4. Dynamical mean field theory

Fock space

We consider the Hilbert space H_N for a system of N identical particles. The wave function $\psi_N(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$ representing the probability amplitude for finding the particles at N positions $\vec{r}_1 \ldots, \vec{r}_N$ must satisfy

$$\langle \psi_N | \psi_N \rangle = \int d^3r_1 \ldots d^3r_N |\psi_N(\vec{r}_1, \ldots, \vec{r}_N)|^2 < +\infty \tag{4.1}$$

H_N is the Nth tensor product of the simple particle spaces $\mathcal{H}$

$$H_N^{(\varepsilon)} = H \otimes H \otimes \cdots \otimes \mathcal{H} \tag{4.2}$$

If $\{|\alpha\rangle\}$ is an orthonormal basis of $\mathcal{H}$, the canonical orthonormal basis of $\mathcal{H}_N$ is constructed from the tensor products:

$$|\alpha_1 \ldots \alpha_N) \equiv |\alpha_1\rangle |\alpha_2\rangle \ldots |\alpha_N\rangle \tag{4.3}$$

The bra/ket have round brackets as long as the symmetry property is not taken into account.
The basis states have wave functions

$$\begin{aligned}\psi_{\alpha_1\alpha_2\ldots\alpha_N}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) &= (\vec{r}_1, \ldots, \vec{r}_N | \alpha_1, \ldots, \alpha_N) \\ &= \big(\langle \vec{r}_1 | \otimes \langle \vec{r}_2 | \otimes \cdots \otimes \langle \vec{r}_N |\big)\big(|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \cdots \otimes |\alpha_N\rangle\big) \\ &= \varphi_{\alpha_1}(\vec{r}_1)\varphi_{\alpha_2}(\vec{r}_2) \ldots \varphi_{\alpha_N}(\vec{r}_N)\end{aligned} \tag{4.4}$$

The overlap of two vectors is

$$\begin{aligned}(\alpha_1\alpha_2 \ldots \alpha_N | \alpha_1'\alpha_2' \ldots \alpha_N') &= \big(\langle \alpha_1 | \otimes \langle \alpha_2 | \otimes \cdots \otimes \langle \alpha_N |\big)\big(|\alpha_1'\rangle \otimes |\alpha_2'\rangle \cdots \otimes |\alpha_N'\rangle\big) \\ &= \langle \alpha_1 | \alpha_1' \rangle \langle \alpha_2 | \alpha_2' \rangle \ldots \langle \alpha_N | \alpha_N' \rangle\end{aligned} \tag{4.5}$$

and the completeness relations of the basis follows from the tensor product of the completeness relations of $\{|\alpha\rangle\}$:

$$\sum_{\alpha_1 \ldots \alpha_N} |\alpha_1\alpha_2 \ldots \alpha_N\rangle\langle \alpha_1\alpha_2 \ldots \alpha_N| = 1 \tag{4.6}$$

1 is the unit operator in H_N. H_N is generated by linear combinations of products of single particle wave functions.
Now we need to account for the symmetry property of the wave function. In nature, for identical particles, only totally symmetric and totally antisymmetric states are observed, corresponding to bosons and fermions, respectively. The wave function for fermions/bosons obeys

$$\psi(\vec{r}_{p_1}, \vec{r}_{p_2}, \ldots, \vec{r}_{p_N}) = \varepsilon^P \psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) \tag{4.7}$$

where $P = (p_1, p_2, \ldots, p_N)$ represents any permutation of the set $(1, 2, \ldots, N)$, and P is the parity (sign) of the permutation P (number of transpositions needed to achieve the permutation). $\varepsilon = -1$ for fermions, $\varepsilon = +1$ for bosons.
This restricts the Hilbert space of the N particle system; a wave function $\psi(\vec{r}_1, \ldots, \vec{r}_N)$ belongs to the Hilbert space $\mathcal{H}_N^{(\varepsilon)}$ of N bosons (fermions) if it is symmetric (antisymmetric) under a permutation of the particles.
We define a symmetrization operator $\mathcal{P}_\varepsilon$ by the action on the wave function:

$$\mathcal{P}_\varepsilon \psi(\vec{r}_1, \ldots, \vec{r}_N) = \frac{1}{N!} \sum_P \varepsilon^P \psi(\vec{r}_{p_1}, \vec{r}_{p_2}, \ldots, \vec{r}_{p_N}) \tag{4.8}$$

E.g. for two fermions

$$P_{-1}\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{2}\big(\psi(\vec{r}_1, \vec{r}_2) - \psi(\vec{r}_2, \vec{r}_1)\big) \tag{4.9}$$

with the group composition of two permutations P and P', the symmetrization operator $\mathcal{P}_\varepsilon$ can be shown to be a projector ($\mathcal{P}_\varepsilon^2 = \mathcal{P}_\varepsilon$). Thus, these projectors project $\mathcal{H}_N$ onto fermionic and bosonic Hilbert spaces:

$$\mathcal{H}_N^{(\varepsilon)} = \mathcal{P}_\varepsilon \mathcal{H}_N \tag{4.10}$$

Now, a system of bosons or fermions with one particle in state α_1, one in state α_2, ... one in state α_N is represented as

$$\begin{aligned} |\alpha_1 \ldots \alpha_N\} &\equiv \sqrt{N!}\mathcal{P}_\varepsilon |\alpha_1 \ldots \alpha_N) \\ &= \frac{1}{\sqrt{N!}} \sum_P \varepsilon^P |\alpha_{p_1}\rangle \otimes |\alpha_{p_2}\rangle \otimes \ldots |\alpha_{p_N}\rangle \end{aligned} \tag{4.11}$$

Symmetrized states are marked with curly bra/ket. The Pauli principle stating that two fermions cannot occupied the same state is automatically satisfied for antisymmetric states; if we take states $|\alpha_1\rangle = |\alpha_2\rangle$ we have

$$|\alpha_1\alpha_2\alpha_3 \ldots \alpha_N\} = \sqrt{N!}\mathcal{P}_{-1}|\alpha_1\alpha_2\alpha_3 \ldots \alpha_N) = -\sqrt{N!}\mathcal{P}_{-1}|\alpha_2\alpha_1\alpha_3 \ldots \alpha_N) = 0$$

(4.12)

Now an occupation number representation can be introduced.

