Abstract

One of the important type of interactions that is ignored in a TB model is the Coulomb energy cost of putting two electrons on the same site. Including such a term leads to important consequences like a Mott insulating state. In this exercise we look at how the inclusion of "a large" on-site coulomb energy effectively translates to a Heisenberg interaction between the electrons.

Exercise 1: Heitler London model

Consider two Hydrogen atoms 'a' and 'b' separated by a finite distance. Taking a Hamiltonian with large Coulomb repulsion, we can ignore the states which contain two electrons on the same orbital(Heitler-London orbitals). A variational state for this system can be written as

$$|c\rangle = \frac{1}{\sqrt{2}}(|ab\rangle + c\,|ba\rangle) \tag{1}$$

where $|ab\rangle$ represents the state with first electron on Hydrogen 'a' and second on 'b'. Representing

$$\langle ab\,|ba\rangle = L^2, \quad \langle ab|\,H\,|ab\rangle = \langle ba|\,H\,|ba\rangle = V, \quad \langle ab|\,H\,|ba\rangle = \langle ba|\,H\,|ab\rangle = X \tag{2}$$

a) Maximize the variational energy $E = \frac{\langle c|H|c\rangle}{\langle c|c\rangle}$ and find the values of 'c' corresponding to the extrema. What are the states corresponding to these values ?

b) Include the spin component of the wavefunction(singlet/triplet) and enforce the antisymmetry of fermion wave function to obtain the final wave functions.

c) Show that the Hamiltonian can be replaced by an effective Heisenberg like Hamiltonian(plus a constant which can be ignored).

$$H = -JS_1 \cdot S_2$$

What is the corresponding coupling constant J?

Hint: for point c), consider that $S_1 \cdot S_2 = \frac{1}{2}(S_{tot}^2 - S_1^2 - S_2^2)$

Exercise 2: Hubbard model

A Hubbard Hamiltonian is given by,

$$H = \underbrace{-t\sum_{ij\sigma} c^\dagger_{i\sigma}c_{j\sigma}}_{T} + \underbrace{U\sum_i c^\dagger_{i\uparrow}c_{i\uparrow}c^\dagger_{i\downarrow}c_{i\downarrow}}_{V} \tag{3}$$

consider a half filled case(one electron per site) with $t/U << 1$. In this scenario the lowest energy sector corresponds to a states with no double occupancies $|\alpha\rangle$,$|\beta\rangle$ such that,

$$V|\alpha\rangle = 0, \qquad V|\beta\rangle = 0$$

a) Considering $|\alpha\rangle$ as ground state and kinetic energy term as a perturbation, what will be the first order perturbation matrix elements between two degenerate ground states $|\alpha\rangle$,$|\beta\rangle$?

b)What is the second order perturbation matrix element? Show that the effective Hamiltonian for this correction, in terms of fermionic operators, becomes:

$$H^{(2)} = \frac{-t^2}{U}\sum_{ij}\sum_{\sigma\sigma'} c^\dagger_{i\sigma}c_{j\sigma}c^\dagger_{j\sigma'}c_{i\sigma'}$$

c) Consider four states $|\alpha_{\sigma\sigma'}\rangle$, where $\{\sigma,\sigma'\} \in \uparrow,\downarrow$ which represent spin σ occupies a site i and σ' occupies a site j. Express the above obtained effective Hamiltonian in matrix form acting on the space spanned by these four states.
Finally, show that the effective Hamiltonian, in this space, becomes a Heisenberg Hamiltonian:

$$H_{eff} = \frac{2t^2}{U}\left(S_i \cdot S_j - \frac{1}{4}\right) \tag{4}$$

Show that the total Hamiltonian becomes,

$$H^{(2)} = \frac{4t^2}{U}\sum_{<i,j>}\left(S_i \cdot S_j - \frac{1}{4}\right) \tag{5}$$

where $< i, j >$ is the sum over all pairs of i,j .

Hint: for point b), the second order correction to a Hamiltonian is given by:

$$\langle\alpha| H^{(2)} |\beta\rangle = \sum_\gamma \frac{\langle\alpha| T |\gamma\rangle \langle\gamma| T |\beta\rangle}{E_\alpha - E_\gamma}$$

Hint: for point c), the following expression is valid for the four states that we are considering

$$S_i \cdot S_j = \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix}$$