6. Dynamical mean field theory

Fock space

We consider the Hilbert space $\mathcal{H}_N$ 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

$$\langle\psi_N|\psi_N\rangle = \int d^3r_1 \ldots d^3r_N |\psi_N(\vec{r}_1, \ldots, \vec{r}_N)|^2 < +\infty \tag{6.1}$$

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

$$\mathcal{H}_N = \mathcal{H} \otimes \mathcal{H} \otimes \cdots \otimes \mathcal{H} \tag{6.2}$$

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

$$|\alpha_1 \ldots \alpha_N) \equiv |\alpha_1\rangle|\alpha_2\rangle \ldots |\alpha_N\rangle \tag{6.3}$$

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

$$\begin{aligned}\psi_{\alpha_1\alpha_2\ldots\alpha_N}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) &= (\vec{r}_1, \ldots, \vec{r}_N|\alpha_1, \ldots, \alpha_N) \\ &= \big(\langle\vec{r}_1| \otimes \langle\vec{r}_2| \otimes \cdots \otimes \langle\vec{r}_N|\big)\big(|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \cdots \otimes |\alpha_N\rangle\big) \\ &= \varphi_{\alpha_1}(\vec{r}_1)\varphi_{\alpha_2}(\vec{r}_2) \ldots \varphi_{\alpha_N}(\vec{r}_N)\end{aligned} \tag{6.4}$$

The overlap of two vectors is

$$\begin{aligned}(\alpha_1\alpha_2 \ldots \alpha_N|\alpha'_1\alpha'_2 \ldots \alpha'_N) &= \big(\langle\alpha_1| \otimes \langle\alpha_2| \otimes \cdots \otimes \langle\alpha_N|\big)\big(|\alpha'_1\rangle \otimes |\alpha'_2\rangle \cdots \otimes |\alpha'_N\rangle\big) \\ &= \langle\alpha_1|\alpha'_1\rangle\langle\alpha_2|\alpha'_2\rangle \ldots \langle\alpha_N|\alpha'_N\rangle\end{aligned} \tag{6.5}$$

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

$$\sum_{\alpha_1\ldots\alpha_N} |\alpha_1\alpha_2 \ldots \alpha_N)(\alpha_1\alpha_2 \ldots \alpha_N| = 1 \tag{6.6}$$

1 is the unit operator in $\mathcal{H}_N$. $\mathcal{H}_N$ 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

$$\psi(\vec{r}_{p_1}, \vec{r}_{p_2}, \dots, \vec{r}_{p_N}) = \varepsilon^P \psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \tag{6.7}$$

where $P = (p_1, p_2, \dots, p_N)$ represents any permutation of the set $(1, 2, \dots, N)$, 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 $\psi(\vec{r}_1, \dots, \vec{r}_N)$ 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:

$$\mathcal{P}_\varepsilon \psi(\vec{r}_1, \dots, \vec{r}_N) = \frac{1}{N!} \sum_P \varepsilon^P \psi(\vec{r}_{p_1}, \vec{r}_{p_2}, \dots, \vec{r}_{p_N}) \tag{6.8}$$

E.g. for two Fermions

$$\mathcal{P}_{-1} \psi(\vec{r}_1, \vec{r}_2) = \frac{1}{2}\big(\psi(\vec{r}_1, \vec{r}_2) - \psi(\vec{r}_2, \vec{r}_1)\big) \tag{6.9}$$

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:

$$\mathcal{H}_N^{(\varepsilon)} = \mathcal{P}_\varepsilon \mathcal{H}_N \tag{6.10}$$

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

$$\begin{aligned} |\alpha_1 \dots \alpha_N\} &\equiv \sqrt{N!}\mathcal{P}_\varepsilon |\alpha_1 \dots \alpha_N) \\ &= \frac{1}{\sqrt{N!}} \sum_P \varepsilon^P |\alpha_{p_1}\rangle \otimes |\alpha_{p_2}\rangle \otimes \dots |\alpha_{p_N}\rangle \end{aligned} \tag{6.11}$$

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

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

$$(6.12)$$

From Eq. (6.10), if $|\alpha_1\alpha_2\ldots\alpha_N)$ is a basis of the Hilbert space $\mathcal{H}_N$, then $\mathcal{P}_\varepsilon|\alpha_1\alpha_2\ldots\alpha_N)$ is a basis of Fermionic or Bosonic Hilbert spaces $\mathcal{H}_N^{(\varepsilon)}$; the completeness (closure) relation Eq. (6.6) becomes the completeness relation in $\mathcal{H}_N^{(-1)}$ or $\mathcal{H}_N^{(1)}$:

$$\sum_{\alpha_1\ldots\alpha_N} \mathcal{P}_\varepsilon|\alpha_1\alpha_2\ldots\alpha_N)(\alpha_1\alpha_2\ldots\alpha_N|\mathcal{P}_\varepsilon = \frac{1}{N!}\sum_{\alpha_1\ldots\alpha_N}|\alpha_1\alpha_2\ldots\alpha_N\}\{\alpha_1\alpha_2\ldots\alpha_N| = 1 \tag{6.13}$$

If a basis $|\alpha\rangle$ is orthogonal in $\mathcal{H}$, then the basis $|\alpha_1\alpha_2\ldots\alpha_N)$ is orthogonal in $\mathcal{H}_N$, and the basis $|\alpha_1\alpha_2\ldots\alpha_N\}$ is orthogonal in $\mathcal{H}_N^{(\varepsilon)}$.
The scalar product of two such vectors constructed from the same basis $|\alpha\rangle$ is

$$\begin{aligned}\{\alpha'_1\alpha'_2\ldots\alpha'_N|\alpha_1\alpha_2\ldots\alpha_N\} &= N!(\alpha'_1\alpha'_2\ldots\alpha'_N|\mathcal{P}_\varepsilon^2|\alpha_1\alpha_2\ldots\alpha_N)\\ &= N!(\alpha'_1\alpha'_2\ldots\alpha'_N|\mathcal{P}_\varepsilon|\alpha_1\alpha_2\ldots\alpha_N)\\ &= \sum_P \varepsilon^P\langle\alpha'_1|\alpha_{p_1}\rangle\langle\alpha'_2|\alpha_{p_2}\rangle\ldots\langle\alpha'_N|\alpha_{p_N}\rangle \end{aligned}\tag{6.14}$$

The basis $|\alpha\rangle$ is orthogonal; therefore, the only nonvanishing terms in this sum are the permutations P such that

$$\alpha'_1 = \alpha_{p_1}, \alpha'_2 = \alpha_{p_2}, \ldots, \alpha'_N = \alpha_{p_N} \tag{6.15}$$

If $\alpha'_1, \alpha'_2, \ldots, \alpha'_N$ is a permutation of $\alpha_1, \alpha_2, \ldots, \alpha_N$, the overlap can be directly evaluated. For Fermions, there is at most one particle per state $|\alpha\rangle$, so that no two identical states can be present in the set $\{\alpha_1, \alpha_2, \ldots, \alpha_N\}$; only one permutation P can transform $\alpha_1, \alpha_2, \ldots, \alpha_N$ into $\alpha'_1, \alpha'_2, \ldots, \alpha'_N$. The sum reduces to one term, and the result is

$$\{\alpha'_1\alpha'_2\ldots\alpha'_N|\alpha_1\alpha_2\ldots\alpha_N\} = (-1)^P \qquad \text{(for Fermions)} \tag{6.16}$$

