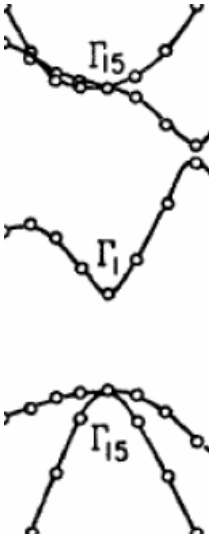
PHY 555 Fall 2007 HW #4

Due Mon.. Oct. 15



1. Electron gas in doped GaAs The bottom of the conduction band of GaAs occurs at the Γ point of the Brillouin zone, labeled Γ_1 in the fragment on the right, excerpted from Lecture 13 p6. Four valence bands are filled: Γ_1 at the bottom, not shown, and the triply degenerate Γ_{15}. The gap between Γ_{15} and Γ_1 is 1.5 eV. The conduction band is spherically symmetric around k=0, with *E(k)* given by $\hbar^2k^2/2m^*$, where m^* is 0.067 m_e, and m_e is the electron mass. This semiconductor can be intentionally doped with "n-type" (or "p-type", but that is a little more complicated) carriers. For example, Se in place of As, or Si in place of Ga, gives excess electrons. A typical doping level is 3 x 10^{18} electrons/cm^3. What is the (a) Fermi wavevector in cm^{-1} and Å^{-1}, (b) Fermi energy in eV, (c) Fermi temperature?

2. **"k dot p" perturbation theory**. (a) Show that a Bloch state for an electron can be written as $\psi_{n\vec{k}} = \exp\left(i\vec{k}\cdot\vec{r}\right)u_{n\vec{k}}\left(\vec{r}\right)$, where $u_{n\vec{k}}\left(\vec{r}\right)$ has the periodicity of the lattice. (b) Show that $u_{n\vec{k}}\left(\vec{r}\right)$ obeys the Schrödinger equation

$$\left[\left(\vec{p}+\hbar\vec{k}\right)^2/2m + V\left(\vec{r}\right) - \varepsilon_n\left(\vec{k}\right)\right]u_{n\vec{k}}\left(\vec{r}\right) = 0\,.$$

(c) Suppose you know a complete set of states at $\vec{k}=0$, labeled as $u_n\left(\vec{r}\right)$ and ε_n. You also need to assume that $V\left(\vec{r}\right)=V\left(-\vec{r}\right)$ and that $u_n\left(-\vec{r}\right)=\pm u_n\left(\vec{r}\right)$, that is, that the $\vec{k}=0$ states are eigenstates of inversion. Use second order Rayleigh- Schrödinger perturbation theory to find $\varepsilon_n\left(\vec{k}\right)$ to second order in $\vec{k}$. Find a formula for *m**, defined through the inverse mass tensor ($\hbar^2/m^*_{\alpha\beta} \equiv \partial^2\varepsilon/\partial k_\alpha \partial k_\beta$) at $\vec{k}=0$, and explain why the electron mass of GaAs is small (remember problem 1).

3. Rocksalt energy band in nearest neighbor LCAO approximation. The most common rocksalt structure materials (like NaCl itself, which gives its name to the crystal structure) have valence bands built mainly from anion *p* states, and conduction bands from cation *s* states. But let us simplify, and assume the material has atoms A and B, with only a single important *s* state per atom, of energy ε_A and ε_B respectively. Let $\left|\vec{\ell}A\right\rangle$ denote the *s* orbital on the A atom in the unit cell $\vec{\ell}$, and let $\left|\vec{\ell}'B\right\rangle$ be the corresponding *s* orbital on the B atom in the same cell, where $\vec{\ell}$ and $\vec{\ell}'$ differ by *a/2* in the *x* direction, which is of course not a translation vector. Let these orbitals be orthonormal to each other. Then we need only know the "ovelap integrals" $\left\langle\vec{\ell}'A\middle|H\middle|\vec{\ell}A\right\rangle$, $\left\langle\vec{\ell}'B\middle|H\middle|\vec{\ell}B\right\rangle$, and $\left\langle\vec{\ell}'A\middle|H\middle|\vec{\ell}B\right\rangle$, in order to construct the LCAO 2 x 2 matrix .

$$H_{ij}\left(\vec{k}\right) = \left\langle\vec{k}i\middle|H\middle|\vec{k}j\right\rangle$$

where $\left|\vec{k}i\right\rangle$ and $\left|\vec{k}j\right\rangle$ are Bloch LCAO's built from the orbitals A,B. The indices i,j refer to A or B. Make the nearest neighbor approximation. Then only a few non-zero numbers determine the H matrix, namely $\left\langle \vec{\ell}A\middle|H\middle|\vec{\ell}A\right\rangle = \varepsilon_A$ and $\left\langle \vec{\ell}'B\middle|H\middle|\vec{\ell}'B\right\rangle = \varepsilon_B$ and $\left\langle \vec{\ell}'A\middle|H\middle|\vec{\ell}B\right\rangle = -t$ for the case where $\vec{\ell}$ and $\vec{\ell}'$ are nearest neighbors (that is, if $\vec{\ell}$ is a translation vector, then $\vec{\ell}'$ is a translation plus a displacement by *a/2* in the *x, y*, or *z* direction) . We expect *t* to have magnitude around 1 eV. (a) Derive formulas for the elements of the matrix $H_{ij}\left(\vec{k}\right)$. (b) Find the two eigenvalues $\varepsilon_n\left(\vec{k}\right)$ and show that there is a gap, which has its minimum value at $\vec{k} = (\pi/a)(1,1,1)$ (the "L" point). Relate the gap to the splitting ε_A-ε_B. (c) Plot the bands for $\vec{k} = (\pi/a)(\zeta,\zeta,\zeta)$ and $0<\zeta<1$ (the Γ to L line in the Brillouin zone.) For plotting purposes you can choose ε_A-ε_B=4*t*.