6. Mean field approximation

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6.1 Hubbard model

The Hubbard model (6.1) is one of the simplest many particle models. However, its ground state is known to be complex. In general, exact solutions are unavailable. The exception are one dimensional systems where there are many possible methods; to cite only some of them: Bethe ansatz, bosonization, Luttinger and Tomonaga method. But these methods can't be used for two or three dimensional systems, and (approximate) numerical methods have to be employed to solve the Hubbard model.
The one band Hubbard model can be written as follows:

$$H = \sum_{\langle i,j\rangle,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \,, \tag{6.1}$$

where t_{ij} is the hopping amplitude, $\langle i, j\rangle$ indicates summation over the nearest neighbors. U is the value of the on-site Coulomb repulsion. $c^{\dagger}_{i\sigma}$, $c_{i\sigma}$ are the creation and annihilation operators, and $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$ is the local density of electrons for spin σ. In this case, the Coulomb interaction doesn't act between electrons of the same spin as the Pauli exclusion principle doesn't allow two electrons two be in identical states, so we can't consider the possibility of two electrons of the same spin on the same site of the lattice.

6.1.1 Simplest mean field approximation

After a direct Hartree-Fock decoupling of the four-operator terms, the mean field Hamiltonian (6.2) can be written as the sum of a Hamiltonian for spin

up, a Hamiltonian for spin down and a constant:

$$\begin{aligned} H^{MF} &= H_\uparrow + H_\downarrow + C. \qquad (6.2) \\ H_\uparrow &= -t \sum_{\langle i,j \rangle} c^\dagger_{i\uparrow} c_{j\uparrow} + U \sum_i n_{i\uparrow} \langle n_{i\downarrow} \rangle, \\ H_\downarrow &= -t \sum_{\langle i,j \rangle} c^\dagger_{i\downarrow} c_{j\downarrow} + U \sum_i \langle n_{i\uparrow} \rangle n_{i\downarrow}, \\ C &= -U \sum_i \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle. \end{aligned}$$

Now the Hamiltonian is reduced to two matrices of size $N \times N$ (where N is the system size), and we have $2N$ mean field parameters (N local densities $\langle n_{i\uparrow} \rangle$ and N local densities $\langle n_{i\downarrow} \rangle$) to determine the ground state.
This approximation allows us to reduce the problem to a one particle problem. There are a number of advantages:

- the study of big system sizes is possible (the size of the Hilbert space is reduced to the size of the system; the Hamiltonian corresponds just to an $N \times N$ matrix);
- the computation can be done in real space;
- there are no restrictions on the shape of the system (open boundary conditions, defects, any type of geometry and lattices); we can even do simulations based on specific experimental systems;
- the model is flexible (it is easy to add some tight-binding or interaction terms to the model, or to study a deformation of the lattice).

But all of this has a high price:

- The $SU(2)$ symmetry is broken.
- Important effects of the electron interaction are not taken into account: only long range order can be considered, and the stability of magnetic order is overestimated.

In general, the mean field approximation is closer to an exact solution of the model at weak U. At larger U, in the best case the mean field approximation can give the qualitative behavior.

6.1.2 Self-consistent solution

An iterative solution of the mean field Hamiltonian (6.2) involves the following steps:

- The initial condition is applied: the mean field parameters are initialized by a local density of electrons of spin σ.
- The following steps are repeated until convergence:
  - Diagonalization of the Hamiltonians for spin up and down:
    $\Rightarrow$ This yields the one particle energy spectrum $\epsilon_{\alpha,\sigma}$.
    $\Rightarrow$ Now the eigenstate can be constructed:

$$|GS\rangle = \prod_{\alpha=1}^{N_\uparrow} d^\dagger_{\alpha\uparrow} \prod_{\beta=1}^{N_\downarrow} d^\dagger_{\beta\downarrow}|0\rangle\,, \quad d_{\alpha,\sigma} = \sum_i Q^\dagger_{\alpha i,\sigma} c_{i\sigma}.$$

$$H^{MF} = \sum_\sigma \sum_\alpha \epsilon_{\alpha,\sigma} d^\dagger_{\alpha,\sigma} d_{\alpha,\sigma} + C$$

  - New mean field parameters are computed using the new eigenstate:

$$\langle n_{i\sigma}\rangle = \sum_{\alpha=1}^{N_\sigma} Q^\dagger_{\alpha i,\sigma} Q_{i\alpha,\sigma}$$

  Convergence means $\langle n_{i\sigma}\rangle_I = \langle n_{i\sigma}\rangle_{I-1}$, where I corresponds to the number of the iteration.

