Physics 601 **Homework Set 3** **Fall, 2007**

Due date: Wednesday, Oct. 17. Recall that lecture has been moved from Wednesday Oct. 17 to Friday Oct. 19 (12:00-1:20 pm in ARC 205), so please leave the homework in my mail slot by the end of the day on Wednesday 10/17.

1) (30 points.) The Wannier function (WF) associated with band n and localized in the vicinity of the lattice vector $\mathbf{R}$ is defined in terms of the Bloch functions $|\psi_{n\mathbf{k}}\rangle$ to be

$$|w_{n\mathbf{R}}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} \, |\psi_{n\mathbf{k}}\rangle$$

a) Show that the WFs are periodic images of one another: $w_{n\mathbf{R}}(\mathbf{r}) = w_{n\mathbf{0}}(\mathbf{r}-\mathbf{R})$, where $|w_{n\mathbf{0}}\rangle$ is the WF in the home unit cell $\mathbf{R} = \mathbf{0}$.

b) Show that $\langle w_{n\mathbf{R}}|w_{n'\mathbf{R}'}\rangle = \delta_{n,n'}\,\delta_{\mathbf{R},\mathbf{R}'}$. Hint: It is easiest to stay in bra-ket notation; you may use the fact that $\langle\psi_{n\mathbf{k}}|\psi_{n'\mathbf{k}'}\rangle = \delta_{n,n'}\,\delta_{\mathbf{k},\mathbf{k}'}$.

c) Show that $\langle w_{n\mathbf{R}}|H|w_{n'\mathbf{R}'}\rangle = \widetilde{E}_n(\mathbf{R}-\mathbf{R}')\delta_{nn'}$, where $\widetilde{E}_n$ is some function which depends only on the relative displacement $\mathbf{R}-\mathbf{R}'$.

d) Show that $\widetilde{E}_n(\mathbf{R})$ is proportional to the Fourier transform of the band-structure function $E_n(\mathbf{k})$. [Here $E_n(\mathbf{k})$ is a periodic function in k-space, and $\widetilde{E}_n(\mathbf{R})$ is its discrete transform in real space, just the reverse of the usual case.]

2) (30 points)
Consider a simple cubic Bravais lattice with lattice constant a. Suppose there is an energy band with the dispersion relation

$$\epsilon(\mathbf{k}) = \epsilon_0 - 2V\cos(k_x a) - 2V\cos(k_y a) - 2V\cos(k_z a) \ ,$$

where $V > 0$, and suppose that this band is almost but not quite completely empty.

(a) Show that the inverse effective mass matrix is diagonal at $\mathbf{k} = \mathbf{0}$ for this band, i.e., m^* is isotropic, and find m^*.

(b) Suppose that the occupied fraction of the band is x (i.e., the average number of electrons per atom in this band is $2x$). In the limit that x is small, so that the effective-mass description of part (a) is applicable, find the Fermi wavevector k_F (the radius of the Fermi surface) and the Fermi velocity v_f (the group velocity at the Fermi surface).

(c) The electronic specific heat of this system will be linear in temperature T at very low T. As T is increased, for a given $x \ll 1$, at roughly what temperature would you expect a breakdown of this linear scaling of the electronic specific heat?

3) (10 points)

(a) In Si, one of the conduction band minima occurs at $\mathbf{k}_0 = \frac{2\pi}{a}\gamma(1,0,0)$ with $\gamma \simeq 0.85$. Suppose some electron states in the valley at $\mathbf{k}_0$ are occupied; does the Pauli exclusion principle then prevent some states in the valley at $-\mathbf{k}_0$ from being occupied?

(b) In Ge, one of the conduction band minima occurs at $\mathbf{k}_0 = \frac{\pi}{a}(1,1,1)$. Suppose some electron states in the valley at $\mathbf{k}_0$ are occupied; does the Pauli exclusion principle then prevent some states in the valley at $-\mathbf{k}_0$ from being occupied?