Strong Coupling Expansion Approach
To
The Hubbard and Periodic Anderson Models

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CHAPTER 1

Introduction and Summary

Though theoretical models containing magnetic moments, related to spins were already known since the $30th$ of the last century (Ising model and Heisenberg model), models for the formation of magnetic moments came up almost 30 years later. In 1961 P.W. Anderson set up what now is called the single impurity Anderson model (SIAM) [3]

$$\mathcal{H}_{\text{SIAM}} = \sum_{\mathbf{k},\sigma} \varepsilon^c_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \varepsilon^f \sum_\sigma f^\dagger_\sigma f_\sigma + \sum_{\mathbf{k},\sigma} \left(V_{\mathbf{k}} f^\dagger_\sigma c_{\mathbf{k}\sigma} + V^*_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} f_\sigma \right) + U n^f_\uparrow n^f_\downarrow. \tag{1.1}$$

It consists of a structureless energy band of a metallic host, which interacts via a hybridization interaction with an impurity, consisting of 4 unperturbed states (empty $|0\rangle$, spin-up $|\uparrow\rangle$, spin-down $|\downarrow\rangle$ and double occupation $|\uparrow\downarrow\rangle$). If the double occupied state is above the Fermi-level or even above the band, corresponding to the large Coulomb interaction U in Hamiltonian, the contribution of it to the physics will be negligible, if the single occupied states are below the Fermi-level.

In particular, if the single occupied states are energetically much below the band, they will be occupied most of the time, interacting quickly with the band electrons via the hybridization, which may lead to a spin-flip from e.g $|\uparrow\rangle$ to $|\downarrow\rangle$. Thus, in this limit the SIAM goes over into the Kondo model [12]

$$\begin{aligned} \mathcal{H}_{\text{Kondo}} = {} & \sum_{\mathbf{k},\sigma} \varepsilon^c_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2} J_{\|} \sum_{\mathbf{k},\mathbf{k}',\sigma} \sigma \; c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma} \boldsymbol{\mathcal{S}}^{f,z} \\ & + J_\perp \sum_{\mathbf{k},\mathbf{k}'} \left(c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}'\downarrow} \boldsymbol{\mathcal{S}}^{f,-} + c^\dagger_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow} \boldsymbol{\mathcal{S}}^{f,+} \right) - h \boldsymbol{\mathcal{S}}^{f,z} \end{aligned} \tag{1.2}$$

In 1964, in $3rd$ order in J, Kondo showed that the quantum mechanical nature of the spin $\boldsymbol{\mathcal{S}}$ caused this model to be a many-particle model with a logarithmic (i.e. infrared) divergent perturbation theory. The relation between the two models (1.1) and (1.2) was given by Schrieffer-Wolff transformation [18] in 1966.

In Kondo-limit, the SIAM has an occupation of the f-level close to 1 $\left(\sum_\sigma f^\dagger_\sigma f_\sigma = 1 - \text{integer valance} \right)$. If the f-level position is higher (i.e. is in the band), all three states come into play, and the valence will be non-integer, i.e. intermediate.

Much later (in the $80th$), the thermodynamics of both models (1.1) and (1.2) could be obtained from a Bethe-Ansatz solution. The dynamical properties of the models, however, up to now were obtained only approximately.

Also the dream of early $60th$ to study 1 magnetic impurity first, then 2, then 3, etc. and then go over to a lattice of magnetic moments, was brutally stopped by the Kondo effect. After one had came to grips with two impurities, experiments showed a spin-glass phase for randomly interacting (antiferromagnetically or ferromagnetically as a function of distance due to a Rudermann-Kittel-like interaction) magnetic impurities. This was the second stop for the dream.

The third stop was the discovery of strongly correlated fermion systems. Alloys with rare-earth impurities showed a specific heat, which, when interpreted in term of a γT-term, γ was three to four order of magnitude larger than in normal metals. So, if $\gamma \propto$ mass, the fermionic excitations had to be really "heavy". Therefore the notion of "heavy fermions" came up.

We will speak of a heavy-fermion system when a metal meets the following conditions:

1. The low-temperature specific heat $C = \gamma T$ has a coefficient γ of order 1 J mol^{-1} K^{-2}, rather than 1 mJ mol^{-1} K^{-2} as, e.g., in the case of sodium metal;
2. The Pauli paramagnetic susceptibility χ_{s} is familiarly enhanced to γ;
3. The ratio $R = \dfrac{\pi^2 k_{\mathrm{B}}^2 \chi_{\mathrm{s}}}{3\mu_{\mathrm{eff}}^2 \gamma}$ is of order unity.

Here μ_{eff} is the effective magnetic moment of quasiparticles. The quantities γ and χ_{s} are both proportional to the quasiparticle density of states at the Fermi level $N^*(0)$. The latter is proportional to m^*, i.e. the effective mass of the fermionic excitations. Large value of γ and χ_{s} can therefore be interpreted by ascribing a large m^* to the quasiparticles. When ratio R (Sommerfeld-Wilson ratio) is calculated, the density of states $N^*(0)$ drops out. For free electrons $R = 1$. Therefore, when conditions 1-3 are met, we may assume a one-to-one correspondence between the quasiparticle excitations of the complex metallic system and those of a free electron gas, provided we use the effective mass m^* instead of the free electron mass. In fact, the effective mass m^* may be as large as several hundred times of the free electron mass. A ratio $R \neq 1$ indicates that quasiparticle interaction are not negligible. As the temperature increases to values above T^* [1] below which a heavy-fermion system shows Fermi liquid behavior with large effective masses m^* of the quasiparticles, the excitations lose their heavy character; the specific heat levels off, and the susceptibility change from Pauli- to Curie-like behavior. With increasing temperature the impurities (rare earth or actinide ions) behave more and more like ions with well-localized f electrons.

Several models for "heavy fermions" have been suggested. The most prominent ones are the Hubbard model, the periodic Anderson model (PAM) and the Kondo-lattice model.

Theoretical progress in the treatments of this class of systems has been impeded, however by extreme difficulty of dealing with even the simplest model Hamiltonians appropriate for these systems, such as the Hubbard model. Only in the one-dimensional case one has a variety of theoretical tools such as Bethe-Ansatz to study these models in a systematic manner. For higher (two- and three-) dimensional model, one is often unable to assess confidently whether a given physical phenomenon is needed captured by a theoretical prediction reflects a true feature of this Hamiltonian, rather than an artifact of the approximation used in its solution. These difficulties originate in unperturbative nature of the problems and reflect the presence of several competing physical mechanisms for even simplest models. The interplay of localization and lattice coherence, of quantum and spatial fluctuations, and of various competing types of long-range order are important examples.

And also several technical treatments, most of them fitted to one of the models, have been suggested.

In the present thesis, an attempt is made to combine all the models and methods into one formalism. For the analogous attempts, functional integrals have been used in quantum field theory at temperature $T = 0$. In statistical and solid state physics, $T > 0$ is needed, and the corresponding field theory is euclidic. The method used for $T > 0$ are called "Martin-Schwinger" methods.

