Quantum Many Body Systems I
Exercise 1

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The Hamiltonian of our two particles systems is:

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

where $t > 0$ and $U \geq 0$. We define the hopping term:

$$\hat{H}_t \equiv -t \sum_{\sigma} \left(c^{\dagger}_{1\sigma} c_{2\sigma} + c^{\dagger}_{2\sigma} c_{1\sigma} \right) \tag{2}$$

and the interaction term:

$$\hat{H}_U \equiv U \hat{D} \tag{3}$$

where $\hat{D} \equiv \sum_{i=1}^{2} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$ is the "Double occupancy" .
First, we need to understand how many states we have in the basis. We can use the general rule and label our basis states

$$|n_{1\uparrow} n_{1\downarrow} n_{2\uparrow} n_{2\downarrow}\rangle \tag{4}$$

where each n= 0,1 depending on whether there is a particle with that spin at that site.
Since we have 2 particles, we need to count how many ways we could put two 1's (two particles) in the 4 different positions of the previous string. Hence we have that the dimension of our space is: $\binom{4}{2} = 6$.
In order to make our notation less cumbersome, we write the spins arrows and the sites numbers in order to indicate the states, e.g. : $|\uparrow_1 \downarrow_2\rangle = |1001\rangle = c^{\dagger}_{1\uparrow} c^{\dagger}_{2\downarrow} |0\rangle$.
Since the Hamiltonian is invariant under the exchange of:

- site 1 $\Leftrightarrow$ site 2
- spin $\uparrow \Leftrightarrow$ spin $\downarrow$

we use a basis invariant under the previous exchanges (except for a global sign) :

$$|\Psi_a\rangle = \frac{|\uparrow_1 \uparrow_2\rangle + |\downarrow_1 \downarrow_2\rangle}{\sqrt{2}} \ , \ |\Psi_b\rangle = \frac{|\uparrow_1 \uparrow_2\rangle - |\downarrow_1 \downarrow_2\rangle}{\sqrt{2}} \ , \ |\Psi_c\rangle = \frac{|\uparrow_1 \downarrow_2\rangle + |\downarrow_1 \uparrow_2\rangle}{\sqrt{2}} \tag{5}$$

$$|\Psi_d\rangle = \frac{|\uparrow_1 \downarrow_1\rangle + |\uparrow_2 \downarrow_2\rangle}{\sqrt{2}} \ , \ |\Psi_e\rangle = \frac{|\uparrow_1 \downarrow_2\rangle - |\downarrow_1 \uparrow_2\rangle}{\sqrt{2}} \ , \ |\Psi_f\rangle = \frac{|\uparrow_1 \downarrow_1\rangle - |\uparrow_2 \downarrow_2\rangle}{\sqrt{2}} \tag{6}$$

In order to make an interpretation of our calculation, we observe that hopping term $\hat{H}_t$ "shifts" a spin σ from a site to another, while $\hat{H}_U$ does not vanish acting on a state only if it is double occupied. Hence, we get: (in the following we largely use the anticommutation relations)

$$\boxed{\hat{H}\left|\uparrow_1\uparrow_2\right\rangle = 0 \quad ; \quad \hat{H}\left|\downarrow_1\downarrow_2\right\rangle = 0} \tag{7}$$

Proof. There cannot be hopping (the site where a spin would do hopping is already occupied) and there are not double occupied sites. ■

$$\boxed{\hat{H}\left|\uparrow_1\downarrow_2\right\rangle = -t\left|\uparrow_2\downarrow_2\right\rangle - t\left|\uparrow_1\downarrow_1\right\rangle} \tag{8}$$

Proof. Since there are not double occupied sites, we have $\hat{H}_U\left|\uparrow_1\downarrow_2\right\rangle = 0$.

$$\hat{H}_t\left|\uparrow_1\downarrow_2\right\rangle = -tc^\dagger_{2\uparrow}c_{1\uparrow}\left|\uparrow_1\downarrow_2\right\rangle - tc^\dagger_{1\downarrow}c_{2\downarrow}\left|\uparrow_1\downarrow_2\right\rangle = \tag{9}$$

$$= -tc^\dagger_{2\uparrow}c_{1\uparrow}c^\dagger_{1\uparrow}c^\dagger_{2\downarrow}\left|0\right\rangle - tc^\dagger_{1\downarrow}c_{2\downarrow}c^\dagger_{1\uparrow}c^\dagger_{2\downarrow}\left|0\right\rangle = \tag{10}$$

$$= -tc^\dagger_{2\uparrow}\{c_{1\uparrow}, c^\dagger_{1\uparrow}\}c^\dagger_{2\downarrow}\left|0\right\rangle + tc^\dagger_{1\downarrow}c^\dagger_{1\uparrow}c_{2\downarrow}c^\dagger_{2\downarrow}\left|0\right\rangle = \tag{11}$$

$$= -t\left|\uparrow_2\downarrow_2\right\rangle + t\left|\downarrow_1\uparrow_1\right\rangle = -t\left|\uparrow_2\downarrow_2\right\rangle - t\left|\uparrow_1\downarrow_1\right\rangle \tag{12}$$

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$$\boxed{\hat{H}\left|\downarrow_1\uparrow_2\right\rangle = +t\left|\uparrow_2\downarrow_2\right\rangle + t\left|\uparrow_1\downarrow_1\right\rangle} \tag{13}$$

Proof. Since there are not double occupied sites, we have $\hat{H}_U\left|\downarrow_1\uparrow_2\right\rangle = 0$.

$$\hat{H}_t\left|\downarrow_1\uparrow_2\right\rangle = -tc^\dagger_{1\uparrow}c_{2\uparrow}\left|\downarrow_1\uparrow_2\right\rangle - tc^\dagger_{2\downarrow}c_{1\downarrow}\left|\downarrow_1\uparrow_2\right\rangle = \tag{14}$$

$$= -tc^\dagger_{1\uparrow}c_{2\uparrow}c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}\left|0\right\rangle - tc^\dagger_{2\downarrow}c_{1\downarrow}c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}\left|0\right\rangle = \tag{15}$$

$$= +t\left|\uparrow_1\downarrow_1\right\rangle - t\left|\downarrow_2\uparrow_2\right\rangle = +t\left|\uparrow_1\downarrow_1\right\rangle + t\left|\uparrow_2\downarrow_2\right\rangle \tag{16}$$

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$$\boxed{\hat{H}\left|\uparrow_1\downarrow_1\right\rangle = t\left|\downarrow_1\uparrow_2\right\rangle - t\left|\uparrow_1\downarrow_2\right\rangle + U\left|\uparrow_1\downarrow_1\right\rangle} \tag{17}$$

Proof. We have $\hat{H}_U\left|\uparrow_1\downarrow_1\right\rangle = U\left|\uparrow_1\downarrow_1\right\rangle$.

$$\hat{H}_t\left|\uparrow_1\downarrow_1\right\rangle = -tc^\dagger_{2\uparrow}c_{1\uparrow}\left|\uparrow_1\downarrow_1\right\rangle - tc^\dagger_{2\downarrow}c_{1\downarrow}\left|\uparrow_1\downarrow_1\right\rangle = \tag{18}$$

$$= -t\left|\uparrow_2\downarrow_1\right\rangle + t\left|\downarrow_2\uparrow_1\right\rangle = \tag{19}$$

$$= +t\left|\downarrow_1\uparrow_2\right\rangle - t\left|\uparrow_1\downarrow_2\right\rangle \tag{20}$$

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$$\boxed{\hat{H}\left|\uparrow_2\downarrow_2\right\rangle = +t\left|\downarrow_1\uparrow_2\right\rangle - t\left|\uparrow_1\downarrow_2\right\rangle + U\left|\uparrow_2\downarrow_2\right\rangle} \tag{21}$$

Proof. We have $\hat{H}_U \left|\uparrow_2\downarrow_2\right\rangle = U \left|\uparrow_2\downarrow_2\right\rangle$.