6.1.3 Frustrated systems

What is frustration?

If we consider the Hubbard model, the on-site Coulomb interaction leads at large U to antiferromagnetic order (for $U \to \infty$, the Hubbard model corresponds to a Heisenberg model with an antiferromagnetic coupling J corresponding to the hopping bond, $J = {}^{4t^2}/_U$). Frustration means that a system is not able to find any magnetic order which satisfies all the couplings of the model.
As illustrated in Figure 6.1, there are at least two types of frustration, geometrical frustration and frustration due to competing interactions.

The classical solution: commensurate spiral order

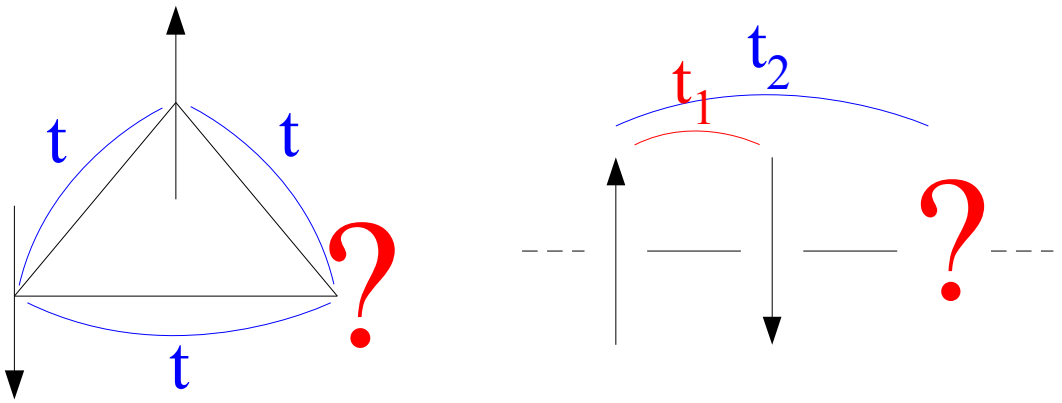

Figure 6.1: Types of frustration: Geometrical frustration (left), and competition between couplings (right).

The classical solution to this problem with periodic boundary conditions (PBC) is a commensurate spiral order (see Figure 6.2).

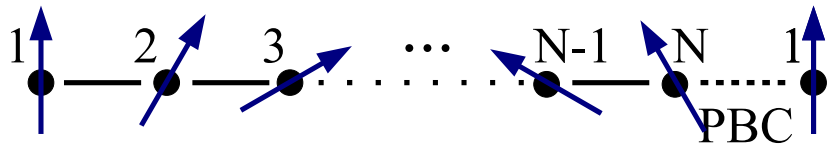

Figure 6.2: Spin spiral that is commensurate with the size of the system due to the periodic boundary condition (PBC).

A spiral order is a magnetic order where the difference of orientation between all first neighbor spins corresponds to a uniform angle θ_a (with a the direction considered). For a system with periodic boundary conditions this angle is not completely free; there is only a finite number of values determined by the system size:

$$\theta_a = \gamma \frac{2\pi}{L_a} \text{ with system size } L_a \text{ in } a \text{ direction and } \gamma \text{ an integer.}$$

For example, in a ring of six sites, θ can only take the values $\pi/3$, $2\pi/3$, and π.