In contrast to normal quantum field theory in which all particles are asymptotically free, for the strongly correlated systems ("heavy fermions") it is advisable, to give up this property and introduce

[1] Usually, the temperature T^* is on the order of a few Kelvin up to few tens Kelvin

cumulants instead of irreducible many-body Green's functions. It is shown that such a program can be successfully carried out.

The present thesis is a self-contained representation of the functional integral formalism for the strong coupling expansion approach to the Hubbard model and the periodic Anderson model.

The general organization of this thesis is as follows:

- This Chapter introduces a brief history of the heavy-fermion systems and the outline of the present thesis.
- Chapter 2 gives model Hamiltonians of the systems considered, for concreteness, the Hubbard model and the periodic Anderson model. Basic definitions for many-particle Green's functions and many-particle cumulants, which are defined instead of connected many-particle Green's functions in the language of functional integral formalism are introduced in this Chapter.
- Chapter 3 sets up the framework for the strong coupling expansion theory where the relationships between the thermodynamical quantities such as the Green's functions, the self-energy, the thermodynamical potential, ... are explicitly established. The Bethe-Salpeter like equations for many-particle cumulants are also found. The results in this Chapter provide a general starting point to reproduce the results obtained in diagrammatical techniques for the Hubbard model which now can be extended to the periodic Anderson model, and the well-known approximations such as XNCA for the periodic Anderson model.
- Chapter 4 discusses some applications obtained from very general results such as constructing a self-consistent and conserving theory in the Baym sense, the Dynamical Mean Field Theory and a way to include non-local contributions to the solution of the Dynamical Mean Field Theory.

CHAPTER 2

The Models and Definitions

In this Chapter the model Hamiltonians of the single band Hubbard model and the periodic Anderson model are represented. Both those model Hamiltonians are subject of our work throughout this thesis. Also, the functional integral formalism is introduced as main mathematical tool applying on the model Hamiltonians to determine the thermodynamical quantities such as the grand partition function, the thermodynamical potential, the many-particle correlation functions related to the systems described by those model Hamiltonians. The many-particle Green's functions and their connected parts called many-particle cumulants are defined in the standard notation of the field theory and in the functional integral formalism.

First, we present the models under consideration and some definitions. In condensed matter physics, the Hubbard model presents the simplest theoretical framework for describing interacting electrons in crystal lattices. It is frequently used to investigate many physical behaviors of strongly correlated electron systems ranging from metallic to insulating and from magnetism to superconductivity. The single band Hubbard model is given by the Hamiltonian [9]

$$\mathcal{H}_{\text{Hubbard}} = \sum_{\mathbf{ij},\sigma} \varepsilon^f_{\mathbf{ij}} f^\dagger_{\mathbf{i}\sigma} f_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n^f_{\mathbf{i}\uparrow} n^f_{\mathbf{i}\downarrow}. \tag{2.1}$$

The periodic Anderson model (PAM) by another one [19]

$$\mathcal{H}_{\text{PAM}} = \sum_{\mathbf{ij},\sigma} \varepsilon^c_{\mathbf{ij}} c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + \varepsilon^f \sum_{\mathbf{i},\sigma} f^\dagger_{\mathbf{i}\sigma} f_{\mathbf{i}\sigma} + \sum_{\mathbf{ij},\sigma} \left(V_{\mathbf{ij}} f^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + V^*_{\mathbf{ij}} c^\dagger_{\mathbf{j}\sigma} f_{\mathbf{i}\sigma} \right) + U \sum_{\mathbf{i}} n^f_{\mathbf{i}\uparrow} n^f_{\mathbf{i}\downarrow}. \tag{2.2}$$

The periodic Anderson model consists of a band of conduction electrons that hybridize with localized f-electrons states at each lattice site. This model Hamiltonian is widely considered to be relevant for description of a large class of strongly correlated electron systems, most notably the heavy fermion compounds and the so-called "Kondo insulators".

In the model Hamiltonians, the operator $f_{\mathbf{i}\sigma}$ ($c_{\mathbf{i}\sigma}$) destroys an electron of spin σ at site $\mathbf{i}$. Its adjoint $f^\dagger_{\mathbf{i}\sigma}$ ($c^\dagger_{\mathbf{i}\sigma}$) creates an electron and the number operator is defined by $n^f_{\mathbf{i}\sigma} = f^\dagger_{\mathbf{i}\sigma} f_{\mathbf{i}\sigma}$ ($n^c_{\mathbf{i}\sigma} = c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{i}\sigma}$). The symmetric hopping matrices $\varepsilon^f_{\mathbf{ij}}$ and $\varepsilon^c_{\mathbf{ij}}$ determine the band structure, which can be arbitrary. Double occupation of a site costs an energy U due to the screened Coulomb interaction. The hybridization matrix $V_{\mathbf{ij}}$ in the Hamiltonian of the periodic Anderson model is an overlap of the conduction c-electron wavefunction at site $\mathbf{i}$ and the localized f-electron wavefunction at site $\mathbf{j}$.

SECTION 2.1

Green's functions, Self-Energy and Cumulants

We will use a "four"-vector notation $k \equiv (\mathbf{k}, i\omega_n)$ for momentum-frequency space, and $x \equiv (\mathbf{i}, \tau)$ for position-imaginary time. In the quantum field theory, the definition of the n-particle Green's function is given by

$$\begin{aligned} &G^{(n)}_{\sigma_1,\ldots\sigma_n;\sigma'_1\ldots\sigma'_n}\left(x_1,\ldots,x_n;x'_1,\ldots,x'_n\right) \\ &\qquad = (-1)^n \left\langle \mathscr{T}_\tau \left(f_{\sigma_1}(x_1)\ldots f_\sigma(x_n)\, f^\dagger_{\sigma_n}(x'_n)\ldots f^\dagger_{\sigma_1}(x'_1)\right)\right\rangle , \end{aligned} \tag{2.3a}$$

it is equivalent to

$$\begin{aligned} &\equiv (-1)^n \left\langle \mathscr{T}_\tau \left(f_{\mathbf{i}_1,\sigma_1}(\tau_1)\ldots f_{\mathbf{i}_n,\sigma_n}(\tau_n)\, f^\dagger_{\mathbf{i}'_n,\sigma'_n}(\tau'_n)\ldots f^\dagger_{\mathbf{i}'_1,\sigma_1}(\tau'_1)\right)\right\rangle \\ &\equiv G^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n\right) \end{aligned} \tag{2.3b}$$

where the brackets $\langle\rangle$ represent expectation value with respect to the grand canonical ensemble, $\mathscr{T}_\tau$ is the time-ordering operator, and τ is imaginary time. The operators used in the definition of the many-particle Green's function can refer to conduction or localized electrons.

