3.23 Electrical, Optical, and Magnetic Properties of Materials
Fall 2007

3.23 Quiz 1 **3.23**
23.10.07 **Fall 2007**
100 points total

Give as much written explanation as possible of your reasoning, and write clearly and legibly.

Time yourself carefully – do not spend most of your time on a single question. Remember, you have from 10.05 am to 11.30 am.

1) **Question 1 [20 points]**

Define and explain the following concepts, and for each of them explain their relevance with an example.

a) Commuting operators

b) Acoustic and optical phonons

c) Time-dependent Schroedinger equation

d) Hartree equations

2) **Question 2 [50 points]: one dimensional metals and Peierls distortions**

Let us consider an infinite, one-dimensional periodic system, with one atom per unit cell. When isolated, each atom has one valence electron, described by an atomic wavefunction $\varphi_s(x)$ and an atomic energy eigenvalue ε_s.

a) What are the real and reciprocal space primitive basis vectors for such infinite system with a lattice spacing *a* between atoms ?

b) For a finite but large *a* such that the overlap between φ_s orbitals at neighboring atoms is zero, what are the wavefunctions of the system that satisfy Bloch theorem ? Prove explicitly that Bloch theorem is satisfied.

c) What is the band diagram for the electronic states in b) ? Suppose that we apply Born-von-Karman boundary conditions so that any wavefunction has a periodicity of 10 units cells. How does that affect the band diagram with respect to the case in which the periodicity is over macroscopic distances (i.e. >> 10 a) ?

d) Show analytically how the band dispersion in b) changes If *a* is decreased further so that there is overlap between the atomic orbitals at neighboring sites.

e) Calculate the density of states for the band dispersion in d), taking into account spin degeneracy. Is the system metallic or insulator ? Where is the Fermi energy ?

f) Calculate the total energy of the system, using the information in e).

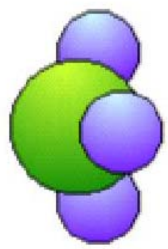
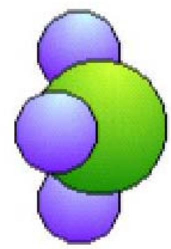
g) Consider the same identical system, but describe it now using a unit cell of length 2*a*, containing 2 atoms. What will be the band dispersion in this case, and how does it relate to the one discussed in d) ?

h) If we have used a free-electron gas model instead of a tight-binding model, how different would have been the bands for the system described in g) ?

i) Let's use the free-electron gas model for the system in g). If we displace the second atom by a small amount, what will be the G vector of the dominant component of the perturbing potential ? How will the band structure change (show it both analytically and graphically) ?

j) What will (qualitatively) happen to the total energy of the system ? Can you draw some general conclusions on the stability of one-dimensional metallic systems ?

3) Question 3 [30 points]: The ammonia maser

$|L\rangle =$  $|R\rangle =$ 

a) Let us consider the NH_3 ammonia molecule. It can exist in the two states pictured above, and the nitrogen atom has a finite probability of tunneling from one side to the other, with respect to the plane of hydrogen atoms. So, the molecule spends half of its time in one form and half in the other. We call these two quantum states representing the entire molecule $|R\rangle$ and $|L\rangle$; these two states are orthonormal. Explain why the 2x2 Hamiltonian for the molecule in this base cannot be diagonal.

b) The 2x2 Hamiltonian for the molecule in the basis of the states $|R\rangle$ and $|L\rangle$ is $\begin{pmatrix} E_0 & V \\ V & E_0 \end{pmatrix}$, where all the elements are real. What are the eigenvalues and eigenvectors of this matrix ? Give the eigenvectors in the basis of $|R\rangle$ and $|L\rangle$.

c) Express $|L\rangle$ in terms of the eigenvectors of the Hamiltonian given in b). If at time t=0 the molecule is found in the state $|L\rangle$, what is the time evolution of the wavefunction ?

d) What is the probability of finding the system in state $|L\rangle$ at time t ?