PHYSICS 555 FALL 2003
problem set 5
due Friday Nov. 7

1. Properties of a simple metal. Aluminum is trivalent and has the fcc structure. The lattice constant is \( a = 4.05 \text{Å} \).
   
   a. Make a choice for the three primitive translation vectors. Try to make a symmetrical choice. What is the volume of the primitive cell?
   
   b. What is the corresponding choice of reciprocal lattice vectors? What is the symmetrical shape of the Brillouin zone. What is the smallest distance from the zone center to the zone boundary, and what is the largest distance?
   
   c. What is the Fermi wavevector \( k_F \) (use cm\(^{-1}\)) and the Fermi energy \( \epsilon_F \) (use eV)?
   
   d. The measured low temperature specific heat is \( C_P = \gamma T \) where the measured coefficient \( \gamma \) is 1.35 mJ mol\(^{-1}\) K\(^{-2}\). Interpreting this as the specific heat of an electron gas (same density as Al) with an effective electron mass \( m^* \), find the value of \( m^* \).

2. Tight-binding model for NaCl. NaCl has the rocksalt (NaCl) structure, which has the fcc translational lattice with a basis which can be taken to be a Cl (approximately a Cl\(^-\) ion) at the origin, and a Na (approximately Na\(^+\)) at \( \vec{r} = (a/2, 0, 0) \) where the lattice constant (edge of the “conventional cube”) is \( a \). Let us make a tight-binding model with a minimal basis of a single Na s-orbital, and three Cl p-orbitals. We can write Bloch orbitals as

\[
| \vec{k}s > = \sqrt{\frac{1}{N}} \sum \ell e^{i\vec{k} \cdot \vec{\ell}} \psi_A(\vec{r} - \vec{\ell} - \vec{r})
\]

\[
| \vec{k}x > = \sqrt{\frac{1}{N}} \sum \ell e^{i\vec{k} \cdot \vec{\ell}} \psi_x(\vec{r} - \vec{\ell})
\]

and similarly for \( |\vec{k}y > \) and \( |\vec{k}z > \). These Bloch orbitals will be assumed to be an orthonormal basis, and the Hamiltonian matrix will be truncated (to 4 × 4) at this point.
a. You will need to know the value of integrals like

\[ \int d\vec{r} \psi_a(\vec{r} + \vec{\tau}) \hat{H} \psi_a(\vec{r} + \vec{\tau}) \]

\[ \int d\vec{r} \psi_x(\vec{r}) \hat{H} \psi_x(\vec{r}) \]

\[ \int d\vec{r} \psi_x(\vec{r}) \hat{H} \psi_x(\vec{r} \pm a\hat{x}/2) \]

\[ \int d\vec{r} \psi_x(\vec{r}) \hat{H} \psi_x(\vec{r} \pm a\hat{y}/2) \]

\[ \int d\vec{r} \psi_x(\vec{r}) \hat{H} \psi_x(\vec{r} \pm a\hat{z}/2) \]

\[ \int d\vec{r} \psi_x(\vec{r}) \hat{H} \psi_x(\vec{r} \pm a\hat{x}/2) \]

All farther-distance Hamiltonian matrix elements will be set to zero. Set the first to a positive value \(\epsilon_a\) (maybe 3 eV, to have a number) and the second to zero (why is this OK?) Some of the remaining ones are zero by symmetry, and the rest which are non-zero, can be parameterized in terms of a number \(t\) (about 0.6 eV), defined as

\[ \int d\vec{r} \psi_x(\vec{r}) \hat{H} \psi_x(\vec{r} - a\hat{x}/2) = -t \]

Using these definitions and being careful about signs etc., write the 4 \(\times\) 4 Hamiltonian matrix.

b. Find eigenvalues and eigenvectors.

c. Sketch the dispersion relations along the two directions (1) the “Δ” direction, from \(\vec{k} = 0\) (the “I” point) to \(\vec{k} = (2\pi/a,0,0)\) (the “X” point), and (2) the “Λ” direction from \(\vec{k} = 0\) to \(\vec{k} = (\pi/a,\pi/a,\pi/a)\) (the “L” point).