Grassmann algebra

We need anticommuting numbers for constructing coherent states for fermions which are eigenstates of annihilation operators because nticommutation relations of annihilation operators a_i lead to anticommutation relations of the eigenvalues χ_i. Algebras of anticommuting numbers are called **Grassmann algebras**. For the present purpose, it is sufficient to consider Grassmann algebra with its definition of differentiation and integration as clever constructs that take care of the minus signs that arise from the antisymmetry of fermions.
An algebra is a linear space in which, besides the usual operations of addition and multiplication by numbers, a product of elements is defined with the usual distributive law:

$$\chi(a\zeta + b\xi) = a\chi\zeta + b\chi\xi \qquad (a\zeta + b\xi)\chi = a\zeta\chi + b\xi\chi \tag{4.13}$$

with numbers a, $b \in \mathbb{K}$ (here $\mathbb{K} = \mathbb{C}$) and elements of the algebra χ, ζ and ξ. The algebra is associative if for any three elements

$$\chi(\zeta\xi) = (\chi\zeta)\xi \tag{4.14}$$

A Grassmann algebra is defined by a set of generators $\{\chi_i\}$, $i = 1 \dots n$. These generators anticommute

$$\chi_i\chi_j + \chi_j\chi_i = 0 \tag{4.15}$$

so that in particular (for $i = j$)

$$\xi_i^2 = 0 \tag{4.16}$$

The basis of the Grassmann algebra is made up of all distinct products of the generators. Thus, a number in the Grassmann algebra is a linear combination, with complex coefficients, of the numbers $\{1, \chi_{\alpha_1}, \chi_{\alpha_1}\chi_{\alpha_2}, \dots, \chi_{\alpha_1}\chi_{\alpha_2} \cdot \cdot \cdot \chi_{\alpha_n}\}$ with indices α_i ordered, by convention, as $\alpha_1 < \alpha_2 < \cdots < \alpha_n$. The dimension of the algebra with n generators is 2^n since distinct basis elements are produced by the two possibilities of including a generator 0 or 1 times for each of the n generators.

A conjugation operation can be defined in an algebra with an even number $n = 2p$ of generators. We select a set of p generators χ_i and to each we associate a generator called χ_i^*. Then the conjugation is defined by

$$(\chi_i)^* = \chi_i^* \qquad (\chi_i^*)^* = \chi_i \tag{4.17}$$

Then, for complex λ

$$(\lambda\chi_i)^* = \lambda^*\chi_i^* \tag{4.18}$$

and for products of generators

$$(\chi_{\alpha_1}\chi_{\alpha_2}\cdots\chi_{\alpha_n})^* = \chi_{\alpha_n}^*\chi_{\alpha_{n-1}}^*\cdots\chi_{\alpha_1}^* \tag{4.19}$$

We now consider a Grassmann algebra with two generators, χ and χ^*. The algebra is generated by $\{1, \chi, \chi^*, \chi^*\chi\}$. Because of $\chi_i^2 = 0$, any analytic function of f defined on this algebra is a linear function:

$$f(\chi) = f_0 + f_1\chi \tag{4.20}$$

An operator A has the form

$$A(\chi^*, \chi) = a_0 + a_1\chi + \bar{a}_1\chi^* + a_{12}\chi^*\chi \tag{4.21}$$

Now a derivative can be defined for Grassmann variable functions; it is like the complex derivative, but for the operator $\frac{\partial}{\partial\chi}$ to act on χ, χ has to be anticommuted until it is adjacent to χ. For example:

$$\frac{\partial}{\partial\chi}(\chi^*\chi) = \frac{\partial}{\partial\chi}(-\chi\chi^*) = -\chi^*$$

Then

$$\begin{aligned} &\frac{\partial}{\partial\chi}A(\chi^*, \chi) = a_1 - a_{12}\chi^* \qquad \frac{\partial}{\partial\chi^*}A(\chi^*, \chi) = \bar{a}_1 + a_{12}\chi \\ &\frac{\partial}{\partial\chi^*}\frac{\partial}{\partial\chi}A(\chi^*, \chi) = -a_{12} = -\frac{\partial}{\partial\chi}\frac{\partial}{\partial\chi^*}A(\chi^*, \chi) \end{aligned} \tag{4.22}$$

Thus, $\frac{\partial}{\partial\chi}$ and $\frac{\partial}{\partial\chi^*}$ anticommute.
In defining an integral, there is no analog of the Riemann sum; rather, it is defined as a linear mapping which has the fundamental property

$$\int_{-\infty}^{\infty}\frac{df(x)}{dx} = 0 \qquad \text{in case } f(x\to\infty) = f(x\to-\infty) = 0 \tag{4.23}$$

of ordinary integrals over functions vanishing at infinity that the integral of an exact differential form is zero. This implies

$$\int d\chi \, 1 = 0 \tag{4.24}$$

The only nonvanishing integral is that of χ since χ is not a derivative. Thus we define

$$\int d\chi \, \chi = 1 \tag{4.25}$$

and again in order to apply this, one has to anticommute χ to bring it next to $d\chi$. Grassmann integration turns out to be equivalent to Grassmann differentiation. As we arbitrarily defined half the generators χ_i^* to be conjugate variables but otherwise they are equivalent to χ_i, we define integration for conjugate variables in the same way:

$$\int d\chi^* \, 1 = 0 \qquad \int d\chi^* \, \chi^* = 1 \tag{4.26}$$

Examples for integration rules are:

$$\begin{aligned}
&\int d\chi \, f(\chi) = \int d\chi (f_0 + f_1\chi) = f_1 \\
&\int d\chi \, A(\chi^*, \chi) = \int d\chi \, (a_0 + a_1\chi + \bar{a}_1\chi^* + a_{12}\chi^*\chi) = a_1 - a_{12}\chi^* \\
&\int d\chi^* \, A(\chi^*, \chi) = \bar{a}_1 + a_{12}\chi \\
&\int d\chi^* \int d\chi \, A(\chi^*, \chi) = \, - a_{12} = \, - \int d\chi \int d\chi^* \, A(\chi^*, \chi)
\end{aligned} \tag{4.27}$$

Functional integral representation

We now introduce coherent states as a basis of Fock space $\mathcal{F}$. They are eigenstates of fermionic annihilation operators (creation operators would not work as they don't have eigenstates)[1]:

$$a_i|\chi\rangle = \chi_i|\chi\rangle \tag{4.28}$$

[1] see J. W. Negele and H. Orland, *Quantum Many-Particle Systems*, Perseus Publishing, Cambridge 1998, p. 20.

This leads to the definition of a generalized Fermion Fock space as now complex as well as Grassmann coefficients are allowed for a state[2]. A vector in this space can be expanded as

$$|\psi\rangle = \sum_i \chi_i |\phi_i\rangle \tag{4.29}$$

with χ_i part of the Grassmann algebra $\mathcal{G}$ and $|\phi_i\rangle$ element of the Fock space $\mathcal{F}$. For calculating with expressions mixing Grassmann variables and creation or annihilation operators, commutation rules are necessary:

$$[\tilde{\chi}, \tilde{a}]_+ = 0 \tag{4.30}$$

and

$$(\tilde{\chi}\tilde{a})^\dagger = \tilde{a}^\dagger \tilde{\chi}^* \tag{4.31}$$

with $\tilde{\chi}$ any Grassmann variable in $\{\chi_i, \chi_i^*\}$ and $\tilde{a}$ is any operator in $\{a_i, a_i^\dagger\}$. A Fermi coherent state is defined as

$$|\chi\rangle = \exp\Big\{-\sum_i \chi_i a_i^\dagger\Big\}|0\rangle = \prod_i \big(1 - \chi_i a_i^\dagger\big)|0\rangle \tag{4.32}$$

