ph 135

Problem set - 4

Due: Nov. 6th by 5pm in TA box.

1. Phonons.

   Consider a chain made out of a unit cell with two atoms in each unit cell. The atoms can move only in one direction, and have masses m_A and m_B. If the distance between the atoms change, there is an elastic energy cost of $E_{pot} = \frac{1}{2}k(\Delta x - a/2)^2$ with a being the lattice constant, and $a/2$ the distance between the two atoms.

   (a) What is the dispersion of phonons in the chain? Identify an optical and acoustic branch.

   (b) What is the speed of sound?

   (c) What is the heat capacity of the system at low temperatures?
   Note that in the limit of $m_A = m_B$ we obtain a chain with lattice constant $a/2$.

2. Tight binding approximation preview.

   Consider a chain of N atoms, with electrons described by an Hamiltonian H. We would like to find the lowest lying states of this hamiltonian using the ground state orbital in each atom. Mark the lowest orbital in the atom i as $|i\rangle$.

   By minimizing the energy of the states, show that the best lowest-energy N solutions that are superpositions of the form $|\psi\rangle = \sum_{i=1}^{N} \alpha_i |i\rangle$ have energies that given by eigenvalues of the matrix:

$$H_{eff} = M^{-1/2} h M^{-1/2} \qquad (1)$$

   with $M_{ij} = \langle i| j\rangle$, and $h = \langle i| H |j\rangle$. How are the corresponding eigenstates relate to the $|\psi\rangle$ states and the α's defined above?

   In a tight-binding approximation we assume that h_{ij} and M_{ij} are nonzero only if $|i - j| \leq 1$.