For Bosons, one has to count the permutations that transform $\{\alpha_1, \alpha_2, \ldots, \alpha_N\}$ into $\{\alpha'_1, \alpha'_2, \ldots, \alpha'_N\}$. The result is (for n_1 Bosons in state α_1, n_2 in state α_2, ..., n_p in state α_p where states $\alpha_1, \alpha_2, \ldots, \alpha_p$ are distinct):

$$\{\alpha'_1\alpha'_2\ldots\alpha'_N|\alpha_1\alpha_2\ldots\alpha_N\} = n_1!n_2!\ldots n_p! \qquad \text{(for Bosons)} \tag{6.17}$$

The two results can be efficiently combined by specifying a state with particles in states $\alpha_1, \alpha_2, \dots, \alpha_N$ in terms of occupation numbers α of each state of the basis $|\alpha\rangle$; n_α is unrestricted for Bosons and can only be 0 or 1 for Fermions. In both cases, the total number of occupied states equals the total number of particles:

$$N = \sum_\alpha n_\alpha \tag{6.18}$$

Example: A three-Boson state with particles in states α_1, α_1, α_2 would be characterized as $n_1 = 2$, $n_2 = 1$, $n_i = 0 \forall i \geqslant 3$. A three-Fermion state with particles in states α_1, α_2, α_3 would be written as $n_1 = 1$, $n_2 = 1$, $n_3 = 1$, $n_i = 0 \forall i \geqslant 4$. With the convention $0! = 1$ we then have

$$\{\alpha_1'\alpha_2' \dots \alpha_N' | \alpha_1 \alpha_2 \dots \alpha_N\} = \varepsilon^P \prod_\alpha n_\alpha! \tag{6.19}$$

With this expression we obtain an orthonormalized basis for the Hilbert spaces $\mathcal{H}_N^{(\varepsilon)}$ as

$$\begin{aligned} |\alpha_1 \alpha_2 \dots \alpha_N\rangle &= \frac{1}{\prod_\alpha n_\alpha!} |\alpha_1 \alpha_2 \dots \alpha_N\} \\ &= \frac{1}{N! \prod_\alpha n_\alpha!} \sum_P \varepsilon^P |\alpha_{p_1}\rangle \otimes |\alpha_{p_2}\rangle \otimes \dots \otimes |\alpha_{p_N}\rangle \end{aligned} \tag{6.20}$$

(angular brackets $|\ \rangle$ are now used for normalized symmetric or antisymmetric states).
The overlap between a tensor product $|\beta_1, \beta_2, \dots, \beta_N)$ and a symmetrized (antisymmetrized) state $|\alpha_1 \alpha_2 \dots \alpha_N\rangle$ is

$$\begin{aligned} (\beta_1 \beta_2 \dots \beta_N | \alpha_1 \alpha_2 \dots \alpha_N\rangle &= \frac{1}{\sqrt{N! \prod_\alpha n_\alpha!}} \sum_P \varepsilon^P \langle \beta_1 | \alpha_{p_1}\rangle \langle \beta_2 | \alpha_{p_2}\rangle \dots \langle \beta_N | \alpha_{p_N}\rangle \\ &\equiv \frac{1}{\sqrt{N! \prod_\alpha n_\alpha!}} S\big(\langle \beta_i | \alpha_j \rangle\big) \end{aligned} \tag{6.21}$$

where $S(M_{ij})$ denotes a permanent (analogon of determinant without signs) for Bosons

$$\mathrm{perm}(M_{ij}) \equiv \sum_P M_{1,p_1} M_{2,p_2} \dots M_{N,p_N} \tag{6.22}$$

and a determinant for Fermions

$$\det(M_{ij}) \equiv \sum_P (-1)^P M_{1,p_1} M_{2,p_2} \dots M_{N,p_N} \tag{6.23}$$

In coordinate representation, we obtain in this way a basis of permanent wave functions for Bosons

$$\begin{aligned}\psi_{\beta_1\beta_2\dots\beta_N}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) &= (\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N|\beta_1\beta_2\dots\beta_N\rangle \\ &= \frac{1}{\sqrt{N!\prod_\alpha n_\alpha!}} \mathrm{perm}(\varphi_{\beta_i}(\vec{r}_j))\end{aligned} \tag{6.24}$$

and a basis of Slater determinants for Fermions

$$\begin{aligned}\psi_{\beta_1\beta_2\dots\beta_N}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) &= (\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N|\beta_1\beta_2\dots\beta_N\rangle \\ &= \frac{1}{\sqrt{N!}} \det(\varphi_{\beta_i}(\vec{r}_j))\end{aligned} \tag{6.25}$$

The overlap of two normalized Boson or Fermion states is

$$\langle\beta_1\beta_2\dots\beta_N|\alpha_1\alpha_2\dots\alpha_N\rangle = \frac{1}{\sqrt{\prod_\beta n_\beta! \prod_\alpha n_\alpha!}} S\big(\langle\beta_i|\alpha_j\rangle\big) \tag{6.26}$$

The completeness relation in $\mathcal{H}_N^{(\varepsilon)}$ becomes

$$\sum_{\alpha_1\dots\alpha_N} \frac{\prod_\alpha n_\alpha!}{N!} |\alpha_1\alpha_2\dots\alpha_N\rangle\langle\alpha_1\alpha_2\dots\alpha_N| = 1 \tag{6.27}$$

Creation and annihilation operators

Creation and annihilation operators provide a convenient representation of the many-particle states (and manybody operators). They generate the entire Hilbert space by their action on a single reference state and provide a basis of the algebra of operators of the Hilbert space. For each single particle state $|\lambda\rangle$ of the single particle space $\mathcal{H}$, a Boson or Fermion creation operator $a_\lambda^\dagger$ is defined by its action on any symmetrized or antisymmetrized state $|\lambda_1, \lambda_2, \dots, \lambda_N\}$ of $\mathcal{H}_N^{(\varepsilon)}$:

$$a_\lambda^\dagger|\lambda_1, \lambda_2, \dots, \lambda_N\} \equiv |\lambda\lambda_1, \lambda_2, \dots, \lambda_N\} \tag{6.28}$$

We use an orthonormal basis $\{|\lambda_i\rangle\}$ so that $a_\lambda^\dagger$ can also be defined as

$$a_\lambda^\dagger|\lambda_1, \lambda_2, \dots, \lambda_N\rangle = \sqrt{n_\lambda + 1}|\lambda\lambda_1, \lambda_2, \dots, \lambda_N\rangle \tag{6.29}$$

with occupation number n_λ of state $|\lambda\rangle$ in $|\lambda_1, \lambda_2, \ldots, \lambda_N\rangle$. $a_\lambda^\dagger$ adds a particle in state $|\lambda\rangle$ to the state on which it operates and symmetrizes or antisymmetrizes the new state. For Fermions:

$$a_\lambda^\dagger|\lambda_1, \lambda_2, \ldots, \lambda_N\} = \begin{cases} |\lambda\lambda_1, \lambda_2, \ldots, \lambda_N\} & \text{if state } |\lambda\rangle \text{ not present in } |\lambda_1, \lambda_2, \ldots, \lambda_N\} \\ 0 & \text{otherwise} \end{cases} \tag{6.30}$$

