MEEN 5900: Special Topics on Nanotechnology
Homework 2
Due by Oct 15, 2007

1. Solve 2.2, 2.6, and 2.8 in the textbook.

2. Solve 3.1, 3.3, 3.6, 3.11, and 3.14 in the textbook.

3. A 5 kg mass attached to a spring of spring constant k = 400 N/m is undergoing simple harmonic motion on a flat frictionless surface with an amplitude of 10 cm. If we assume the energy levels are quantized according to the Planck relation $E = nhf$, what is the corresponding quantum number n ?

4. Suppose visible light of wavelength $\lambda = 5 \times 10^{-7}$ m is used to determine the position of an electron to within the wavelength of the light. What is the minimum uncertainty in the electron's speed?

5. Given a two-dimensional electron gas (mass m, spin ½ and charge e) of N particles confined in a square of size L,

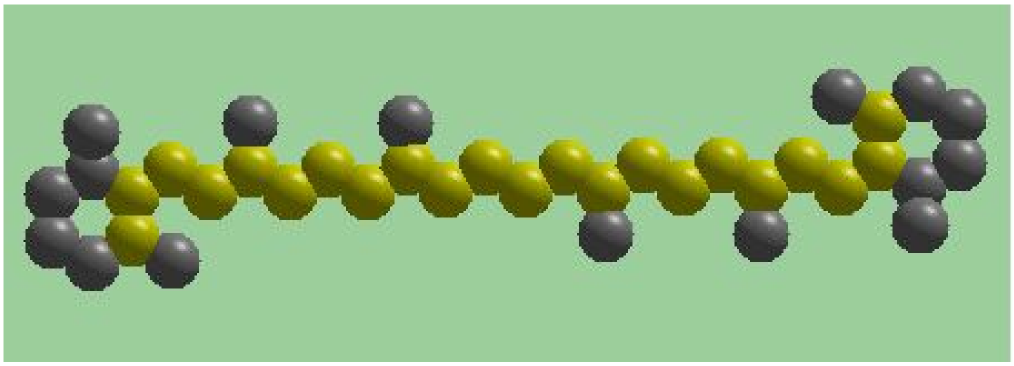
a. calculate its density of states (per unit energy)
b. calculate its Fermi energy
c. Using only simple physical arguments predict how the heat capacity of this 2D electron gas will depend on temperature T at low T (i.e. $k_B T$ << Fermi energy)

6. The main application of most of simple 1D model for a particle in a box (1D PIAB) is in their pedagodical utility. By seeing how quantum systems perform in cases where we can solve the problem exactly, we can subsequently apply the intuitive feel we obtain to systems which are less straightforward to solve. The principle concept to take away from the 1D PIAB is that "confinement leads to quantization". The general solutions for this problem are identical to those for the Free Particle except that most specific solutions are rejected because they do not satisfy the boundary conditions. Only those survive which meet the specified boundary conditions and the quantum number - the index of these remaining solutions - is born. Each solution is identified by its unique quantum number.

One type of problem that is an application of this formalism is that of the problem of the UV-Vis absorption spectrum of long-chain, conjugated polyenes. The π-electrons of such a molecule are modeled as particles in a box, which is defined by the carbon atom framework that makes up the conjugated section of the molecule. Some concepts need to be recalled when setting up these problems.

1. The carbon-carbon length of the conjugated double bond. Add these up to determine the length of the box. Often, to obtain better agreement with experiment, the length of the box is increased by 1 additional bond length, allowing the electrons to "spill" over the ends. An average bond length in the conjugated network can be taken as 0.140 nm, so that the box length is L = (N+1)*0.140 nm, where N is the number of bonds making up the box.
2. Each double bond contributes two electrons to the box, or in otherwords, each carbon atom in the chain contributes 1 electron.
3. Each energy level of the box accepts two electrons, as explained in the Aufbau Principle, as required by the Pauli Exclusion Principle.

4. The lowest spectroscopic transition would be expected to promote an electron in the highest filled state to the lowest empty state. A careful analysis of the spectroscopic selection rules show that the quantum number must change by 1, 3, 5, etc. so that the transition to the next highest state is allowed while a transition up two states is not allowed.



β-carotene molecule in carrots

An example of this type of problem would be to identify the lowest energy absorption of the β-carotene molecule. A carbon framework outline is given above. Determine the length of the box by adding up the number of bonds and calculate the number of π-electrons present - 2 from each double bond. We can easily count to see that there are 21 bonds in the conjugated bond network. This indicates that we have a box that is (21+1)*0.140 nm = 3.08 nm = L. Furthermore, since there are 11 double bonds in the system, there must be 22 π-electrons.

As these electrons enter the box, they must pair up in the energy levels (a consequence of spin), so that the lowest 11 energy levels will be filled. The lowest energy transition will be when an electron in the 11th state is promoted to the 12th state by the absorption of a photon. The energy of that transition is given by the difference in the two energy levels.

$$E_{12} - E_{11} = \frac{h^2}{8mL^2}\left(12^2 - 11^2\right) = \frac{23h^2}{8mL^2}$$

Knowing the value for Planck's constant, the mass of the electron, and the size of the box calculated above we can find the value for the energy of the absorbed photon, and from there, its wavelength.

$$\Delta E = \frac{23\left(6.626 \times 10^{-34}\ \mathrm{J\ s}\right)^2}{8\left(9.109 \times 10^{-31}\ \mathrm{kg}\right)\left(3.08 \times 10^{-9}\ \mathrm{m}\right)^2} = 1.461 \times 10^{-19}\ \mathrm{J}$$

$$E = h\nu = h\frac{c}{\lambda} \qquad \therefore \lambda = \frac{hc}{E}$$

$$\lambda = \frac{\left(6.626 \times 10^{-34}\ \mathrm{J\ s}\right)\left(2.9979 \times 10^{8}\ \mathrm{m/s}\right)}{1.461 \times 10^{-19}\ \mathrm{J}} = 1.359 \times 10^{-6}\ \mathrm{m} = 1359\ nm$$

This wavelength is in the infrared. Carrots are orange because the absorption of the short wavelength (blue) light leaves only the red-orange to reflect. This first absorption wavelength is clearly inadequate to describe the colour of carrots. A smaller box or more electrons would shift the absorption wavelength towards the blue as needed to agree with experiment.

Now, the problem is:

An electron in a one-dimensional box undergoes a transition from the n=3 level to the n=6 level by absorbing a photon of wavelength 500 nm. What is the width of the box?