Noting that pairs of Grassmann variables and creation or annihilation operators commute:

$$\begin{aligned}[\chi_i a_i^\dagger, \chi_j a_j^\dagger] &= \chi_i a_i^\dagger \chi_j a_j^\dagger - \chi_j a_j^\dagger \chi_i a_i^\dagger = -\chi_i \chi_j a_i^\dagger a_j^\dagger + \chi_j \chi_i a_j^\dagger a_i^\dagger \\ &= \chi_j \chi_i a_i^\dagger a_j^\dagger - \chi_j \chi_i a_i^\dagger a_j^\dagger = 0 \end{aligned}\tag{4.33}$$

we can show that the two definitions of Eq. (4.32) are really the same:

$$|\chi\rangle = \exp\Big\{-\sum_i \chi_i a_i^\dagger\Big\}|0\rangle = \prod_i \exp\{-\chi_i a_i^\dagger\}|0\rangle = \prod_i \big(1 - \chi_i a_i^\dagger\big)|0\rangle \tag{4.34}$$

We show that $|\chi\rangle$ is indeed an eigenstate for a_i with eigenvalue χ_i:

$$\begin{aligned} a_i|\chi\rangle &= a_i \prod_j \big(1 - \chi_j a_j^\dagger\big)|0\rangle \\ &= \prod_{j\neq i} \big(1 - \chi_j a_j^\dagger\big) a_i \big(1 - \chi_i a_i^\dagger\big)|0\rangle = \prod_{j\neq i} \big(1 - \chi_j a_j^\dagger\big)\chi_i a_i a_i^\dagger|0\rangle \quad \text{using Eq. (4.30)} \\ &= \prod_{j\neq i} \big(1 - \chi_j a_j^\dagger\big)\chi_i|0\rangle = \prod_{j\neq i} \big(1 - \chi_j a_j^\dagger\big)\chi_i(1 - \chi_i a_i^\dagger)|0\rangle \quad \text{because } \chi_i^2 = 0 \\ &= \chi_i|\chi\rangle \end{aligned}$$

[2] see *ibid.*, p. 29.

(4.35)

The adjoint of a coherent state is

$$\langle\chi| = \langle 0|\exp\Big\{-\sum_j \big(\chi_j a_j^\dagger\big)^\dagger\Big\} = \langle 0|\exp\Big\{\sum_j \chi_j^* a_j\Big\} = \langle 0|\prod_j \big(1+\chi_j^* a_j\big) \tag{4.36}$$

This state is a left eigenfunction of $a_i^\dagger$

$$\langle\chi|a_i^\dagger = \langle\chi|\chi_i^* \tag{4.37}$$

The effect of a creation operator $a_i^\dagger$ on a state $|\chi\rangle$ is

$$\begin{aligned} a_i^\dagger|\chi\rangle &= a_i^\dagger \prod_j \big(1-\chi_j a_j^\dagger\big)|0\rangle = \prod_{j\neq i}\big(1-\chi_j a_j^\dagger\big)\, a_i^\dagger \big(1-\chi_i a_i^\dagger\big)|0\rangle \\ &= \prod_{j\neq i}\big(1-\chi_j a_j^\dagger\big)\, a_i^\dagger|0\rangle \quad \text{because } a_i^\dagger a_i^\dagger = 0 \\ &= -\frac{\partial}{\partial\chi_i}\big(1-\chi_i a_i^\dagger\big)\prod_{j\neq i}\big(1-\chi_j a_j^\dagger\big)|0\rangle = -\frac{\partial}{\partial\chi_i}|\chi\rangle \end{aligned} \tag{4.38}$$

and in the same way

$$\langle\chi|a_i = \frac{\partial}{\partial\chi_i^*}\langle\chi| \tag{4.39}$$

The coherent states now form an overcomplete basis of the generalized Fock space, and two states $|\chi\rangle$ and $|\chi'\rangle$ have an overlap:

$$\begin{aligned} \langle\chi'|\chi\rangle &= \langle 0|\prod_i \big(1+\chi_i^* a_i\big)\prod_j\big(1-\chi_j a_j^\dagger\big)|0\rangle = \langle 0|\prod_i\big(1+\chi_i^* a_i\big)\big(1-\chi_i a_i^\dagger\big)|0\rangle \\ &= \langle 0|\prod_i\big(1-\chi_i^* a_i \chi_i a_i^\dagger\big)|0\rangle = \prod_i\big(1+\chi_i^*\chi_i\big) = \exp\Big\{\sum_i \chi_i^*\chi_i\Big\} \end{aligned} \tag{4.40}$$

One can then prove that the unit of the physical Fock space $\mathcal{F}$ can be written as[3]

$$\int\prod_i d\chi_i^* d\chi_i e^{\sum_i \chi_i^*\chi_i}|\chi\rangle\langle\chi| = 1 \tag{4.41}$$

[3]for the proof see *ibid.*, p. 31.

4.1 DMFT self consistency condition for the Hubbard model

We consider the Hubbard Hamiltonian

$$H = -\sum_{ij\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} - \mu \sum_{i\sigma} c^+_{i\sigma} c_{i\sigma} + \frac{U}{2} \sum_{\substack{i\sigma\sigma' \\ \sigma\neq\sigma'}} c^+_{i\sigma} c_{i\sigma} c^+_{i\sigma'} c_{i\sigma'} \tag{4.42}$$

where the spin and orbital index σ runs from 1 to N. The partition function corresponding to this Hamiltonian is

$$Z = \int \prod_i \mathcal{D}\bar{c}_{i\sigma} \mathcal{D}c_{i\sigma} e^{-S} \tag{4.43}$$

with the action

$$\begin{aligned} S = \int_0^\beta d\tau \sum_{i\sigma} \bar{c}_{i\sigma}(\tau) \frac{\partial}{\partial\tau} c_{i\sigma}(\tau) + \int_0^\beta d\tau \Big[&- \sum_{ij\sigma} t_{ij} \bar{c}_{i\sigma}(\tau) c_{j\sigma}(\tau) - \mu \sum_{i\sigma} \bar{c}_{i\sigma}(\tau) c_{i\sigma}(\tau) \\ &+ \frac{U}{2} \sum_{\substack{i\sigma\sigma' \\ \sigma\neq\sigma'}} \bar{c}_{i\sigma}(\tau) c_{i\sigma}(\tau) \bar{c}_{i\sigma'}(\tau) c_{i\sigma'}(\tau) \Big] \end{aligned} \tag{4.44}$$

where the fermion operators $c^+_{i\sigma}$, $c_{i\sigma}$ of the Hamiltonian have been replaced by Grassmann variables $\bar{c}_{i\sigma}(\tau)$, $c_{i\sigma}(\tau)$.
The cavity method now requires that we focus on one site $i = o$ and separate the Hamiltonian (4.42) into three parts, one relating to site o only, one connecting this site to the lattice and one for the lattice with site o removed:

$$H = H_o + H_c + H^{(o)} \tag{4.45}$$

$$H_o = -\mu \sum_{\sigma} c^+_{o\sigma} c_{o\sigma} + \frac{U}{2} \sum_{\substack{\sigma\sigma' \\ \sigma\neq\sigma'}} c^+_{o\sigma} c_{o\sigma} c^+_{o\sigma'} c_{o\sigma'} \tag{4.46}$$

$$H_c = -\sum_{i\sigma} \left[t_{io} c^+_{i\sigma} c_{o\sigma} + t_{oi} c^+_{o\sigma} c_{i\sigma} \right] \tag{4.47}$$

$$H^{(o)} = -\sum_{i\neq o\, j\neq o\, \sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} - \mu \sum_{i\neq o\, \sigma} c^+_{i\sigma} c_{i\sigma} + \frac{U}{2} \sum_{\substack{i\neq o\, \sigma\sigma' \\ \sigma\neq\sigma'}} c^+_{i\sigma} c_{i\sigma} c^+_{i\sigma'} c_{i\sigma'} \tag{4.48}$$