Grassmann algebra

We need anticommuting numbers for constructing coherent states for Fermions which are eigenstates of annihilation operators because anticommutation 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:

$$\chi(a\zeta + b\xi) = a\chi\zeta + b\chi\xi \qquad (a\zeta + b\xi)\chi = a\zeta\chi + b\xi\chi \tag{6.31}$$

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

$$\chi(\zeta\xi) = (\chi\zeta)\xi \tag{6.32}$$

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

$$\chi_i\chi_j + \chi_j\chi_i = 0 \tag{6.33}$$

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

$$\xi_i^2 = 0 \tag{6.34}$$

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 $\{1, \chi_{\alpha_1}, \chi_{\alpha_1}\chi_{\alpha_2}, \cdots, \chi_{\alpha_1}\chi_{\alpha_2}\cdot$

$\cdots\chi_{\alpha_n}\}$ 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

$$(\chi_i)^* = \chi_i^* \qquad (\chi_i^*)^* = \chi_i \tag{6.35}$$

Then, for complex λ

$$(\lambda\chi_i)^* = \lambda^*\chi_i^* \tag{6.36}$$

and for products of generators

$$(\chi_{\alpha_1}\chi_{\alpha_2}\cdots\chi_{\alpha_n})^* = \chi_{\alpha_n}^*\chi_{\alpha_{n-1}}^*\cdots\chi_{\alpha_1}^* \tag{6.37}$$

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:

$$f(\chi) = f_0 + f_1\chi \tag{6.38}$$

An operator A has the form

$$A(\chi^*, \chi) = a_0 + a_1\chi + \bar{a}_1\chi^* + a_{12}\chi^*\chi \tag{6.39}$$

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

$$\begin{aligned}
&\frac{\partial}{\partial\chi}A(\chi^*, \chi) = a_1 - a_{12}\chi^* \qquad \frac{\partial}{\partial\chi^*}A(\chi^*, \chi) = \bar{a}_1 + a_{12}\chi \\
&\frac{\partial}{\partial\chi^*}\frac{\partial}{\partial\chi}A(\chi^*, \chi) = -a_{12} = -\frac{\partial}{\partial\chi}\frac{\partial}{\partial\chi^*}A(\chi^*, \chi)
\end{aligned} \tag{6.40}$$

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

$$\int_{-\infty}^{\infty} \frac{df(x)}{dx} = 0 \qquad \text{in case } f(x \to \infty) = f(x \to -\infty) = 0 \tag{6.41}$$

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

$$\int d\chi \, 1 = 0 \tag{6.42}$$

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

$$\int d\chi \, \chi = 1 \tag{6.43}$$

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:

$$\int d\chi^* \, 1 = 0 \qquad \int d\chi^* \, \chi^* = 1 \tag{6.44}$$

Examples for integration rules are:

$$\begin{aligned}
&\int d\chi \, f(\chi) = \int d\chi (f_0 + f_1 \chi) = f_1 \\
&\int d\chi \, A(\chi^*, \chi) = \int d\chi \, (a_0 + a_1 \chi + \bar{a}_1 \chi^* + a_{12} \chi^* \chi) = a_1 - a_{12} \chi^* \\
&\int d\chi^* \, A(\chi^*, \chi) = \bar{a}_1 + a_{12} \chi \\
&\int d\chi^* \int d\chi \, A(\chi^*, \chi) = -a_{12} = -\int d\chi \int d\chi^* \, A(\chi^*, \chi)
\end{aligned} \tag{6.45}$$

<u>**Coherent states**</u>

We now introduce **coherent states** as a basis of Fock space $\mathcal{F}$; this is an alternative to Slater determinants in analogy to position eigenstates in quantum mechanics where $|\mathbf{r}\rangle$ is defined as eigenstate of $\hat{\mathbf{r}}$. They are eigenstates of Fermionic annihilation operators (creation operators would not work as they don't have eigenstates)[1]:

$$a_i|\chi\rangle = \chi_i|\chi\rangle \tag{6.46}$$

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

$$|\psi\rangle = \sum_i \chi_i|\phi_i\rangle \tag{6.47}$$

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:

$$[\tilde{\chi}, \tilde{a}]_+ = 0 \tag{6.48}$$

and

$$(\tilde{\chi}\tilde{a})^\dagger = \tilde{a}^\dagger\tilde{\chi}^* \tag{6.49}$$

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

$$|\chi\rangle = \exp\Big\{-\sum_i \chi_i a_i^\dagger\Big\}|0\rangle = \prod_i \big(1 - \chi_i a_i^\dagger\big)|0\rangle\,. \tag{6.50}$$

Any physical Fermion state of Fock space $\mathcal{F}$ can be expanded in terms of $|\chi\rangle$. Noting that pairs of Grassmann variables and creation or annihilation operators commute:

$$\begin{aligned}[\chi_i a_i^\dagger, \chi_j a_j^\dagger] &= \chi_i a_i^\dagger \chi_j a_j^\dagger - \chi_j a_j^\dagger \chi_i a_i^\dagger = -\chi_i\chi_j a_i^\dagger a_j^\dagger + \chi_j\chi_i a_j^\dagger a_i^\dagger \\ &= \chi_j\chi_i a_i^\dagger a_j^\dagger - \chi_j\chi_i a_i^\dagger a_j^\dagger = 0\end{aligned} \tag{6.51}$$

we can show that the two definitions of Eq. (6.50) are really the same:

$$|\chi\rangle = \exp\Big\{-\sum_i \chi_i a_i^\dagger\Big\}|0\rangle = \prod_i \exp\{-\chi_i a_i^\dagger\}|0\rangle = \prod_i \big(1 - \chi_i a_i^\dagger\big)|0\rangle \tag{6.52}$$

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

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

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

$$\begin{aligned}
a_i|\chi\rangle &= a_i \prod_j \big(1-\chi_j a_j^\dagger\big)|0\rangle \\
&= \prod_{j\neq i}\big(1-\chi_j a_j^\dagger\big)\, a_i\big(1-\chi_i a_i^\dagger\big)|0\rangle = \prod_{j\neq i}\big(1-\chi_j a_j^\dagger\big)\chi_i a_i a_i^\dagger|0\rangle \quad \text{using Eq. (6.48)} \\
&= \prod_{j\neq i}\big(1-\chi_j a_j^\dagger\big)\chi_i|0\rangle = \prod_{j\neq i}\big(1-\chi_j a_j^\dagger\big)\chi_i\big(1-\chi_i a_i^\dagger\big)|0\rangle \quad \text{because } \chi_i^2=0 \\
&= \chi_i|\chi\rangle
\end{aligned} \tag{6.53}$$

The adjoint of a coherent state is

$$\langle\chi| = \langle 0|\exp\Big\{-\sum_j \big(\chi_j a_j^\dagger\big)^\dagger\Big\} = \langle 0|\exp\Big\{\sum_j \chi_j^* a_j\Big\} = \langle 0|\prod_j \big(1+\chi_j^* a_j\big) \tag{6.54}$$