From the general definition (2.3), the one-particle Green's function is written as follows

$$G_\sigma\left(x,x'\right) = -\left\langle \mathscr{T}_\tau\left(f_\sigma(x)\, f^\dagger_\sigma(x')\right)\right\rangle . \tag{2.4}$$

In zero external field and in the absence of symmetry breaking the one-particle Green's function is translation invariance i.e. $G_\sigma(x,x') = G_\sigma(x-x')$ and the Fourier-Matsubara transforms of the one-particle Green's function are

$$\begin{aligned} G_\sigma(\mathbf{k}, i\omega_n) &= \sum_{\mathbf{i}} \mathrm{e}^{-i\mathbf{k}\mathbf{i}} \int_0^\beta \mathrm{d}\tau\ \mathrm{e}^{i\omega_n\tau}\ G_\sigma(\mathbf{i},\tau) \\ &\equiv \int \mathrm{d}x\ \mathrm{e}^{-ikx}\ G_\sigma(x) \\ &\equiv G_\sigma(k) \end{aligned} \tag{2.5a}$$

$$G_\sigma(x) = \frac{1}{N\beta}\sum_k \mathrm{e}^{ikx}\ G_\sigma(k) \tag{2.5b}$$

where $\beta = (k_B T)^{-1}$ is the inverse of temperature.

The self-energy obeys Dyson's equation, leading to

$$G_\sigma(\mathbf{k}, i\omega_n) \ = \frac{1}{\left(G^0\right)^{-1}_\sigma(\mathbf{k}, i\omega_n) - \Sigma_\sigma(\mathbf{k}, i\omega_n)} \tag{2.6}$$

where $G^0_\sigma(\mathbf{k}, i\omega_n)$ is the unperturbed Green's functions of the models.

Normal field theory, where the unperturbed Hamiltonian is quadratic, deals with asymptotically free particles. The cumulants or in other words, connected diagram part of many-particle Green's functions in the language of the normal field theory, can be also defined for the case in which the particles are not asymptotically free i.e. the unperturbed Hamiltonian is non-quadratic. In such case the n-particle Green's function $G^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}(x_1,\ldots,x_n;x'_1,\ldots,x'_n)$ in (2.3) can be expressed as a sum of products of cumulants $\mathcal{G}^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}(x_1,\ldots,x_n;x'_1,\ldots,x'_n)$, where each term of the sum corresponds to a partition of $(x_1,\ldots,x_n;x'_1,\ldots,x'_n)$ in subsets containing equal numbers of primed and unprimed variables, e.g.[1],

$$\begin{aligned} &G^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}(x_1,\ldots,x_n;x'_1,\ldots,x'_n) \\ &\quad= \sum_{\substack{\varsigma_1,\ldots,\varsigma_n\\ \varsigma'_1,\ldots,\varsigma'_n}} \int \mathrm{d}y_1\cdots\mathrm{d}y_n\mathrm{d}y'_1\cdots\mathrm{d}y'_n \Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varsigma_1,\ldots,\varsigma_n}(x_1,\ldots,x_n;y_1,\ldots,y_n) \\ &\qquad\qquad \left(\mathrm{e}^X\right)^{(n)}_{\varsigma_1,\ldots,\varsigma_n;\varsigma'_1,\ldots,\varsigma'_n}(y_1,\ldots,y_n;y'_1,\ldots,y'_n)\, \Delta^{(n)}_{\varsigma'_1,\ldots,\varsigma'_n;\sigma'_1,\ldots,\sigma'_n}(y'_1,\ldots,y'_n;x'_1,\ldots,x'_n) \end{aligned} \tag{2.7b}$$

where the exponential function notation $\left(\mathrm{e}^X\right)^{(n)}_{\varsigma_1,\ldots,\varsigma_n;\varsigma'_1,\ldots,\varsigma'_n}(y_1,\ldots,y_n;y'_1,\ldots,y'_n)$ is defined in Section A.2 (page 60) and variable X is chosen

$$X^{(n)} = \frac{1}{(n!)^2}\,\mathcal{G}^{(n)}_{\varsigma_1,\ldots,\varsigma_n;\varsigma'_1,\ldots,\varsigma'_n}\left(y_1,\ldots,y_n;y'_1,\ldots,y'_n\right). \tag{2.7c}$$

Each term of the function $\Delta^{(n)}$ defined in (A.1) determines the signs attached to a product in the sum. These functions $\Delta^{(n)}$, in general, contain the parity of the permutation of the primed variables with respect to the unprimed variables [2].

For the connection between the many-particle Green's functions and the physical properties of a given system, one may consult any book on many particle physics like Abrikosov, Gor'kov and Dzyaloshinskii [1], Fetter and Walecka [5]. Therefore, only a few general remarks seem to be in place here.

From the grand partition function, one can obtain the thermodynamical potential via

$$\Omega = -\beta^{-1}\ln\mathcal{Z} \tag{2.8}$$

and for thermodynamical potential Ω one obtains all the information on the thermodynamics of the system under consideration.

The one-particle Green's function is useful for the one-particle quantities such as the number density

$$\langle n(\mathbf{i})\rangle = \lim_{\substack{\mathbf{i}'\longrightarrow\mathbf{i}\\ \tau'\longrightarrow\tau+0}} \mathbf{Tr}\, G^{(1)}\left(\mathbf{i}\ \tau;\mathbf{i}'\ \tau'\right), \tag{2.9a}$$

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[1]Here, some first orders of Green's functions are written down

$$G^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}(x_1,\ldots,x_n;x'_1,\ldots,x'_n) = \begin{cases} \mathcal{G}^{(1)}_{\sigma_1;\sigma'_1}(x_1;x'_1) & \text{for } n=1 \\ \mathcal{G}^{(2)}_{\sigma_1,\sigma_2;\sigma'_1,\sigma'_2}(x_1,x_2;x'_1,x'_2) + & \\ \quad \mathcal{G}^{(1)}_{\sigma_1;\sigma'_1}(x_1;x'_1)\,\mathcal{G}^{(1)}_{\sigma_2;\sigma'_2}(x_2;x'_2) - & \\ \quad \mathcal{G}^{(1)}_{\sigma_1;\sigma'_2}(x_1;x'_2)\,\mathcal{G}^{(1)}_{\sigma_2;\sigma'_1}(x_2;x'_1) & \text{for } n=2 \\ \ldots & \ldots \end{cases} \tag{2.7a}$$

[2]Function $\Delta^{(n)}$ contains $n!$ terms and has the following explicit form

$$\Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varsigma_1,\ldots,\varsigma_n}(x_1,\ldots,x_n;y_1,\ldots,y_n) = \begin{cases} \delta_{\sigma_1\varsigma_1}\delta_{x_1y_1} & \text{for } n=1 \\ \delta_{\sigma_1\varsigma_1}\delta_{x_1y_1}\delta_{\sigma_2\varsigma_2}\delta_{x_2y_2} - \delta_{\sigma_1\varsigma_2}\delta_{x_1y_2}\delta_{\sigma_2\varsigma_1}\delta_{x_2y_1} & \text{for } n=2 \\ \ldots & \ldots \end{cases} \tag{2.7d}$$

the current density

$$\langle \boldsymbol{\mathcal{J}}(\mathbf{i})\rangle = \lim_{\substack{\mathbf{i}' \longrightarrow \mathbf{i} \\ \tau' \longrightarrow \tau+0}} \mathbf{Tr}\left[\boldsymbol{\mathcal{J}}(\mathbf{i})\, G^{(1)}\left(\mathbf{i}\ \tau; \mathbf{i}'\ \tau'\right)\right], \tag{2.9b}$$

or the spin density

$$\langle \boldsymbol{\mathcal{S}}(\mathbf{i})\rangle = \lim_{\substack{\mathbf{i}' \longrightarrow \mathbf{i} \\ \tau' \longrightarrow \tau+0}} \mathbf{Tr}\left[\boldsymbol{\sigma} G^{(1)}\left(\mathbf{i}\ \tau; \mathbf{i}'\ \tau'\right)\right]. \tag{2.9c}$$