The three parts of the Hamiltonian correspond to the action S_o of site o, the action ΔS for the interaction between site o and the lattice, and the action $S^{(o)}$ of the lattice without site o:

$$S_o = \int_0^\beta d\tau \Big[\sum_\sigma \bar{c}_{o\sigma}(\tau) \Big(\frac{\partial}{\partial\tau} - \mu \Big) c_{o\sigma}(\tau) + \frac{U}{2} \sum_{\substack{\sigma\sigma' \\ \sigma\neq\sigma'}} \bar{c}_{o\sigma}(\tau) c_{o\sigma}(\tau) \bar{c}_{o\sigma'}(\tau) c_{o\sigma'}(\tau) \Big] \tag{4.49}$$

$$\Delta S = -\int_0^\beta d\tau \Big[\sum_{i\sigma} t_{io} \bar{c}_{i\sigma}(\tau) c_{o\sigma}(\tau) + t_{oi} \bar{c}_{o\sigma}(\tau) c_{i\sigma}(\tau) \Big] \tag{4.50}$$

$$\begin{aligned} S^{(o)} = \int_0^\beta d\tau \Big[& \sum_{i\neq o\,\sigma} \bar{c}_{i\sigma}(\tau) \Big(\frac{\partial}{\partial\tau} - \mu \Big) c_{i\sigma}(\tau) - \sum_{i\neq o\, j\neq o\,\sigma} t_{ij} \bar{c}_{i\sigma}(\tau) c_{j\sigma}(\tau) \\ & + \frac{U}{2} \sum_{\substack{i\neq o\,\sigma\sigma' \\ \sigma\neq\sigma'}} \bar{c}_{i\sigma}(\tau) c_{i\sigma}(\tau) \bar{c}_{i\sigma'}(\tau) c_{i\sigma'}(\tau) \Big] \end{aligned} \tag{4.51}$$

The aim is now to integrate out all lattice degrees of freedom except those of site o in order to find the effective dynamics at site o. In that process, the action S_o remains unchanged, the terms of ΔS are expanded in terms of the hopping t which becomes small with increasing dimension and averaged with respect to the action $S^{(o)}$. Defining $\Delta S(\tau)$ via $\Delta S = \int_0^\beta d\tau\, \Delta S(\tau)$ the partition function is

$$Z = \int \mathcal{D}\bar{c}_{o\sigma} \mathcal{D}c_{o\sigma} e^{-S_o} \int \prod_{i\neq o} \mathcal{D}\bar{c}_{i\sigma} \mathcal{D}c_{i\sigma} e^{-S^{(o)}} e^{-\int_0^\beta d\tau\, \Delta S(\tau)} \tag{4.52}$$

Now we can expand the last exponential function as

$$e^{-\int_0^\beta d\tau\, \Delta S(\tau)} = 1 - \int_0^\beta d\tau\, \Delta S(\tau) + \frac{1}{2!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2\, \Delta S(\tau_1) \Delta S(\tau_2) - \dots \tag{4.53}$$

Taking into account that in general an operator average with respect to an action S can be expressed as

$$\langle A \rangle_S = \frac{\int \prod_i \mathcal{D}\bar{c}_\alpha \mathcal{D}c_\alpha e^{-S} A[\bar{c}_\alpha, c_\alpha]}{\int \prod_i \mathcal{D}\bar{c}_\alpha \mathcal{D}c_\alpha e^{-S}} = Z_s^{-1} \int \prod_i \mathcal{D}\bar{c}_\alpha \mathcal{D}c_\alpha e^{-S} A[\bar{c}_\alpha, c_\alpha]$$

$$(4.54)$$

we can consider the second functional integral in (4.52) to average the terms of the expansion (4.53) with respect to the lattice action $S^{(o)}$:

$$Z = \int \prod_i \mathcal{D}\bar{c}_{o\sigma}\mathcal{D}c_{o\sigma} e^{-S_o} Z_{S^{(o)}} \Big\{ 1 - \int_0^\beta d\tau \, \langle \Delta S(\tau) \rangle_{S^{(o)}} + \frac{1}{2!}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \, \langle \Delta S(\tau_1)\Delta S(\tau_2) \rangle_{S^{(o)}} - \dots \Big\} \tag{4.55}$$

Here, the partition function of the lattice without site o is abbreviated as

$$Z_{S^{(o)}} = \int \prod_i \mathcal{D}\bar{c}_\alpha \mathcal{D}c_\alpha e^{-S^{(o)}} . \tag{4.56}$$

Now the terms in (4.55) with odd powers of ΔS will average to zero. For example,

$$\langle \Delta S(\tau) \rangle_{S^{(o)}} = \sum_{i\sigma} t_{io} \langle \bar{c}_{i\sigma}(\tau) \rangle_{S^{(o)}} c_{o\sigma}(\tau) + t_{oi}\bar{c}_{o\sigma}(\tau) \langle c_{i\sigma}(\tau) \rangle_{S^{(o)}} = 0 \, , \tag{4.57}$$

because the average $\langle \dots \rangle_{S^{(o)}}$ acts on all sites except o. The next average in (4.55) yields