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

$$\langle\chi|a_i^\dagger = \langle\chi|\chi_i^* \tag{6.55}$$

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

$$\begin{aligned}
a_i^\dagger|\chi\rangle &= a_i^\dagger \prod_j \big(1-\chi_j a_j^\dagger\big)|0\rangle = \prod_{j\neq i}\big(1-\chi_j a_j^\dagger\big)\, a_i^\dagger\big(1-\chi_i a_i^\dagger\big)|0\rangle \\
&= \prod_{j\neq i}\big(1-\chi_j a_j^\dagger\big)\, a_i^\dagger|0\rangle \quad \text{because } a_i^\dagger a_i^\dagger = 0 \\
&= -\frac{\partial}{\partial\chi_i}\big(1-\chi_i a_i^\dagger\big)\prod_{j\neq i}\big(1-\chi_j a_j^\dagger\big)|0\rangle = -\frac{\partial}{\partial\chi_i}|\chi\rangle
\end{aligned} \tag{6.56}$$

and in the same way

$$\langle\chi|a_i = \frac{\partial}{\partial\chi_i^*}\langle\chi| \tag{6.57}$$

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

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

(6.58)

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

$$\int \prod_i d\chi_i^* d\chi_i e^{-\sum_i \chi_i^* \chi_i} |\chi\rangle\langle\chi| = 1 \tag{6.59}$$

The completeness relation leads to an expression for the trace of an operator. Matrix elements between $|\psi_i\rangle$ in Fock space and coherent states $|\chi_i\rangle$ contain Grassmann numbers; therefore, anticommutation rules imply for the matrix elements $\langle\psi_i|\chi\rangle$ and $\langle\chi|\psi_i\rangle$ that

$$\langle\psi_i|\chi\rangle\langle\chi|\psi_i\rangle = \langle-\chi|\psi_i\rangle\langle\psi_i|\chi\rangle \tag{6.60}$$

Thus, if we have a complete set of states $\{|n\rangle\}$ in Fock space, the trace of an operator becomes

$$\begin{aligned}\mathrm{Tr}A = \sum_n \langle n|A|n\rangle &= \int \prod_i d\chi_i^* d\chi_i e^{-\sum_i \chi_i^* \chi_i} \sum_n \langle n|\chi\rangle\langle\chi|A|n\rangle \\ &= \int \prod_i d\chi_i^* d\chi_i e^{-\sum_i \chi_i^* \chi_i} \langle-\chi|A \sum_n |n\rangle\langle n|\chi\rangle \\ &= \int \prod_i d\chi_i^* d\chi_i e^{-\sum_i \chi_i^* \chi_i} \langle-\chi|A|\chi\rangle \end{aligned} \tag{6.61}$$

The overcompleteness of the Fermion coherent states allow for a Grassmann coherent state representation:

$$|\psi\rangle = \int \prod_i d\chi_i^* d\chi_i e^{-\sum_i \chi_i^* \chi_i} \psi(\chi^*)|\chi\rangle \quad \text{with } \langle\chi|\psi\rangle = \psi(\chi^*) \tag{6.62}$$

in analogy to position eigenstates in quantum mechanics when a state can be written as $|\psi\rangle = \int dx \psi(x)|x\rangle$ with the coordinate representation $\psi(x) = \langle x|\psi\rangle$ of $|\psi\rangle$. $\psi(\chi^*)$ means the wavefunction of the state $|\psi\rangle$ in the coherent state representation, *i.e.* the probability amplitude for finding the system in the coherent state $|\chi\rangle$.
From Eqs. (6.55) and (6.57) we obtain

$$\begin{aligned}\langle\chi|a_i|\psi\rangle &= \frac{\partial}{\partial\chi_i^*}\psi(\chi^*) \\ \langle\chi|a_i^\dagger|\psi\rangle &= \chi_i^*\psi(\chi^*)\,. \end{aligned} \tag{6.63}$$

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

Thus, the annihilation and creation operators a_i and $a_i^\dagger$ are represented by operators $\frac{\partial}{\partial \chi_i^*}$ and χ_i^*, respectively; Fermion anticommutation relations are represented by

$$\left[\frac{\partial}{\partial \chi_i^*}, \chi_i^*\right] = \delta_{ij} \tag{6.64}$$

The matrix element of a normal ordered operator $A(a_i^\dagger, a_i)$ between two coherent states is

$$\langle \chi | A(a_i^\dagger, a_i) | \chi' \rangle = e^{\sum_i \chi_i^* \chi_i'} A(\chi_i^*, \chi_i') \tag{6.65}$$

but the expectation value of the number operator is not a real number:

$$\langle \chi | N | \chi \rangle \langle \chi | \chi \rangle = \sum_i \chi_i^* \chi_i \tag{6.66}$$

and the average number of particles in a Fermion coherent state has no meaning.

Gaussian integrals

In the evaluation of the path integrals appearing in the derivation of the DMFT equations, we will have to perform integrals of exponential functions with polynomials of complex or Grassmann variables as argument. For quadratic forms, standard Gaussian integrals can be generalized. For real variables, with a real symmetric positive definite matrix and summation over repeated Latin indices we have

$$\int \frac{dx_1 dx_2 \ldots dx_n}{(2\pi)^{n/2}} e^{-\frac{1}{2} x_i A_{ij} x_j + x_i J_i} = (\det A)^{-1/2} e^{\frac{1}{2} J_i A_{ij}^{-1} J_j} \tag{6.67}$$

This can be proven by changing variables to diagonalize A and using the Gaussian integral

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2} = \sqrt{\frac{\pi}{a}} \tag{6.68}$$

We transform $y_i - A_{ij}^{-1} J_j$, $z_k = O_{ki}^{-1} y_i$ with the orthogonal transofrmation

O diagonalizing A:

$$
\begin{aligned}
&\int dx_1 \ldots dx_n e^{-\frac{1}{2}x_i A_{ik} x_k + J_k x_k - \frac{1}{2} J_i A^{-1}_{ik} J_k} \\
&\qquad = \int dy_1 \ldots dy_n e^{-\frac{1}{2} y_i A_{ik} y_k} = \int dz_1 \ldots dz_n e^{\sum_m \frac{1}{2} a_m z_m^2} \\
&\qquad = \prod_{m=1}^{n} \sqrt{\frac{2\pi}{a_m}} = \frac{(2\pi)^{n/2}}{(\det A)^{1/2}}
\end{aligned}
\tag{6.69}
$$

For a Hermitian matrix H and pairs of complex conjugate variable x_i, x_i^* one can prove

$$
\int \prod_{i=1}^{n} \frac{dx_i^* dx_i}{2\pi i} e^{-x_i^* H_{ij} x_j + J_i^* x_i + J_i x_i^*} = (\det H)^{-1} e^{J_i^* H^{-1}_{ij} J_j} \tag{6.70}
$$

in the same way. Finally, for Grassmann variable

$$
\int \prod_{i=1}^{n} d\chi_i^* d\chi_i e^{-\chi_i^* H_{ij} \chi_j + \zeta_i^* \chi_i + \zeta_i \chi_i^*} = (\det H) e^{\zeta_i^* H^{-1}_{ij} \zeta_j} \tag{6.71}
$$

with H Hermitian (not necessarily positive definite) and Grassmann variables $\{\chi_i, \chi_i^*, \zeta_i, \zeta_i^*\}$.