Mean field approximation for a spiral state

The Hartree-Fock decoupling of the Hubbard model used in the previous section is not unique. The one chosen previously allows only magnetic order of Ising type (ferromagnetic or antiferromagnetic order). For frustrated systems, we want to have at least the possibility to study spiral states. To

achieve this, we should choose a mean field approximation including the x and y components of the spin:

$$\begin{aligned} H^{MF2} &= -t\sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i\sigma}c_{j\sigma} + U\sum_{i}\left[\langle n_{i\downarrow}\rangle n_{i\uparrow} + \langle n_{i\uparrow}\rangle n_{i\downarrow} - \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle\right] \\ &\quad -U\sum_{i}\left[\langle S^{+}_{i}\rangle c^{\dagger}_{i\downarrow}c_{i\uparrow} + \langle S^{-}_{i}\rangle c^{\dagger}_{i\uparrow}c_{i\downarrow} - \langle S^{+}_{i}\rangle\langle S^{-}_{i}\rangle\right] \qquad (6.3) \\ &= C^{\dagger}\begin{pmatrix} H^{\uparrow\uparrow} & H^{\uparrow\downarrow} \\ H^{\downarrow\uparrow} & H^{\downarrow\downarrow} \end{pmatrix}_{2N\times 2N} C + \text{constant}, \end{aligned}$$

with:

$$\begin{aligned} S^{-}_{i} &= c^{\dagger}_{i\downarrow}c_{i\uparrow} \\ S^{+}_{i} &= c^{\dagger}_{i\uparrow}c_{i\downarrow} \\ C^{\dagger} &= \left(c^{\dagger}_{1\uparrow},...,c^{\dagger}_{N\uparrow},c^{\dagger}_{1\downarrow},...,c^{\dagger}_{N\downarrow}\right) \\ H^{\uparrow\uparrow}_{ij} &= \left(U\langle n_{i\downarrow}\rangle - \mu\right)\delta_{ij} + T_{ij} \\ H^{\uparrow\downarrow}_{ij} &= -U\langle S^{-}_{i}\rangle\delta_{ij} \\ H^{\downarrow\uparrow}_{ij} &= -U\langle S^{+}_{i}\rangle\delta_{ij} \\ H^{\downarrow\downarrow}_{ij} &= \left(U\langle n_{i\uparrow}\rangle - \mu\right)\delta_{ij} + T_{ij} \\ \text{constant} &= U\sum_{i}\left[\langle S^{+}_{i}\rangle\langle S^{-}_{i}\rangle - \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle\right] \end{aligned}$$

We have now a Hamiltonian of size $2N\times 2N$ and $4N$ mean field parameters to compute (N values for the local operators $\langle S^{+}_{i}\rangle$, $\langle S^{-}_{i}\rangle$, $\langle n_{i\uparrow}\rangle$ and $\langle n_{i\downarrow}\rangle$). But we can easily reduce the number of parameters by assuming that the spins are coplanar. We can choose the spin to lie in the xy plane or in the xz (yz) plane:

- To have the spin in the xy plane we should enforce:

$$\langle n_{i\uparrow}\rangle = \langle n_{i\downarrow}\rangle \Leftrightarrow \langle S^{z}_{i}\rangle = \langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle = 0.$$

- And to have them in the xz plane we should enforce:

$$\langle S^{+}_{i}\rangle = \langle S^{-}_{i}\rangle = \langle S^{x}_{i}\rangle \Leftrightarrow \langle S^{y}_{i}\rangle = \frac{i}{2}\left(\langle S^{+}_{i}\rangle - \langle S^{-}_{i}\rangle\right) = 0.$$

Computation of the mean field parameters

From the diagonalization of H^{MF2}, we obtain:

- the one particle spectrum for spin up and down ϵ_α,
- and the ground state:

$$|GS\rangle = \Pi_\alpha d^\dagger_\alpha |0\rangle \tag{6.4}$$
$$\text{with } d_\alpha = \sum_i Q^\dagger_{\alpha i} c_i, \text{ and } H^{MF2} = \sum_\alpha \epsilon_\alpha d^\dagger_\alpha d_\alpha + \text{Constant}$$

