Phys 506 lecture 39: Two-Site Hubbard model

1 Introduction and counting states

Consider the two-site Hubbard model Hamiltonian:

$$H = -t \sum_{\sigma} (c_{1\sigma}^{\dagger} c_{2\sigma} + c_{2\sigma}^{\dagger} c_{1\sigma}) + U \sum_{i=1}^{2} n_{i\uparrow} n_{i\downarrow}$$

If there are N sites, then we claim that there will be 4^N possible states since each site needs to be specified as either $0, \uparrow, \downarrow, \uparrow\downarrow$, i.e. vacant, one spin up particle, one spin down particle, or two particles with opposite spin. If we have a total of m electrons ($0 \leq m \leq 2N$), the number of states is given by:

$$\binom{2N}{m} = \frac{(2N)!}{m!(2N-m)!}$$

states with exactly m electrons. This follows since each electron can be spin-up or spin-down on each site. Hence, there are $2N$ choices, and we choose m of them. As a verification, we can check that

$$\sum_{m=0}^{2N} \binom{2N}{m} = 2^{2N} = 4^N$$

using the binomial theorem and if we choose $N = 2$, then we can count the number of states to be:

- $m = 0 : \binom{4}{0} = 1$ state.
- $m = 1 : \binom{4}{1} = 4$ states.
- $m = 2 : \binom{4}{2} = 6$ states.
- $m = 3 : \binom{4}{3} = 4$ states.
- $m = 4 : \binom{4}{4} = 1$ state.

Thus, adding up all states, we get 16 states which equals $4^N = 4^2$. Let's study each case more specifically.

2 Energy Eigenstates

1. $m = 0$: $J = 1, m_J = -1, S = 0$ is the ground state $|0\rangle$ with energy $E = 0$
2. $m = 1$: $J = 1/2, m_J = -1/2, S = 1/2$, considering spatial symmetry, this case has two states:
   - $|1\rangle = \frac{1\uparrow+2\uparrow}{\sqrt{2}}$ which is shorthand for $\frac{1}{\sqrt{2}}(c^\dagger_{1\uparrow}|0\rangle + c^\dagger_{2\uparrow}|0\rangle)$
   - $|2\rangle = \frac{1\uparrow-2\uparrow}{\sqrt{2}}$

   The energies can be found as:
   - $\hat{T}|1\rangle = -t|1\rangle$, so $E = -t$. Note that this state has a two fold degeneracy with $\uparrow$ and $\downarrow$ cases.
   - $\hat{T}|2\rangle = t|2\rangle$, so $E = t$. This state also has a two fold degeneracy as above.
3. $m = 2$:
   (a) $J = 1, m_J = 0, S = 0$. Here we have $J^\dagger|0\rangle = \frac{1}{\sqrt{2}}(1\uparrow 1\uparrow -2\uparrow 2\uparrow) = |1\rangle$ and $\hat{T}|1\rangle = -t\frac{1}{\sqrt{2}}(2\uparrow 1\downarrow +1\uparrow 2\downarrow -1\uparrow 2\downarrow -2\uparrow 1\downarrow) = 0$ and $\hat{U}|1\rangle = U|1\rangle$ which implies $E = U$ as it must since $J^\dagger$ raises E by U.

   (b) $J = 0, m_J = 0, S = 1$. Here we have $1\uparrow 2\uparrow = |1\rangle$ and $H|\uparrow\rangle = 0$ so $E = 0$ with a threefold degeneracy.

   (c) $J = 0, m_J = 0, S = 0$. Here we have two states:
   - $|1\rangle = \frac{1}{\sqrt{2}}(1\uparrow 1\downarrow +2\uparrow 2\downarrow)$ with $\hat{H}|1\rangle = -t\frac{1}{\sqrt{2}}(2\uparrow 1\downarrow +1\uparrow 2\downarrow +1\uparrow 2\downarrow +2\uparrow 1\downarrow) + U|1\rangle = -2t|2\rangle + U|1\rangle$
   - $|2\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ with $\hat{H}|2\rangle = -t\frac{1}{\sqrt{2}}(2\uparrow 2\downarrow +1\uparrow 1\downarrow +2\downarrow 2\uparrow +1\downarrow 1\uparrow) = -2t|1\rangle$

   Putting the two together, we get:

$$H = \begin{pmatrix} U & -2t \\ -2t & 0 \end{pmatrix}$$

   which has eigenvalues given by $E^2 - UE - 4t^2 = 0$, which implies:

$$E = \frac{U}{2} \pm \frac{1}{2}\sqrt{U^2 + 16t^2}.$$

3 Summary

Thus, we can summarize the results above in the following table:

m	J	S	E	Number of States
0	1	0	$E = 0$	1 state
1	$\frac{1}{2}$	$\frac{1}{2}$	$E = \pm t$ (twofold)	4 states
2	1	0	$E = 0$	1 state
	0	1	$E = 0$ (threefold)	3 states
	0	0	$E = \frac{U}{2} \pm \frac{1}{2}\sqrt{U^2 + 16t^2}$	2 states

Note that the ground state always has the minimal J and minimal S. In general, one finds minimal S for $U < 0$ and minimal J for $U > 0$.