Functional integral representation

We jump over a number of steps explaining the functional integral formulation: representing the partition function by an integral over field configurations as physically intuitive description of the system and as starting point for approximations: perturbation expansions, loop expansions around stationary solutions, stochastic approximations. Steps left out here are the Feynman path integral in real time; path integrals automatically represent time ordered products; the analytic continuation to imaginary time to represent partition functions.

$$
Z = \mathrm{Tr} e^{-\beta H} = \int dx \langle x | e^{-\beta H} | x \rangle \tag{6.72}
$$

can be understood as a sum of diagonal matrix elements of the imaginary time evolution operator

$$
\mathcal{U}(x_f \tau_f, x_i \tau_i) = \langle x_f | e^{-(\tau_f - \tau_i)\frac{\hat{H}}{\hbar}} | x_i \rangle \quad \text{for time interval } \tau_f - \tau_i = \beta\hbar
$$

(6.73)

The coherent state functional integral is introduced to deal with the general many-particle Hamiltonian using the manybody evolution operator; coherent states $|\chi\rangle$ replace position and momentum eigenstates.
For the many-particle system, we now express the partition function as the trace of the imaginary time evolution operator:

$$Z = \mathrm{Tr} e^{-\beta(\hat{H} - \mu\hat{N})} = \int \prod_i d\chi_i^* d\chi_i \langle \eta\chi | e^{-\beta(\hat{H} - \mu\hat{N})} | \chi\rangle \quad (6.74)$$

where $\eta = -1$ for Fermions. Upon continuation of Eq. (6.72) to imaginary time, the trace imposes periodic or antiperiodic boundary conditions $\chi_{i,0} = \chi_i$ and $\chi_{i,M}^* = \eta\chi_i^*$; relabelling $\chi_i \equiv \eta\chi_{i,M}$ leads to

$$Z = \lim_{M\to\infty} \int \prod_{k=1}^{M} \prod_i \frac{1}{\mathcal{N}} d\chi_{i,k}^* d\chi_{i,k} e^{-S(\chi^*, \chi)} \quad \text{with } \mathcal{N} = \begin{cases} 2\pi i & \text{Bosons} \\ 0 & \text{Fermions} \end{cases} \quad (6.75)$$

where

$$\begin{aligned} S(\chi^*, \chi) = {} & \varepsilon \sum_{k=2}^{M} \left[\sum_i \chi_{i,k}^* \left\{ \frac{\chi_{i,k} - \chi_{i,k-1}}{\varepsilon} - \mu\chi_{i,k-1} \right\} + H(\chi_{i,k}^*, \chi_{i,k-1}) \right] \\ & + \varepsilon \left[\sum_i \chi_{i,1}^* \left\{ \frac{\chi_{i,1} - \eta\chi_{i,M}}{\varepsilon} - \mu\eta\chi_{i,M} \right\} + H(\chi_{i,1}^*, \eta\chi_{i,M}) \right] \end{aligned} \quad (6.76)$$

In trajectory notation, this becomes

$$Z = \int_{\chi_i(\beta)=\eta\chi_i(0)} \mathcal{D}\big(\chi_i^*(\tau)\chi_i(\tau)\big) e^{-\int_0^\beta d\tau \left\{ \sum_i \chi_i^*(\tau)\left(\frac{\partial}{\partial\tau} - \mu\right)\chi_i(\tau) + H\left(\chi_i^*(\tau), \chi_i(\tau)\right) \right\}} \quad (6.77)$$

where

$$\int_{\chi_i(\beta)=\eta\chi_i(0)} \mathcal{D}\big(\chi_i^*(\tau)\chi_i(\tau)\big) = \lim_{M\to\infty} \int \prod_{k=1}^{M} \prod_i \frac{1}{\mathcal{N}} d\chi_{i,k}^* d\chi_{i,k} \quad (6.78)$$

The imaginary time Greens functions now have a simple form in terms of a coherent state path integral:

$$
\begin{aligned}
G^{(n)}&(i_1\tau_1,\dots,i_n\tau_n|i'_1\tau'_1,\dots,i'_n\tau'_n)\\
&= \left\langle T\left[a^{(H)}_{i_1}(\tau_1),\dots,a^{(H)}_{i_n}(\tau_n)a^{(H)}_{i'_1}(\tau'_1),\dots,a^{(H)}_{i'_n}(\tau'_n)\right]\right\rangle\\
&= \frac{1}{Z}\int \mathcal{D}\big(\chi_i^*(\tau)\chi_i(\tau)\big)\Big[e^{-\int_0^\beta d\tau\left[\sum_i \chi_i^*(\tau)\left(\frac{\partial}{\partial\tau}-\mu\right)\chi_i(\tau)+H\left(\chi_i^*(\tau),\chi_i(\tau)\right)\right]}\times\\
&\quad\times \chi_{i_1}(\tau_1)\dots\chi_{i_n}(\tau_n)\chi_{i_{n+1}}(\tau_{n+1})\dots\chi_{i_{2n}}(\tau_{2n})\Big]
\end{aligned}
\tag{6.79}
$$

6.1 DMFT self consistency condition for the Hubbard model

We consider the Hubbard Hamiltonian

$$
H = -\sum_{ij\sigma} t_{ij}c^+_{i\sigma}c_{j\sigma} - \mu\sum_{i\sigma} c^+_{i\sigma}c_{i\sigma} + \frac{U}{2}\sum_{\substack{i\sigma\sigma'\\ \sigma\neq\sigma'}} c^+_{i\sigma}c_{i\sigma}c^+_{i\sigma'}c_{i\sigma'}
\tag{6.80}
$$

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

$$
Z = \int\prod_i \mathcal{D}\bar{c}_{i\sigma}\mathcal{D}c_{i\sigma}e^{-S}
\tag{6.81}
$$

with the action

$$
\begin{aligned}
S = \int_0^\beta d\tau \sum_{i\sigma}\bar{c}_{i\sigma}(\tau)\frac{\partial}{\partial\tau}c_{i\sigma}(\tau) + \int_0^\beta d\tau\Big[&-\sum_{ij\sigma} t_{ij}\bar{c}_{i\sigma}(\tau)c_{j\sigma}(\tau) - \mu\sum_{i\sigma}\bar{c}_{i\sigma}(\tau)c_{i\sigma}(\tau)\\
&+\frac{U}{2}\sum_{\substack{i\sigma\sigma'\\ \sigma\neq\sigma'}}\bar{c}_{i\sigma}(\tau)c_{i\sigma}(\tau)\bar{c}_{i\sigma'}(\tau)c_{i\sigma'}(\tau)\Big]
\end{aligned}
\tag{6.82}
$$

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 (6.80) 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:

$$H = H_o + H_c + H^{(o)} \tag{6.83}$$

$$H_o = -\mu \sum_{\sigma} c^+_{o\sigma} c_{o\sigma} + \frac{U}{2} \sum_{\substack{\sigma\sigma' \\ \sigma\neq\sigma'}} c^+_{o\sigma} c_{o\sigma} c^+_{o\sigma'} c_{o\sigma'} \tag{6.84}$$

$$H_c = -\sum_{i\sigma} \left[t_{io} c^+_{i\sigma} c_{o\sigma} + t_{oi} c^+_{o\sigma} c_{i\sigma} \right] \tag{6.85}$$

$$H^{(o)} = -\sum_{i\neq o\, j\neq o\, \sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} - \mu \sum_{i\neq o\, \sigma} c^+_{i\sigma} c_{i\sigma} + \frac{U}{2} \sum_{\substack{i\neq o\, \sigma\sigma' \\ \sigma\neq\sigma'}} c^+_{i\sigma} c_{i\sigma} c^+_{i\sigma'} c_{i\sigma'} \tag{6.86}$$

