Tight binding bands - DOS

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:

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

   where $\gamma = -\int \phi_{1s}(\mathbf{r})\,\Delta U(\mathbf{r})\,\phi_{1s}(\mathbf{r}-\mathbf{R})$; $\mathbf{R}$ 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 $E(\mathbf{k})$ 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: $E(\mathbf{k}) - E_{1s} = -\left[E\left(\mathbf{k} - \frac{\pi}{a}(1,1)\right) - E_{1s}\right]$

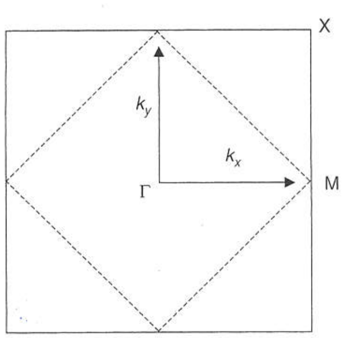
3. Show that the Fermi energy coincides with E_{1s} in case of half-filled band.

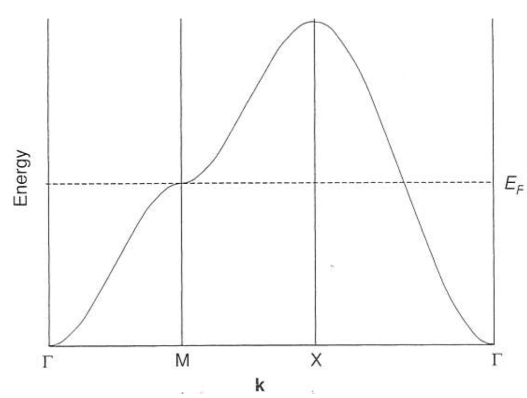
4. Plot the Brillouin zone and the Fermi surface in case of half-filled band.

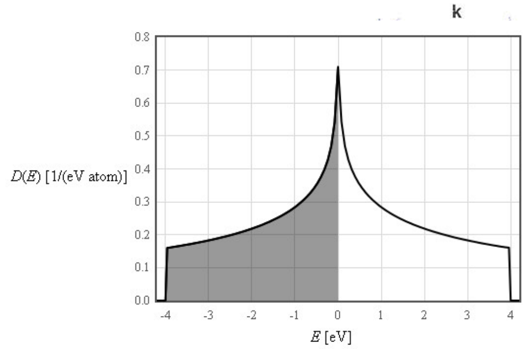
5. Plot $E(\mathbf{k})$ along Γ-M-X-Γ, where $M = \frac{\pi}{a}(1,0)$ and $X = \frac{\pi}{a}(1,1)$.

6. Show that: Γ 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*).

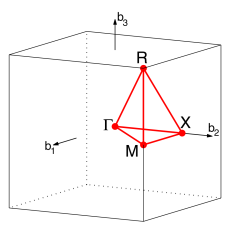
1. Show that the expression of the tight binding s-band is:

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

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

2. Plot $E(\mathbf{k})$ along Γ-X-M-Γ-R, where $X = \dfrac{\pi}{a}(1,0,0)$, $M = \dfrac{\pi}{a}(1,1,0)$ and $R = \dfrac{\pi}{a}(1,1,1)$.

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



CUB path: Γ-X-M-Γ-R-X|M-R

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