Homework 1, 620 Many body

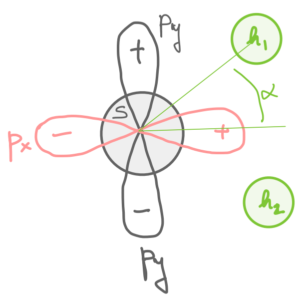
September 27, 2022

1) Using canonical transformation show that at half-filling and large interaction U the Hubbard model is approximately mapped to the Heisenberg model with the form

$$H = J \sum_{<ij>} \vec{S}_i \vec{S}_j - 1/4 \tag{1}$$

where $J = 4t^2/U$. Solution is in A&S page 63.

2) Obtain energy spectrum and the ground state wave function for water molecule in the tight-binding approximation. You can use the following tight-binding values $\varepsilon_s = -1.5$ Ry, $\varepsilon_p = -1.2$ Ry $\varepsilon_H = -1$ Ry t_s = -0.4 Ry t_p = -0.3 Ry $\alpha = 52°$



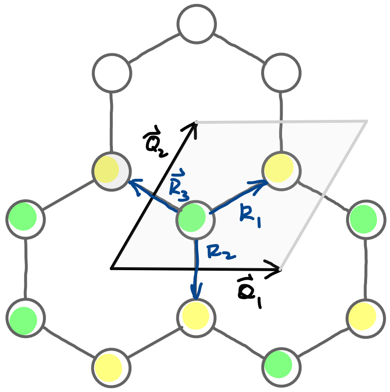
- Determine eigenvalue spectrum from tight-binding Hamiltonian
- The oxygen configuration is $2s^2\ 2p^4$ and hydrogen is $1s^1$, hence we have 8 electrons in the system. Which states are occupied in this model?
- What is the ground state wave function?

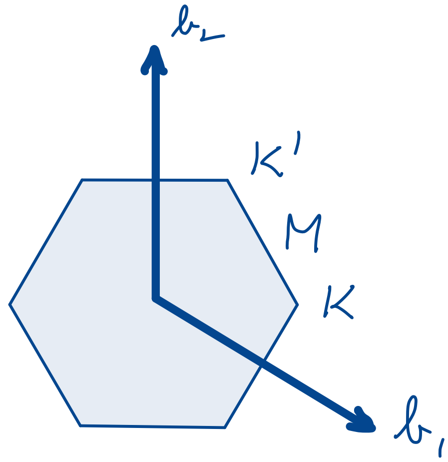
3) Obtain the band structure of graphene and plot it in the path $\Gamma - K - M - \Gamma$. The hooping integral is t.

   Show that expansion around the K point in momentum space leads to the following Hamiltonian

$$H_{\mathbf{k}} = \frac{\sqrt{3}}{2} t\, (\mathbf{k} - \mathbf{K}) \cdot \vec{\sigma} \tag{2}$$

   where $\vec{\sigma} = (\sigma^x, \sigma^y)$ and σ^α are Pauli matrices. From that argue that the energy spectrum around the K point has Dirac form.





Let's use the standard notation

$$\vec{a}_1 = a(1, 0) \tag{3}$$

$$\vec{a}_2 = a(\frac{1}{2}, \frac{\sqrt{3}}{2}) \tag{4}$$

$$\vec{b}_1 = \frac{2\pi}{a}(1, -\frac{1}{\sqrt{3}}) \tag{5}$$

$$\vec{b}_2 = \frac{2\pi}{a}(0, \frac{2}{\sqrt{3}}) \tag{6}$$

Here $r_1 = \frac{1}{3}\vec{a}_1 + \frac{1}{3}\vec{a}_2$ and $r_2 = \frac{2}{3}\vec{a}_1 + \frac{2}{3}\vec{a}_2$. The K point is at $\mathbf{K} = \frac{1}{3}\vec{b}_2 + \frac{2}{3}\vec{b}_1$ and M point is at $\vec{M} = \frac{1}{2}(\vec{b}_1 + \vec{b}_2)$.