The next class of problems arises if the given system is perturbed by a time-dependent external field

$$\mathcal{H}_U(t) = \sum_{\mathbf{i}} U(\mathbf{i}\ t)\, \mathcal{O}_1(\mathbf{i}) \tag{2.10a}$$

where the external field couples to the system through an operator denoted $\mathcal{O}_1$. In this case, the response function of a measurement of $\langle \mathcal{O}_2(\mathbf{i}_2\ t_2)\rangle$ to a perturbation coupled to $\mathcal{O}_1$ is specified by the response function

$$\begin{aligned} \mathcal{D}(\mathbf{i}_2\ t_2, \mathbf{i}_1\ t_1) &\equiv \frac{\delta \langle \mathcal{O}_2(\mathbf{i}_2\ t_2)\rangle}{\delta U(\mathbf{i}_1\ t_1)} \\ &= -i\theta(t_2 - t_1)\langle[\mathcal{O}_2(\mathbf{i}_2\ t_2), \mathcal{O}_1(\mathbf{i}_1\ t_1)]\rangle \end{aligned} \tag{2.10b}$$

where the operator $\mathcal{O}(\mathbf{i}\ t)$ in the Heisenberg representation is related to the operator $\mathcal{O}(\mathbf{i})$ by

$$\mathcal{O}(\mathbf{i}\ t) = \mathrm{e}^{iHt}\mathcal{O}(\mathbf{i})\,\mathrm{e}^{-iHt}. \tag{2.10c}$$

In the imaginary-time representation the response function is given by

$$\mathcal{D}(\mathbf{i}_1\ \tau_1, \mathbf{i}_1\ \tau_2) = -\langle \mathcal{T}_\tau(\mathcal{O}_1(\mathbf{i}_1\ \tau_1)\,\mathcal{O}_2(\mathbf{i}_2\ \tau_2))\rangle. \tag{2.10d}$$

The physical response of a system to an external potential is thus characterized by correlation functions of the form $\langle \mathcal{O}_2(\mathbf{i}_2\ t_2)\,\mathcal{O}_1(\mathbf{i}_1\ t_1)\rangle$. This result that a transport coefficient characterizing the dissipation in a system is specified by a matrix element of the thermodynamic or ground state fluctuations of an operator is often called the fluctuation-dissipation theorem. For example, consider measuring the magnetization of a spin system in presence of a time a spatially varying magnetic field. Since the magnetic field couples to the spin through scalar product $\boldsymbol{\mathcal{S}}(\mathbf{r}).\mathbf{H}(\mathbf{r}\ t)$, the operator $\mathcal{O}_1$ and $\mathcal{O}_2$ are spin operators $\boldsymbol{\mathcal{S}}$ and the response function is given by in terms of the spin-spin correlation function $\langle \boldsymbol{\mathcal{S}}(\mathbf{r}_1, t_1)\,\boldsymbol{\mathcal{S}}(\mathbf{r}_2, t_2)\rangle$. Fourier transforming to momentum and frequency then directly specifies the dynamic magnetic susceptibility $\chi(\mathbf{k}, \omega)$. Similarly, an electromagnetic field couples to a system of charged particle through the vector potential $\boldsymbol{\mathcal{J}}(\mathbf{r}).\mathbf{A}(\mathbf{r}\ t)$ and in a gauge in which $\Phi = 0$, $\mathbf{E} = -\frac{\partial}{\partial t}\mathbf{A}$. Thus, the response of the current to a variation in the electric field, that is the electrical conductivity tensor, is given by the current-current correlation function $\langle \boldsymbol{\mathcal{J}}(\mathbf{r}_1, t_1)\,\boldsymbol{\mathcal{J}}(\mathbf{r}_2, t_2)\rangle$. The current-current and higher correlation functions are especially useful in the investigation of many effects in condensed matter physics such as photoemission, Hall effect where the electrical resistivity tensor is directly determined by the inversion of electrical conductivity tensor, ...

These examples reflect the role of many-particle Green's functions in condensed matter physics. They on one hand are the expectation values of time-ordered products of operators that are the most convenient to calculate in perturbation theory and on the other hand can be related by suitable analytic continuation to quantities arising from experimental observables.

SECTION 2.2

Grand partition function and Generating functional

The techniques presented in the following, were first used in field theory by Schwinger and coworkers. In the imaginary time formalism they are called Martin-Schwinger methods. The aim of this Section and of Chapter 3 is to show that they allow for a very general formulation.

The grand partition function of a many-particle system given by Hamiltonian $\mathcal{H}$ is defined by

$$\mathcal{Z} = \mathrm{Tr}\ \exp\left\{-\beta\left(\mathcal{H} - \mu\mathcal{N}\right)\right\}, \tag{2.11}$$

which can be represented via a functional integral with the imaginary-time [17]

$$\mathcal{Z} = \int \left[\mathcal{D}\varphi\right]\left[\mathcal{D}\bar{\varphi}\right]\ \exp\left\{-\int_0^\beta \mathrm{d}\tau\ \mathcal{L}\left[\varphi\left(\tau\right), \bar{\varphi}\left(\tau\right)\right]\right\} \tag{2.12}$$

where

$$\mathcal{L}\left[\varphi\left(\tau\right), \bar{\varphi}\left(\tau\right)\right] = \sum_{\mathbf{i},\sigma} \bar{\varphi}_{\mathbf{i}\sigma}\left(\tau\right)\left(\partial_\tau - \mu_\sigma\right)\varphi_{\mathbf{i}\sigma}\left(\tau\right) + \mathcal{H}\left[\varphi\left(\tau\right), \bar{\varphi}\left(\tau\right)\right] \tag{2.13}$$

and φ and $\bar{\varphi}$ are field variables of particles, which can be complex or Grassmannian corresponding to boson or fermion particles of the system, resp., and the imaginary-time dependence of an operator is determined by

$$\mathcal{O}\left(\tau\right) = \mathrm{e}^{\tau\left(\mathcal{H}-\mu\mathcal{N}\right)}\mathcal{O}\ \mathrm{e}^{-\tau\left(\mathcal{H}-\mu\mathcal{N}\right)}. \tag{2.14}$$

In functional integral formalism the expectation value of the operator $\mathcal{O}\left(\tau\right)$ is read as

$$\left\langle\mathcal{O}\right\rangle = \frac{1}{\mathcal{Z}}\int \left[\mathcal{D}\varphi\right]\left[\mathcal{D}\bar{\varphi}\right]\ \mathcal{O}\left(\tau\right)\ \exp\left\{-\int_0^\beta \mathrm{d}\tau\ \mathcal{L}\left[\varphi\left(\tau\right), \bar{\varphi}\left(\tau\right)\right]\right\} \tag{2.15}$$

where the time ordering symbol is implicitly included in the functional integral.