Let us now examine the ground state wavefunction for $m = 2$ as follows:

$$\begin{pmatrix} U - \frac{U}{2} + \frac{1}{2}\sqrt{U^2 + 16t^2} & -2t \\ -2t & -\frac{U}{2} + \frac{1}{2}\sqrt{U^2 + 16t^2} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0$$

Thus, we get the equation:

$$\left(\frac{U}{2} + \frac{1}{2}\sqrt{U^2 + 16t^2}\right)\alpha - 2t\beta = 0$$

Rearranging, we get when solving for β:

$$\beta = \left(\frac{U}{4t} + \frac{1}{4t}\sqrt{U^2 + 16t^2}\right)\alpha$$

Using the normalization $\alpha^2 + \beta^2 = 1$, we get when substituting in for β:

$$\alpha^2(1 + \beta^2) = \alpha^2\left(1 + \left(\left(\frac{U}{4t} + \frac{1}{4t}\sqrt{U^2 + 16t^2}\right)\alpha\right)^2\right) = 1$$

Expanding out:

$$\alpha^2\left(1 + \frac{U^2}{16t^2} + \frac{2U}{16t^2}\sqrt{U^2 + 16t^2} + \frac{U^2 + 16t^2}{16t^2}\right) = 1$$

and solving for α:

$$\alpha = \frac{1}{\sqrt{2\left(1 + \frac{U^2}{16t^2} + \frac{2U}{16t^2}\sqrt{U^2 + 16t^2}\right)}} = \frac{1}{\sqrt{\frac{2\sqrt{U^2+16t^2}}{16t^2}\left(U + \sqrt{U^2 + 16t^2}\right)}}$$

Hence, β is:

$$\beta = \frac{\sqrt{2t}\sqrt{\frac{U}{4t} + \frac{1}{4t}\sqrt{U^2 + 16t^2}}}{(U^2 + 16t^2)^{1/4}}$$

Now let the quantum state vector be:

$$|\psi\rangle = \alpha|1\rangle + \beta|2\rangle$$

4 Limiting cases

We can study it in the following limits:

- $U \to 0$: $\alpha \to \frac{1}{\sqrt{2}}$, $\beta \to \frac{1}{\sqrt{2}}$.

  $$|\psi\rangle \to \frac{1}{\sqrt{2}}\left(|1\rangle + |2\rangle\right) = \frac{1}{2}\left(1\uparrow 1\downarrow + 2\uparrow 2\downarrow + 1\uparrow 2\downarrow + 1\downarrow 2\uparrow\right) = \frac{1}{\sqrt{2}}\left(1\uparrow + 2\uparrow\right)\frac{1}{\sqrt{2}}\left(1\downarrow + 2\downarrow\right)$$

  When $U = 0$, we fill the lowest states of the band structure:

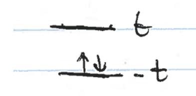

Figure 1: In this figure, we show the two noninteracting energy levels of the band structure at t and $-t$. The ground state fills in the lowest level with one up spin electron and one down spin electron.

- $U \to \infty$: $\alpha \to 0$, $\beta \to 1$.

  $$|\psi\rangle \to |2\rangle = \frac{1}{\sqrt{2}}\left(1\uparrow 2\downarrow - 1\downarrow 2\uparrow\right)$$

  This state is degenerate with $\frac{1}{\sqrt{2}}\left(1\uparrow 2\downarrow + 1\downarrow 2\uparrow\right)$, $1\uparrow 2\uparrow$, and $1\downarrow 2\downarrow$ with $E = 0$. When $U = \infty$, there is no double occupancy so $E \to 0$. As $U \to \infty$, all singly occupied states are degenerate as U decreases and the $S = 0$ state is the lowest.

- $U \to -\infty$: $\alpha \to 1$, $\beta \to 0$.

  $$|\psi\rangle \to |1\rangle = \frac{1}{\sqrt{2}}\left(1\uparrow 1\downarrow + 2\uparrow 2\downarrow\right)$$

  This state is degenerate with $\frac{1}{\sqrt{2}}\left(1\uparrow 1\downarrow - 2\uparrow 2\downarrow\right)$. As $U \to -\infty$, only doubly occupied states are allowed. and both degnerate states have $E = U \to -\infty$

For the more general cases, we have the following. For $U = \infty$ at half-filling, all singly occupied states are degenerate. The system is frozen in an insulator. As $U < \infty$ but large, on a bipartite lattice, the $S = 0$ state is the lowest in energy. By performing a partial particle-hole transformation $S \leftrightarrow J$, the ground state for $U = -\infty$ has all doubly occupied states degenerate. For $U > -\infty$ but large and negative, on a bipartite lattice, one has $J = 0$ as the ground state.

In the article, you can learn about other approximations to the ground-state exact solution and see how accurate they are for different U values. We won't examine further here.