Problem Set 6

Instructions:

1. Answer all questions below. Show your work for full credit.
2. Read partial derivative symbols, e.g., $\partial/\partial x$, as d/dx if you are unfamiliar.
3. The first problem is due at the start of class on 25 Oct 2013
4. The second problem is due at the start of class on 28 Oct 2013
5. The remaining problems are due by the end of the day on 30 Oct 2013
6. You may collaborate, but everyone must turn in their own work.

Daily problem for 25 Oct On last week's homework, you proved (presumably) that in quantum mechanics one can find the average force from the average gradient of the potential:

$$\langle F_x \rangle = \left\langle -\frac{\partial V}{\partial x} \right\rangle \tag{1}$$

Use this result to verify that the average force on a particle in a simple harmonic oscillator potential ($V = \frac{1}{2}m\omega^2 x^2$) is zero. You may restrict your solution to the ground state, whose wave function you can find readily in your text.

Daily problem for 28 Oct (a) How many different sets of quantum numbers (n, l, m_l, m_s) are possible for an electron on the $4f$ level? **(b)** Suppose a certain atom has three electrons in the $4f$ level. What is the maximum possible value of the total m_s of the three electrons? **(c)** What is the maximum possible total m_l of three $4f$ electrons? **(d)** Suppose an atom has ten electrons in the $4f$ level. What is the maximum possible value of the total m_s of the ten $4f$ electrons? **(e)** What is the maximum possible total m_l of ten $4f$ electrons?

The remaining problems are due 30 Oct 2013

1. *Variational Principle I.* The energy of a system with wave function ψ is given by

$$E[\psi] = \frac{\int \psi^* H \psi \, dV}{\int |\psi|^2 \, dV} \tag{2}$$

where H is the energy operator. The variational principle is a method by which we guess a trial form for the wave function ψ, with adjustable parameters, and minimize the resulting energy with respect to the adjustable parameters. This essentially chooses a "best fit" wave function based on our guess. Since the energy of the system with the correct wave function will always be minimum, our guess will always lead to an energy which is slightly too high, but the variational principle allows us to get as close as possible to the correct energy with our trial wave function.

Use the variational principle to estimate the ground state energy for the anharmonic oscillator,

$$H = \frac{p^2}{2m} + \lambda x^4 \qquad \text{i.e., } H\psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + \lambda x^4 \psi \tag{3}$$

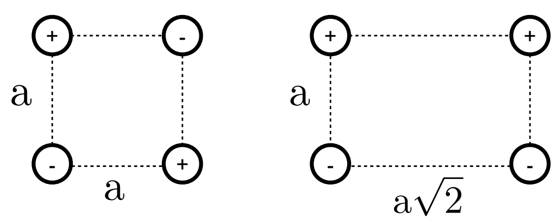
Compare your result with the exact result

$$E_o = 1.060\lambda^{1/3}\left(\frac{\hbar^2}{2m}\right)^{2/3} \tag{4}$$

Note that this is a one-dimensional problem, so take $dV = dx$. The wavefunction for the *harmonic* oscillator ground state might not be a bad choice, $\psi = e^{-cx^2}$, though many other choices are possible.

2. *Variational Principle II.* Repeat the problem above with a different trial wave function. You know physically a trial function must be peaked around $x = 0$ and must be normalizable (i.e., $\int_{-\infty}^{\infty} \psi^2\,dx$ is finite). Such functions would include $e^{-c|x|}$ or $1/(c + x^2)$, for instance. Choose wisely, and the mathematics will be far simpler.

3. The two figures below show small sections of two different possible surfaces of a NaCl surface. In the left arrangement, the NaCl(100) surface, charges of $+e$ and $-e$ are arranged on a square lattice as shown. In the right arrangement, the NaCl(110) surface, the same charges are arranged in a rectangular lattice. **(a)** What is the potential energy of each arrangement (symbolic answer)? **(b)** Which is more stable?



4. *Energetics of diatomic systems* An approximate expression for the potential energy of two ions as a function of their separation is (treating the problem one dimensionally),

$$V = -\frac{ke^2}{x} + \frac{b}{x^9} \tag{5}$$

The first term is the usual Coulomb interaction, while the second term is introduced to account for the repulsive effect of the two ions at small distances. **(a)** What is the equilibrium spacing x_o? **(b)** Find b as a function of the equilibrium spacing x_o. **(c)** For NaCl, with an equilibrium spacing of $r_o = 0.236\,\text{nm}$, calculate the frequency of small oscillations about $x = x_o$. *Hint: do a Taylor expansion of the potential energy to make it look like a harmonic oscillator for small $x = x_o$.*

5. A collection of hydrogen atoms is placed in a magnetic field of 3.50 T. Ignoring the effects of electron spin, find the wavelengths of the three normal Zeeman components of **(a)** the $3d$ to $2p$ transition, **(b)** the $3s$ to $2p$ transition.

6. Consider a hydrogen atom and a singly-ionized helium atom (i.e., Bohr-like). Which atom has the lower ground state energy, and how big is the difference? Justify your answer with an explicit calculation, even if it is just an order-of-magnitude estimate.