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:

$$S_o = \int_0^\beta d\tau \left[\sum_{\sigma} \bar{c}_{o\sigma}(\tau) \left(\frac{\partial}{\partial\tau} - \mu \right) c_{o\sigma}(\tau) + \frac{U}{2} \sum_{\substack{\sigma\sigma' \\ \sigma\neq\sigma'}} \bar{c}_{o\sigma}(\tau) c_{o\sigma}(\tau) \bar{c}_{o\sigma'}(\tau) c_{o\sigma'}(\tau) \right] \tag{6.87}$$

$$\Delta S = -\int_0^\beta d\tau \left[\sum_{i\sigma} t_{io} \bar{c}_{i\sigma}(\tau) c_{o\sigma}(\tau) + t_{oi} \bar{c}_{o\sigma}(\tau) c_{i\sigma}(\tau) \right] \tag{6.88}$$

$$\begin{aligned} S^{(o)} = \int_0^\beta d\tau \Bigg[& \sum_{i\neq o\, \sigma} \bar{c}_{i\sigma}(\tau) \left(\frac{\partial}{\partial\tau} - \mu \right) c_{i\sigma}(\tau) - \sum_{i\neq o\, j\neq o\, \sigma} t_{ij} \bar{c}_{i\sigma}(\tau) c_{j\sigma}(\tau) \\ & + \frac{U}{2} \sum_{\substack{i\neq o\, \sigma\sigma' \\ \sigma\neq\sigma'}} \bar{c}_{i\sigma}(\tau) c_{i\sigma}(\tau) \bar{c}_{i\sigma'}(\tau) c_{i\sigma'}(\tau) \Bigg] \end{aligned} \tag{6.89}$$

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

$$Z = \int \mathcal{D}\bar{c}_{o\sigma}\mathcal{D}c_{o\sigma}e^{-S_o} \int \prod_{i\neq o} \mathcal{D}\bar{c}_{i\sigma}\mathcal{D}c_{i\sigma}e^{-S^{(o)}} e^{-\int_0^\beta d\tau\, \Delta S(\tau)} \tag{6.90}$$

Now we can expand the last exponential function as

$$e^{-\int_0^\beta d\tau\, \Delta S(\tau)} = 1 - \int_0^\beta d\tau\, \Delta S(\tau) + \frac{1}{2!}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2\, \Delta S(\tau_1)\Delta S(\tau_2) - \dots \tag{6.91}$$

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

$$\langle A \rangle_S = \frac{\int \prod_i \mathcal{D}\bar{c}_\alpha \mathcal{D}c_\alpha e^{-S} A[\bar{c}_\alpha, c_\alpha]}{\int \prod_i \mathcal{D}\bar{c}_\alpha \mathcal{D}c_\alpha e^{-S}} = Z_s^{-1} \int \prod_i \mathcal{D}\bar{c}_\alpha \mathcal{D}c_\alpha e^{-S} A[\bar{c}_\alpha, c_\alpha] \tag{6.92}$$

we can consider the second functional integral in (6.90) to average the terms of the expansion (6.91) with respect to the lattice action $S^{(o)}$:

$$\begin{aligned} Z = \int \prod_i \mathcal{D}\bar{c}_{o\sigma}\mathcal{D}c_{o\sigma}e^{-S_o} Z_{S^{(o)}} \Big\{ 1 - \int_0^\beta d\tau\, \langle \Delta S(\tau) \rangle_{S^{(o)}} \\ + \frac{1}{2!}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2\, \langle \Delta S(\tau_1)\Delta S(\tau_2) \rangle_{S^{(o)}} - \dots \Big\} \end{aligned} \tag{6.93}$$

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

$$Z_{S^{(o)}} = \int \prod_i \mathcal{D}\bar{c}_\alpha \mathcal{D}c_\alpha e^{-S^{(o)}} . \tag{6.94}$$

Now the terms in (6.93) with odd powers of ΔS will average to zero. For example,

$$\langle \Delta S(\tau) \rangle_{S^{(o)}} = \sum_{i\sigma} t_{io} \langle \bar{c}_{i\sigma}(\tau) \rangle_{S^{(o)}} c_{o\sigma}(\tau) + t_{oi} \bar{c}_{o\sigma}(\tau) \langle c_{i\sigma}(\tau) \rangle_{S^{(o)}} = 0 \,, \tag{6.95}$$

because the average $\langle \dots \rangle_{S^{(o)}}$ acts on all sites except o. The next average in (6.93) yields

$$\langle \Delta S(\tau_1)\Delta S(\tau_2)\rangle_{S^{(o)}} = \Big\langle T_\tau \Big[\sum_{i\sigma} t_{io}\bar{c}_{i\sigma}(\tau_1)c_{o\sigma}(\tau_1) + t_{oi}\bar{c}_{o\sigma}(\tau_1)c_{i\sigma}(\tau_1)\Big]\times$$
$$\times \Big[\sum_{j\sigma'} t_{jo}\bar{c}_{j\sigma'}(\tau_2)c_{o\sigma'}(\tau_2) + t_{oj}\bar{c}_{o\sigma'}(\tau_2)c_{j\sigma'}(\tau_2)\Big]\Big\rangle_{S^{(o)}}$$
$$= \sum_{ij\sigma\sigma'} t_{io}t_{oj}c_{o\sigma}(\tau_1)\langle T_\tau \bar{c}_{i\sigma}(\tau_1)c_{j\sigma'}(\tau_2)\rangle_{S^{(o)}}\ \bar{c}_{o\sigma'}(\tau_2)$$
$$+ \sum_{ij\sigma\sigma'} t_{oi}t_{jo}\bar{c}_{o\sigma}(\tau_1)\langle T_\tau c_{i\sigma}(\tau_1)\bar{c}_{j\sigma'}(\tau_2)\rangle_{S^{(o)}}\ c_{o\sigma'}(\tau_2)$$
$$= 2\sum_{ij\sigma\sigma'} t_{io}t_{oj}\bar{c}_{o\sigma}(\tau_1)\langle T_\tau c_{i\sigma}(\tau_1)\bar{c}_{j\sigma'}(\tau_2)\rangle_{S^{(o)}}\ c_{o\sigma'}(\tau_2)$$
$$= 2\sum_{ij\sigma} t_{io}t_{oj}\bar{c}_{o\sigma}(\tau_1)\langle T_\tau c_{i\sigma}(\tau_1)\bar{c}_{j\sigma}(\tau_2)\rangle_{S^{(o)}}\ c_{o\sigma}(\tau_2)$$
$$= -2\sum_{ij\sigma} t_{io}t_{oj}\bar{c}_{o\sigma}(\tau_1)G^{(o)}_{ij\,\sigma}(\tau_1-\tau_2)c_{o\sigma}(\tau_2) \tag{6.96}$$

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

$$Z = \int \prod_\sigma \mathcal{D}\bar{c}_{o\sigma}\mathcal{D}c_{o\sigma}e^{-S_o}Z_{S^{(o)}}\times$$
$$\times\left\{1 - \int_0^\beta d\tau_1\int_0^\beta d\tau_2 \sum_{ij\sigma} t_{io}t_{oj}\bar{c}_{o\sigma}(\tau_1)c_{o\sigma}(\tau_2)G^{(o)}_{ij\,\sigma}(\tau_1-\tau_2) + \dots\right\} \tag{6.97}$$

We would like to write the bracket $\{\dots\}$ in (6.97) again as an exponential function in order to identify an effective action S_{eff}:

$$Z = \int \prod_\sigma \mathcal{D}\bar{c}_{o\sigma}\mathcal{D}c_{o\sigma}e^{-S_{\text{eff}}} \tag{6.98}$$

