1 Two-site Hubbard model: Antiferromagnetism

a. Calculate the spectrum

Solution: We start by substituting

$$\begin{aligned} H &= H_0 + H_u \\ &= -t\sum_\sigma [c^\dagger_{1\sigma}c_{2\sigma} + c^\dagger_{2\sigma}c_{1\sigma}] + U\hat{n}_{1\uparrow}\langle\hat{n}_{1\downarrow}\rangle + U\hat{n}_{1\downarrow}\langle\hat{n}_{1\uparrow}\rangle - U\langle\hat{n}_{1\downarrow}\rangle\langle\hat{n}_{1\uparrow}\rangle \\ &+ U\hat{n}_{2\uparrow}\langle\hat{n}_{2\downarrow}\rangle + U\hat{n}_{2\downarrow}\langle\hat{n}_{2\uparrow}\rangle - U\langle\hat{n}_{2\downarrow}\rangle\langle\hat{n}_{2\uparrow}\rangle. \end{aligned} \tag{1}$$

Now if we use the fact that $n_{1\sigma} = n_{2-\sigma}$, and $m = (n_{1\uparrow} - n_{1\downarrow})/2$, $n = n_{1\uparrow} + n_{1\downarrow}$, H_u changes to

$$\begin{aligned} H_u &= U\hat{n}_{1\uparrow}\langle\hat{n}_{2\uparrow}\rangle + U\hat{n}_{1\downarrow}\langle\hat{n}_{2\downarrow}\rangle + U\hat{n}_{2\uparrow}\langle\hat{n}_{1\uparrow}\rangle + U\hat{n}_{2\downarrow}\langle\hat{n}_{1\downarrow}\rangle - 2U\langle\hat{n}_{1\uparrow}\rangle\langle\hat{n}_{1\downarrow}\rangle \\ &= \sum_\sigma U(\hat{n}_{1\sigma}\langle\hat{n}_{2\sigma}\rangle + \hat{n}_{1\sigma}\langle\hat{n}_{2\sigma}\rangle) - 2U\langle\hat{n}_{1\uparrow}\rangle\langle\hat{n}_{1\downarrow}\rangle \end{aligned} \tag{2}$$

Hence the system to solve is

$$H = \sum_\sigma (c^\dagger_{1\sigma}c^\dagger_{2\sigma}) \begin{pmatrix} U\langle n_{1-\sigma}\rangle & -t \\ -t & U\langle n_{1\sigma}\rangle \end{pmatrix} \begin{pmatrix} c_{1\sigma} \\ c_{2\sigma} \end{pmatrix} - 2U\langle\hat{n}_{1\uparrow}\rangle\langle\hat{n}_{1\downarrow}\rangle \tag{3}$$

To get the energies we require to compute

$$\begin{vmatrix} U\langle n_{1-\sigma}\rangle - \epsilon & -t \\ -t & U\langle n_{1\sigma}\rangle - \epsilon \end{vmatrix} = 0, \tag{4}$$

and solve for $\epsilon_{i\sigma}, i = 1, 2$, therefore

$$\begin{aligned} \epsilon_{i\sigma} &= \frac{U}{2}(\langle\hat{n}_{i\sigma}\rangle + \langle\hat{n}_{i-\sigma}\rangle) \pm \sqrt{\frac{U^2}{4}(\langle\hat{n}_{i\sigma}\rangle + \langle\hat{n}_{i-\sigma}\rangle)^2 - U^2\langle\hat{n}_{i\sigma}\rangle\langle\hat{n}_{i-\sigma}\rangle + t^2} \\ &= \frac{U}{2}n_i \pm \sqrt{\frac{U^2}{4}(\langle\hat{n}_{i\sigma}\rangle - \langle\hat{n}_{i-\sigma}\rangle)^2 + t^2} \\ &= \frac{U}{2}n_i \pm \sqrt{U^2m^2 + t^2}. \end{aligned} \tag{5}$$