$$\hat{H}_t \left|\uparrow_2\downarrow_2\right\rangle = -tc^\dagger_{1\uparrow}c_{2\uparrow}\left|\uparrow_2\downarrow_2\right\rangle - tc^\dagger_{1\downarrow}c_{2\downarrow}\left|\uparrow_2\downarrow_2\right\rangle = \tag{22}$$

$$= -t\left|\uparrow_1\downarrow_2\right\rangle + t\left|\downarrow_1\uparrow_2\right\rangle \tag{23}$$

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Hence, if we apply the Hamiltonian to our basis, we get:

$$\hat{H}\left|\Psi_a\right\rangle = 0\ ,\ \hat{H}\left|\Psi_b\right\rangle = 0\,,\ \hat{H}\left|\Psi_c\right\rangle = 0 \tag{24}$$

$$\hat{H}\left|\Psi_d\right\rangle = -2t\left|\Psi_e\right\rangle + U\left|\Psi_d\right\rangle\ ,\ \hat{H}\left|\Psi_e\right\rangle = -2t\left|\Psi_d\right\rangle\ ,\ \hat{H}\left|\Psi_f\right\rangle = U\left|\Psi_f\right\rangle \tag{25}$$

Therefore, we have to diagonalize only the 2×2 matrix (written in the subspace basis given by $\left|\Psi_d\right\rangle$ and $\left|\Psi_e\right\rangle$):

$$\hat{H}_{d,e} = \begin{pmatrix} \left\langle\Psi_d\right|\hat{H}\left|\Psi_d\right\rangle & \left\langle\Psi_d\right|\hat{H}\left|\Psi_e\right\rangle \\ \left\langle\Psi_e\right|\hat{H}\left|\Psi_d\right\rangle & \left\langle\Psi_e\right|\hat{H}\left|\Psi_e\right\rangle \end{pmatrix} = \begin{pmatrix} U & -2t \\ -2t & 0 \end{pmatrix} \tag{26}$$

So, we have:

$$\hat{H}_{d,e} - \mathrm{E}\,\mathrm{Id} = \begin{pmatrix} U-E & -2t \\ -2t & -E \end{pmatrix} \tag{27}$$

In order to find the eigenvalues we find the solution of :

$$0 = \det\left(\hat{H}_{d,e} - \mathrm{E}\,\mathrm{Id}\,\right) = -E(U-E) - 4t^2 = E^2 - UE - 4t^2 \tag{28}$$

Therefore:

$$E = \frac{U}{2} \pm \frac{\sqrt{U^2+16t^2}}{2} \tag{29}$$

In order to deal with adimensional quantities, let me define:

$$e \equiv \frac{E}{t}\quad ,\quad u \equiv \frac{U}{t} \tag{30}$$

$$e^2 - ue - 4 = 0 \tag{31}$$

$$e = \frac{u}{2} \pm \frac{\sqrt{u^2+16}}{2} \tag{32}$$

Hence, we consider:

$$\left(\hat{H}_{d,e} - \mathrm{E}\,\mathrm{Id}\right)\left|\Psi\right\rangle = \begin{pmatrix} U-E & -2t \\ -2t & -E \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} \tag{33}$$

$$\begin{cases} (U-E)\,a - 2tb = 0 \\ -2ta - Eb = 0 \\ a^2 + b^2 = 1 \end{cases} \Rightarrow \begin{cases} a = -\dfrac{Eb}{2t} \\ b^2\left(1 + \dfrac{E^2}{4t^2}\right) = 1 \end{cases} \tag{34}$$

$$\Rightarrow \begin{cases} a = -\dfrac{E}{(4t^2+E^2)^{\frac{1}{2}}} \\ b = \dfrac{2t}{(4t^2+E^2)^{\frac{1}{2}}} \end{cases} \tag{35}$$

Therefore:

$$|\Psi\rangle = a\,|\Psi_d\rangle + b\,|\Psi_e\rangle = -\frac{E}{(4t^2+E^2)^{\frac{1}{2}}}\frac{|\uparrow_1\downarrow_1\rangle + |\uparrow_2\downarrow_2\rangle}{\sqrt{2}} + \frac{2t}{(4t^2+E^2)^{\frac{1}{2}}}\frac{|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle}{\sqrt{2}} \quad (36)$$

For future discussions (in order to see better the limits of the ground state), it is useful to observe that:

$$\frac{b}{a} = -\frac{2t}{E} \quad (37)$$

Hence, our spectrum is :

$E_0 = \frac{U}{2} - \frac{\sqrt{U^2+16t^2}}{2}$	$\|\Psi_0\rangle = -\frac{E_0}{(4t^2+E_0^2)^{\frac{1}{2}}}\frac{\|\uparrow_1\downarrow_1\rangle+\|\uparrow_2\downarrow_2\rangle}{\sqrt{2}} + \frac{2t}{(4t^2+E_0^2)^{\frac{1}{2}}}\frac{\|\uparrow_1\downarrow_2\rangle-\|\downarrow_1\uparrow_2\rangle}{\sqrt{2}}$
$E_1 = 0$	$\|\Psi_1\rangle = \frac{\|\uparrow_1\uparrow_2\rangle+\|\downarrow_1\downarrow_2\rangle}{\sqrt{2}}$
$E_2 = 0$	$\|\Psi_2\rangle = \frac{\|\uparrow_1\uparrow_2\rangle-\|\downarrow_1\downarrow_2\rangle}{\sqrt{2}}$
$E_3 = 0$	$\|\Psi_3\rangle = \frac{\|\uparrow_1\downarrow_2\rangle+\|\downarrow_1\uparrow_2\rangle}{\sqrt{2}}$
$E_4 = U$	$\|\Psi_4\rangle = \frac{\|\uparrow_1\downarrow_1\rangle-\|\uparrow_2\downarrow_2\rangle}{\sqrt{2}}$
$E_5 = \frac{U}{2} + \frac{\sqrt{U^2+16t^2}}{2}$	$\|\Psi_5\rangle = -\frac{E_5}{(4t^2+E_5^2)^{\frac{1}{2}}}\frac{\|\uparrow_1\downarrow_1\rangle+\|\uparrow_2\downarrow_2\rangle}{\sqrt{2}} + \frac{2t}{(4t^2+E_5^2)^{\frac{1}{2}}}\frac{\|\uparrow_1\downarrow_2\rangle-\|\downarrow_1\uparrow_2\rangle}{\sqrt{2}}$

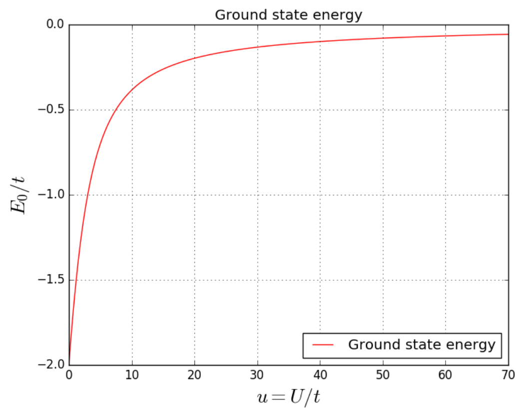

Figure 1: Ground state energy at different values of U/t.

The previous results make sense in fact, for example, the ground state assumes the form for U=0 ($E_0(U=0) = -2t$) : $|\Psi_0\rangle = \frac{|\uparrow_1\downarrow_1\rangle+|\uparrow_2\downarrow_2\rangle}{2} + \frac{|\uparrow_1\downarrow_2\rangle-|\downarrow_1\uparrow_2\rangle}{2}$ which means that with probability $1/2$ both electrons are at the same site (the first two terms), and with probability $1/2$ there is one electron in each orbital that is what we expect for zero coupling U. Moreover, the fact that $|\Psi_1\rangle$ and $|\Psi_2\rangle$ have 0 energy makes sense because there cannot be hopping (the site where a spin would do hopping is already occupied) and there are not double occupied sites. The state $|\Psi_3\rangle$ has 0 energy because the "total hopping" vanishes and there are not double occupied sites. The fact that state $|\Psi_4\rangle$ has U energy makes also sense because there is no total hopping and there are occupied sites.