Noting that the next term in the expansion of (6.97) would read

$$\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \int_0^\beta d\tau_4 \sum_{i_1\, i_2\, j_1\, j_2\, \sigma} \bar{c}_{o\sigma}(\tau_1)\bar{c}_{o\sigma}(\tau_3)c_{o\sigma}(\tau_2)c_{o\sigma}(\tau_4)\times$$
$$\times\, t_{i_1\, o} t_{i_2\, o} t_{o\, j_1} t_{o\, j_2} G^{(o)}_{i_1\, i_2\, j_1\, j_2\, \sigma}(\tau_1\, \tau_3, \tau_2\, \tau_4)\,. \tag{6.99}$$

We can write for the partion function (6.97)

$$Z = \int \prod_\sigma \mathcal{D}\bar{c}_{o\sigma}\mathcal{D}c_{o\sigma} e^{-S_o} Z_{S^{(o)}} \times$$
$$\times \exp\Big\{ -\sum_{n=1}^{\infty}\sum_\sigma \int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_{2n}\, \bar{c}_{o\sigma}(\tau_1)\dots\bar{c}_{o\sigma}(\tau_{2n-1})c_{o\sigma}(\tau_2)\dots c_{o\sigma}(\tau_{2n})\times$$
$$\times \sum_{\substack{i_1,\dots,i_n\\ j_1,\dots,j_n}} t_{i_1\, o}\dots t_{i_n\, o} t_{o\, j_1}\dots t_{o\, j_n} G^{(o)}_{i_1\dots i_n\, j_1\dots j_n\, \sigma}(\tau_1\dots\tau_{2n-1}, \tau_2\dots\tau_{2n})\Big\} \tag{6.100}$$

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

$$\begin{aligned} S_{\text{eff}} &= S_o + \sum_\sigma \int_0^\beta d\tau_1 \int_0^\beta d\tau_2\, \bar{c}_{o\sigma}(\tau_1)c_{o\sigma}(\tau_2) \sum_{ij} t_{io}t_{oj} G^{(o)}_{ij\,\sigma}(\tau_1 - \tau_2) \\ &= \int_0^\beta d\tau \Big[\sum_\sigma \bar{c}_{o\sigma}(\tau)\Big(\frac{\partial}{\partial\tau} - \mu\Big)c_{o\sigma}(\tau) + \frac{U}{2}\sum_{\substack{\sigma\sigma'\\ \sigma\neq\sigma'}} \bar{c}_{o\sigma}(\tau)c_{o\sigma}(\tau)\bar{c}_{o\sigma'}(\tau)c_{o\sigma'}(\tau)\Big] \\ &\quad + \sum_\sigma \int_0^\beta d\tau_1 \int_0^\beta d\tau_2\, \bar{c}_{o\sigma}(\tau_1)c_{o\sigma}(\tau_2) \sum_{ij} t_{io}t_{oj} G^{(o)}_{ij\,\sigma}(\tau_1 - \tau_2) \end{aligned} \tag{6.101}$$

and introducing the Weiss field

$$\mathcal{G}^{-1}_\sigma(\tau_1 - \tau_2) = -\Big(\frac{\partial}{\partial\tau_1} - \mu\Big)\delta_{\tau_1\,\tau_2} - \sum_{ij} t_{io}t_{oj} G^{(o)}_{ij\,\sigma}(\tau_1 - \tau_2) \tag{6.102}$$

we finally get

$$S_{\text{eff}} = -\sum_{\sigma} \int_0^{\beta} d\tau_1 \int_0^{\beta} d\tau_2\, \bar{c}_{o\sigma}(\tau_1) \mathcal{G}_{\sigma}^{-1}(\tau_1 - \tau_2) c_{o\sigma}(\tau_2)$$
$$+ \int_0^{\beta} d\tau\, \frac{U}{2} \sum_{\sigma\sigma' \sigma\neq\sigma'} \bar{c}_{o\sigma}(\tau) c_{o\sigma}(\tau) \bar{c}_{o\sigma'}(\tau) c_{o\sigma'}(\tau) \tag{6.103}$$

The equation

$$G_{ij\,\sigma}^{(o)} = G_{ij\,\sigma} - G_{io\,\sigma} G_{oo\,\sigma}^{-1} G_{oj\,\sigma} \tag{6.104}$$

is needed to relate the cavity Greens function to the Greens function of the lattice $G_{ij\,\sigma}$. This equation can already be found in the Appendix of J. Hubbard, Proc. Roy. Soc. A **281**, 401 (1964). It is explained in A. Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996) by the following argument: When the Greens function is expanded in hopping matrix elements t_{kl}, additional paths contributing to $G_{ij\,\sigma}$ but not to $G_{ij\,\sigma}^{(o)}$ connect i to j through o. In the $d = \infty$ limit, only paths going once through o need to be considered, so that these paths constitute a term proportional to $G_{io\,\sigma} G_{oj\,\sigma}$; but this needs to be divided by $G_{oo\,\sigma}$ in order not to double count paths from o to o.

Going from imaginary time to imaginary frequency and combining with (6.104), the Weiss function (6.102) reads

$$\begin{aligned}\mathcal{G}_{\sigma}^{-1}(i\omega_n) &= i\omega_n + \mu - \sum_{ij} t_{io} t_{oj} G_{ij\,\sigma}^{(o)}(i\omega_n) \\ &= i\omega_n + \mu - \sum_{ij} t_{io} t_{oj} \Big[G_{ij\,\sigma}(i\omega_n) - G_{io\,\sigma}(i\omega_n) G_{oo\,\sigma}^{-1}(i\omega_n) G_{oj\,\sigma}(i\omega_n) \Big]\end{aligned} \tag{6.105}$$

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

$$G_{ij\,\sigma}(i\omega_n) = \sum_{k} e^{ikR_{ij}} G_{k\,\sigma}(i\omega_n) \tag{6.106}$$

we find

$$
\begin{aligned}
\sum_i t_{io} G_{io\,\sigma}(i\omega_n) &= \sum_i t_{io} \sum_k e^{ikR_{io}} G_{k\,\sigma}(i\omega_n) = \sum_k \varepsilon_k G_{k\,\sigma}(i\omega_n) \\
\sum_{ij} t_{io} t_{oj} G_{ij\,\sigma}(i\omega_n) &= \sum_{ij} t_{io} t_{oj} \sum_k e^{ikR_{ij}} G_{k\,\sigma}(i\omega_n) \\
&= \sum_k \sum_i t_{io} e^{ikR_{io}} \sum_j t_{oj} e^{ikR_{oj}} G_{k\,\sigma}(i\omega_n) = \sum_k \varepsilon_k^2 G_{k\,\sigma}(i\omega_n)
\end{aligned}
\tag{6.107}
$$

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

$$
\begin{aligned}
\sum_k \varepsilon_k G_{k\,\sigma}(i\omega_n) &= \sum_k \frac{\varepsilon_k}{\xi - \varepsilon_k} = \sum_k \frac{\varepsilon_k - \xi + \xi}{\xi - \varepsilon_k} = -1 + \sum_k \frac{\xi}{\xi - \varepsilon_k} \\
&= -1 + \xi \sum_k G_{k\,\sigma}(i\omega_n) = -1 + \xi G_{oo\,\sigma}(i\omega_n) \\
\sum_k \varepsilon_k^2 G_{k\,\sigma}(i\omega_n) &= \sum_k \frac{\varepsilon_k^2}{\xi - \varepsilon_k} = \sum_k \frac{\varepsilon_k(\varepsilon_k - \xi) + \varepsilon_k \xi}{\xi - \varepsilon_k} = \sum_k \varepsilon_k + \xi \sum_k \frac{\varepsilon_k}{\xi - \varepsilon_k} \\
&= \xi\big(-1 + \xi G_{oo\,\sigma}(i\omega_n)\big) = -\xi + \xi^2 G_{oo\,\sigma}(i\omega_n)
\end{aligned}
\tag{6.108}
$$