If we define

$$\theta = tan^{-1}\left(\frac{-t}{Um}\right), \tag{6}$$

then we can express the eigenvectors in a much simpler way, as

$$\boldsymbol{v}_1 = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) \end{pmatrix}, \qquad \boldsymbol{v}_2 = \begin{pmatrix} \sin\left(\frac{\theta}{2}\right) \\ -\cos\left(\frac{\theta}{2}\right) \end{pmatrix}. \tag{7}$$

Now we are in position to obtain our eigenstates, they will be

$$|\psi_{1\sigma}\rangle = \left(\cos\left(\frac{\theta}{2}\right)c^\dagger_{1\sigma} + \sin\left(\frac{\theta}{2}\right)c^\dagger_{2\sigma}\right)|0\rangle, \tag{8}$$

$$|\psi_{2\sigma}\rangle = \left(\sin\left(\frac{\theta}{2}\right)c^\dagger_{1\sigma} - \cos\left(\frac{\theta}{2}\right)c^\dagger_{2\sigma}\right)|0\rangle. \tag{9}$$

Up to this point we got the single particle states. In order to get the ground state, what we need to do is to fill up the states with lowest energies to get the salter determinant. So let's do that

$$\epsilon_{GS} = \epsilon_{2\uparrow} + \epsilon_{2\downarrow} = Un_2 + 2\sqrt{U^2m^2 + t^2} - 2U\langle\hat{n}_{1\uparrow}\rangle\langle\hat{n}_{1\downarrow}\rangle \tag{10}$$

So the ground state is

$$|GS\rangle = |\psi_{2\uparrow}\rangle \otimes |\psi_{2\downarrow}\rangle = \sin^2\left(\frac{\theta}{2}\right)|\uparrow\downarrow, 0\rangle - \frac{1}{2}\sin\left(\frac{\theta}{2}\right)(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle) + \cos^2\left(\frac{\theta}{2}\right)|0,\uparrow\downarrow\rangle \tag{11}$$

Now we need to solve the original hamiltonian exactly.

$$|\uparrow\downarrow,\uparrow\downarrow\rangle = c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}|0\rangle \tag{12}$$

The energy for $|\uparrow,\uparrow\rangle$ and $|\downarrow,\downarrow\rangle$ is zero. For the remaining ones we need to solve for the next hamiltonian

$$\begin{pmatrix} 0 & 0 & -t & -t \\ 0 & 0 & t & t \\ -t & t & U & 0 \\ -t & -t & 0 & U \end{pmatrix} \tag{13}$$

For the solution we can propose a basis of covalent and ionic states

$$|cov_\pm\rangle = \frac{1}{\sqrt{2}}\left(c^\dagger_{1\uparrow}c^\dagger_{2\downarrow} \pm c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}\right)|0\rangle\,, \tag{14}$$

$$|ion_\pm\rangle = \frac{1}{\sqrt{2}}\left(c^\dagger_{1\uparrow}c^\dagger_{1\downarrow} \pm c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}\right)|0\rangle\,. \tag{15}$$

Two of the eigenstates are easy to find. The state $|cov_+\rangle$ has energy equal to zero and it corresponds to

$$|cov_+\rangle = 0\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}. \tag{16}$$

The state $|ion_-\rangle$ has energy U and it corresponds to

$$|ion_-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \end{pmatrix}. \tag{17}$$

To solve the remaining two we construct the new matrix in the space spanned by $|cov_-\rangle$,$|ion_+\rangle$ we get

$$H = \begin{pmatrix} 0 & -2t \\ -2t & U \end{pmatrix}. \tag{18}$$

We use Mathematica to solve the eigenproblem for the energy and we find

$$\epsilon_{c/i} = \frac{U}{2} \pm \frac{1}{2}\sqrt{U^2 + 16t^2}, \tag{19}$$

if we define $\theta = \tan^{-1}\left(\frac{4t}{U}\right)$, we can now write the ground state as

$$|GS\rangle = \cos\frac{\theta}{2}|cov_-\rangle + \sin\frac{\theta}{2}|ion_+\rangle\,. \tag{20}$$