We are going to compute the expectation value at T=0 of some quantities. We define $e_0 \equiv \frac{E_0}{t}$.

We have:

$$\langle\Psi_0|\,\hat{D}\,|\Psi_0\rangle = \frac{E_0^2}{4t^2+E_0^2} = \frac{e_0^2}{4+e_0^2} \quad (38)$$

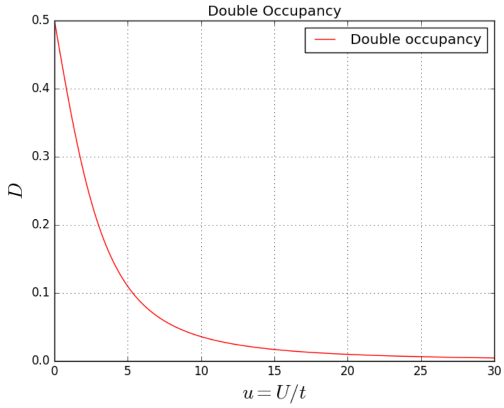

Figure 2: Double Occupancy at different values of U/t. It starts by $\frac{1}{2}$ at 0 coupling (that is what we expected in the case of no interaction term (more on this you can find in the last section)) and approaches to 0 for large U as it is expected since in the limit of large coupling we don't have double occupied sites.

Proof.

$$\langle\Psi_0|\hat{D}|\Psi_0\rangle = -\frac{E_0}{(4t^2+E_0^2)^{\frac{1}{2}}}\langle\Psi_0|\left(\frac{|\uparrow_1\downarrow_1\rangle+|\uparrow_2\downarrow_2\rangle}{\sqrt{2}}\right) = \frac{E_0^2}{4t^2+E_0^2} = \frac{e_0^2}{4+e_0^2} \tag{39}$$

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For the expectation value of the hopping term we get:

$$\langle\Psi_0|\hat{H}_t|\Psi_0\rangle = \frac{8t^2E_0}{4t^2+E_0^2} = \frac{8e_0}{4+e_0^2}t \tag{40}$$

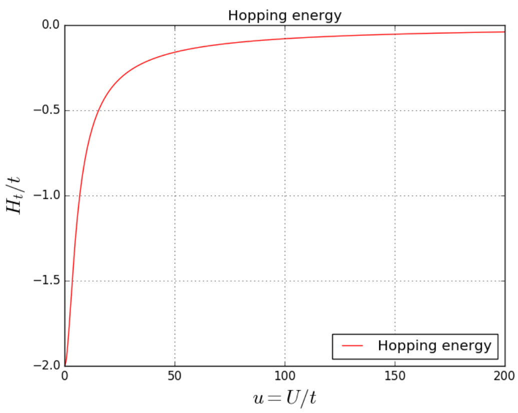

Figure 3: Hopping energy at different values of U/t. It starts by $-2t$ at 0 coupling (which is also the value of the total energy U=0) and approaches to 0 for large U as it is expected since in the limit of large coupling we don't have hopping.

Proof.

$$\langle\Psi_0|\,\hat{H}_t\,|\Psi_0\rangle = \langle\Psi_0|\,(\frac{2tE_0}{(4t^2+E_0^2)^{\frac{1}{2}}}\frac{|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle}{\sqrt{2}} - \frac{4t^2}{(4t^2+E_0^2)^{\frac{1}{2}}}\frac{|\uparrow_1\downarrow_1\rangle + |\uparrow_2\downarrow_2\rangle}{\sqrt{2}}) = \quad (41)$$

$$= \frac{4t^2E_0}{4t^2+E_0^2} + \frac{4t^2E_0}{4t^2+E_0^2} = \frac{8t^2E_0}{4t^2+E_0^2} = \frac{8e_0}{4+e_0^2}t \quad (42)$$

$$(43)$$

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As a check of the previous results, we compute the expectation value of the ground energy:

$$\langle\Psi_0|\,\frac{\hat{H}}{t}\,|\Psi_0\rangle = \langle\Psi_0|\,\frac{\hat{H}_t}{t}\,|\Psi_0\rangle + \langle\Psi_0|\,u\hat{D}\,|\Psi_0\rangle = \frac{8e_0}{4+e_0^2} + u\frac{e_0^2}{4+e_0^2} = \frac{8e_0+ue_0^2}{4+e_0^2} = \quad (44)$$

$$= \frac{e_0(8+ue_0)}{4+e_0^2} = \frac{e_0(4+e_0^2)}{4+e_0^2} = e_0 \quad (45)$$

where we have used the eq(31): $e^2 - ue - 4 = 0$.
For the expectation value of $\vec{S}_1 \cdot \vec{S}_2$ we get:

$$\langle\Psi_0|\,\vec{S}_1\cdot\vec{S}_2\,|\Psi_0\rangle = -\frac{3t^2}{4t^2+E_0^2} = -\frac{3}{4+e_0^2} \quad (46)$$

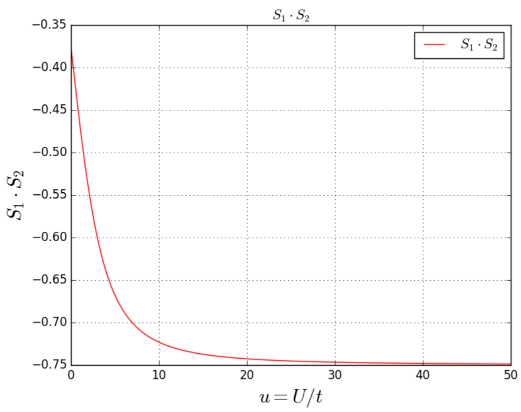

Figure 4: $\vec{S}_1 \cdot \vec{S}_2$ at different values of U/t. The fact that it starts by $-3/8$ makes sense because we can check easily that $-3/8$ is the expectation value of $\vec{S}_1 \cdot \vec{S}_2$ on the U=0 ground state $|\Psi_0\rangle = \frac{|\uparrow_1\downarrow_1\rangle+|\uparrow_2\downarrow_2\rangle}{2} + \frac{|\uparrow_1\downarrow_2\rangle-|\downarrow_1\uparrow_2\rangle}{2}$. The asymptotic value is $-3/4$ which is the value expected for a singlet of two electrons $\frac{|\uparrow_1\downarrow_2\rangle-|\downarrow_1\uparrow_2\rangle}{\sqrt{2}}$ which is the ground state for $u \to \infty$ as we can see by eq.(36).

Proof. We have:

$$S_1^xS_2^x + S_1^yS_2^y = \frac{1}{2}S_1^+S_2^- + \frac{1}{2}S_1^-S_2^+ \quad (47)$$

$$\langle\Psi_0|\,\vec{S}_1\cdot\vec{S}_2\,|\Psi_0\rangle = \langle\Psi_0|\,S_1^zS_2^z\,|\Psi_0\rangle + \frac{1}{2}\langle\Psi_0|\,S_1^+S_2^-\,|\Psi_0\rangle + \frac{1}{2}\langle\Psi_0|\,S_1^-S_2^+\,|\Psi_0\rangle \quad (48)$$

