AP 295a **Problem Set 2** **Due: Wednesday, March 5, 2003**

Problem 1

Assume we have a two-dimensional nearly free-electron system on a square lattice of lattice spacing a. The Fourier transform of the weak lattice potential is $V(\vec{G})$. We want to investigate the band structure around the $(\frac{\pi}{a}, \frac{\pi}{a})$ point in the reciprocal lattice. The unperturbed spectrum has a fourfold degeneracy at this point. Only the $\vec{G} = (0, \frac{2\pi}{a})$ and the $\vec{G} = (\frac{2\pi}{a}, \frac{2\pi}{a})$ components of $V(\vec{G})$ are important. Find the electron energies at $k = (\frac{\pi}{a}, \frac{\pi}{a})$ if:
a) $V(0, \frac{2\pi}{a}) = V_0$ and $V(\frac{2\pi}{a}, \frac{2\pi}{a}) = 0$;
b) $V(0, \frac{2\pi}{a}) = 0$ and $V(\frac{2\pi}{a}, \frac{2\pi}{a}) = V_1$.

Problem 2

An electron of mass m moves in a square lattice of lattice spacing a. The nearly free electron approximation applies

(a) With one electron per site in the crystal, draw the Fermi surface on the k_x, k_y plane. Is this a metal or an insulator?

(b) With two electrons per site, draw the Fermi surface. Is this a metal or an insulator?

Problem 3

Consider electrons on a two-dimensional square lattice (lattice constant a) in the tight binding approximation (assume that the next band is very high in energy),

$$E = -E_0(cosk_x a + cosk_y a)$$

(a) With one electron per site in this crystal, draw the Fermi surface. Is this a metal or an insulator?

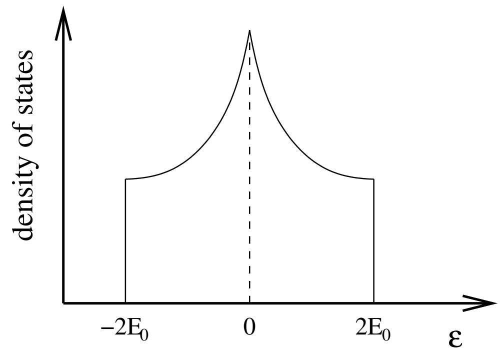
(b) With two electrons per site, draw the Fermi surface. Is this a metal or an insulator?

Problem 4

The density of states for a two-dimensional system of electrons with the "tight-binding" band structure

$$E(k) = -E_0(cosk_x a + cosk_y a)$$

is shown in the figure below. Investigate the density of states in the neighborhood of $E = 0$



Problem 5

For the problem 4c from PS1, consider the case $V_0 < 0$ $|V_0| \gg \frac{\hbar^2}{ma^2}$. Calculate the bandwidth and compare the result to the bandwidth obtained in the tight-binding approximation.

Problem 6

In the Thomas-Fermi theory one approximates the kinetic energy by the local functional of density and neglects the exchange term in the interaction. This gives an equation on the density

$$n(\vec{r})\,\frac{\hbar^2}{2m}\,(3\pi^2)^{\frac{2}{3}}\,n^{\frac{2}{3}}\,(\vec{r})\;+U(\vec{r})\;+\int d^3\vec{r}\,'\;\frac{e^2 n(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|} = \mu$$

with the constraint $\int d^3\vec{r}\,n(\vec{r}) = N$, where N is the total number of electrons. Consider an atom with nuclear charge Z and Z electrons, so that the potential is

$$U(\vec{r}) = -\,\frac{ze^2}{|\vec{r}|}$$

Take the density $n(r)$ in the form

$$\frac{n(r) = [2mV(r)]^{\frac{3}{2}}}{3\pi^2\hbar^3}$$

with $V(r) = \frac{Ze^2}{r}\,\chi(r)$

(a) Show that $\chi(r)$ satisfies an equation

$$s^{\frac{1}{2}}\,\frac{d^2\chi}{ds^2}\;=\;\chi^{\frac{3}{2}}$$

where $s = \frac{r}{b}$, $b = \frac{a_0}{z}(\frac{3\pi}{4})^{\frac{2}{3}}\,Z^{-\frac{1}{3}}$, and a_0 is the Bohr radius

(b) Show that the boundary conditions on χ require that $\chi(0) = 1$ and $\chi(\infty) = 0$