We need to express this as a function of m, so let's do it. Using $n_{1\uparrow} = n_1/2 + m$ and $n_{1\downarrow} = n_1/2 - m$ the energy of the ground state is

$$\epsilon_{GS} = Un - 2\sqrt{U^2m^2 + t^2} - U(n^2/2 - 2m^2). \tag{21}$$

for the following analysis I'm going to be using eq. 19 just because some things are easier to see there. We can see that when $t \gg U$ is like we have $U = 0$ the spectrum and the ground state are the same, in this case the electrons are not interacting so our ground states looks like

$$|GS\rangle = \frac{1}{2}\left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle + |\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right). \tag{22}$$

On the other hand, if we have $t << U$ then the energy is either zero. The ground state looks like

$$|GS\rangle = |\uparrow,\downarrow\rangle. \tag{23}$$

This means that when the interaction is really strong, the ground state takes the form of a singlet that can also be written as a product of two single states. Basically this means no quantum-correlation on the ground state.

2 Effect of intersite Coulomb interaction

a. What effect does V has

Solution: The hamiltonian we need to diagonalize now is (using the ordered basis $|\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\uparrow\downarrow,0\rangle, |0,\uparrow\downarrow\rangle$)

$$H = \begin{pmatrix} V & 0 & -t & -t \\ 0 & V & t & t \\ -t & t & U & 0 \\ -t & t & 0 & U \end{pmatrix} \tag{24}$$

Again making the assumption that the eigenstates are covalent and ionic states

$$|cov_\pm\rangle = \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle \pm |\downarrow,\uparrow\rangle), \tag{25}$$

$$|ion_\pm\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow,0\rangle \pm |0,\uparrow\downarrow\rangle). \tag{26}$$

Using this states what we found is that the state $|cov_+\rangle$ has energy $\epsilon = V$, and the state $|ion_-\rangle$ has energy $\epsilon = U$. For the remaining ones, as we did before we construct the hamiltonian and find

$$H = \begin{pmatrix} V & -2t \\ -2t & U \end{pmatrix}, \tag{27}$$

Therefore

$$\epsilon_\pm = \frac{V+U}{2} \pm \frac{1}{2}\sqrt{(U-V)^2 + 16t^2}. \tag{28}$$

Defining $\theta = \tan^{-1}(4t/(U-V))$, the ground state will be

$$|GS\rangle = \cos\left(\frac{\theta}{2}\right)|cov_-\rangle + \sin\left(\frac{\theta}{2}\right)|ion_+\rangle. \tag{29}$$

If we make $V = 0$ we can see that eq. 28 is the same as the one we calculated on the previous exercise, eq. 19. This should not be a surprise. So the effect of V here is something like damping U a little bit.

3 Dimensionless units

a. All depends only on one ratio

Solution: Basically that is going to work because is like dividing the original equation by t and solving the new one

$$\frac{H}{t} = -\sum_{\sigma}[c^{\dagger}_{1\sigma}c_{2\sigma} + c^{\dagger}_{2\sigma}c_{1\sigma}] + rn_{1\uparrow}n_{1\downarrow} + rn_{2\uparrow}n_{2\downarrow}. \tag{30}$$

So at first glance it seems that the only parameter we have is actually r, this is why.

Does this means we solve the same problem? Not exactly. We can see this by looking at the changes it introduces to the energies

$$\epsilon'_1 = \frac{\epsilon_1}{t} = 0, \tag{31}$$

$$\epsilon'_2 = \frac{\epsilon_2}{t} = r, \tag{32}$$

$$\epsilon'_i = \frac{\epsilon_i}{t} = \frac{r}{2} \pm \frac{1}{2}\sqrt{r^2 + 16}, \quad i = 3, 4. \tag{33}$$

If r is the same for different systems the spectrum willl have the same form basically, because we didn't change the topological properties of it. But the non-rescaled energies will change, since we are going to multiply by t in order to get them. So in conclusion, the shape does not change but the value of the energies does.