Let's compute the three pieces of the last equation. Since:

$$S_i^z = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}) \tag{49}$$

we have:

$$\langle\Psi_0| S_1^z S_2^z |\Psi_0\rangle = \langle\Psi_0| (\frac{2t}{\left(4t^2+E_0^2\right)^{\frac{1}{2}}} \frac{S_1^z S_2^z |\uparrow_1\downarrow_2\rangle - S_1^z S_2^z |\downarrow_1\uparrow_2\rangle}{\sqrt{2}}) = \tag{50}$$

$$= -\frac{1}{4}\frac{4t^2}{4t^2+E_0^2} = -\frac{t^2}{4t^2+E_0^2} = -\frac{1}{4+e_0^2} \tag{51}$$

$$\tag{52}$$

We have:

$$S_i^+ = c_{i\uparrow}^\dagger c_{i\downarrow} \ , \quad S_i^- = c_{i\downarrow}^\dagger c_{i\uparrow} \tag{53}$$

$$\langle\Psi_0| S_1^+ S_2^- |\Psi_0\rangle = \langle\Psi_0| S_1^+ S_2^- (-\frac{E_0}{(4t^2+E_0^2)^{\frac{1}{2}}} \frac{|\uparrow_1\downarrow_1\rangle + |\uparrow_2\downarrow_2\rangle}{\sqrt{2}} + \frac{2t}{\left(4t^2+E_0^2\right)^{\frac{1}{2}}} \frac{|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle}{\sqrt{2}}) = \tag{54}$$

$$= \langle\Psi_0| (\frac{2t}{\left(4t^2+E_0^2\right)^{\frac{1}{2}}} \frac{S_1^+ S_2^- |\uparrow_1\downarrow_2\rangle - S_1^+ S_2^- |\downarrow_1\uparrow_2\rangle}{\sqrt{2}}) = \tag{55}$$

$$= -\frac{2t}{\left(4t^2+E_0^2\right)^{\frac{1}{2}}} \frac{\langle\Psi_0|\uparrow_1\downarrow_2\rangle}{\sqrt{2}} = -\frac{2t^2}{4t^2+E_0^2} = -\frac{2}{4+e_0^2} \tag{56}$$

$$\tag{57}$$

$$\langle\Psi_0| S_1^- S_2^+ |\Psi_0\rangle = \langle\Psi_0| (\frac{2t}{\left(4t^2+E_0^2\right)^{\frac{1}{2}}} \frac{S_1^- S_2^+ |\uparrow_1\downarrow_2\rangle - S_1^- S_2^+ |\downarrow_1\uparrow_2\rangle}{\sqrt{2}}) = \tag{58}$$

$$= \frac{2t}{\left(4t^2+E_0^2\right)^{\frac{1}{2}}} \frac{\langle\Psi_0|\downarrow_1\uparrow_2\rangle}{\sqrt{2}} = -\frac{2t^2}{4t^2+E_0^2} = -\frac{2}{4+e_0^2} \tag{59}$$

$$\tag{60}$$

Therefore:

$$\langle\Psi_0| \vec{S}_1 \cdot \vec{S}_2 |\Psi_0\rangle = \langle\Psi_0| S_1^z S_2^z |\Psi_0\rangle + \frac{1}{2}\langle\Psi_0| S_1^+ S_2^- |\Psi_0\rangle + \frac{1}{2}\langle\Psi_0| S_1^- S_2^+ |\Psi_0\rangle = \tag{61}$$

$$= -\frac{3t^2}{4t^2+E_0^2} = -\frac{3}{4+e_0^2} \tag{62}$$

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Hartree-Fock

We are going to minimize the energy functional with:

$$|\Psi_{HF}\rangle = \left(\cos\alpha c_{1\uparrow}^\dagger + \sin\alpha c_{2\uparrow}^\dagger\right)\left(\cos\beta c_{1\downarrow}^\dagger + \sin\beta c_{2\downarrow}^\dagger\right)|0\rangle \tag{63}$$

where α and β are our variational parameters. We are using a two opposite spins state as trial wavefunction because the two spin up or two spin down eigenstates have E=0 (in fact, becauce of Pauli principle, the two particles have to occupy two different sites and so the interaction energy is 0 while there cannot be hopping due to the same spin), therefore, with this choice, we hope to find a negative value of energy functional.

$$E(\alpha,\beta) \equiv \langle\Psi_{HF}|\,\hat{H}\,|\Psi_{HF}\rangle = -2t\sin(\alpha+\beta)\cos(\alpha-\beta) + \frac{U}{2}\left[\cos^2(\alpha+\beta)+\cos^2(\alpha-\beta)\right] \tag{64}$$

Proof.

$$\begin{aligned}
|\Psi_{HF}\rangle = \left(\cos\alpha c^\dagger_{1\uparrow} + \sin\alpha c^\dagger_{2\uparrow}\right)\left(\cos\beta c^\dagger_{1\downarrow} + \sin\beta c^\dagger_{2\downarrow}\right)|0\rangle = \quad (65)\\
= \cos\alpha\cos\beta\,|\uparrow_1\downarrow_1\rangle + \cos\alpha\sin\beta\,|\uparrow_1\downarrow_2\rangle + \sin\alpha\cos\beta\,|\uparrow_2\downarrow_1\rangle + \sin\alpha\sin\beta\,|\uparrow_2\downarrow_2\rangle \quad (66)\\
= \cos\alpha\cos\beta\,|\uparrow_1\downarrow_1\rangle + \cos\alpha\sin\beta\,|\uparrow_1\downarrow_2\rangle - \sin\alpha\cos\beta\,|\downarrow_1\uparrow_2\rangle + \sin\alpha\sin\beta\,|\uparrow_2\downarrow_2\rangle \quad (67)\\
(68)
\end{aligned}$$

Using eq.(8), (13), (17), (21):

$$\begin{aligned}
\hat{H}\,|\Psi_{HF}\rangle = &+\cos\alpha\cos\beta\hat{H}\,|\uparrow_1\downarrow_1\rangle + \cos\alpha\sin\beta\hat{H}\,|\uparrow_1\downarrow_2\rangle + && (69)\\
&-\sin\alpha\cos\beta\hat{H}\,|\downarrow_1\uparrow_2\rangle + \sin\alpha\sin\beta\hat{H}\,|\uparrow_2\downarrow_2\rangle = && (70)\\
= &+\cos\alpha\cos\beta(t\,|\downarrow_1\uparrow_2\rangle - t\,|\uparrow_1\downarrow_2\rangle + U\,|\uparrow_1\downarrow_1\rangle)+ && (71)\\
&+\cos\alpha\sin\beta(-t\,|\uparrow_2\downarrow_2\rangle - t\,|\uparrow_1\downarrow_1\rangle)+ && (72)\\
&-\sin\alpha\cos\beta(+t\,|\uparrow_2\downarrow_2\rangle + t\,|\uparrow_1\downarrow_1\rangle)+ && (73)\\
&+\sin\alpha\sin\beta(+t\,|\downarrow_1\uparrow_2\rangle - t\,|\uparrow_1\downarrow_2\rangle + U\,|\uparrow_2\downarrow_2\rangle) = && (74)\\
= &+(U\cos\alpha\cos\beta - t\cos\alpha\sin\beta - t\sin\alpha\cos\beta)\,|\uparrow_1\downarrow_1\rangle + && (75)\\
&+(-t\cos\alpha\cos\beta - t\sin\alpha\sin\beta)\,|\uparrow_1\downarrow_2\rangle + && (76)\\
&+(t\cos\alpha\cos\beta + t\sin\alpha\sin\beta)\,|\downarrow_1\uparrow_2\rangle + && (77)\\
&+(-t\cos\alpha\sin\beta - t\sin\alpha\cos\beta + U\sin\alpha\sin\beta)\,|\uparrow_2\downarrow_2\rangle && (78)
\end{aligned}$$

