6.728 Applied Quantum and Statistical Physics

Department of Electrical Engineering and Computer Science
Massachusetts Institute of Technology

PROBLEM SET 6

Issued: 10-17-02 Due: 10-23-02, in-class

Problem 6.1

Do problem 15.1 of Chapter 15 of the 6.728 Class Notes. Only do parts (b) and (c); you can accept as given the integrals done in part (a). Hint: Don't forget to normalize the wavefuntion.

Problem 6.2

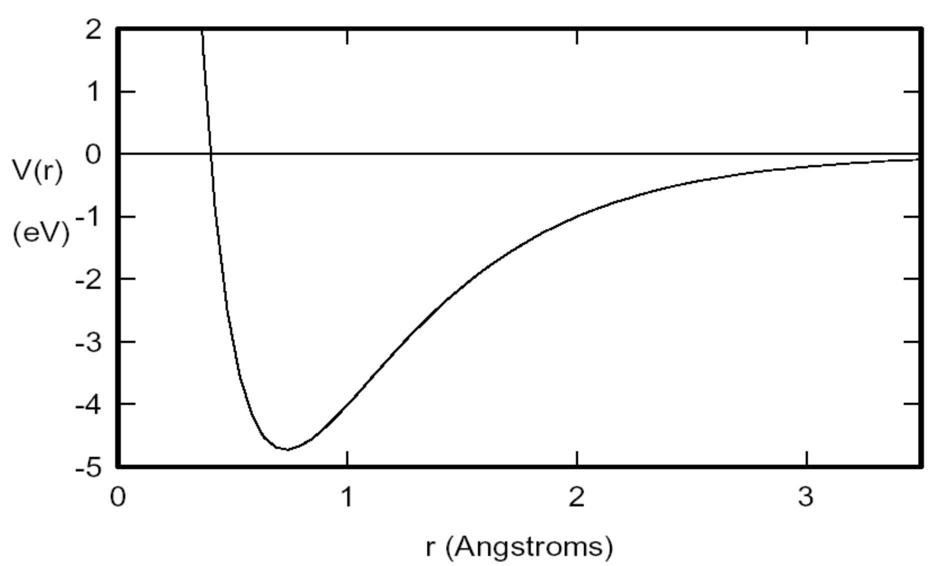
Do problem 16.1 of Chapter 16 of the 6.728 Class Notes. Only do parts (b) and (c); you can accept as given the integrals done in part (a). Hint: Use matlab (or any other numerical package) to numerically find the eigen values and eigen vectors.

Problem 6.3

The potential between two hydrogen atoms in an H_2 molecule is well approximated by

$$V(r) = 2e^{-ar}\left(\frac{a_0}{r} - b\right) I_H$$

where I_H = 13.6 eV, $a = 0.886/a_0$, $b = 1.315$, and $a_0 = 0.529$ Å is the Bohr radius.



The time-independent Schrödinger equation in this case is

$$E\,\psi(r) = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial r^2}\psi(r) + V(r)\,\psi(r)$$

where M is the reduced mass $M_P/2$ (recall that proton mass, M_P, is equal to ~$1836 m_e$). (Note :We will discuss this expression in detail later in the semester.)

(a) Estimate the energies of the two lowest vibrational quantum states. Note that near the bottom of the potential

$$V(r) \sim V(R_0) + \frac{1}{2}(r - R_0)^2 \left.\frac{\partial^2 V}{\partial r^2}\right|_{R_0}$$

Give your answer numerically in eV above the minimum potential. The energy difference between the ground state and the first excited vibrational state is known from experiments to be 0.516 eV. Compare your answer against this result.

(b) Now use the WKB approximation to estimate the energies of these two lowest vibrational quantum states (you may use your favorite computer program for this).