$$\begin{aligned}
\langle \Delta S(\tau_1)\Delta S(\tau_2) \rangle_{S^{(o)}} &= \Big\langle T_\tau \Big[\sum_{i\sigma} t_{io}\bar{c}_{i\sigma}(\tau_1)c_{o\sigma}(\tau_1) + t_{oi}\bar{c}_{o\sigma}(\tau_1)c_{i\sigma}(\tau_1) \Big] \times \\
&\qquad \times \Big[\sum_{j\sigma'} t_{jo}\bar{c}_{j\sigma'}(\tau_2)c_{o\sigma'}(\tau_2) + t_{oj}\bar{c}_{o\sigma'}(\tau_2)c_{j\sigma'}(\tau_2) \Big] \Big\rangle_{S^{(o)}} \\
&= \sum_{ij\sigma\sigma'} t_{io}t_{oj} c_{o\sigma}(\tau_1) \langle T_\tau \bar{c}_{i\sigma}(\tau_1) c_{j\sigma'}(\tau_2) \rangle_{S^{(o)}} \; \bar{c}_{o\sigma'}(\tau_2) \\
&\quad + \sum_{ij\sigma\sigma'} t_{oi}t_{jo} \bar{c}_{o\sigma}(\tau_1) \langle T_\tau c_{i\sigma}(\tau_1) \bar{c}_{j\sigma'}(\tau_2) \rangle_{S^{(o)}} \; c_{o\sigma'}(\tau_2) \\
&= 2\sum_{ij\sigma\sigma'} t_{io}t_{oj} \bar{c}_{o\sigma}(\tau_1) \langle T_\tau c_{i\sigma}(\tau_1) \bar{c}_{j\sigma'}(\tau_2) \rangle_{S^{(o)}} \; c_{o\sigma'}(\tau_2) \\
&= 2\sum_{ij\sigma} t_{io}t_{oj} \bar{c}_{o\sigma}(\tau_1) \langle T_\tau c_{i\sigma}(\tau_1) \bar{c}_{j\sigma}(\tau_2) \rangle_{S^{(o)}} \; c_{o\sigma}(\tau_2) \\
&= -2\sum_{ij\sigma} t_{io}t_{oj} \bar{c}_{o\sigma}(\tau_1) G^{(o)}_{ij\,\sigma}(\tau_1 - \tau_2) c_{o\sigma}(\tau_2)
\end{aligned}$$

$$(4.58)$$

The imaginary time ordering operatore T_τ enters because the path integral leads to imaginary time ordering. Only terms with $\sigma = \sigma'$ contribute as we are considering a paramagnetic state and thus $\langle T_\tau c_{i\sigma}(\tau_1)\bar{c}_{j\sigma'}(\tau_2)\rangle_{S^{(o)}} = \delta_{\sigma\sigma'}\langle T_\tau c_{i\sigma}(\tau_1)\bar{c}_{j\sigma}(\tau_2)\rangle_{S^{(o)}}$. We have identified the average with the cavity Greens function $G^{(o)}_{ij\,\sigma}(\tau_1-\tau_2) = -\langle T_\tau c_{i\sigma}(\tau_1)c^+_{j\sigma}(\tau_2)\rangle_{S^{(o)}}$, *i. e.* the Greens function of the Hubbard model without the site o. Now we have for the partition function

$$Z = \int \prod_\sigma \mathcal{D}\bar{c}_{o\sigma}\mathcal{D}c_{o\sigma}e^{-S_o}Z_{S^{(o)}} \times \\ \times \left\{1 - \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{ij\sigma} t_{io}t_{oj}\bar{c}_{o\sigma}(\tau_1)c_{o\sigma}(\tau_2)G^{(o)}_{ij\,\sigma}(\tau_1-\tau_2) + \dots\right\} \tag{4.59}$$

We would like to write the bracket $\{\dots\}$ in (4.59) again as an exponential function in order to identify an effective action S_{eff}:

$$Z = \int \prod_i \mathcal{D}\bar{c}_{o\sigma}\mathcal{D}c_{o\sigma}e^{-S_{\text{eff}}} \tag{4.60}$$

Noting that the next term in the expansion of (4.59) would read

$$\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \int_0^\beta d\tau_4 \sum_{i_1\, i_2\, j_1\, j_2\, \sigma} \bar{c}_{o\sigma}(\tau_1)\bar{c}_{o\sigma}(\tau_3)c_{o\sigma}(\tau_2)c_{o\sigma}(\tau_4) \times \\ \times t_{i_1\,o}t_{i_2\,o}t_{o\,j_1}t_{o\,j_2}G^{(o)}_{i_1\,i_2\,j_1\,j_2\,\sigma}(\tau_1\,\tau_3,\tau_2\,\tau_4)\,. \tag{4.61}$$

We can write for the partion function (4.59)

$$Z = \int \prod_i \mathcal{D}\bar{c}_{o\sigma}\mathcal{D}c_{o\sigma}e^{-S_o}Z_{S^{(o)}} \times \\ \times \exp\Bigg\{-\sum_{n=1}^{\infty}\sum_\sigma \int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_{2n}\, \bar{c}_{o\sigma}(\tau_1)\dots\bar{c}_{o\sigma}(\tau_{2n-1})c_{o\sigma}(\tau_2)\dots c_{o\sigma}(\tau_{2n}) \times \\ \times \sum_{\substack{i_1,\dots,i_n \\ j_1,\dots,j_n}} t_{i_1\,o}\dots t_{i_n\,o}t_{o\,j_1}\dots t_{o\,j_n}G^{(o)}_{i_1\dots i_n\,j_1\dots j_n\,\sigma}(\tau_1\dots\tau_{2n-1},\tau_2\dots\tau_{2n})\Bigg\}$$

$$ \tag{4.62} $$

All terms but the first in this sum over n turn out to be at least of order $1/d$ so that they vanish in the limit of infinite dimension $d = \infty$. Thus, in this limit we find for the effective action

$$
\begin{aligned}
S_{\text{eff}} &= S_o + \sum_\sigma \int_0^\beta d\tau_1 \int_0^\beta d\tau_2\, \bar{c}_{o\sigma}(\tau_1) c_{o\sigma}(\tau_2) \sum_{ij} t_{io} t_{oj} G^{(o)}_{ij\,\sigma}(\tau_1 - \tau_2) \\
&= \int_0^\beta d\tau \Big[\sum_\sigma \bar{c}_{o\sigma}(\tau) \Big(\frac{\partial}{\partial\tau} - \mu\Big) c_{o\sigma}(\tau) + \frac{U}{2} \sum_{\substack{\sigma\sigma' \\ \sigma\neq\sigma'}} \bar{c}_{o\sigma}(\tau) c_{o\sigma}(\tau) \bar{c}_{o\sigma'}(\tau) c_{o\sigma'}(\tau) \Big] \\
&\quad + \sum_\sigma \int_0^\beta d\tau_1 \int_0^\beta d\tau_2\, \bar{c}_{o\sigma}(\tau_1) c_{o\sigma}(\tau_2) \sum_{ij} t_{io} t_{oj} G^{(o)}_{ij\,\sigma}(\tau_1 - \tau_2)
\end{aligned}
\tag{4.63}
$$

and introducing the Weiss field

$$
\mathcal{G}_\sigma^{-1}(\tau_1 - \tau_2) = -\Big(\frac{\partial}{\partial\tau_1} - \mu\Big) \delta_{\tau_1\,\tau_2} - \sum_{ij} t_{io} t_{oj} G^{(o)}_{ij\,\sigma}(\tau_1 - \tau_2) \tag{4.64}
$$

we finally get

$$
\begin{aligned}
S_{\text{eff}} &= -\sum_\sigma \int_0^\beta d\tau_1 \int_0^\beta d\tau_2\, \bar{c}_{o\sigma}(\tau_1) \mathcal{G}_\sigma^{-1}(\tau_1 - \tau_2) c_{o\sigma}(\tau_2) \\
&\quad + \int_0^\beta d\tau \frac{U}{2} \sum_{\sigma\sigma'\sigma\neq\sigma'} \bar{c}_{o\sigma}(\tau) c_{o\sigma}(\tau) \bar{c}_{o\sigma'}(\tau) c_{o\sigma'}(\tau)
\end{aligned}
\tag{4.65}
$$