Therefore:

$$\begin{aligned}
\langle\Psi_{HF}|\,\hat{H}\,|\Psi_{HF}\rangle =&+(U\cos\alpha\cos\beta - t\cos\alpha\sin\beta - t\sin\alpha\cos\beta)\cos\alpha\cos\beta+ &(79)\\
&+(-t\cos\alpha\cos\beta - t\sin\alpha\sin\beta)\cos\alpha\sin\beta+ &(80)\\
&-(t\cos\alpha\cos\beta + t\sin\alpha\sin\beta)\sin\alpha\cos\beta+ &(81)\\
&+(-t\cos\alpha\sin\beta - t\sin\alpha\cos\beta + U\sin\alpha\sin\beta)\sin\alpha\sin\beta = &(82)\\
=&+U\cos^2\alpha\cos^2\beta - t\cos^2\alpha\sin\beta\cos\beta - t\sin\alpha\cos^2\beta\cos\alpha+ &(83)\\
&-t\cos^2\alpha\cos\beta\sin\beta - t\sin\alpha\sin^2\beta\cos\alpha+ &(84)\\
&-t\cos\alpha\cos^2\beta\sin\alpha - t\sin^2\alpha\sin\beta\cos\beta+ &(85)\\
&-t\cos\alpha\sin^2\beta\sin\alpha - t\sin^2\alpha\cos\beta\sin\beta + U\sin^2\alpha\sin^2\beta = &(86)\\
=&+U(\cos^2\alpha\cos^2\beta + \sin^2\alpha\sin^2\beta) &(87)\\
&-t\cos^2\alpha\sin\beta\cos\beta - t\sin\alpha\cos^2\beta\cos\alpha+ &(88)\\
&-t\cos^2\alpha\cos\beta\sin\beta - t\sin\alpha\sin^2\beta\cos\alpha+ &(89)\\
&-t\cos\alpha\cos^2\beta\sin\alpha - t\sin^2\alpha\sin\beta\cos\beta+ &(90)\\
&-t\cos\alpha\sin^2\beta\sin\alpha - t\sin^2\alpha\cos\beta\sin\beta = &(91)\\
=&+\frac{U}{2}\left[\cos^2(\alpha+\beta)+\cos^2(\alpha-\beta)\right]+ &(92)\\
&-2t\cos^2\alpha\sin\beta\cos\beta - 2t\sin\alpha\cos^2\beta\cos\alpha+ &(93)\\
&-2t\sin\alpha\sin^2\beta\cos\alpha - 2t\sin^2\alpha\sin\beta\cos\beta = &(94)\\
=&+\frac{U}{2}\left[\cos^2(\alpha+\beta)+\cos^2(\alpha-\beta)\right]+ &(95)\\
&-2t\alpha\sin\beta\cos\beta - 2t\sin\alpha\cos\alpha = &(96)\\
=&+\frac{U}{2}\left[\cos^2(\alpha+\beta)+\cos^2(\alpha-\beta)\right] - 2t\sin(\alpha+\beta)\cos(\alpha-\beta) &(97)
\end{aligned}$$

■

Using the previous computation, it is straightforward to deduce also:

$$\langle\Psi_{HF}|\,\hat{D}\,|\Psi_{HF}\rangle = \frac{1}{2}\left[\cos^2(\alpha+\beta)+\cos^2(\alpha-\beta)\right] \tag{98}$$

$$\langle\Psi_{HF}|\,\hat{H}_t\,|\Psi_{HF}\rangle = -2t\sin(\alpha+\beta)\cos(\alpha-\beta) \tag{99}$$

Moreover, we have:

$$\begin{aligned}
\langle\Psi_{HF}|\,\vec{S}_1\cdot\vec{S}_2\,|\Psi_{HF}\rangle =&-\frac{1}{8}\left[\sin^2(\alpha+\beta)+\sin^2(\alpha-\beta)\right]+ &(100)\\
&-\frac{1}{8}\left[\cos^2(\alpha-\beta)-\sin^2(\alpha-\beta)-\cos^2(\alpha+\beta)+\sin^2(\alpha+\beta)\right] &(101)
\end{aligned}$$

Proof.

$$\langle\Psi_{HF}|\,\vec{S}_1\cdot\vec{S}_2\,|\Psi_{HF}\rangle = \langle\Psi_{HF}|\,S_1^zS_2^z\,|\Psi_{HF}\rangle + \frac{1}{2}\langle\Psi_{HF}|\,S_1^+S_2^-\,|\Psi_{HF}\rangle + \frac{1}{2}\langle\Psi_{HF}|\,S_1^-S_2^+\,|\Psi_{HF}\rangle \tag{102}$$

$$\langle\Psi_{HF}|\, S_1^z S_2^z \,|\Psi_{HF}\rangle = \langle\Psi_{HF}|\, S_1^z S_2^z (\cos\alpha\sin\beta\,|\uparrow_1\downarrow_2\rangle - \sin\alpha\cos\beta\,|\downarrow_1\uparrow_2\rangle) = \tag{103}$$

$$= -\frac{1}{4}\,\langle\Psi_{HF}|\,(\cos\alpha\sin\beta\,|\uparrow_1\downarrow_2\rangle - \sin\alpha\cos\beta\,|\downarrow_1\uparrow_2\rangle) = \tag{104}$$

$$= -\frac{1}{4}(\cos^2\alpha\sin^2\beta + \sin^2\alpha\cos^2\beta) = \tag{105}$$

$$= -\frac{1}{8}\left[\sin^2(\alpha+\beta) + \sin^2(\alpha-\beta)\right] \tag{106}$$

$$\langle\Psi_{HF}|\, S_1^+ S_2^- \,|\Psi_{HF}\rangle = \langle\Psi_{HF}|\, S_1^+ S_2^- (\cos\alpha\sin\beta\,|\uparrow_1\downarrow_2\rangle - \sin\alpha\cos\beta\,|\downarrow_1\uparrow_2\rangle) = \tag{107}$$

$$= -\,\langle\Psi_{HF}|\,\sin\alpha\cos\beta\,|\uparrow_1\downarrow_2\rangle = -\sin\alpha\cos\beta\sin\beta\cos\alpha \tag{108}$$

$$\tag{109}$$

$$\langle\Psi_{HF}|\, S_1^- S_2^+ \,|\Psi_{HF}\rangle = \langle\Psi_{HF}|\, S_1^- S_2^+ (\cos\alpha\sin\beta\,|\uparrow_1\downarrow_2\rangle - \sin\alpha\cos\beta\,|\downarrow_1\uparrow_2\rangle) = \tag{110}$$

$$= \langle\Psi_{HF}|\,\cos\alpha\sin\beta\,|\downarrow_1\uparrow_2\rangle = -\sin\alpha\cos\beta\sin\beta\cos\alpha \tag{111}$$

$$\tag{112}$$

$$\langle\Psi_{HF}|\, \vec{S}_1\cdot\vec{S}_2 \,|\Psi_{HF}\rangle = \langle\Psi_{HF}|\, S_1^z S_2^z \,|\Psi_{HF}\rangle + \frac{1}{2}\,\langle\Psi_{HF}|\, S_1^+ S_2^- \,|\Psi_{HF}\rangle + \frac{1}{2}\,\langle\Psi_{HF}|\, S_1^- S_2^+ \,|\Psi_{HF}\rangle = \tag{113}$$

$$= -\frac{1}{8}\left[\sin^2(\alpha+\beta) + \sin^2(\alpha-\beta)\right] - \sin\alpha\cos\beta\sin\beta\cos\alpha = \tag{114}$$

$$= -\frac{1}{8}\left[\sin^2(\alpha+\beta) + \sin^2(\alpha-\beta)\right] + \tag{115}$$

$$-\frac{1}{8}\left[\cos(2\alpha-2\beta) - \cos(2\alpha+2\beta)\right] = \tag{116}$$

$$= -\frac{1}{8}\left[\sin^2(\alpha+\beta) + \sin^2(\alpha-\beta)\right] + \tag{117}$$

$$-\frac{1}{8}\left[\cos^2(\alpha-\beta) - \sin^2(\alpha-\beta) - \cos^2(\alpha+\beta) + \sin^2(\alpha+\beta)\right] \tag{118}$$

■

Let me call:

$$\begin{cases} x = \sin(\alpha+\beta) \\ y = \cos(\alpha-\beta) \end{cases} \tag{119}$$

Therefore:

$$E(\alpha,\beta) = -2t\sin(\alpha+\beta)\cos(\alpha-\beta) + \frac{U}{2}\left[1 - \sin^2(\alpha+\beta) + \cos^2(\alpha-\beta)\right] = \tag{120}$$

$$= -2txy + \frac{U}{2}\left[1 - x^2 + y^2\right] \equiv \mathrm{E}(x,y) \quad \text{with } |x|\le 1, |y|\le 1 \tag{121}$$

$$\langle\Psi_{HF}|\,\hat{D}\,|\Psi_{HF}\rangle = \frac{1}{2}\left[\cos^2(\alpha+\beta)+\cos^2(\alpha-\beta)\right] = \tag{122}$$

$$= \frac{1}{2}\left[1-x^2+y^2\right] \tag{123}$$

$$\langle\Psi_{HF}|\,\hat{H}_t\,|\Psi_{HF}\rangle = -2t\sin(\alpha+\beta)\cos(\alpha-\beta) = -2txy \tag{124}$$

$$\langle\Psi_{HF}|\,\vec{S}_1\cdot\vec{S}_2\,|\Psi_{HF}\rangle = \frac{1}{8}\left[-3x^2-y^2+1\right] \tag{125}$$