And we can compute from the eigenstates the different mean field parameters:

$$\begin{aligned}
\langle n_{i\uparrow}\rangle &= \sum_{\alpha \leqslant N_e} Q^\dagger_{\alpha i} Q_{i\alpha} \\
\langle n_{i\downarrow}\rangle &= \sum_{\alpha \leqslant N_e} Q^\dagger_{\alpha i+N} Q_{i+N\alpha} \\
\langle S^+_i\rangle &= \sum_{\alpha \leqslant N_e} Q^\dagger_{\alpha i} Q_{i+N\alpha} \\
\langle S^-_i\rangle &= \sum_{\alpha \leqslant N_e} Q^\dagger_{\alpha i+N} Q_{i\alpha}
\end{aligned}$$

Be careful: the indices now don't correspond anymore to the lattice indices, but to the ones you choose in $C^\dagger$, so here the formulas correspond to $C^\dagger = (c^\dagger_{1\uparrow}, ..., c^\dagger_{N\uparrow}, c^\dagger_{1\downarrow}, ..., c^\dagger_{N\downarrow})$.

6.1.4 Some methods to solve convergence issues

Self-consistent solution and ground state

One important point is to notice the difference between a self-consistent solution and the ground state. The ground state will be the the self-consistent solution of lowest total energy. To be sure that your solution is the ground state and not an exited state, repeat the whole procedure several times (varying the initial conditions) and take the solution of lowest energy. In most cases you will mostly converge to the ground state. But in the case of frustrated systems, the first exited states are really close in energy to the ground state, which can therefore be difficult to find.

Choice of the initial condition

Here you have several possibilities:

- Random initial condition: choose random numbers for your mean field parameter. This is probably the best method, but the convergence process can be really slow and difficult.
- Paramagnetic state: $\langle n_{i\sigma}\rangle = N_\sigma/N$. This state is a special one but in combination with the annealing method for the first iterations, it will give you a more or less "physical" random initial condition.
- Special initial conditions: choose a specific state (for example the classical antiferromagnetic order). This type of choice is dangerous as it will reduce the number of self-consistent solutions which would be reachable. In the case of frustrated systems, it can be a good way to investigate the whole set of possible spiral states by searching the self-consistent solutions corresponding to each classical spiral (reachable for the system size) as initial condition. Be careful: you are probably reducing your solution to the spiral state only and potentially missing the true ground state.

Annealing

In some cases the symmetry of the system makes the convergence difficult. A good solution in this case is to add a small temperature to the first iteration. In this case, the computation of your mean field parameter is a bit modified and takes the following shape:

$$\langle n_{i\sigma}\rangle = \sum_{\alpha\in\Omega} Q^{\dagger}_{\alpha i,\sigma} Q_{i\alpha,\sigma}\,,$$

where Ω is a set of N_σ one-particle states chosen with a probability : $n(\epsilon_{\alpha,\sigma}) = 1/(1+e^{\beta(\epsilon_{\alpha,\sigma}-\epsilon_F)})$ with Fermi energy ϵ_F.
In this method you have several possibilities:

- A fixed temperature during a fixed number of iterations (for example 10 iterations at $\beta = t$),
- or you can smoothly reduce the value of β, until you reach zero temperature corresponding to your regular iterations.

Damping

A usual problem of convergence is the oscillation between two states:

$$\langle n_{i\sigma}\rangle_I \to \langle n_{i\sigma}\rangle_{I+1} \text{ and } \langle n_{i\sigma}\rangle_{I+1} \to \langle n_{i\sigma}\rangle_I.$$

So in this case a simple solution is to introduce a form of damping by averaging the results of an iteration with a previous one.

- the simplest possibility is : $\langle n_{i\sigma}\rangle_I = 0.5\langle n_{i\sigma}\rangle_I + 0.5\langle n_{i\sigma}\rangle_{I-1}$. But this is in general not sufficient to solve your problem.
- a better solution is to introduce a variable weight: $\langle n_{i\sigma}\rangle_I = P_I\langle n_{i\sigma}\rangle_I + (1 - P_I)\langle n_{i\sigma}\rangle_{I-1}$ where P_I evolves with the number of iteration I.
- And you can imagine more complicated possibilities; any linear combination of previous solutions could work.

