1 Two-site Hubbard model, particle-hole symmetry

a. Show that the model is particle hole symmetric

Solution: Starting from the point

$$H = \varepsilon_e \sum_{\sigma}\sum_{i=1}^{2} \hat{n}_{i\sigma} - t\sum_{\sigma}\left[c_{1\sigma}^{\dagger}c_{2\sigma} + c_{2\sigma}^{\dagger}c_{1\sigma}\right] + U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} \tag{1}$$

If we make the change

$$c_{i\sigma} \rightarrow (-1)^i d_{i\sigma}^{\dagger}, \tag{2}$$
$$c_{i\sigma}^{\dagger} \rightarrow (-1)^i d_{i\sigma}, \tag{3}$$

Then we will have

$$c_{i\sigma}^{\dagger}c_{j\sigma} = (-1)^{i+j} d_{i\sigma}^{\dagger}d_{j\sigma} = (-1)^{i+j+1} d_{j\sigma}d_{i\sigma}^{\dagger}. \tag{4}$$

Where in the last step we used the anti-commutation relations, using this equation in the original hamiltoninan we get the following result

$$\begin{aligned}
H &= \varepsilon_e \sum_{\sigma}\sum_{i=1}^{2} \hat{n}_{i\sigma} - t\sum_{\sigma}\left[c_{1\sigma}^{\dagger}c_{2\sigma} + c_{2\sigma}^{\dagger}c_{1\sigma}\right] + U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow},\\
&= \varepsilon_e \sum_{\sigma}\sum_{i=1}^{2} \hat{n}_{i\sigma} - t\sum_{\sigma}\left[(-1)^{1+2+1}d_{1\sigma}^{\dagger}d_{2\sigma} + (-1)^{2+1+1}d_{2\sigma}^{\dagger}d_{1\sigma}\right] + U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow},\\
&= \varepsilon_e \sum_{\sigma}\sum_{i=1}^{2} \hat{n}_{i\sigma} - t\sum_{\sigma}\left[d_{1\sigma}^{\dagger}d_{2\sigma} + d_{2\sigma}^{\dagger}d_{1\sigma}\right] + U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow},
\end{aligned} \tag{5}$$

But we still need to make the changes for the $\hat{n}$ operators. This transformation implies that $\tilde{n}_{i\sigma} = 1-\hat{n}_{i\sigma}$ where the tilde operator is the number operator for the holes. So let's do these transformations further.

$$\begin{aligned}
-\frac{U}{2}\sum_{\sigma}\sum_{i=1}^{2} \hat{n}_{i\sigma} &= \frac{U}{2}(\hat{n}_{1\uparrow} + \hat{n}_{1\downarrow} + \hat{n}_{2\uparrow} + \hat{n}_{2\downarrow})\\
&= \frac{U}{2}(1-\tilde{n}_{1\uparrow} + 1-\tilde{n}_{1\downarrow} + 1-\tilde{n}_{2\uparrow} + 1-\tilde{n}_{2\downarrow})\\
&= -2U + \frac{U}{2}(\tilde{n}_{1\uparrow} + \tilde{n}_{1\downarrow} + \tilde{n}_{2\uparrow} + \tilde{n}_{2\downarrow}).
\end{aligned} \tag{6}$$

Also

$$\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = (1-\tilde{n}_{i\uparrow})(1-\tilde{n}_{i\downarrow}) = 1 - \tilde{n}_{i\uparrow} - \tilde{n}_{i\downarrow} + \tilde{n}_{i\uparrow}\tilde{n}_{i\downarrow}. \tag{7}$$

If we add these last two terms we get

$$\begin{aligned}
&-2U + \frac{U}{2}(\tilde{n}_{1\uparrow} + \tilde{n}_{1\downarrow} + \tilde{n}_{2\uparrow} + \tilde{n}_{2\downarrow}) + U(1 - \tilde{n}_{1\uparrow} - \tilde{n}_{1\downarrow} + \tilde{n}_{1\uparrow}\tilde{n}_{1\downarrow} + 1 - \tilde{n}_{2\uparrow} - \tilde{n}_{2\downarrow} + \tilde{n}_{2\uparrow}\tilde{n}_{2\downarrow}),\\
&-\frac{U}{2}(\tilde{n}_{1\uparrow} + \tilde{n}_{1\downarrow} + \tilde{n}_{2\uparrow} + \tilde{n}_{2\downarrow}) + U(\tilde{n}_{1\uparrow}\tilde{n}_{1\downarrow} + \tilde{n}_{2\uparrow}\tilde{n}_{2\downarrow})
\end{aligned} \tag{8}$$