The equation

$$
G^{(o)}_{ij\,\sigma} = G_{ij\,\sigma} - G_{io\,\sigma} G^{-1}_{oo\,\sigma} G_{oj\,\sigma} \tag{4.66}
$$

is needed to relate the cavity Greens function to the Greens function of the lattice $G_{ij\,\sigma}$. Going from imaginary time to imaginary frequency and combining with (4.66), the Weiss function (4.64) reads

$$
\begin{aligned}
\mathcal{G}_\sigma^{-1}(i\omega_n) &= i\omega_n + \mu - \sum_{ij} t_{io} t_{oj} G^{(o)}_{ij\,\sigma}(i\omega_n) \\
&= i\omega_n + \mu - \sum_{ij} t_{io} t_{oj} \Big[G_{ij\,\sigma}(i\omega_n) - G_{io\,\sigma}(i\omega_n) G^{-1}_{oo\,\sigma}(i\omega_n) G_{oj\,\sigma}(i\omega_n) \Big]
\end{aligned}
$$

$$(4.67)$$

If we now go from real space to k space we can simplify this equation. Introducing the Fourier transform $G_{k\,\sigma}$ via

$$G_{ij\,\sigma}(i\omega_n) = \sum_k e^{ikR_{ij}} G_{k\,\sigma}(i\omega_n) \tag{4.68}$$

we find

$$\begin{aligned}
\sum_i t_{io} G_{io\,\sigma}(i\omega_n) &= \sum_i t_{io} \sum_k e^{ikR_{io}} G_{k\,\sigma}(i\omega_n) = \sum_k \varepsilon_k G_{k\,\sigma}(i\omega_n) \\
\sum_{ij} t_{io} t_{oj} G_{ij\,\sigma}(i\omega_n) &= \sum_{ij} t_{io} t_{oj} \sum_k e^{ikR_{ij}} G_{k\,\sigma}(i\omega_n) \\
&= \sum_k \sum_i t_{io} e^{ikR_{io}} \sum_j t_{oj} e^{ikR_{oj}} G_{k\,\sigma}(i\omega_n) = \sum_k \varepsilon_k^2 G_{k\,\sigma}(i\omega_n)
\end{aligned} \tag{4.69}$$

In the general form of the Greens function $G^{-1}_{k\,\sigma}(i\omega_n) = i\omega_n + \mu - \varepsilon_k - \Sigma_\sigma(i\omega_n)$ we introduce the abbreviation $\xi = i\omega_n + \mu - \Sigma_\sigma(i\omega_n)$ to get $G^{-1}_{k\,\sigma}(i\omega_n) = \xi - \varepsilon_k$ and determine the sums

$$\begin{aligned}
\sum_k \varepsilon_k G_{k\,\sigma}(i\omega_n) &= \sum_k \frac{\varepsilon_k}{\xi - \varepsilon_k} = \sum_k \frac{\varepsilon_k - \xi + \xi}{\xi - \varepsilon_k} = -1 + \sum_k \frac{\xi}{\xi - \varepsilon_k} \\
&= -1 + \xi \sum_k G_{k\,\sigma}(i\omega_n) = -1 + \xi G_{oo\,\sigma}(i\omega_n) \\
\sum_k \varepsilon_k^2 G_{k\,\sigma}(i\omega_n) &= \sum_k \frac{\varepsilon_k^2}{\xi - \varepsilon_k} = \sum_k \frac{\varepsilon_k(\varepsilon_k - \xi) + \varepsilon_k \xi}{\xi - \varepsilon_k} = \sum_k \varepsilon_k + \xi \sum_k \frac{\varepsilon_k}{\xi - \varepsilon_k} \\
&= \xi\big(-1 + \xi G_{oo\,\sigma}(i\omega_n)\big) = -\xi + \xi^2 G_{oo\,\sigma}(i\omega_n)
\end{aligned} \tag{4.70}$$

With this, the Weiss function (4.67) becomes

$$\begin{aligned}
\mathcal{G}^{-1}_\sigma(i\omega_n) &= i\omega_n + \mu - \sum_k \varepsilon_k^2 G_{k\,\sigma}(i\omega_n) + \Big(\sum_k \varepsilon_k G_{k\,\sigma}(i\omega_n)\Big)^2 G^{-1}_{oo\,\sigma}(i\omega_n) \\
&= i\omega_n + \mu + \xi - \xi^2 G_{oo\,\sigma}(i\omega_n) \\
&\quad + \big(-1 + \xi G_{oo\,\sigma}(i\omega_n)\big)\big(-G^{-1}_{oo\,\sigma}(i\omega_n) + \xi\big) \\
&= i\omega_n + \mu - \xi + G^{-1}_{oo\,\sigma}(i\omega_n) = \Sigma_\sigma(i\omega_n) + G^{-1}_{oo\,\sigma}(i\omega_n)
\end{aligned}$$

(4.71)

The effective action (4.65) can now be interpreted in terms of the Anderson impurity model, *i. e.* the Anderson impurity model gives rise to an action which becomes identical to (4.65) if an additional self consistency condition is fulfilled. The Hamiltonian for the Anderson impurity model is

$$H = \sum_{k\sigma} \varepsilon_k c^+_{k\sigma} c_{k\sigma} + \sum_{k\sigma} \left(V_k c^+_{k\sigma} f_\sigma + V^*_k f^+_\sigma c_{k\sigma} \right) - \sum_{\sigma} \mu f^+_\sigma f_\sigma + \frac{U}{2} \sum_{\substack{\sigma\sigma' \\ \sigma\neq\sigma'}} f^+_\sigma f_\sigma f^+_{\sigma'} f_{\sigma'} \tag{4.72}$$

where σ runs from 1 to the degeneracy N. The action corresponding to this Hamiltonian will consist of a purely local part S_o concerning only the f electrons

$$S_o = \int_0^\beta d\tau \left[\sum_\sigma \bar{f}_\sigma(\tau) \left(\frac{\partial}{\partial\tau} - \mu \right) f_\sigma(\tau) + \frac{U}{2} \sum_{\substack{\sigma\sigma' \\ \sigma\neq\sigma'}} \bar{f}_\sigma(\tau) f_\sigma(\tau) \bar{f}_{\sigma'}(\tau) f_{\sigma'}(\tau) \right] \tag{4.73}$$

and a part involving conduction band electrons that can be integrated out:

$$S = S_o + \int_0^\beta d\tau \sum_{k\sigma} \left[\bar{c}_{k\sigma}(\tau) \left(\frac{\partial}{\partial\tau} + \varepsilon_k \right) c_{k\sigma}(\tau) + V_k \bar{c}_{k\sigma}(\tau) f_\sigma(\tau) + V^*_k \bar{f}_\sigma(\tau) c_{k\sigma}(\tau) \right] \tag{4.74}$$