Be careful: The weight assigned to your new mean field parameters should not be lower that your criterion of convergence ($P_I > \delta$ if δ is the demanded precision).

Reduction of the number of parameters

Normally you have a number of mean field parameter proportional to the size of your system. You can reduce this number to the number of sublattices of your system (for example two sublattices for the square lattice with periodic boundary condition). To achieve this goal it is enough to enforce that $\langle n_{i\sigma}\rangle = n_X$ for all i which belong to the X sublattice. In practice, n_X corresponds to the average on your new $\langle n_{i\sigma}\rangle$ which belongs to the X sublattice:

$$n_X = \frac{1}{N_X}\sum_{i\in X}\langle n_{i\sigma}\rangle \text{ where } N_X \text{ is the number of sites in sublattice } X\,.$$

Be careful: If you didn't choose the appropriate sublattices, you will miss the ground state.

6.1.5 Limits of the mean field approximation

The mean field approximation of the Hubbard model is a powerful method to study large system sizes, compute real space quantities and consider systems with sophisticated geometry. It will give really good results in the case of weak interaction. Now you should keep in mind, that this method allows only long range order and overestimates magnetic order. So if you don't see something it doesn't mean it doesn't exist. In particular exotic phases like a spin liquid, for example, is not accessible by this approximation.

6.2 Details of the computation of $\langle n_{i\sigma}\rangle$.

$$d_{\alpha,\sigma} = \sum_i Q^{\dagger}_{\alpha i,\sigma} c_{i\sigma} \quad \text{and} \quad d^{\dagger}_{\alpha,\sigma} = \sum_i Q_{i\alpha,\sigma} c^{\dagger}_{i\sigma}$$

$$|GS\rangle = \prod_{\alpha=1}^{N_\uparrow} d^{\dagger}_{\alpha\uparrow} \prod_{\beta=1}^{N_\downarrow} d^{\dagger}_{\beta\downarrow}|0\rangle$$

$$\langle n_{i\sigma}\rangle = \langle GS|n_{i,\sigma}|GS\rangle = \langle 0| \prod_{\beta'=1}^{N_\downarrow} d_{\beta'\downarrow} \prod_{\alpha'=1}^{N_\uparrow} d_{\alpha'\uparrow} c^{\dagger}_{i,\sigma} c_{i,\sigma} \prod_{\alpha=1}^{N_\uparrow} d^{\dagger}_{\alpha\uparrow} \prod_{\beta=1}^{N_\downarrow} d^{\dagger}_{\beta\downarrow}|0\rangle \quad (6.5)$$

We will consider here only the special case $\sigma = \uparrow$ but the case $\sigma = \downarrow$ is strictly similar.

$c_{i\uparrow}$ is operator annihilation of electron of spin up and so follow the following rules of commutation: $\{c_{i,\sigma}, c^{\dagger}_{j,\sigma'}\} = \delta_{\sigma,\sigma'}\delta_{i,j}$.
And we can as well derive the relation of commutation between the operator c and d:

$$\begin{aligned} c_{i\uparrow} d^{\dagger}_{\alpha,\downarrow} &= c_{i\uparrow} \sum_j Q_{j\alpha,\downarrow} c^{\dagger}_{j\downarrow} = \sum_j Q_{j\alpha,\downarrow} c_{i\uparrow} c^{\dagger}_{j\downarrow} \\ &= \sum_j Q_{j\alpha,\downarrow} (-c^{\dagger}_{j\downarrow} c_{i\uparrow}) = -d^{\dagger}_{\alpha,\downarrow} c_{i\uparrow} \end{aligned}$$

$$c_{i\uparrow} \prod_{\beta=1}^{N_\downarrow} d^{\dagger}_{\alpha,\downarrow} = (-1)^{N_\downarrow} \prod_{\beta=1}^{N_\downarrow} d^{\dagger}_{\alpha,\downarrow} c_{i\uparrow} \quad (6.6)$$

