

1 HUBBARD MODEL

The Hubbard model is a simple model to understand the interaction of electrons inside a solid. It includes hopping of electrons between the sites of a lattice and the interaction between the electrons on the same site and the last term is the chemical potential term. The Hubbard model takes up the most general form of the Hamiltonian for a system of interacting electrons on a lattice and reduce the interaction only to the same site. In different limits of the model one can derive the tight binding model and the Heisenberg model. Consider a simple model to understand metal insulator transition, the magnetic properties of the system and the superconductivity. The model can be studied in the for different types of particles like fermions and bosons and in this chapter we'll discuss both of them first the The Fermi-Hubbard Model and then the Bose Hubbard Model.

1.1 The Fermi-Hubbard Hamiltonian

I'll simply introduce the Hamiltonian for the Fermi-Hubbard model as

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma}) + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} - \mu \sum_{i,\sigma} \hat{n}_{i,\sigma} \quad (1)$$

The different terms in the Hamiltonian are

1. First term is the hopping term which describes the hopping of electrons between the sites of the lattice.
2. Second term is the interaction term which describes the interaction between the electrons on the same site. Note that electrons of opposite spins can only occupy the same site.
3. Third term is the chemical potential term which describes the energy required to add an electron to the system.

1.1.1 Symmetries of the Hubbard Model

For this part we'll consider the fermi-hubbard model and discuss the symmetries of the model. The model has a lot of symmetries and we'll discuss them one by one.

1.1.2 Strong Interaction limit ($t = 0$)

1.1.3 Weak Interaction limit ($U = 0$)

1.2 The Bose-Hubbard Model

The Hamiltonian for the Bose-Hubbard model can be simply written as

$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i \quad (2)$$

there are few differences between the Fermi-Hubbard model and the Bose-Hubbard model as

1. There is no spin for bosons.
2. All the bosons can occupy the same site unlike the fermions.
3. In the interaction there is interaction of n particles with $n - 1$ particles and interestingly they can be on the same site.

1.2.1 Strong Interaction limit ($t = 0$)

There is no hopping between the sites of the lattice and the Hamiltonian reduces to

$$\hat{H} = \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i \quad (3)$$

where i takes up over all the the number of sites of the lattice, say M .

Now in the absence of the pauli's principle we have an infinite dimensional hilbert space at each site of the lattice and spanned by the fock basis $\beta_i = |n\rangle_j$ and we can take tensor product overall sites to get the full state for M site.

For a single site, we have $|n\rangle$ be the bosons present here, then we have the energy of the system be

$$H|n\rangle = \frac{U}{2}n(n-1) - \mu n = E(n)|n\rangle \quad (4)$$

clearly this grows quadratically for $U < 0$ it is unbounded below, so no ground state but we can fix this by fixing the number of the particles in the system and they all end up settling up in one well.

For repulsive model ($U > 0$), $\frac{dE(n)}{dn} = Un - \frac{U}{2} - \mu = 0$ then we have $\bar{n} = \frac{\mu}{U} + \frac{1}{2}$ in general $\bar{n} \in \mathbb{R}_{>0}$ so we have $\frac{\mu}{U} > -\frac{1}{2}$ and this additionally bounds $\mu \geq -\frac{U}{2}$. If, $\frac{\mu}{U} \in \mathbb{Z}$ then, we have two possibilities $\bar{n} \in \{\frac{\mu}{U}, \frac{\mu}{U} + 1\}$ both these possibilities lie symmetrically around the minima of E vs n curve around $\bar{n} = \frac{\mu}{U} + \frac{1}{2}$. Now every state is unique or doubly degenerate.

In degenerate case, $E_o \sim \frac{U}{2}(\frac{\mu}{U} + \frac{1}{2})(\frac{\mu}{U} - \frac{1}{2}) - \mu(\frac{1}{2} + \frac{\mu}{U}) = -\frac{(U+2\mu)^2}{8}$ and in unique case $E_o \sim \frac{U}{2}(\frac{\mu}{U})(\frac{\mu}{U} - 1) - \mu(\frac{\mu}{U}) = -\frac{\mu(U+\mu)}{2U}$. Now extra $\frac{1}{2}$ can simply change the scaling from $\sim U + \frac{1}{U}$ (non-degenerate) to $\sim \frac{1}{U}$ (degenerate).

Alternatively, we can find a ground state when, $(n-1)U < \mu < nU$, now at $\mu = nU$ we have level crossing between levels of adjacent number of bosons. Far from this point there is gap between the energy levels and they are protected against small perturbations in the system and these states are called **Mott States**.

Exercise 1.1: Show that there is level crossing between the energy levels of adjacent number of bosons(± 1) at $\mu = nU$. *Hint: Start with n_1 and n_2 fock states and show that they have equal energy at some point. Obviously as before level crossing at some point they should become equal so find this point.*

1.2.2 Weak Interaction limit ($U = 0$)

1.2.3 Phase Transition between Superfluid and Mott Insulator