Now the partition function for the Hamiltonian (4.72) is

$$\begin{aligned} Z = {} & \int \mathcal{D}\bar{f}_\sigma \mathcal{D} f_\sigma \int \prod_i \mathcal{D}\bar{c}_{i\sigma} \mathcal{D} c_{i\sigma} e^{-S} = \int \mathcal{D}\bar{f}_\sigma \mathcal{D} f_\sigma \, e^{-S_o} \int \prod_i \mathcal{D}\bar{c}_{i\sigma} \mathcal{D} c_{i\sigma} \times \\ & \times \exp\left\{ \int_0^\beta d\tau \sum_{k\sigma} \left[\bar{c}_{k\sigma}(\tau) \left(\frac{\partial}{\partial\tau} + \varepsilon_k \right) c_{k\sigma}(\tau) + V_k \bar{c}_{k\sigma}(\tau) f_\sigma(\tau) + V^*_k \bar{f}_\sigma(\tau) c_{k\sigma}(\tau) \right] \right\} \\ = {} & \int \mathcal{D}\bar{f}_\sigma \mathcal{D} f_\sigma \, e^{-S_o} \prod_k \det\left(\frac{\partial}{\partial\tau} + \varepsilon_k \right) \times \\ & \times \exp\left\{ \sum_{k\sigma} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \, \bar{f}_\sigma(\tau_1) V^*_k V_k \left(\frac{\partial}{\partial\tau_1} + \varepsilon_k \right)^{-1} \delta_{\tau_1 \tau_2} f_\sigma(\tau_2) \right\} \end{aligned} \tag{4.75}$$

In the last step, the terms involving f electrons $V_k^* \bar{f}_\sigma(\tau)$ and $V_k f_\sigma(\tau)$ were taken as source terms, which makes the term in the exponent a Gaussian integral that can be evaluated directly. The determinant constitutes a constant factor in the partition function that doesn't concern us here. We are left with an action for the f electrons that reads

$$S_f = \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_\sigma \bar{f}_\sigma(\tau_1) \left[\left(\frac{\partial}{\partial \tau_1} - \mu \right) \delta_{\tau_1 \tau_2} - \sum_k |V_k|^2 \left(\frac{\partial}{\partial \tau_1} + \varepsilon_k \right)^{-1} \delta_{\tau_1 \tau_2} \right] f_\sigma(\tau_2)$$
$$+ \int_0^\beta d\tau \frac{U}{2} \sum_{\substack{\sigma\sigma' \\ \sigma \neq \sigma'}} \bar{f}_\sigma(\tau) f_\sigma(\tau) \bar{f}_{\sigma'}(\tau) f_{\sigma'}(\tau) \tag{4.76}$$

If we now compare this to the effective action of the Hubbard model (4.65), we see that they are identical if we require that the Weiss function $\mathcal{G}(\tau_1 - \tau_2)$ fulfils the condition

$$\mathcal{G}^{-1}(\tau_1 - \tau_2) = -\left(\frac{\partial}{\partial \tau_1} - \mu \right) \delta_{\tau_1 \tau_2} + \sum_k |V_k|^2 \left(\frac{\partial}{\partial \tau_1} + \varepsilon_k \right)^{-1} \delta_{\tau_1 \tau_2} \tag{4.77}$$

Going from imaginary time to imaginary frequency, this equation reads

$$\mathcal{G}^{-1}(i\omega_n) = i\omega_n + \mu - \sum_k \frac{|V_k|^2}{i\omega_n - \varepsilon_k} \tag{4.78}$$

Here we can identify the usual definition of the hybridization function $\Delta(i\omega_n)$ in the Anderson impurity model

$$\Delta(i\omega_n) = \sum_k \frac{|V_k|^2}{i\omega_n - \varepsilon_k} \tag{4.79}$$

If we now equate Weiss functions (4.71) and (4.78) we find the DMFT selfconsistency condition in terms of a prescription for $\Delta(i\omega_n)$

$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_\sigma(i\omega_n) - G_{oo\,\sigma}^{-1}(i\omega_n) \tag{4.80}$$

On the Bethe lattice and with a half band width of $2t$, we have a noninteracting density of states

$$\rho_0(\varepsilon) = \frac{1}{2\pi t^2} \sqrt{4t^2 - \varepsilon^2} \tag{4.81}$$

and thus we can write for the local Greens function

$$G_{oo\,\sigma}(\omega) = \sum_k G_k(\omega) = \sum_k \frac{1}{\zeta - \varepsilon_k} \qquad \text{with} \quad \zeta = \omega + \mu - \Sigma_\sigma(\omega)$$
$$= \int d\varepsilon \frac{\rho_0(\varepsilon)}{\zeta - \varepsilon} = \frac{1}{2\pi t^2} \int_{-2t}^{2t} d\varepsilon \frac{\sqrt{4t^2 - \varepsilon^2}}{\zeta - \varepsilon} = \frac{1}{2t^2}\left(\zeta - \mathrm{sgn}(\zeta)\sqrt{\zeta^2 - 4t^2}\right) \tag{4.82}$$

From this we gain the expression

$$t^2 G_{oo\,\sigma}(\omega) - \zeta + G^{-1}_{oo\,\sigma}(\omega) = 0\,, \tag{4.83}$$

which combined with Eq. (4.80) leads to a simplified form of the selfconsistency condition

$$\Delta(i\omega_n) = t^2 G_{oo\,\sigma}(i\omega_n)\,. \tag{4.84}$$

4.2 Semiclassical approximation

The Hamiltonian is given as

$$H = -t \sum_{\langle ij \rangle \sigma} (c^+_{i\sigma} c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{4.85}$$

where t is the hopping matrix between sites and U is the Coulomb repulsion. The partition function Z for many-body system is

$$Z = \mathrm{Tr} e^{-\beta H} = \int D[c^\dagger c] e^{-S_{eff}}, \tag{4.86}$$

where the effective action S_{eff} is

$$S_{eff} = -\int_0^\beta d\tau \int_0^\beta d\tau' c^\dagger(\tau) a(\tau, \tau') c(\tau') + \int_0^\beta d\tau\, U n_{i\uparrow}(\tau) n_{i\downarrow}(\tau). \tag{4.87}$$

Here, $a(\tau, \tau') = G_0^{-1}(\tau - \tau')$ and $\beta = \frac{1}{T}$. We can decompose $n_\uparrow n_\downarrow$ into

$$n_\uparrow n_\downarrow = \frac{1}{4}\left((n_\uparrow + n_\downarrow)^2 - (n_\uparrow - n_\downarrow)^2\right) = \frac{1}{4}(N^2 - M^2), \tag{4.88}$$

where $N(\tau)$ is the particle number and $M(\tau)$ is the magnetization. Now, the effective action is rewritten as

$$S_{eff} = -\int_0^\beta d\tau \int_0^\beta d\tau' c^\dagger(\tau) a(\tau, \tau') c(\tau') + \frac{U}{4} \int_0^\beta d\tau \left(N^2(\tau) - M^2(\tau)\right).$$

$$(4.89)$$

If we substitute $N(\tau)$ by $\langle N\rangle$, where $\langle N\rangle = 1$ at half-filling, the partition function is

$$Z = \int D[c^\dagger c] e^{\int_0^\beta d\tau \int_0^\beta d\tau' c^\dagger(\tau) a(\tau,\tau') c(\tau') + \frac{U}{4}\int_0^\beta d\tau M^2(\tau)} e^{-\frac{\beta U}{4}}, \tag{4.90}$$

where term $\frac{\beta U}{4}$ shifts the energy at $-\frac{U}{4}$ and plays the same role like a chemical potential. It does not affect the Green's function, so we neglect the term $e^{-\frac{\beta U}{4}}$.