The operator $\mathcal{O}\left(\tau\right)$ can be any expression containing field-operators of the system considered. For example, the n-particle Green's function (2.3) has the following form

$$\begin{aligned} &G^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n\right) \\ &\quad= \left(-1\right)^n\left\langle\mathcal{T}_\tau\left(\varphi_{\mathbf{i}_1,\sigma_1}\left(\tau_1\right)\ldots\varphi_{\mathbf{i}_n,\sigma_n}\left(\tau_n\right)\bar{\varphi}_{\mathbf{i}'_n,\sigma'_n}\left(\tau'_n\right)\ldots\bar{\varphi}_{\mathbf{i}'_1,\sigma_1}\left(\tau'_1\right)\right)\right\rangle \\ &\quad\equiv \left(-1\right)^n\ \frac{1}{\mathcal{Z}}\int\left[\mathcal{D}\varphi\right]\left[\mathcal{D}\bar{\varphi}\right]\ \left(\varphi_{\mathbf{i}_1,\sigma_1}\left(\tau_1\right)\ldots\varphi_{\mathbf{i}_n,\sigma_n}\left(\tau_n\right)\bar{\varphi}_{\mathbf{i}'_n,\sigma'_n}\left(\tau'_n\right)\ldots\bar{\varphi}_{\mathbf{i}'_1,\sigma_1}\left(\tau'_1\right)\right) \\ &\qquad\qquad \exp\left\{-\int_0^\beta \mathrm{d}\tau\ \mathcal{L}\left[\varphi\left(\tau\right), \bar{\varphi}\left(\tau\right)\right]\right\} \end{aligned} \tag{2.16}$$

where the symbols $\varphi_{\mathbf{i},\sigma}\left(\tau\right)$ and $\bar{\varphi}_{\mathbf{i},\sigma}\left(\tau\right)$ stand for the original operators of the system considered, for instance $f_{\mathbf{i},\sigma}\left(\tau\right)$ and $f^\dagger_{\mathbf{i},\sigma}\left(\tau\right)$.

The generating functional of the system considered is defined as the expectation value [17]

$$\mathcal{Z}\left[\xi,\bar{\xi}\right] = \left\langle\mathcal{T}_\tau \exp\left\{-\int \mathrm{d}x\ \left[\sum_\sigma\left(\bar{\xi}_\sigma\left(x\right)\varphi_\sigma\left(x\right) + \bar{\varphi}_\sigma\left(x\right)\xi_\sigma\left(x\right)\right)\right]\right\}\right\rangle\ \mathcal{Z}\left[0,0\right] \tag{2.17}$$

with the appearance of external field-operator variables ξ, $\bar{\xi}$, which can be written in functional integral formalism as

$$\mathcal{Z}\left[\xi,\bar{\xi}\right] = \int \left[\mathcal{D}\varphi\right]\left[\mathcal{D}\bar{\varphi}\right]\, \exp\left\{-\int\limits_0^\beta \mathrm{d}\tau\, \left[\sum_{\mathbf{i}\sigma}\left(\bar{\xi}_{\mathbf{i}\sigma}\left(\tau\right)\varphi_{\mathbf{i}\sigma}\left(\tau\right) + \bar{\varphi}_{\mathbf{i}\sigma}\left(\tau\right)\xi_{\mathbf{i}\sigma}\left(\tau\right)\right)\right]\right\} \exp\left\{-\int\limits_0^\beta \mathrm{d}\tau\, \mathcal{L}\left[\varphi\left(\tau\right),\bar{\varphi}\left(\tau\right)\right]\right\}. \tag{2.18}$$

All thermodynamic quantities of a physical system can be obtained by performing functional derivatives on the generating functional (2.18) with respect to external field-operator variables ξ, $\bar{\xi}$. For example, the n-particle Green's function can be defined by the following operation

$$G^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(x_1,\ldots,x_n;x'_1,\ldots,x'_n\right) = (-1)^n \frac{1}{\mathcal{Z}\left[\xi,\bar{\xi}\right]}\frac{\delta}{\delta\xi_{\sigma'_1}\left(x'_1\right)}\cdots\frac{\delta}{\delta\xi_{\sigma'_n}\left(x'_n\right)}\frac{\delta}{\delta\bar{\xi}_{\sigma_n}\left(x_n\right)}\cdots\frac{\delta}{\delta\bar{\xi}_{\sigma_1}\left(x_1\right)}\,\mathcal{Z}\left[\xi,\bar{\xi}\right]\Bigg|_{\xi=\bar{\xi}=0} \tag{2.19a}$$

or the n-particle cumulant by

$$\mathcal{G}^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(x_1,\ldots,x_n;x'_1,\ldots,x'_n\right) = (-1)^n \frac{\delta}{\delta\xi_{\sigma'_1}\left(x'_1\right)}\cdots\frac{\delta}{\delta\xi_{\sigma'_n}\left(x'_n\right)}\frac{\delta}{\delta\bar{\xi}_{\sigma_n}\left(x_n\right)}\cdots\frac{\delta}{\delta\bar{\xi}_{\sigma_1}\left(x_1\right)}\ln\,\mathcal{Z}\left[\xi,\bar{\xi}\right]\Bigg|_{\xi=\bar{\xi}=0}. \tag{2.19b}$$

That is not difficult to see that in the expressions (2.19a) and (2.19b) the expectation values of all terms with an odd number of φ and $\bar{\varphi}$ operators will vanish when the external field-operator variables ξ, $\bar{\xi}$ are going to zero and only the combinations having equal numbers of destruction and creation field-operators as in (2.16) survive.

CHAPTER 3

The Strong-Coupling Expansion

This Chapter presents the main results of the present thesis. In the functional integral formalism the grand partition functions of the Hubbard model and the periodic Anderson model are considered. By integration over the Grassmann variables of the conduction electrons in the grand partition function of the periodic Anderson model one is able to write the grand partition function for the Hubbard model and the periodic Anderson model in the same form involving some parameters characterizing the difference of the model Hamiltonians. That enables one to develop a unique mathematical tool to express all thermodynamic quantities of both model Hamiltonians in the same mathematical formulation.

Next, some less well-known theoretical approaches which are used to investigate the Hubbard model are shortly discussed. The perturbation expansion around the atomic limit of the Hubbard model where the static approximation becomes exact up to one-particle function is chosen as a basics to apply the functional integral formalism. This perturbation expansion is called strong coupling expansion theory.

Later, the Grassmann Hubbard-Stratonovich transformation is introduced to convert the generic grand partition function for both model Hamiltonians to a new auxiliary interacting fermion system which contains infinite interaction terms.

In Section 3.4, the one-particle Green's function and the self-energy of the auxiliary fields are represented as a functional of renormalized local many-particle correlation functions of localized electrons and many-particle cumulants of the auxiliary fields. Moreover, the relationships between many-body cumulants of the localized electrons and those of the auxiliary fields are also explicitly established.

Also, the "self-energy" of renormalized local many-particle correlation functions of the localized electrons are explicitly shown.

Bethe-Salpeter-like equations for many-particle cumulants of the auxiliary fields are found. Those allow for a possibility to construct a self-consistent approximation theory with respect to renormalized many-particle functions where thermodynamic relations and sum rules are fulfilled.