Proof.

$$\langle\Psi_{HF}|\,\vec{S}_1\cdot\vec{S}_2\,|\Psi_{HF}\rangle = -\frac{1}{8}\left[\sin^2(\alpha+\beta)+\sin^2(\alpha-\beta)\right]+ \tag{126}$$

$$-\frac{1}{8}\left[\cos^2(\alpha-\beta)-\sin^2(\alpha-\beta)-\cos^2(\alpha+\beta)+\sin^2(\alpha+\beta)\right] = \tag{127}$$

$$= -\frac{1}{8}\left[x^2+1-y^2\right]+ \tag{128}$$

$$-\frac{1}{8}\left[y^2-1+y^2-1+x^2+x^2\right] = \tag{129}$$

$$= -\frac{1}{8}\left[x^2+1-y^2\right]-\frac{1}{8}\left[2y^2-2+2x^2\right] = \tag{130}$$

$$= -\frac{1}{8}\left[3x^2+y^2-1\right] = \frac{1}{8}\left[-3x^2-y^2+1\right] \tag{131}$$

$$\tag{132}$$

■

In order to optimize the parameters of our wavefunction, we have to minimize the expectation value of the hamiltonian. We have:

$$\min_{|x|\le 1,|y|\le 1} \mathrm{E}(x,y) = \begin{cases} -2t+\frac{U}{2} & ,\ \frac{U}{t}<2 \text{ with } (x,y)_{\min}=(\pm1,\pm1) \\ -\frac{2t^2}{U} & ,\ \frac{U}{t}>2 \text{ with } (x,y)_{\min}=(\pm1,\pm\frac{2t}{U}) \end{cases} \tag{133}$$

Proof. We must find the minimum:

$$\min_{|x|\le 1,|y|\le 1} \mathrm{E}(x,y) \tag{134}$$

which exists because of Weistress theorem since $\mathrm{E}(x,y)$ is a continous function and $(|x|\le 1, |y|\le 1)$ is closed and bounded. Let us start by checking the function gradient:

$$\boldsymbol{\nabla}\mathrm{E}(x,y) = (-2ty-Ux, -2tx+Uy) = (0,0) \tag{135}$$

$$\begin{cases} y = -\frac{U}{2t}x \\ Uy = 2tx \end{cases} \Rightarrow U^2 = -4t^2 \Rightarrow \nexists\ |x|<1, |y|<1 \text{ such that } \boldsymbol{\nabla}E = (0,0) \tag{136}$$

Hence, the minimum must exist on the border.
CASE : $\mathbf{x = 1, |y| \le 1}$:

$$E(1,y) = -2ty + \frac{U}{2}y^2 \ \Rightarrow E'(1,y) = -2t+Uy = 0 \ \Rightarrow y^* = \frac{2t}{U} \tag{137}$$

In this point, we have:

$$E(1, \frac{2t}{U}) = -\frac{4t^2}{U} + \frac{U}{2}\frac{4t^2}{U^2} = -\frac{2t^2}{U} \tag{138}$$

We have that $|y^*| \leq 1$ when $\frac{U}{t} \geq 2$.
CASE : $\mathbf{x = -1, |y| \leq 1}$:

$$E(-1, y) = +2ty + \frac{U}{2}y^2 \ \Rightarrow E'(1, y) = +2t + Uy = 0 \Rightarrow y^* = -\frac{2t}{U} \tag{139}$$

In this point, we have:

$$E(1, -\frac{2t}{U}) = -\frac{4t^2}{U} + \frac{U}{2}\frac{4t^2}{U^2} = -\frac{2t^2}{U} \tag{140}$$

We have that $|y^*| \leq 1$ when $\frac{U}{t} \geq 2$.
CASE : $\mathbf{|x| \leq 1, y = 1}$:

$$E(x, 1) = -2tx + \frac{U}{2}\left[2 - x^2\right] \ \Rightarrow E'(x, 1) = -2t - Ux = 0 \Rightarrow x^* = -\frac{2t}{U} \tag{141}$$

In this point, we have:

$$E(-\frac{2t}{U}, 1) = \frac{4t^2}{U} + \frac{U}{2}\left[2 - \frac{4t^2}{U^2}\right] = U + \frac{2t^2}{U} > 0 \tag{142}$$

But it is larger that the energy values previously found.
CASE : $\mathbf{|x| \leq 1, y = -1}$:

$$E(x, -1) = 2tx + \frac{U}{2}\left[2 - x^2\right] \ \Rightarrow E'(x, 1) = 2t - Ux = 0 \Rightarrow x^* = \frac{2t}{U} \tag{143}$$

In this point, we have:

$$E(\frac{2t}{U}, 1) = \frac{4t^2}{U} + \frac{U}{2}\left[2 - \frac{4t^2}{U^2}\right] = U + \frac{2t^2}{U} > 0 \tag{144}$$

But it is larger that the energy values previously found.
CASE : $\mathbf{x = \pm 1, y = \mp 1}$:

$$E(\pm 1, \mp 1) = +2t + \frac{U}{2} > 0 \tag{145}$$

But it is larger that the energy values previously found.
CASE : $\mathbf{x = \pm 1, y = \pm 1}$:

$$E(\pm 1, \pm 1) = -2t + \frac{U}{2} \tag{146}$$

We have that this point is lower than the one we found ($E^* = -\frac{2t^2}{U}$) before when $\frac{U}{t} < 2$, in fact:

$$-2t + \frac{U}{2} < -\frac{2t^2}{U} \ \Rightarrow U^2 - 4Ut + 4t^2 < 0 \ \Rightarrow \frac{U}{t} < 2 \tag{147}$$

Therefore we have that:

$$\min_{|x|\leq 1, |y|\leq 1} \mathrm{E}(x, y) = \begin{cases} -2t + \frac{U}{2} & , \ \frac{U}{t} < 2 \text{ with } (x, y)_{\min} = (\pm 1, \pm 1) \\ -\frac{2t^2}{U} & , \ \frac{U}{t} > 2 \text{ with } (x, y)_{\min} = (\pm 1, \pm \frac{2t}{U}) \end{cases} \tag{148}$$

■

In addition we can observe that:

$$|\Psi_{HF}\rangle = \frac{1}{\sqrt{2}}\left(c^\dagger_{1\uparrow} + c^\dagger_{2\uparrow}\right)\frac{1}{\sqrt{2}}\left(c^\dagger_{1\downarrow} + c^\dagger_{2\downarrow}\right)|0\rangle \quad \text{for } \frac{U}{t} < 2 \tag{149}$$

(we can have other states where only the signes in front of the various creation operators change, but all the creation operators must have $\sqrt{1/2}$ as factor)

$$|\Psi_{HF}\rangle = |\uparrow_1\downarrow_2\rangle \text{ or } |\Psi_{HF}\rangle = |\uparrow_2\downarrow_1\rangle \text{ for } \frac{U}{t} > 2 \tag{150}$$

Proof. From previous calculation we have for $U/t < 2$:

$$(\sin(\alpha+\beta), \cos(\alpha-\beta))_{\min} = (x, y)_{\min} = (\pm 1, \pm 1) \Rightarrow (\alpha, \beta) = (\frac{\pi}{4}, \frac{\pi}{4}), (-\frac{3\pi}{4}, \frac{\pi}{4}), ... \tag{151}$$

