$ at $x = \pm a/2$.

Show that this leads to the following transcendental equation, which is effectively the *quantization condition* for the energy *E*:

$$\cot(\frac{\sqrt{2mE}a}{2\hbar}) = -\sqrt{\frac{V_0 - E}{E}} \qquad [1]$$

c) To analyze this equation further, introduce dimensionless versions of the system energy and the barrier height. In particular, recall the ground state energy eigenvalue of a particle in an particle in an infinitely deep box of width *a*, namely $E_{gs}^{\infty} = \frac{\hbar^2\pi^2}{2ma^2}$. Then, let $\varepsilon \equiv E / E_{gs}^{\infty}$ and $v_0 = V_0 / E_{gs}^{\infty}$.

Substituting into Eq. [1] gives the equivalent equation:

$$-\cot(\frac{\pi}{2}\sqrt{\varepsilon}) = \sqrt{\frac{v_0 - \varepsilon}{\varepsilon}} \qquad [2]$$

Plot the left hand side of Eq. 2 and the right hand side of Eq. 2 on the same graph for the case that $v_0 = 30$. How many odd-parity energy eigenfunction are there in a finite-depth box characterized by this value of v_0?

[Note: you may wish to consult Engel P5.1 for guidance.]

The following two problems are to be handing in for grading:

(1) **Basic Features of Rotational Spectra**: Engel P8.19.

(2) **Quantum Mechanical Tunneling through a 1D Potential Energy Barrier**: Engel P5.6.

In addition to the questions asked in the statement of the problem in the book, show that the tunneling probability formula derived in this problem reduces to the one asserted in class when $\kappa a \gg 1$, i.e.:

$$\frac{1}{1+[(k^2+\kappa^2)^2 \sinh^2(\kappa a)]/4(\kappa k)^2} \cong \frac{16k^2\kappa^2 e^{-2\kappa a}}{(k^2+\kappa^2)^2} \quad , \quad \kappa a \gg 1 .$$