Last, the thermodynamical potential of the system considered is calculated. It can be expressed as a sum of site-dependent functionals of fully renormalized many-particle quantities.

We start with the grand partition functions of the Hubbard model (2.1) and the periodic Anderson model (PAM) (2.2). From the formal representation of functional integral formalism (2.12) and (2.13) one can easily write out the grand partition function for the Hubbard model as

$$\begin{aligned}\mathcal{Z}_{\text{Hubbard}} &= \text{Tr}\ \exp\{-\beta(\mathcal{H}_{\text{Hubbard}}-\mu\mathcal{N})\}\\ &\equiv \int [\mathcal{D}\zeta][\mathcal{D}\bar{\zeta}]\ \exp\left\{-\int_0^\beta \mathrm{d}\tau\ \mathcal{L}_{\text{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]\right\}\end{aligned} \tag{3.1}$$

and the grand partition function for the periodic Anderson model

$$\begin{aligned}\mathcal{Z}_{\text{PAM}} &= \text{Tr}\ \exp\{-\beta(\mathcal{H}_{\text{PAM}}-\mu\mathcal{N})\}\\ &\equiv \int [\mathcal{D}\zeta][\mathcal{D}\bar{\zeta}][\mathcal{D}\eta][\mathcal{D}\bar{\eta}]\ \exp\left\{-\int_0^\beta \mathrm{d}\tau\ \mathcal{L}_{\text{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau);\eta(\tau),\bar{\eta}(\tau)\right]\right\}\end{aligned} \tag{3.2}$$

where $\mathcal{L}_{\text{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]$ and $\mathcal{L}_{\text{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau);\eta(\tau),\bar{\eta}(\tau)\right]$ are the Lagrangians for the Hubbard model and for the PAM, resp.

$$\mathcal{L}_{\text{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right] = \sum_{\mathbf{i},\sigma}\bar{\zeta}_{\mathbf{i}\sigma}(\tau)(\partial_\tau-\mu_\sigma)\zeta_{\mathbf{i}\sigma}(\tau)+\mathcal{H}_{\text{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right] \tag{3.3}$$

$$\begin{aligned}\mathcal{L}_{\text{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau);\eta(\tau),\bar{\eta}(\tau)\right] = &\sum_{\mathbf{i},\sigma}\bar{\zeta}_{\mathbf{i}\sigma}(\tau)(\partial_\tau-\mu_\sigma)\zeta_{\mathbf{i}\sigma}(\tau)+\sum_{\mathbf{i},\sigma}\bar{\eta}_{\mathbf{i}\sigma}(\tau)(\partial_\tau-\mu_\sigma)\eta_{\mathbf{i}\sigma}(\tau)\\ &+\mathcal{H}_{\text{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau);\eta(\tau),\bar{\eta}(\tau)\right]\end{aligned} \tag{3.4}$$

and the Grassmann variables $\zeta_{\mathbf{i}\sigma}$, $\bar{\zeta}_{\mathbf{i}\sigma}$ stand for fermionic operators of localized electrons $f_{\mathbf{i}\sigma}$, $f^\dagger_{\mathbf{i}\sigma}$ and the Grassmann variables $\eta_{\mathbf{i}\sigma}$, $\bar{\eta}_{\mathbf{i}\sigma}$ for fermionic operators of conduction electrons $c_{\mathbf{i}\sigma}$, $c^\dagger_{\mathbf{i}\sigma}$, resp..
For later use we separate the expressions (3.3) and (3.4) into local parts which contain only field-operators at a certain site $\mathbf{i}$ and non-local (inter-site) parts which describe non-local processes such as hopping and hybridization in the systems considered. Then for the Hubbard model the Lagrangian is given by

$$\mathcal{L}_{\text{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right] = \mathcal{L}^0_{\text{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]+\mathcal{L}^1_{\text{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right], \tag{3.5}$$

where the local part $\mathcal{L}^0_{\text{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]$ corresponds to the atomic limit of the system considered, that is

$$\begin{aligned}\mathcal{L}^0_{\text{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right] &= \sum_{\mathbf{i}}\mathcal{L}^0_{\text{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]_{\mathbf{i}}\\ \mathcal{L}^0_{\text{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]_{\mathbf{i}} &= \sum_{\sigma}\bar{\zeta}_{\mathbf{i}\sigma}(\tau)(\partial_\tau-\mu_\sigma)\zeta_{\mathbf{i}\sigma}(\tau)+U\bar{\zeta}_{\mathbf{i}\uparrow}(\tau)\zeta_{\mathbf{i}\uparrow}(\tau)\bar{\zeta}_{\mathbf{i}\downarrow}(\tau)\zeta_{\mathbf{i}\downarrow}(\tau)\end{aligned} \tag{3.6a}$$

and the non-local part $\mathcal{L}^1_{\text{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]$ is hopping term

$$\mathcal{L}^1_{\text{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right] = \sum_{\mathbf{ij},\sigma}\varepsilon^f_{\mathbf{ij}}\ \bar{\zeta}_{\mathbf{i}\sigma}(\tau)\zeta_{\mathbf{j}\sigma}(\tau)\,. \tag{3.6b}$$

For the PAM, the Lagrangian has the following parts

$$\mathcal{L}_{\text{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau);\eta(\tau),\bar{\eta}(\tau)\right] = \mathcal{L}^0_{\text{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]+\mathcal{L}^1_{\text{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau);\eta(\tau),\bar{\eta}(\tau)\right], \tag{3.7}$$

where the local part $\mathcal{L}^0_{\mathrm{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]$ corresponds to the atomic limit of the localized electrons, depending only on the Grassmann variables $\bar{\zeta}$ and ζ, that is

$$\begin{aligned}\mathcal{L}^0_{\mathrm{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right] &= \sum_{\mathbf{i},\sigma}\mathcal{L}^0_{\mathrm{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]_{\mathbf{i}}\\ \mathcal{L}^0_{\mathrm{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]_{\mathbf{i}} &= \sum_{\sigma}\bar{\zeta}_{\mathbf{i}\sigma}(\tau)\left(\partial_\tau+\varepsilon^f-\mu_\sigma\right)\zeta_{\mathbf{i}\sigma}(\tau)+U\bar{\zeta}_{\mathbf{i}\uparrow}(\tau)\,\zeta_{\mathbf{i}\uparrow}(\tau)\,\bar{\zeta}_{\mathbf{i}\downarrow}(\tau)\,\zeta_{\mathbf{i}\downarrow}(\tau)\end{aligned} \tag{3.8a}$$

and the non-local part $\mathcal{L}^1_{\mathrm{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau);\eta(\tau),\bar{\eta}(\tau)\right]$ contains the hopping term of conduction electrons and the hybridization term between conduction electrons and localized electrons

$$\begin{aligned}\mathcal{L}^1_{\mathrm{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau);\eta(\tau),\bar{\eta}(\tau)\right] &= \sum_{\mathbf{ij},\sigma}\bar{\eta}_{\mathbf{i}\sigma}(\tau)\left(\left(\partial_\tau-\mu_\sigma\right)\delta_{\mathbf{ij}}+\varepsilon^c_{\mathbf{ij}}\right)\eta_{\mathbf{i}\sigma}(\tau)\\ &\quad+\sum_{\mathbf{ij},\sigma}\left(V_{\mathbf{ij}}\,\bar{\zeta}_{\mathbf{i}\sigma}(\tau)\,\eta_{\mathbf{j}\sigma}(\tau)+V^*_{\mathbf{ij}}\,\bar{\eta}_{\mathbf{j}\sigma}(\tau)\,\zeta_{\mathbf{i}\sigma}(\tau)\right).\end{aligned} \tag{3.8b}$$

Note that in the expressions (3.6a) and (3.8a) the local parts $\mathcal{L}^0_{\mathrm{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]$ and $\mathcal{L}^0_{\mathrm{PAM}}[\zeta(\tau),\bar{\zeta}(\tau)]$ contain the Coulomb interaction term i.e. they are non-quadratic in the Grassmann fields of localized electrons.

