Problem Set 6
Physics 520

Fall 2005
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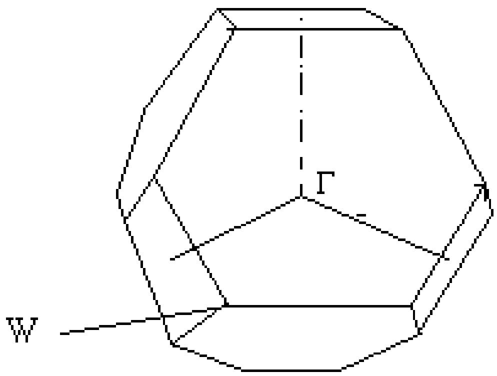
11/15/05 due 11/22/05

1.) a.) Consider the point W; where $\mathbf{k}_W = (2\pi/a)\,[1, 0.5, 0]$ in the Brillouin zone of a fcc metal.



The free electron bands are four-fold degenerate at W. Prove this, i.e., find 3 **G**'s such that $\hbar^2 \mathbf{k}_W{}^2/2m = \hbar^2[\mathbf{k}_W + \mathbf{G}]^2/2m$. One of the solutions is $\mathbf{G} = 2\pi/a[1,1,1]$.
b.) Set up the 4x4 determinant for the $\varepsilon_{\mathbf{k}}$'s near $\mathbf{k}_W$ in terms of the V_G's. Assume that V_G is real and that $V[2\pi/a(111)] = V[2\pi/a(11\text{-}1)]$
Solve for the energies within the manifold spanned by the four degenerate **G**'s and sketch the band structure for a short distance along the line leading from W to the center of the zone. (See Ashcroft and Mermin, prob. 9.3)

2. a.) Show that the charge density for a wavefunction of the Bloch form is periodic.
b.) Define the Wannier function for the nth band as follows:

$$w_n(\mathbf{r},\mathbf{R}) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}}\psi_{n,\mathbf{k}}(\mathbf{r}).$$

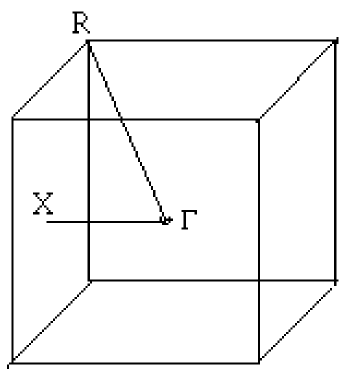
The sum is over the Brillouin zone, **R** is a lattice vector. Show that w depends only on **r - R**.
c.) Show that $\langle w_n(\mathbf{r},\mathbf{R}) | w_m(\mathbf{r},\mathbf{S})\rangle = \delta_{m,n}\,\delta_{R,S}$
d.) Suppose that $\psi_{n,k}(r)$ is a tight-binding wavefunction made from a single atomic wavefunction $\phi(r)$. What is the relationship between w and ϕ?
e.) Consider a one dimensional crystal of lattice constant a. Suppose the Bloch function is of the form $u_o(x)e^{ikx}$, where u_o is independent of k. Find w and show that the charge density associated with w is peaked near one lattice site.

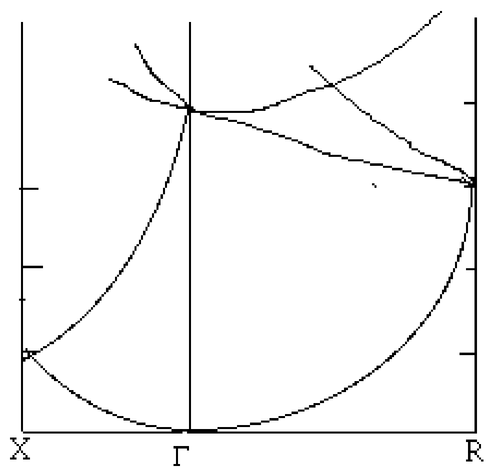
3.) a.) Suppose there are several identical atoms in a unit cell each having an identical potential of interaction $v(\mathbf{r})$ with the electrons. Put
$V_{tot} = \Sigma_{lm}\, v(\mathbf{r} - \mathbf{R}_l - \rho_m)$ $\mathbf{R}_l$ = Bravais lattice point; ρ_m runs over basis
Show that the quantity that determines the gaps in the nearly free electron model is

$V_{\mathbf{G}} = S(\mathbf{G})\, v_{\mathbf{G}}$ where $S(\mathbf{G}) = \Sigma_m\, e^{i\,\mathbf{G}\cdot\rho_m}$. i.e. the geometric structure factor.
b.) Prove that a monovalent element with the hexagonal close packed structure (hence with 2 electrons per unit cell) *must* be a metal.

4. Work out the spin susceptibility of the electron gas to order $(k_BT)^2$. (Hint: in a magnetic field each electron has kinetic energy and Zeeman energy: $\varepsilon \pm g\mu H$, where g is the g factor (near to 2), μ is the Bohr magneton, and H the magnetic field. You need a separate integral over the spin-up electrons and spin-down ones. But the chemical potential is the same for both. For the T=0 part, see Kittel).

5.) Consider a divalent simple cubic metal. Sketch the energy bands up to the Fermi energy for the two directions shown.in the free electron model.





I give a partial answer here. Locate the Fermi energy and put a scale on the picture. Be sure that you write each band in the form: $\varepsilon_{\mathbf{k}} = (\hbar^2/ 2m)[\mathbf{k}+\mathbf{G}]^2$ and find the $\mathbf{G}$'s and put them on the picture.

6.) a.) Find the tight-binding band structure for a bcc lattice with nearest neighbor overlaps. b.) Find the effective mass near the bottom of the band.