Physics 506 lecture 37

The two-site Hubbard model

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

Counting: N sites 4^N possible states (0, ↑, ↓, ↑↓ on each site)

If we have a total of m electrons $(0 \le m \le 2N)$ then there are

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

states with exactly m electrons. This follows since each electron can be spin up or spin down on each site. So there are $2N$ choices and we choose m of them.

Check: $\displaystyle\sum_{m=0}^{2N} \binom{2N}{m} = 2^{2N} = 4^N$ (binomial theorem.)

$N=2$

$m=0 \quad \binom{4}{0} = 1$ state

$m=1 \quad \binom{4}{1} = 4$ states

$m=2 \quad \binom{4}{2} = 6$ states

$m=3 \quad \binom{4}{3} = 4$ states

$m=4 \quad \binom{4}{4} = 1$ state

16 states $= 4^2$ ✓

$m=0$, $J=1$ $m_J=-1$ $S=0$ $|0\rangle$ $E=0$

$m=1$, $J=\frac{1}{2}$ $m_J=-\frac{1}{2}$ $S=\frac{1}{2}$ consider spatial symmetry

$|1\rangle = (1\uparrow + 2\uparrow)/\sqrt{2}$ shorthand $\frac{1}{\sqrt{2}}\left(c^{+}_{1\uparrow}|0\rangle + c^{+}_{2\uparrow}|0\rangle\right)$

$|2\rangle = (1\uparrow - 2\uparrow)/\sqrt{2}$

$\hat{T}|1\rangle = -t|1\rangle \qquad E = -t \qquad$ (two fold degenerate $\uparrow \Leftrightarrow \downarrow$)

$\hat{T}|2\rangle = t|2\rangle \qquad E = t \qquad$ (two fold)

$m=2$: $\quad J=1 \quad m_J=0 \quad S=0 \qquad J^+|0\rangle = \frac{1}{\sqrt{2}}(1\uparrow 1\downarrow - 2\uparrow 2\downarrow) = |1\rangle$

$\hat{T}|1\rangle = -t\frac{1}{\sqrt{2}}(2\uparrow 1\downarrow + 1\uparrow 2\downarrow - 1\uparrow 2\downarrow - 2\uparrow 1\downarrow) = 0$

$\hat{U}|1\rangle = U|1\rangle \Rightarrow \boxed{E = U}$ as it must since J^+ raises E by U.

$J=0 \quad m_J=0 \quad S=1$

$1\uparrow 2\uparrow = |1\rangle \qquad H|\uparrow\rangle = 0 \qquad \boxed{E=0}$ (threefold deg)

$J=0 \quad m_J=0 \quad S=0$

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

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

$\hat{H}|1\rangle = -t\frac{1}{\sqrt{2}}(2\uparrow 1\downarrow + 1\uparrow 2\downarrow + 1\uparrow 2\downarrow + 2\uparrow 1\downarrow) + U|1\rangle$

$= -2t|2\rangle + U|1\rangle$

$\hat{H}|2\rangle = -t\frac{1}{\sqrt{2}}(2\uparrow 2\downarrow + 1\uparrow 1\downarrow - 2\downarrow 2\uparrow - 1\downarrow 1\uparrow) = -2t|1\rangle$

$$H = \begin{pmatrix} U & -2t \\ -2t & 0 \end{pmatrix} \qquad E^2 - UE - 4t^2 = 0 \qquad \boxed{E = \frac{U}{2} \pm \frac{1}{2}\sqrt{U^2 + 16t^2}}$$

summary

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

~~[illegible]~~ ground state always has minimal J and minimal S

In general, one finds minimal S for $U<0$

minimal J for $U>0$

examine GS wave function for $m=0$

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

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

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

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

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

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

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

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

$U\to 0$ $\quad \alpha\to\frac{1}{\sqrt{2}}$ $\quad \beta\to\frac{1}{\sqrt{2}}$

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

$$= \frac{1}{\sqrt{2}}\left(1\!\uparrow+2\!\uparrow\right)\frac{1}{\sqrt{2}}\left(1\!\downarrow+2\!\downarrow\right)$$

$U\to\infty$ $\quad \alpha\to 0$ $\quad \beta\to 1$

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

$U\to-\infty$ $\quad \alpha\to 1$ $\quad \beta\to 0$

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

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

$$\underline{\quad\quad} \; t$$

$$\underline{\uparrow\downarrow} \; -t$$

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

when $U=\infty$ no double occupancy

$$|\psi\rangle = \frac{1}{\sqrt{2}}(1\uparrow 2\downarrow - 1\downarrow 2\uparrow) \Rightarrow E \to 0$$

but $\frac{1}{\sqrt{2}}(1\uparrow 2\downarrow + 1\downarrow 2\uparrow)$, $1\uparrow 2\downarrow$ and $1\downarrow 2\uparrow$

are also degenerate with $E=0$

As $U \to +\infty$ all singly occupied states are degenerate

as U decreases, the $S=0$ state is lowest,

As $U \to -\infty$ only doubly occupied is allowed

$$\frac{1}{\sqrt{2}}(1\uparrow 1\downarrow + 2\uparrow 2\downarrow)$$

is degenerate with $\frac{1}{\sqrt{2}}(1\uparrow 1\downarrow - 2\uparrow 2\downarrow)$

Both have $E = U \to -\infty$

General case

Find for $U=\infty$ at half filling - all singly occupied states are degenerate. 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
$S \leftrightarrow J$

So the ground state for $U = -\infty$ has all doubly occupied states degenerate - ~~[illegible]~~
~~[illegible]~~

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.