Comparing the form of the local parts in (3.6a) and in (3.8a), one finds that they are identical if ε^f in (3.8a) is zero, so it is more convenient to denote them by a unique form as

$$\mathcal{L}^0_{\mathbf{i}}\left[\zeta(\tau),\bar{\zeta}(\tau);\varepsilon\right] = \sum_{\sigma}\bar{\zeta}_{\mathbf{i}\sigma}(\tau)\left(\partial_\tau+\varepsilon-\mu_\sigma\right)\zeta_{\mathbf{i}\sigma}(\tau)+U\bar{\zeta}_{\mathbf{i}\uparrow}(\tau)\,\zeta_{\mathbf{i}\uparrow}(\tau)\,\bar{\zeta}_{\mathbf{i}\downarrow}(\tau)\,\zeta_{\mathbf{i}\downarrow}(\tau)\,. \tag{3.9}$$

It would be useful to rewrite $\mathcal{L}^0_{\mathrm{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]_{\mathbf{i}}$ and $\mathcal{L}^0_{\mathrm{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]_{\mathbf{i}}$ in the new short notation of (3.9)

$$\mathcal{L}^0_{\mathrm{Hubbard}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]_{\mathbf{i}} = \mathcal{L}^0_{\mathbf{i}}\left[\zeta(\tau),\bar{\zeta}(\tau);\varepsilon=0\right] \tag{3.10a}$$

and

$$\mathcal{L}^0_{\mathrm{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]_{\mathbf{i}} = \mathcal{L}^0_{\mathbf{i}}\left[\zeta(\tau),\bar{\zeta}(\tau);\varepsilon=\varepsilon^f\right]. \tag{3.10b}$$

SECTION 3.1

Formal Equivalence between the Hubbard Model and the periodic Anderson Model

Now one can put the expressions (3.10b), (3.8b) and (3.7) into the given form of the grand partition function for the PAM (3.2)

$$\begin{aligned}\mathcal{Z}_{\mathrm{PAM}} = \int\left[\mathcal{D}\zeta\right]\left[\mathcal{D}\bar{\zeta}\right]\left[\mathcal{D}\eta\right]\left[\mathcal{D}\bar{\eta}\right]\exp&\left\{-\int_0^\beta \mathrm{d}\tau\;\mathcal{L}^1_{\mathrm{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau);\eta(\tau),\bar{\eta}(\tau)\right]\right\}\\ \exp&\left\{-\int_0^\beta\mathrm{d}\tau\;\sum_{\mathbf{i}}\mathcal{L}^0_{\mathbf{i}}\left[\zeta(\tau),\bar{\zeta}(\tau);\varepsilon=\varepsilon^f\right]\right\}.\end{aligned} \tag{3.11}$$

The integration over the Grassmann variables $\eta_{\mathbf{i}\sigma}$, $\bar{\eta}_{\mathbf{i}\sigma}$ of the conduction electrons in (3.11) is easily performed due to the quadratic form of the non-local part $\mathcal{L}^1_{\mathrm{PAM}}\left[\zeta(\tau),\bar{\zeta}(\tau);\eta(\tau),\bar{\eta}(\tau)\right]$ (3.8b) with respect to the field-operator variables, then the grand partition function $\mathcal{Z}_{\mathrm{PAM}}$ is rewritten as the grand partition function of an effective system which has only one kind of electrons $\zeta_{\mathbf{i}\sigma}$ and $\bar{\zeta}_{\mathbf{i}\sigma}$

$$\mathcal{Z}_{\mathrm{PAM}} = \mathcal{Z}_0^c \int [\mathcal{D}\zeta]\,[\mathcal{D}\bar{\zeta}]\ \exp\left\{ - \int_0^\beta \mathrm{d}\tau\ \mathcal{L}^{\mathrm{eff}}_{\mathrm{PAM}}\left[\zeta(\tau), \bar{\zeta}(\tau)\right] \right\} \tag{3.12}$$

where $\mathcal{Z}_0^c$ is the partition function of free conduction electrons, and the effective Lagrangian $\mathcal{L}^{\mathrm{eff}}_{\mathrm{PAM}}\big[\zeta(\tau), \bar{\zeta}(\tau)\big]$ is

$$\begin{aligned} \mathcal{L}^{\mathrm{eff}}_{\mathrm{PAM}}\left[\zeta(\tau), \bar{\zeta}(\tau)\right] = \sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'} \int_0^\beta \mathrm{d}\tau'\ \bar{\zeta}_{\mathbf{i}\sigma}(\tau)\, \Omega_{\sigma;\sigma'}\left(\mathbf{i}\ \tau; \mathbf{i}'\ \tau'\right) \zeta_{\mathbf{i}'\sigma'}\left(\tau'\right) \\ + \sum_{\mathbf{i}} \mathcal{L}^0_{\mathbf{i}}\left[\zeta(\tau), \bar{\zeta}(\tau); \varepsilon = \varepsilon^f\right] \end{aligned} \tag{3.13}$$

with

$$\Omega_{\sigma;\sigma'}\left(\mathbf{i}\ \tau; \mathbf{i}'\ \tau'\right) = \sum_{\mathbf{i}_1\mathbf{i}'_1,\sigma_1\sigma'_1} V_{\mathbf{i}\mathbf{i}'_1} G^{(1),c}_{\sigma\sigma'}\left(\mathbf{i}'_1\ \tau; \mathbf{i}_1\ \tau'\right) V_{\mathbf{i}_1\mathbf{i}'}, \tag{3.14}$$

$G^{(1),c}_{\sigma\sigma'}\left(\mathbf{i}'_1\ \tau; \mathbf{i}_1\ \tau'\right)$ is the unperturbed Green's function of conduction electrons.
It is obvious that the effective Lagrangian $\mathcal{L}^{\mathrm{eff}}_{\mathrm{PAM}}\left[\zeta(\tau), \bar{\zeta}(\tau)\right]$ in (3.13) and the Lagrangian for the Hubbard model $\mathcal{L}_{\mathrm{Hubbard}}\left[\zeta(\tau), \bar{\zeta}(\tau)\right]$ in (3.5) have the same form by replacement of non-local parts in both equations

$$\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}\mathbf{j},\sigma} \varepsilon^f_{\mathbf{i}\mathbf{j}}\ \bar{\zeta}_{\mathbf{i}\sigma}(\tau)\, \zeta_{\mathbf{j}\sigma}(\tau) \longleftrightarrow \int_0^\beta \mathrm{d}\tau\ \mathrm{d}\tau' \sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'} \bar{\zeta}_{\mathbf{i}\sigma}(\tau)\, \Omega_{\sigma;\sigma'}\left(\mathbf{i}\ \tau; \mathbf{i}'\ \tau'\right) \zeta_{\mathbf{i}'\sigma'}\left(\tau'\right). \tag{3.15}$$

