

PHYS 4310, Homework 3 due on September 23<sup>th</sup>, 2015

Griffiths (2<sup>nd</sup> edition): 2.10 (10 points), 2.11 (15 points), 2.12 (10 points), 2.17 (20 points)

5. Problem 4-13, parts (a) through (f) of attached backside sheet (25 points). Part (g) of this problem is a 5 point bonus question.

(Classical analog: two gliders on a linear air track connected by a flexible but inextensible string.) By what factor do the permitted energies increase as  $m_2$  is decreased from  $m_2 = \infty$  to  $m_2 = m_1$  while the value of  $m_1$  remains constant?

(b) Perform the same analysis for a harmonic interaction:

$$V(x) = \frac{1}{2} C(x - x_0)^2$$

(Classical analog: two gliders on a linear air track connected by a spring of relaxed length  $x_0$ .) [Hint: Write the Schrödinger equation using the variable  $x' = x - x_0$ .]

(c) Why is the variation of energy with reduced mass different for the two potentials used above? Discuss the physical basis for the difference, not only the mathematical results.

4-13 *A simple model of ionic bonding in the sodium chloride molecule.* The molecular bonding in the compound sodium chloride (NaCl) is predominantly ionic, so to a good approximation we can model a sodium chloride molecule as consisting of two units—an  $\text{Na}^+$  ion and a  $\text{Cl}^-$  ion—bound together. Assume that the attractive potential between the ions is electrostatic in nature:  $-e^2/r$ , where  $r$  is the internuclear distance. Assume that the repulsive term in the potential energy function  $V(r)$ , which rises steeply for contact between the electron structures of the two ions, has the form  $+A/r^n$ .  $A$  and  $n$  are constants to be determined.

(a) Using  $V(r) = -e^2/r + A/r^n$ , find the equilibrium separation  $r_0$  of the nuclei in the NaCl molecule. (That is, find the value of  $r$  for which  $V$  is a minimum.)

(b) Find the value  $V_{\min}$  of the potential energy at this equilibrium separation  $r_0$ .

(c) Evaluate the second derivative of  $V$  at  $r = r_0$ . This is the “spring constant” in the SHO approximation to the potential energy near the equilibrium separation.

(d) Using the reduced mass (for the isotopes  $\text{Na}^{23}$  and  $\text{Cl}^{35}$ ), calculate the energy spacing of the vibrational levels in the harmonic approximation. Find also the zero-point energy of the vibrational motion.

(e) The equilibrium separation  $r_0$  of the nuclei in  $\text{Na}^{23}\text{Cl}^{35}$  is 2.51 Å, and the frequency of the radiation for transitions between adjacent vibrational levels is  $1.14 \times 10^{13}$  Hz. Use these experimental values to determine the parameters  $n$  and  $A$ . [Hint: Determine  $n$  and then  $A$ .]

(f) Using the results from (b), (d), and (e), calculate the energy (in eV) needed to dissociate an NaCl molecule from its ground state into an  $\text{Na}^+$  ion and a  $\text{Cl}^-$  ion.

(g) The ionization energy of the Na atom is 5.1 eV, while the ionization energy of the  $\text{Cl}^-$  ion is only 3.7 eV. This means that at large separations of the two nuclei of the NaCl molecule, the neutral atoms Na and Cl are a more stable pair than the ions  $\text{Na}^+$  and  $\text{Cl}^-$ . Use this information, together with your result from (f), to find the energy required to dissociate an NaCl molecule into an Na atom and a Cl atom. Compare your result with the experimental value of 4.3 eV. The discrepancy is not very large considering the simple model we have used.

4-14 *Computer normalization of computer-generated wave functions.* Suppose you have just used a computer program to calculate the wave function for a particle in one of the energy states of a given one-dimensional potential. The wave “function” is in the form of a set of values  $\psi_j$ , one for each point  $z_j$  on the spatial axis. Given this set of values, write a computer program to normalize the wave function. Is this normalization exact or approximate?

4-15 *Machine solution of the finite square-well potential.* Modify the computer program of Table 4-3 to calculate wave functions for the one-dimensional finite square well of width  $L$  and height  $V_0$ .

*Discussion:* The first step is to convert the Schrödinger equation to dimensionless units for this potential. The well width  $L$  is an obvious natural unit of length. One might think of  $V_0$  as a natural unit of energy, but this choice does not eliminate the factors  $\hbar$  and particle mass  $m$  from the Schrödinger equation. Unfortunately, the lowest energy of the system depends on  $V_0$  in a complicated way, or that might be an easy unit of energy. Instead, think of using the lowest energy of the corresponding infinite well, namely  $\hbar^2/(8mL^2)$ . Substituting this natural unit, together with  $x = Lz$  for length, still leaves some factors of  $\pi$  in the result. The equation can be still further simplified by modifying the unit of energy to be  $\hbar^2/(2mL^2)$ . Derive the difference equation (4-30) for your choice of natural units and modify the program of Table 4-3 accordingly. If computer facilities are available, rewrite the program in the local computer language and run it.