Tight binding bands - DOS - cyclotron orbits

Exercise 1: Tight binding bands in the square lattice

Consider a square lattice with one $s$ orbital per site, only nearest-neighbor interactions and neglect overlap.

1. Show that the expression of the tight binding $s$-band is:

$$E(k) = E_{1s} - 2\gamma (\cos k_x a + \cos k_y a)$$

where $\gamma = -\int \phi_{1s}(r) \Delta U(r) \phi_{1s}(r - R) \, dr$; $R$ are Bravais lattice vectors joining the nearest-neighbour sites to the origin, and $\gamma > 0$.

2. Show that the band has remarkable symmetry properties: the band $E(k)$ is symmetric with respect to $E_{1s}$, in the sense that every state at $E - E_{1s}$ has a corresponding state at $-(E - E_{1s})$, and, more precisely:

$$E(k) - E_{1s} = -\left[ E \left( k - \frac{\pi}{a}(1,1) \right) - E_{1s} \right]$$

3. Show that the Fermi energy coincides with $E_{1s}$ in case of half-filled band.

4. Plot the Brillouin zone and the Fermi surface in case of half-filled band.

5. Plot $E(k)$ along $\Gamma$-$M$-$X$-$\Gamma$, where $M = \frac{\pi}{a}(1,0)$ and $X = \frac{\pi}{a}(1,1)$.

6. Show that: $\Gamma$ corresponds to the minimum, $X$ to the maximum, $M$ to a saddle point.

7. Plot the density of states $g(E)$ and show that it diverges at $E_F$ (set to 0 in the figure below) with a logarithmic divergence. The figure also shows the occupied states in case of half filling of the band.
Exercise 2: Tight binding bands of "cubium"

Similarly as above, consider now the 3D case. Consider a simple cubic lattice with one s orbital per site, only nearest-neighbor interactions and neglect overlap (a toy model known also as cubium).

1. Show that the expression of the tight binding s-band is:

\[ E(k) = E_{1s} - 2\gamma (\cos k_x a + \cos k_y a + \cos k_z a) \]

where \( \gamma = -\int \phi_{1s}(r) \Delta U(r) \phi_{1s}(r-R); R \) are Bravais lattice vectors joining the nearest-neighbour sites to the origin, and \( \gamma > 0 \).

2. Plot \( E(k) \) along \( \Gamma-X-M-\Gamma-R \), where \( X = \frac{\pi}{a}(1,0,0), M = \frac{\pi}{a}(1,1,0) \) and \( R = \frac{\pi}{a}(1,1,1) \).

3. Plot the density of states \( g(E) \).

Exercise 3: Semiclassical theory of electron dynamics: cyclotron orbits

Consider the problem of a cyclotron orbit in the \((k_x,k_y)\) plane (suppose an external uniform magnetic field \( H \) applied in the z direction, and \( k_z(t=0) = \dot{k}_z(t=0) = 0 \)) for a SC crystal with band structure:

\[ \mathcal{E}(k) = \mathcal{E}_0 - 2A[\cos(ak_x) + \cos(ak_y) + \cos(ak_z)] \]

1. Show that the equation for the orbit with a given energy \( \mathcal{E} \) close to the minimum \( \mathcal{E}_{min} \) is: \( \mathcal{E} = \mathcal{E}_{min} + Aa^2 (k_x^2 + k_y^2) \).

2. Calculate the period of the orbit as a function of the parameter \( A \).

3. Describe the orbit in real space.

4. Generalize your result to a crystal with band structure:

\[ \mathcal{E}(k) = \mathcal{E}_0 - 2[A \cos(ak_x) + B \cos(ak_y) + C \cos(ak_z)] \]