For $U/t \to \infty$:

$$(\sin(\alpha+\beta), \cos(\alpha-\beta))_{\min} = (x, y)_{\min} = (\pm 1, \pm\frac{2t}{U} \sim 0) \Rightarrow (\alpha, \beta) = (0, \frac{\pi}{2}), (\frac{\pi}{2}, 0) \tag{152}$$

And we can easily conclude by considering the initial form of the state:

$$|\Psi_{HF}\rangle = \left(\cos\alpha c^\dagger_{1\uparrow} + \sin\alpha c^\dagger_{2\uparrow}\right)\left(\cos\beta c^\dagger_{1\downarrow} + \sin\beta c^\dagger_{2\downarrow}\right)|0\rangle \tag{153}$$

■

Since now we have found our optimized parameters, we can compute the expectation values on the HF wavefunction of the following observables:

$$\langle\Psi_{HF}|\hat{D}|\Psi_{HF}\rangle = \frac{1}{2}\left[1 - x^2 + y^2\right] = \begin{cases} \frac{1}{2} & , \frac{U}{t} < 2 \text{ with } (x,y)_{\min} = (\pm 1, \pm 1) \\ \frac{2t^2}{U^2} & , \frac{U}{t} > 2 \text{ with } (x,y)_{\min} = (\pm 1, \pm\frac{2t}{U}) \end{cases} \tag{154}$$

$$\langle\Psi_{HF}|\hat{H}_t|\Psi_{HF}\rangle = -2txy = \begin{cases} -2t & , \frac{U}{t} < 2 \text{ with } (x,y)_{\min} = (\pm 1, \pm 1) \\ -\frac{4t^2}{U} & , \frac{U}{t} > 2 \text{ with } (x,y)_{\min} = (\pm 1, \pm\frac{2t}{U}) \end{cases} \tag{155}$$

$$\langle\Psi_{HF}|\vec{S}_1 \cdot \vec{S}_2|\Psi_{HF}\rangle = \frac{1}{8}\left[-3x^2 - y^2 + 1\right] = \begin{cases} -\frac{3}{8} & , \frac{U}{t} < 2 \text{ with } (x,y)_{\min} = (\pm 1, \pm 1) \\ \frac{1}{4}(-1 - \frac{2t^2}{U^2}) & , \frac{U}{t} > 2 \text{ with } (x,y)_{\min} = (\pm 1, \pm\frac{2t}{U}) \end{cases} \tag{156}$$

Comparing Hartee-Fock with exact results

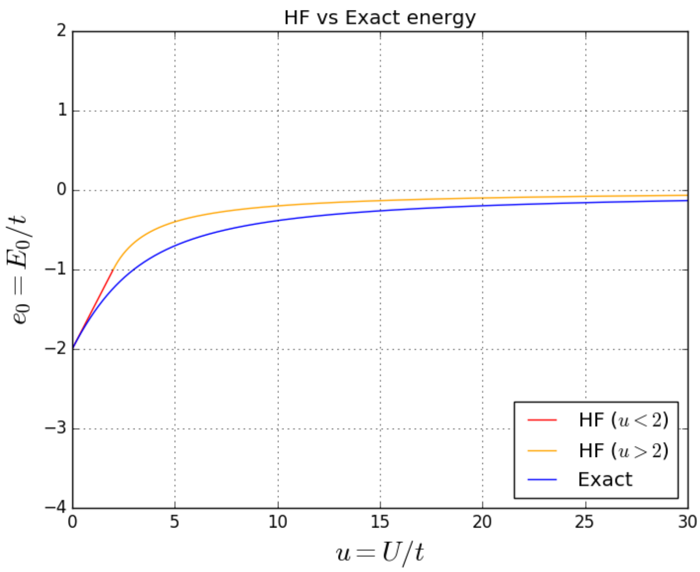

Figure 5: Plot of HF vs Exact ground state energy. The exact ground energy is below HF one as it must be because of variational principle.

We got ground state energy:

$$E_0 = \frac{U}{2} - \frac{\sqrt{U^2 + 16t^2}}{2} \tag{157}$$

$$e_0 = \frac{u}{2} - \frac{\sqrt{u^2 + 16}}{2} \tag{158}$$

where $e \equiv \frac{E}{t}$, $u \equiv \frac{U}{t}$. We have that:

$$e_0 = \frac{u}{2} - \frac{\sqrt{u^2 + 16}}{2} = \begin{cases} -2 + \frac{u}{2} - \frac{u^2}{16} + o(u^2) & , \ u \to 0 \\ -\frac{4}{u} + o(u) & , \ u \to \infty \end{cases} \tag{159}$$

Proof. For $u = \frac{U}{t} \ll 1$ we have:

$$e_0 = \frac{u}{2} - \frac{\sqrt{u^2 + 16}}{2} = \frac{u}{2} - 4\frac{\sqrt{\frac{u^2}{16} + 1}}{2} = \frac{u}{2} - 2(\frac{u^2}{32} + 1) + o(u^2) = -2 + \frac{u}{2} - \frac{u^2}{16} + o(u^2) \tag{160}$$

For $u = \frac{U}{t} \gg 1$ we have:

$$e_0 = \frac{u}{2} - \frac{\sqrt{u^2 + 16}}{2} = \frac{u}{2} - \frac{u\sqrt{1 + \frac{16}{u^2}}}{2} = \frac{u}{2} - \frac{u}{2}(1 + \frac{8}{u^2}) + o(u) = -\frac{4}{u} + o(u) \tag{161}$$

■

With HF we found:

$$E_{0\,HF} = \begin{cases} -2t + \frac{U}{2} & , \ \frac{U}{t} < 2 \\ -\frac{2t^2}{U} & , \ \frac{U}{t} > 2 \end{cases} \Rightarrow \ e_{0\,HF} = \begin{cases} -2 + \frac{u}{2} & , \ u < 2 \\ -\frac{2}{u} & , \ u > 2 \end{cases} \tag{162}$$

Hence for $u \to 0$ the exact energy is below the HF energy (as it must be by the variational principle) but the difference is a function of order $o(u^2)$, so the two results agree in this case.

Moreover, we have that for $u \to 0$ the exact ground state also agrees with the HF solution, in fact for the exact state, by eq. (37), we have $b/a = -2t/E \to 1$ and so $|\Psi_0\rangle = \frac{|\uparrow_1\downarrow_1\rangle + |\uparrow_2\downarrow_2\rangle}{2} + \frac{|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle}{2}$, while for HF we have the form of state written in eq.(149). This means that any electron has the same probability to be found at any site.

In the limit $u \to \infty$, ground state exact energy is twice smaller than HF one. In this case, for exact state, (by eq.(37)) $a/b = -E/2t \to 2/u \to 0$ which means that the probability to have both electrons at the same site vanishes like $\sim 1/u^2$.

We also see that, in this limit of strong interaction, the true ground state is a singlet $\frac{|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle}{\sqrt{2}}$, not the HF prediction that one electron is on the left ion and the other one on the right one, or viceversa (which follows from eq.(150)). The singlet makes better sense because there is nothing to distinguish the two ions, hence there is no reason why they would have different permanent magnetic moments associated with their electrons. Nonetheless, the singlet state is not a Slater determinant, so the best HF can do is to imitate the tendency for antiferromagnetic order (singlet) by putting electrons with opposite spins on the two sites. This also explains why HF energy is twice bigger than exact one.

So we see that HF predicts that the system is "metallic" at small U/t, but becomes "insulating" at large U/t, where the wavefunction has one electron per site. Even if the electrons are localized at one per site (which is now favourable in order to avoid the large cost U of having two electrons per site), they tend to order in a singlet, as if there is antiferromagnetic coupling between the electrons. As said before, with HF we don't get this completely right, but at least we imitate the antiferromagnet tendency. HF also predicts a transition between the two regimes, in fact there is a discontinuity of E_{HF}/t at $U/t = 2$. This is not correct precisely in the exact case, but it's the best HF can do to imitate this "phase transition".

