Assignment 4
Physics/ECE 176

Made available: Saturday, February 5, 2011
Due: Thursdays, February 10, 2011, by 5pm

Problem 1: Harmonic Oscillator Approximation to the Morse Potential of a Diatomic Molecule

A useful simple approximation for the intermolecular potential of two atoms in a diatomic molecule is the Morse potential

$$V(l) = D \left(1 - e^{-\beta(l-l_0)} \right)^2, \tag{1}$$

where l is the distance between the nuclei, l_0 is the the equilibrium (minimum energy) distance between the nuclei, D is the dissociation energy of the molecule measured from the minimum value of $V(l)$, and β is a measure of the curvature of the potential at its minimum.

1. A harmonic oscillator approximation to the potential $V(l)$ about its minimum at $l = l_0$ will have the form $V(x) = c + (1/2)kx^2$ where $x = l - l_0$, k is the spring constant, and c is the minimum value of V. This is none other than the Taylor series of $V(x)$ with up to 2nd-order terms retained in the small quantity x. Given this insight and the fact that $e^x \approx 1 + x$ for sufficiently small x (the first two terms of its Taylor series), show that the spring constant k for the Morse potential is given by

$$k = 2D\beta^2. \tag{2}$$

2. For diatomic hydrogen, empirical fits of the Morse potential to vibrational spectroscopic lines give the approximate values

$$D \approx 7.6 \times 10^{-19} \, \text{J}, \qquad \beta = 0.0193 \, \text{pm}^{-1}, \qquad l_0 = 74.1 \, \text{pm}, \tag{3}$$

   where a picometer, pm, is $10^{-12} \, \text{m} = 10^{-3} \, \text{nm}$. From these data, deduce the effective spring constant k for diatomic hydrogen. Then use Google to determine whether the electronic attraction between nuclei in H_2 is a strong or weak spring compared to day-to-day mechanical springs.

3. Use the Mathematica command `Plot[ { f1[x], f2[x] }, {x, 0, xmax} ]` to plot the Morse potential with its harmonic oscillator approximation $c_0 + c_2(l-l_0)^2$. From your plot, discuss qualitatively and briefly over what range in l the quantum levels of a harmonic oscillator give a good description of the vibrational states of diatomic hydrogen.

4. Use the value of your spring constant and the mass of a hydrogen atom $m_H \approx 2 \times 10^{-27} \, \text{kg}$ to **estimate to one significant digit the energy spacing $\Delta E = hf$ between successive vibrational quantum levels of diatomic hydrogen** by using the formula

$$f = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}, \tag{4}$$

   for the frequency f of an oscillator with spring constant k. A subtlety related to how one converts a two-particle diatomic molecule AB into a single-particle spring problem is that you need to calculate the frequency f using the *reduced mass* μ of the molecule, which is defined by

$$\frac{1}{\mu} = \frac{1}{m_A} + \frac{1}{m_B}, \tag{5}$$

1

where m_A and m_B are the masses of the atoms A and B.

Is your spacing ΔE large or small compared to the disassociation energy D in Eq. (3) above? Or visually: is the spacing between energy levels large or small compared to the depth of the potential well for diatomic hydrogen?

Problem 2: Schroeder Problems

1. Problem 1.16 on pages 8-9. When you consider the horizontal slab of air of thickness dz, it will help if you further assume it has a finite area A and that the bottom of the slab is at height z above the ground. Then the pressure pushing down on the top of the slab will be $P(z + dz)A$.

   For part (d) of this problem, only calculate the answers for Ogden, Utah, and Mt. Everest, Tibet.

   Note: I should have assigned this problem earlier, it should help you to understand how the pressure can vary in an equilibrium system in the presence of an external gravitational field in such a way that mechanical equilibrium is everywhere satisfied.

2. Problem 2.5 on page 55 but only parts (e), (f), and (g).

3. Problem 2.7 on page 55.

4. Problem 2.8 on page 59.

5. Problem 2.12 on page 61. This problem should help you review some basic but important properties of the logarithm function $\ln(x)$.

   For part (d), get the answer in *three* ways:

   (a) by using the first two terms in the known Taylor series of e^x about $x = 0$ that $e^x \approx 1 + x$.

   (b) by using the fact that one can integrate a convergent power series term by term, applied to the convergent geometric series

   $$\frac{1}{1-x} = 1 + x + x^2 + \dots, \qquad |x| < 1. \tag{6}$$

   (c) by a direct computation of the Taylor series of $\ln(1 + x)$ about $x = 0$.

   Naturally, I like approach (b) the best, since we already know the geometric series.

   Also for part (d), instead of checking the accuracy of the approximation for $x = 0.1$ and $x = 0.01$ as asked by Schroeder, use your Mathematica skills to deduce over what range of x values the approximation $\ln(1 + x) \approx x$ gives a 10% relative error and a 1% relative error.

6. Problem 2.13(b) on page 62.

Problem 3: Time to Finish This Homework Assignment

Please tell me the approximate time in hours that it took you to complete this homework assignment.