$$\begin{aligned} c_{i\uparrow} d^{\dagger}_{\alpha,\uparrow} &= \sum_j Q_{j\alpha,\uparrow} c^{\dagger}_{j\uparrow} = \sum_j Q_{j\alpha,\uparrow} c_{i,\uparrow} c^{\dagger}_{j\uparrow} \\ &= \sum_j Q_{j\alpha,\uparrow} (\delta_{ij} - c^{\dagger}_{j\uparrow} c_{i,\uparrow}) = Q_{i\alpha,\uparrow} - d^{\dagger}_{\alpha,\uparrow} c_{i,\uparrow} \end{aligned}$$

$$
\begin{aligned}
c_{i,\uparrow}\prod_{\alpha=1}^{N_\uparrow} d^\dagger_{\alpha,\uparrow} &= (Q_{i1,\uparrow} - d^\dagger_{1,\uparrow}c_{i,\uparrow})\prod_{\alpha=2}^{N_\uparrow} d^\dagger_{\alpha,\uparrow} \\
&= Q_{i1,\uparrow}\prod_{\alpha=2}^{N_\uparrow} d^\dagger_{\alpha,\uparrow} - d^\dagger_{1,\uparrow}c_{i,\uparrow}\prod_{\alpha=2}^{N_\uparrow} d^\dagger_{\alpha,\uparrow} \\
&= Q_{i1,\uparrow}\prod_{\alpha=2}^{N_\uparrow} d^\dagger_{\alpha,\uparrow} - d^\dagger_{1,\uparrow}(Q_{i2,\uparrow} - d^\dagger_{2,\uparrow}c_{i,\uparrow})\prod_{\alpha=3}^{N_\uparrow} d^\dagger_{\alpha,\uparrow} \\
&= Q_{i1,\uparrow}\prod_{\alpha=2}^{N_\uparrow} d^\dagger_{\alpha,\uparrow} - Q_{i2,\uparrow}\prod_{\alpha\neq 2}^{N_\uparrow} d^\dagger_{\alpha,\uparrow} + d^\dagger_{1,\uparrow}d^\dagger_{2,\uparrow}c_{i,\uparrow}\prod_{\alpha=3}^{N_\uparrow} d^\dagger_{\alpha,\uparrow} \\
&= \ldots \\
&= \sum_{\beta}^{N_\uparrow}(-1)^{\beta+1}Q_{i\beta,\uparrow}\prod_{\alpha\neq\beta}^{N_\uparrow} d^\dagger_{\alpha,\uparrow} + (-1)^{N_\uparrow}\prod_{\alpha=1}^{N_\uparrow} d^\dagger_{\alpha,\uparrow}c_{i,\uparrow} \quad (6.7)
\end{aligned}
$$

Using (6.6) and (6.7) and $c_{i,\sigma}|0\rangle = 0$ we obtain:

$$
\begin{aligned}
c_{i,\uparrow}|GS\rangle &= c_{i,\uparrow}\prod_{\alpha=1}^{N_\uparrow} d^\dagger_{\alpha\uparrow}\prod_{\gamma=1}^{N_\downarrow} d^\dagger_{\gamma\downarrow}|0\rangle \\
&= \left(\sum_{\beta}^{N_\uparrow}(-1)^{\beta+1}Q_{i\beta,\uparrow}\prod_{\alpha\neq\beta}^{N_\uparrow} d^\dagger_{\alpha,\uparrow} + (-1)^{N_\uparrow}\prod_{\alpha=1}^{N_\uparrow} d^\dagger_{\alpha,\uparrow}c_{i,\uparrow}\right)\prod_{\gamma=1}^{N_\downarrow} d^\dagger_{\gamma\downarrow}|0\rangle \\
&= \sum_{\beta}^{N_\uparrow}(-1)^{\beta+1}Q_{i\beta,\uparrow}\prod_{\alpha\neq\beta}^{N_\uparrow} d^\dagger_{\alpha,\uparrow}\prod_{\gamma=1}^{N_\downarrow} d^\dagger_{\gamma\downarrow}|0\rangle + \\
&\qquad + (-1)^{N_\uparrow}(-1)^{N_\downarrow}\prod_{\alpha=1}^{N_\uparrow} d^\dagger_{\alpha,\uparrow}\prod_{\gamma=1}^{N_\downarrow} d^\dagger_{\gamma\downarrow}c_{i,\uparrow}|0\rangle \\
&= \sum_{\beta}^{N_\uparrow}(-1)^{\beta+1}Q_{i\beta,\uparrow}\prod_{\alpha\neq\beta}^{N_\uparrow} d^\dagger_{\alpha,\uparrow}\prod_{\gamma=1}^{N_\downarrow} d^\dagger_{\gamma\downarrow}|0\rangle
\end{aligned}
$$

