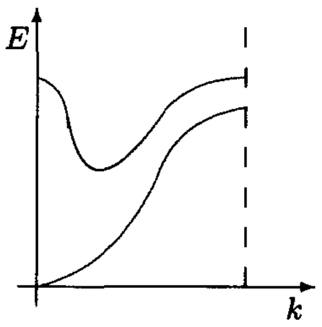
Condensed Matter Physics (I): Homework 5
Due: December 30, 2019

Exercises in Ashcroft/Mermin

9-1,9-3

Ex.1 10% Is it possible to have band overlap as shown in the following figure for one dimensional lattice with inversion symmetry ? Prove your answer.



Ex.2 20% Graphene has a two-dimensional regular hexagonal reciprocal lattice whose primitive translations are $b_1 = \frac{2\pi}{a}(1, -\frac{1}{\sqrt{3}})$ and $b_2 = \frac{2\pi}{a}(0, \frac{2}{\sqrt{3}})$.

(a) List the operations of point groups that make Γ point [$= (0,0)$ in k space], K point [$= \frac{2\pi}{a}(\frac{2}{3}, 0)$], and M point [$= \frac{2\pi}{a}(\frac{1}{2}, \frac{1}{2\sqrt{3}})$] invariant.

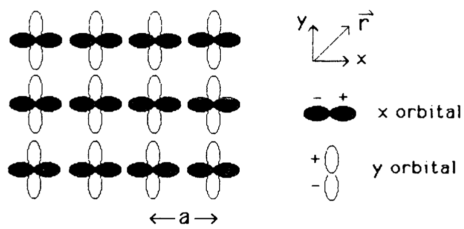
(b) Write down the empty lattice wave functions and energies $\Psi_l(k,r)$ and $E_l(k)$ at Γ and K.

(c) Tabulate the energies at Γ and K for $(l_1, l_2) = (0,0), (0,\pm 1), (\pm 1, 0), (-1,-1), (1,1)$.

(d) Sketch E vs. k along the line from Γ to K for these bands.

Ex.3 25% Tight binding p bands on a square lattice

Electronic bands on a simple square lattice are formed out of the two atomic $2p$ orbitals, energy E_p, which have the wavefunctions $\phi_1 = x\phi(r)$, $\phi_2 = y\phi(r)$, where $\phi(r)$ is real, positive and depends only magnitude of the vectors $\vec{r} = (x, y)$, decreasing as r increases.



The Bloch solution can be written as

$$\psi_{\vec{k}}(\vec{r}) = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \left[\sum_{i=1}^{2} b_i \phi_i(\vec{r} - \vec{R}) \right], \tag{1}$$

with the equation for b_i and the eigenvalue $\epsilon(\vec{k})$ be given by

$$(\epsilon(\vec{k}) - E_p) b_i = \sum_{j=1}^{2} (\beta_{ij} + \bar{\gamma}_{ij}(\vec{k})) b_j. \tag{2}$$

Here we define

$$\begin{aligned} \bar{\gamma}_{ij}(\vec{k}) &= \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \gamma_{ij}(\vec{R}) \\ \gamma_{ij}(\vec{R}) &= -\int d^3\vec{r} \phi_i^*(\vec{r}) \phi_j(\vec{r} - \vec{R}) \Delta U(\vec{r}) \\ \beta_{ij} &= \gamma_{ij}(\vec{R} = 0), \end{aligned}$$

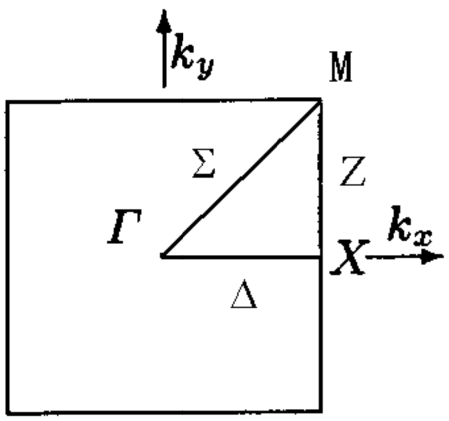
where $\Delta U(\vec{r})$ is the crystal potential and we neglected overlap of ϕ at different site.

(a) Show $\beta_{11} = \beta_{22}$ and $\beta_{12} = 0$.

(b) Assume that $\gamma_{ij}(\vec{R})$ are negligible except for nearest neighbors. Calculate the energy bands $\epsilon_1(\vec{k})$ and $\epsilon_2(\vec{k})$ in terms of the overlaps to nearest neighbors in the x and y directions $\gamma_1 = \gamma_{11}(a\hat{x})$ and $\gamma_2 = \gamma_{11}(a\hat{y})$.

(c) Sketch the energy contours in the 1st Brillouin zone for the band formed from ϕ_1. (Note that γ_1 is positive and γ_2 is negative. You may take them to be roughly equal in magnitude.)

Ex.4 40% Consider a two dimensional square lattice of lattice constant a. The 1st Brillouin zone is shown in the below.



(a)If the electron can be described by a tight binding model with only nearest neighboring hopping amplitude t, on a plot, show the energy of the electron $\epsilon(k)$ from Γ to M along Σ, then from M to X along Z and then from X back to Γ along Δ.

(b)Following (a), draw the density of states per area $g(\epsilon)$. How does $g(\epsilon)$ change for ϵ being close to $\epsilon = 0$?

(c)Now suppose that the electron is in the potential

$$U(\vec{r}) = -4U_0 \cos\frac{2\pi x}{a}\cos\frac{2\pi y}{a} \tag{3}$$

Find the Fourier transformation of U.

(d) From (c), by using the 4-fold symmetry of square lattice and considering the largest component of U, find energies at M point. Sketch $\epsilon(\vec{k})$ from Γ to M along Σ.

Ex.5 10% Consider the generalization of square lattice ($d = 2$) and cubic lattice ($d = 3$) to general a d-dimension lattice with each lattice point being surrounding by $2d$ nearest neighbors. If the electron can be described by a tight binding model with only nearest neighboring hopping amplitude t, find the asymptotic form of density of states for the electron at $d \to \infty$ (neglect spin degree of freedom).