And at this point we can end with all the transformations to our system by substituting this last equation into the hamiltonian

$$H = -\frac{U}{2}\sum_{\sigma}\sum_{i=1}^{2} \tilde{n}_{i\sigma} - t\sum_{\sigma}\left[d_{1\sigma}^{\dagger}d_{2\sigma} + d_{2\sigma}^{\dagger}d_{1\sigma}\right] + U\tilde{n}_{1\uparrow}\tilde{n}_{1\downarrow} + U\tilde{n}_{2\uparrow}\tilde{n}_{2\downarrow}, \tag{9}$$

So now we can see that the Hubbard Hamiltonian with $\varepsilon_e = -U/2$ is invariant to the hole transformation.

For the holes, I think the vacuum states are the ones without holes, so at half filling, we will have four states $|\uparrow,\uparrow\rangle, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$.

And finally, for the last question. I have absolutely no idea.

2 Atomic limit

a. Exact solution

Solution: The hamiltonian looks like this

$$\begin{aligned} H_U = \Delta E\hat{n}_2 + U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} + (U-2J)\hat{n}_{1\uparrow}\hat{n}_{2\downarrow} \\ + (U-2J)\hat{n}_{1\downarrow}\hat{n}_{2\uparrow} + (U-3J)\hat{n}_{1\uparrow}\hat{n}_{2\uparrow} + (U-3J)\hat{n}_{1\downarrow}\hat{n}_{2\downarrow}. \end{aligned} \tag{10}$$

The states that are going to yield a non-zero energy are $|\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle$, $|\downarrow\uparrow,0\rangle, |0,\downarrow\uparrow\rangle, |\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$, $|0,\downarrow\rangle, |0,\uparrow\rangle$. Using the basis with this specific order we see

$$H_U|\uparrow,\downarrow\rangle = \Delta E + U - 2J, \tag{11}$$
$$H_U|\downarrow,\uparrow\rangle = \Delta E + U - 2J, \tag{12}$$
$$H_U|\downarrow\uparrow,0\rangle = U, \tag{13}$$
$$H_U|0,\downarrow\uparrow\rangle = \Delta E + U, \tag{14}$$
$$H_U|\uparrow,\uparrow\rangle = \Delta E + U - 3J, \tag{15}$$
$$H_U|\downarrow,\downarrow\rangle = \Delta E + U - 3J, \tag{16}$$
$$H_U|0,\downarrow\rangle = \Delta E, \tag{17}$$
$$H_U|0,\uparrow\rangle = \Delta E. \tag{18}$$

So our matrix H_U looks like

$$\begin{pmatrix} \Delta E + U - 2J & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \Delta E + U - 2J & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & U & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \Delta E + U & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \Delta E + U - 3J & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \Delta E + U - 3J & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \Delta E & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta E \end{pmatrix} \tag{19}$$

If we remember that the Hubbard model has the following form

$$\begin{aligned} H &= H_d + H_T + H_U \\ &= \varepsilon \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + H_U \end{aligned} \tag{20}$$

This turns into a complicated matrix. Luckily for us we just need to diagonalize H_U and it's already diagonal. So the eigenstates is the basis we use to get this matrix form of the operator.

The ground state depends actually on some quantities, for example it depends on whether $U - 3J$ is positive or negative. The ground state will be the eigenstate associated with the smaller diagonal terms. But if we suppose $U - 3J < 0$ then the ones with spins pointing in the same direction (5th and 6th row) $|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$ have the smallest energies and their energies (coming from H_U) are going to be $\Delta E + U - 3J$. So the ground state is going to be any linear combination of this two states.

If $\Delta E/J \to 0$ then $J \gg \Delta E$ so we can basically drop the ΔE term from the energy, for there are no qualitative changes. Maybe we can also ignore the last two terms because their energies are really small compared to the other ones.

If $\Delta E/J \to \infty$ then $J \ll \Delta E$ so we can drop the J terms and now we have a 5-fold degeneracy in the ground state. Now the states $|\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, \ , |0,\downarrow\uparrow\rangle, |\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$, have also the energy of the ground state, so any linear combination of this states it is going to be the ground state.

3 Project exercise