Now, let us use a Hubbard-Stratonovich (HS) transformation. The HS transformation introduces a new auxiliary field. The HS transformation is given as

$$\int_{-\infty}^{\infty} dx e^{-\pi x^2 + 2\sqrt{\pi} A x} = e^{A^2}, \tag{4.91}$$

where A is a number and x is an auxiliary field. Using the HS transformation, we obtain the partition function with auxiliary field ϕ:

$$Z = \int D[c^\dagger c] D[\phi] e^{\int_0^\beta d\tau \int_0^\beta d\tau' c^\dagger(\tau) a(\tau,\tau') c(\tau') - \int_0^\beta d\tau \left(\frac{\phi^2(\tau)}{4U} - \frac{\phi(\tau) M(\tau)}{2}\right)}, \tag{4.92}$$

where $A = \frac{\sqrt{U}M}{2}$ and $x = \frac{\phi}{\sqrt{4U\pi}}$ from Eq. (7). In general, the semiclassical field ϕ is a function of the imaginary time τ, but in this approximation we assume it to be τ-independent (why we call semiclassical approximation). Let us employ $M(\tau) = \int_0^\beta d\tau' c^\dagger(\tau) \sigma_z \delta(\tau - \tau') c(\tau')$ in Eq. (8), where σ_z is the Pauli matrix. In that case, the partition function is given as

$$Z = \int D[c^\dagger c] \int_{-\infty}^{\infty} d\phi e^{-\frac{\beta\phi^2}{4U} + \int_0^\beta d\tau \int_0^\beta d\tau' c^\dagger(\tau)\left(a(\tau,\tau') + \frac{1}{2}\phi\sigma_z\delta(\tau-\tau')\right)c(\tau')} \tag{4.93}$$

After a Fourier transformation from imaginary time τ to Matsubara frequency ω_n, we can rewrite the partition function in the Matsubara frequency space:

$$Z = \int D[c^\dagger c] \int_\infty^\infty d\phi e^{-\frac{\phi^2\beta}{4U} + \beta \sum_{\omega_n} c^\dagger(\omega_n)\left(a(\omega_n) + \frac{1}{2}\phi\sigma_z\right)c(\omega_n)} . \tag{4.94}$$

Using $e^{\sum_{\omega_n} c^\dagger(\omega_n)} = \prod_{\omega_n}\left(1+c^\dagger(\omega_n)c(\omega_n)\right)$, we can express the partition function:

$$Z = \int D[c^\dagger c] \int_\infty^\infty d\phi e^{-\frac{\beta\phi^2}{4U}} \prod_{\omega_n}\left(1 + c^\dagger(\omega_n)c(\omega_n)\right) \tag{4.95}$$

With Grassmann integration $\int dc^\dagger dc = 0$ and $\int dc^\dagger dc\, ac^\dagger c = -a\int c^\dagger dc^\dagger = -a$, the partition function is

$$Z = \int_\infty^\infty d\phi e^{-\frac{\beta\phi^2}{4U} + \sum_{\omega_n} \ln\det\left[-\beta(a(\omega_n) + \frac{1}{2}\phi\sigma_z)\right]} . \tag{4.96}$$

The general partition function for single-site calculations is

$$Z = \int_{-\infty}^\infty d\phi e^{-\beta V(\phi)}, \tag{4.97}$$

with $V(\phi) = \frac{\phi^2}{4U} - T\sum_{\omega_n} \ln\det[-\beta(a(\omega_n) + \Lambda(\phi, s))]$. Note that $a(\omega_n)$ and $\Lambda(\phi, s)$ are 2×2 matrices, where $s = \frac{1}{2}, -\frac{1}{2}$. Some permutations of the rows and the columns matrix lead to a diagonal matrix, which looks $\mathrm{diag}(a_\uparrow, a_\downarrow)$, where $a_\uparrow(a_\downarrow)$ is a 1×1 matrix. In that case, the potential can be rewritten as

$$V(\phi) = \frac{1}{U}\phi^2 - T\sum_{\omega_n,\sigma=\uparrow,\downarrow} \ln\det\left[-\beta(a(\omega_n) + \Lambda_\sigma(\phi))\right], \tag{4.98}$$

where $\sigma_z = 1(-1)$ if $\sigma =\uparrow (\downarrow)$. Finally, the impurity Green's function is

$$G_\sigma^{imp}(i\omega_n) = \frac{1}{Z}\int_{-\infty}^\infty d\phi\, e^{-\beta V(\phi)}\left(a_\sigma(\omega_n) + \Lambda_\sigma(\phi)\right), \tag{4.99}$$

from $G_\sigma^{imp}(i\omega_n) = \frac{\partial \ln Z}{\partial a}$.

The dynamical mean field theory (DMFT) self-consistent loop:

(1) Set the self-energy $\Sigma(i\omega_n) = 0$ and $\Sigma(\omega) = 0$, where ω_n and ω are the Matsubara frequency and real frequency, respectively.

(2) Using DMFT self-consistent equation (Hilbert transformation) and Dyson's equation, the Weiss field $G^0(i\omega_n)$ and $G^0(\omega)$. The DMFT self-consistent equation is given as

$$G^{\mathrm{imp}}(i\omega_n) = \int^{\mathrm{BZ}} dk \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma(i\omega_n)}, \tag{4.100}$$

and

$$\frac{1}{G^0(i\omega_n)} = \Sigma(i\omega_n) + \frac{1}{G^{\mathrm{imp}}(i\omega_n)}. \tag{4.101}$$

(3) Insert $G^0(i\omega_n)$ into the semiclassical approximation impurity solver and calculate the new self-energy by Dyson's equation.

$$\Sigma^{\mathrm{new}}(i\omega_n) = \frac{1}{G^0(i\omega_n)} - \frac{1}{G^{\mathrm{imp}}(i\omega_n)}. \tag{4.102}$$

(4) The new self-energy are inserted into (2) process. This DMFT iterations are repetitive and after several iterations, we can obtain the converged self-energy $\Sigma(i\omega_n)$.

It is recommended to write a code for the semiclassical approximation by solving only Eqs. (4.97), (4.98) and (4.99).