Now we compare the expectation values of the other observables. By the results obtained in the previous sections we have (where $|\Psi_0\rangle$ is the exact ground state solution):

$$\langle \Psi_{HF} | \hat{D} | \Psi_{HF} \rangle = \begin{cases} \frac{1}{2} & , \ \frac{U}{t} < 2 \\ \frac{2t^2}{U^2} & , \ \frac{U}{t} > 2 \end{cases} \tag{163}$$

$$\langle \Psi_0 | \hat{D} | \Psi_0 \rangle = \frac{e_0^2}{4 + e_0^2} = \begin{cases} \frac{1}{2} & , \ u \to 0 \\ \frac{4}{u^2} & , \ u \to \infty \end{cases} \tag{164}$$

For small u we obtain the same result, while for large u we obtain a factor 2 of difference for the same reason explained before.

$$\langle \Psi_{HF} | \hat{H}_t/t | \Psi_{HF} \rangle = \begin{cases} -2 & , \ \frac{U}{t} < 2 \\ -\frac{4t}{U} & , \ \frac{U}{t} > 2 \end{cases} \tag{165}$$

$$\langle \Psi_0 | \hat{H}_t/t | \Psi_0 \rangle = \frac{8e_0}{4 + e_0^2} = \begin{cases} -2 & , \ u \to 0 \\ -\frac{8}{u} & , \ u \to \infty \end{cases} \tag{166}$$

We obtain the same we argued before: for small u same result, for large u we obtain a factor 2 of difference.

$$\langle\Psi_{HF}|\,\vec{S}_1\cdot\vec{S}_2\,|\Psi_{HF}\rangle = \begin{cases} -\dfrac{3}{8} & , \frac{U}{t} < 2 \\ \dfrac{1}{4}(-1-\dfrac{2t^2}{U^2}) & , \frac{U}{t} > 2 \end{cases} \tag{167}$$

$$\langle\Psi_0|\,\vec{S}_1\cdot\vec{S}_2\,|\Psi_0\rangle = -\frac{3}{4+e_0^2} = \begin{cases} -\frac{3}{8} & , u\to 0 \\ -\frac{3}{4}(1-\dfrac{4}{u^2}) & , u\to\infty \end{cases} \tag{168}$$

For small coupling u we get the same result, but different for large u. The fact that for $u\to 0$ we have $\langle\vec{S}_1\cdot\vec{S}_2\rangle = -3/8$ makes sense because we can check easily that $-3/8$ is the expectation value of $\vec{S}_1\cdot\vec{S}_2$ on the U=0 ground state $|\Psi_0\rangle = \frac{|\uparrow_1\downarrow_1\rangle+|\uparrow_2\downarrow_2\rangle}{2} + \frac{|\uparrow_1\downarrow_2\rangle-|\downarrow_1\uparrow_2\rangle}{2}$ that it what we found also with HF.

We can observe that, in the exact case for large u, we have $\langle\Psi_0|\,\vec{S}_1\cdot\vec{S}_2\,|\Psi_0\rangle \to -3/4$ which makes sense besause it is the eigenvalue of $\vec{S}_1\cdot\vec{S}_2$ for the singlet state as it must be (according to the previous result, the ground state approaches to singles state for strong coupling limit).

In conclusion, in the "metallic" regime (for small u), we can trust HF approximation.

Comparing 2 sites Hubbard model with general case

In this case of two sites Hubbard model, we have that the double occupancy for number of particles is:

$$\langle\Psi_0|\,\frac{\hat{D}}{2}\,|\Psi_0\rangle = \frac{1}{2}\frac{e_0^2}{4+e_0^2} = \begin{cases} \frac{1}{4} & , u\to 0 \\ \frac{2}{u^2} & , u\to\infty \end{cases} \tag{169}$$

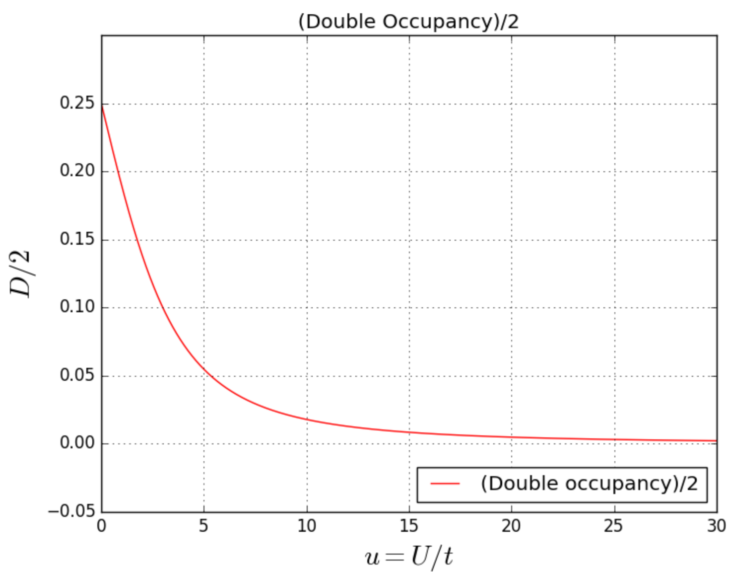

Figure 6: Double occupancy for number of particles. It starts by 1/4 as in the general case.

which is in agreement with what we have in the general case. In fact, in the general case of Hubbard model at half filling, we have for $u = 0$:

$$\langle \hat{D} \rangle = \sum_{i=1}^{N} \langle \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \rangle = \sum_{i=1}^{N} \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle = \sum_{i=1}^{N} \frac{n}{2} \frac{n}{2} = N \frac{n^2}{4} \Rightarrow \frac{\langle \hat{D} \rangle}{N} = \frac{n^2}{4} = \frac{1}{4} \tag{170}$$

Hence this result is general but it is not surprising because when $u = 0$ there is no coupling between different spins and each configuration for a site (empty, $\uparrow$, $\downarrow$ and $\uparrow\downarrow$) has the same probability to occur. Operator $\hat{D}$ is the one that appears in the Hamiltonian when the interaction is turned on and so, in general, for $u \neq 0$ we have a different value of $\frac{\langle \hat{D} \rangle}{N}$. For $u \to \infty$ we have $\frac{\langle \hat{D} \rangle}{N} = 0$ because all electrons tend to stay on different sites. Since in this limit there is no hopping, we have an insulator. This tell us that Hubbard model must feature a metal-insulator phase transition (Mott transition). This is also what we have found with our two sites problem in fact we can observe the two different regimes for $u \to 0$ and $u \to \infty$ as largely described previously for our case. To sum up what we have obtained previously, for $u \to 0$ the exact ground state is $|\Psi_0\rangle = \frac{|\uparrow_1\downarrow_1\rangle + |\uparrow_2\downarrow_2\rangle}{2} + \frac{|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle}{2}$ which means that any electron has the same probability to be found at any site and hopping is allowed (metallic behaviour).

In the limit $u \to \infty$, for exact state we have that the true ground state is a singlet $\frac{|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle}{\sqrt{2}}$ and there is no hopping in this limit (insulator behaviour).

In addition, as explained in the previous section, the excistence of these two different regimes is also emphasized by the result of HF energy that we got (which show a discontinuity).

In the general case we have the emergence of an antiferromagnetic ordering which arises also in our two sites results. The fact that the spins of the electrons would prefer AFM order in the insulating phase makes sense because when there is one electron per ion in fact for parallel spins, Pauli principle forbids any electron from hopping to its neighbour and the energy is zero $E_{\uparrow\uparrow} = E_{\downarrow\downarrow} = 0$. On the other hand, if the spins are antiparallel, then each electron can make short "visits" to the other site. The "visit" (virtual hopping) is short so as to avoid paying the large cost U (indeed, in our case, by eq.(37), $a/b = -E/2t \to 2/u \to 0$) but the energy is lowered a bit because the electron moves so the kinetic energy contributes a bit. This is what we can observe in our two sites case, where we have the ground state that for $u \to \infty$ approach to a singlet state (AFM ordering) and, moreover, we can observe that $\langle\Psi_0| \vec{S}_1 \cdot \vec{S}_2 |\Psi_0\rangle \to -3/4$ which is the value that it should be for the singlet state.