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Exercise Set 10
(Due date: Tuesday, January 19, 2010)

Exercise 21 (**Tight binding for two-dimensional lattice**) (25 points)

Consider a system of N electrons in a two-dimensional square lattice with lattice constant a. The tight binding matrix elements for a single band n are given by

$$\langle n\vec{R}|H|n\vec{R}'\rangle = \begin{cases} \varepsilon_0\,, & \vec{R} = \vec{R}' \\ -t\,, & \vec{R} - \vec{R}' = \vec{\rho} = \text{nearest neighbour vector} \\ 0\,, & \text{otherwise.} \end{cases}$$

a) Find the dispersion relation $\varepsilon(\vec{k})$ for this system in tight binding approximation.

b) Plot a few constant energy lines on the (k_x, k_y) plane.

c) Show that most of the constant energy lines cross the Brillouin zone boundary at a right angle.

d) Sketch $\varepsilon(\vec{k})$ along the $W - X$ line of the Brillouin zone where $W = (\pi/a, \pi/a)$ and $X = (\pi/a, 0)$.

e) Assuming that the crystal has only one electron per lattice site, draw the Fermi surface. Is this a metal or an insulator?

f) Consider now the case of two electrons per site. Is this a metal or an insulator?

g) Calculate the density of states as a function of energy close to $\varepsilon = \varepsilon_0$. Discuss your result.