With this, the Weiss function (6.105) becomes

$$
\begin{aligned}
\mathcal{G}^{-1}_\sigma(i\omega_n) &= i\omega_n + \mu - \sum_k \varepsilon_k^2 G_{k\,\sigma}(i\omega_n) + \Big(\sum_k \varepsilon_k G_{k\,\sigma}(i\omega_n)\Big)^2 G^{-1}_{oo\,\sigma}(i\omega_n) \\
&= i\omega_n + \mu + \xi - \xi^2 G_{oo\,\sigma}(i\omega_n) \\
&\quad + \big(-1 + \xi G_{oo\,\sigma}(i\omega_n)\big)\big(-G^{-1}_{oo\,\sigma}(i\omega_n) + \xi\big) \\
&= i\omega_n + \mu - \xi + G^{-1}_{oo\,\sigma}(i\omega_n) = \Sigma_\sigma(i\omega_n) + G^{-1}_{oo\,\sigma}(i\omega_n)
\end{aligned}
\tag{6.109}
$$

The effective action (6.103) 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 (6.103) if an additional self consistency condition is fulfilled. The Hamiltonian for the Anderson impurity model is

$$H = \sum_{k\sigma} \varepsilon_k c^+_{k\sigma} c_{k\sigma} + \sum_{k\sigma} \left(V_k c^+_{k\sigma} f_\sigma + V^*_k f^+_\sigma c_{k\sigma} \right) - \sum_\sigma \mu f^+_\sigma f_\sigma + \frac{U}{2} \sum_{\substack{\sigma\sigma' \\ \sigma \neq \sigma'}} f^+_\sigma f_\sigma f^+_{\sigma'} f_{\sigma'} \tag{6.110}$$

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

$$S_o = \int_0^\beta d\tau \left[\sum_\sigma \bar{f}_\sigma(\tau) \left(\frac{\partial}{\partial \tau} - \mu \right) f_\sigma(\tau) + \frac{U}{2} \sum_{\substack{\sigma\sigma' \\ \sigma \neq \sigma'}} \bar{f}_\sigma(\tau) f_\sigma(\tau) \bar{f}_{\sigma'}(\tau) f_{\sigma'}(\tau) \right] \tag{6.111}$$

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

$$S = S_o + \int_0^\beta d\tau \sum_{k\sigma} \left[\bar{c}_{k\sigma}(\tau) \left(\frac{\partial}{\partial \tau} + \varepsilon_k \right) c_{k\sigma}(\tau) + V_k \bar{c}_{k\sigma}(\tau) f_\sigma(\tau) + V^*_k \bar{f}_\sigma(\tau) c_{k\sigma}(\tau) \right] \tag{6.112}$$

Now the partition function for the Hamiltonian (6.110) is

$$\begin{aligned} Z = &\int \mathcal{D}\bar{f}_\sigma \mathcal{D} f_\sigma \int \prod_i \mathcal{D}\bar{c}_{i\sigma} \mathcal{D} c_{i\sigma} e^{-S} = \int \mathcal{D}\bar{f}_\sigma \mathcal{D} f_\sigma \, e^{-S_o} \int \prod_i \mathcal{D}\bar{c}_{i\sigma} \mathcal{D} c_{i\sigma} \times \\ &\times \exp\left\{ \int_0^\beta d\tau \sum_{k\sigma} \left[\bar{c}_{k\sigma}(\tau) \left(\frac{\partial}{\partial \tau} + \varepsilon_k \right) c_{k\sigma}(\tau) + V_k \bar{c}_{k\sigma}(\tau) f_\sigma(\tau) + V^*_k \bar{f}_\sigma(\tau) c_{k\sigma}(\tau) \right] \right\} \\ = &\int \mathcal{D}\bar{f}_\sigma \mathcal{D} f_\sigma \, e^{-S_o} \prod_k \det\left(\frac{\partial}{\partial \tau} + \varepsilon_k \right) \times \\ &\times \exp\left\{ \sum_{k\sigma} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \, \bar{f}_\sigma(\tau_1) V^*_k V_k \left(\frac{\partial}{\partial \tau_1} + \varepsilon_k \right)^{-1} \delta_{\tau_1 \tau_2} f_\sigma(\tau_2) \right\} \end{aligned} \tag{6.113}$$

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

$$S_f = \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_\sigma \bar{f}_\sigma(\tau_1) \left[\left(\frac{\partial}{\partial \tau_1} - \mu \right) \delta_{\tau_1 \tau_2} - \sum_k |V_k|^2 \left(\frac{\partial}{\partial \tau_1} + \varepsilon_k \right)^{-1} \delta_{\tau_1 \tau_2} \right] f_\sigma(\tau_2)$$
$$+ \int_0^\beta d\tau \frac{U}{2} \sum_{\substack{\sigma\sigma' \\ \sigma \neq \sigma'}} \bar{f}_\sigma(\tau) f_\sigma(\tau) \bar{f}_{\sigma'}(\tau) f_{\sigma'}(\tau) \tag{6.114}$$

If we now compare this to the effective action of the Hubbard model (6.103), we see that they are identical if we require that the Weiss function $\mathcal{G}(\tau_1 - \tau_2)$ fulfils the condition

$$\mathcal{G}^{-1}(\tau_1 - \tau_2) = -\left(\frac{\partial}{\partial \tau_1} - \mu \right) \delta_{\tau_1 \tau_2} + \sum_k |V_k|^2 \left(\frac{\partial}{\partial \tau_1} + \varepsilon_k \right)^{-1} \delta_{\tau_1 \tau_2} \tag{6.115}$$

Going from imaginary time to imaginary frequency, this equation reads

$$\mathcal{G}^{-1}(i\omega_n) = i\omega_n + \mu - \sum_k \frac{|V_k|^2}{i\omega_n - \varepsilon_k} \tag{6.116}$$

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

$$\Delta(i\omega_n) = \sum_k \frac{|V_k|^2}{i\omega_n - \varepsilon_k} \tag{6.117}$$

If we now equate Weiss functions (6.109) and (6.116) we find the DMFT selfconsistency condition in terms of a prescription for $\Delta(i\omega_n)$

$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_\sigma(i\omega_n) - G^{-1}_{oo\,\sigma}(i\omega_n) \tag{6.118}$$

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

$$\rho_0(\varepsilon) = \frac{1}{2\pi t^2} \sqrt{4t^2 - \varepsilon^2} \tag{6.119}$$

and thus we can write for the local Greens function

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

$$(6.120)$$

From this we gain the expression

$$t^2 G_{oo\,\sigma}(\omega) - \zeta + G^{-1}_{oo\,\sigma}(\omega) = 0\,, \tag{6.121}$$

which combined with Eq. (6.118) leads to a simplified form of the selfconsistency condition

$$\Delta(i\omega_n) = t^2 G_{oo\,\sigma}(i\omega_n)\,. \tag{6.122}$$