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

$$H = J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j - 1/4$$  \hspace{1cm} (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 $\alpha = 52^\circ$

- 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

$$H_k = \frac{\sqrt{3}}{2} t (k - K) \cdot \vec{\sigma}$$  \hspace{1cm} (2)

where $\vec{\sigma} = (\sigma_x, \sigma_y)$ and $\sigma^a$ are Pauli matrices. From that argue that the energy spectrum around the $K$ point has Dirac form.
Let’s use the standard notation

\[
\begin{align*}
\vec{a}_1 &= a(1, 0) \quad (3) \\
\vec{a}_2 &= a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right) \quad (4) \\
\vec{b}_1 &= \frac{2\pi}{a}(1, -\frac{1}{\sqrt{3}}) \quad (5) \\
\vec{b}_2 &= \frac{2\pi}{a}(0, \frac{2}{\sqrt{3}}) \quad (6)
\end{align*}
\]

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 \( \vec{K} = \frac{1}{3}\vec{b}_2 + \frac{2}{3}\vec{b}_1 \) and \( M \) point is at \( \vec{M} = \frac{1}{2}(\vec{b}_1 + \vec{b}_2) \).