Using this equation and its Hermitian conjugate we can at last compute

$\langle n_{i,\sigma}\rangle$:

$$\begin{aligned}\langle n_{i\uparrow}\rangle = \langle GS|n_{i,\sigma}|GS\rangle &= \langle 0|\prod_{\gamma'=1}^{N_\downarrow} d_{\gamma'\downarrow}\prod_{\alpha'=1}^{N_\uparrow} d_{\alpha'\uparrow}c^\dagger_{i,\sigma}c_{i,\sigma}\prod_{\alpha=1}^{N_\uparrow} d^\dagger_{\alpha\uparrow}\prod_{\gamma=1}^{N_\downarrow} d^\dagger_{\gamma\downarrow}|0\rangle \\ &= \langle 0|\prod_{\gamma'=1}^{N_\downarrow} d_{\gamma'\downarrow}\Bigg(\sum_{\beta'}^{N_\uparrow}(-1)^{\beta'+1}Q^\dagger_{\beta' i,\uparrow}\prod_{\alpha\neq\beta'}^{N_\uparrow} d_{\alpha',\uparrow}\Bigg)\times \\ &\qquad \times\Bigg(\sum_{\beta}^{N_\uparrow}(-1)^{\beta+1}Q_{i\beta,\uparrow}\prod_{\alpha\neq\beta}^{N_\uparrow} d^\dagger_{\alpha,\uparrow}\Bigg)\prod_{\gamma=1}^{N_\downarrow} d^\dagger_{\gamma\downarrow}|0\rangle \\ &= \sum_{\beta'}^{N_\uparrow}\sum_{\beta}^{N_\uparrow}(-1)^{\beta+1+\beta'+1}Q^\dagger_{\beta' i,\uparrow}Q_{i\beta,\uparrow}\langle 0|\prod_{\gamma'=1}^{N_\downarrow} d_{\gamma'\downarrow}\prod_{\alpha\neq\beta'}^{N_\uparrow} d_{\alpha',\uparrow}\prod_{\alpha\neq\beta}^{N_\uparrow} d^\dagger_{\alpha,\uparrow}\prod_{\gamma=1}^{N_\downarrow} d^\dagger_{\gamma\downarrow}|0\rangle\end{aligned}$$

The eigenvector are orthogonal and normalized so:

$$\langle 0|\prod_{\gamma'=1}^{N_\downarrow} d_{\gamma'\downarrow}\prod_{\alpha\neq\beta'}^{N_\uparrow} d_{\alpha',\uparrow}\prod_{\alpha\neq\beta}^{N_\uparrow} d^\dagger_{\alpha,\uparrow}\prod_{\gamma=1}^{N_\downarrow} d^\dagger_{\gamma\downarrow}|0\rangle = \delta_{\beta\beta'}$$

And at the end:

$$\begin{aligned}\langle n_{i\uparrow}\rangle &= \sum_{\beta'}\sum_{\beta}(-1)^{\beta+1+\beta'+1}Q^\dagger_{\beta' i,\uparrow}Q_{i\beta,\uparrow}\delta_{\beta\beta'} \\ &= \sum_{\alpha=1}^{N_\uparrow} Q_{i\alpha,\uparrow}Q^\dagger_{\alpha i,\uparrow} \qquad (6.8)\end{aligned}$$