As a direct consequence of (3.15) one can rewrite both grand partition functions for the Hubbard model and the periodic Anderson model in the unique form as

$$\begin{aligned} \mathcal{Z} &= \mathcal{Z}_0 \int [\mathcal{D}\zeta]\,[\mathcal{D}\bar{\zeta}]\ \exp\left\{ - \int_0^\beta \mathrm{d}\tau\ \mathcal{L}\left[\zeta(\tau), \bar{\zeta}(\tau)\right] \right\} \\ &\equiv \mathcal{Z}_0 \int [\mathcal{D}\zeta]\,[\mathcal{D}\bar{\zeta}]\ \exp\left\{ - \int_0^\beta \mathrm{d}\tau \Big(\mathcal{L}^1\left[\zeta(\tau), \bar{\zeta}(\tau)\right] + \mathcal{L}^0\left[\zeta(\tau), \bar{\zeta}(\tau)\right] \Big) \right\} \end{aligned} \tag{3.16}$$

where coefficient $\mathcal{Z}_0$

$$\mathcal{Z}_0 = \begin{cases} 1 & \text{for the Hubbard model} \\ \mathcal{Z}_0^c & \text{for the PAM} \end{cases} \tag{3.17a}$$

the local part $\mathcal{L}^0\left[\zeta(\tau), \bar{\zeta}(\tau)\right]$ of $\mathcal{L}\left[\zeta(\tau), \bar{\zeta}(\tau)\right]$

$$\mathcal{L}^0\left[\zeta(\tau), \bar{\zeta}(\tau)\right] = \begin{cases} \sum_{\mathbf{i}} \mathcal{L}^0_{\mathbf{i}}\left[\zeta(\tau), \bar{\zeta}(\tau); \varepsilon = 0\right] & \text{for the Hubbard model} \\ \sum_{\mathbf{i}} \mathcal{L}^0_{\mathbf{i}}\left[\zeta(\tau), \bar{\zeta}(\tau); \varepsilon = \varepsilon^f\right] & \text{for the PAM} \end{cases} \tag{3.17b}$$

and the non-local part $\mathcal{L}^1\left[\zeta(\tau),\bar{\zeta}(\tau)\right]$

$$\mathcal{L}^1\left[\zeta(\tau),\bar{\zeta}(\tau)\right]=\int_0^\beta \mathrm{d}\tau' \sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'} \bar{\zeta}_{\mathbf{i}\sigma}(\tau)\,\Omega^{(0)}_{\sigma;\sigma'}\left(\mathbf{i}\ \tau;\mathbf{i}'\ \tau'\right)\zeta_{\mathbf{i}'\sigma'}\left(\tau'\right) \tag{3.17c}$$

with

$$\Omega^{(0)}_{\sigma;\sigma'}\left(\mathbf{i}\ \tau;\mathbf{i}'\ \tau'\right)=\begin{cases}\delta_{\sigma,\sigma'}\,\delta\left(\tau-\tau'\right)\varepsilon^{c}_{\mathbf{i}\mathbf{i}'} & \text{for the Hubbard model}\\ \sum\limits_{\mathbf{i}_1\mathbf{i}'_1} V_{\mathbf{i}\mathbf{i}'_1}G^{(1),c}_{\sigma\sigma'}\left(\mathbf{i}'_1\ \tau;\mathbf{i}_1\ \tau'\right)V_{\mathbf{i}_1\mathbf{i}'} & \text{for the PAM}\end{cases} \tag{3.17d}$$

The formal equivalence between the Hubbard model and the periodic Anderson model in functional integral formalism allows one to apply unique mathematical approaches to achieve relevant physical quantities of both models in a mathematically equivalent formulation. However, the difference of the non-local parts in thus models (imaginary-time independence for the Hubbard model and imaginary-time dependence for the PAM) causes the differently physical behaviors of each model in certain conditions. Apparently, because of (3.17d), the dynamics of the PAM is richer than that of the Hubbard model.

In further representation the generic grand partition function (3.16) will take into place for that of the Hubbard model and of the periodic Anderson model.

SECTION 3.2

Some Available Field-Theoretical Approaches

For the generic grand partition function (3.16) one may use many different field-theoretical approaches to treat the functional integral. We will list here some of those approaches, that are playing a dominant role in the investigation of strongly correlated electron systems.

Treating The Coulomb Interaction as a Perturbation where the quadratic form of the localized electrons is treated as a unperturbed Hamiltonian.

In order to do that one writes $\mathcal{L}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]$ again explicitly in the form of one-body and Coulomb interaction parts

$$\begin{aligned}\mathcal{L}\left[\zeta(\tau),\bar{\zeta}(\tau)\right]=&\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\int_0^\beta \mathrm{d}\tau'\ \bar{\zeta}_{\mathbf{i}\sigma}(\tau)\Big(\left(\partial_{\tau'}+\varepsilon-\mu_\sigma\right)\delta_{\sigma,\sigma'}\delta_{\mathbf{i}\mathbf{i}'}+\Omega^{(0)}_{\sigma;\sigma'}\left(\mathbf{i}\ \tau;\mathbf{i}'\ \tau'\right)\Big)\zeta_{\mathbf{i}'\sigma'}\left(\tau'\right)\\&+U\sum_{\mathbf{i}}\bar{\zeta}_{\mathbf{i}\uparrow}(\tau)\,\zeta_{\mathbf{i}\uparrow}(\tau)\,\bar{\zeta}_{\mathbf{i}\downarrow}(\tau)\,\zeta_{\mathbf{i}\downarrow}(\tau)\,,\end{aligned} \tag{3.18}$$

To decompose the Coulomb interaction term in (3.18), one can start from a bosonic auxiliary functional integral

$$\mathcal{W}_0=\int\left[\mathcal{D}\varphi\right]\exp\left\{-\int_0^\beta \mathrm{d}\tau\ \varphi_\uparrow(\tau)\,\varphi_\downarrow(\tau)\right\} \tag{3.19a}$$

then performing the shift transformation for the bosonic auxiliary field $\varphi_\sigma(\tau)$ as

$$\varphi_\sigma(\tau)\longrightarrow\varphi_\sigma(\tau)+\bar{\sigma}\sqrt{U}\bar{\zeta}_{\bar{\sigma}}(\tau)\,\zeta_{\bar{\sigma}}(\tau)\,, \tag{3.19b}$$

with $\sigma = 1$ for spin-up $\uparrow$, $\sigma = -1$ for spin-down $\downarrow$ and $\bar{\sigma} = -\sigma$. Under the shift transformation (3.19b) the auxiliary functional integral is invariant and one can get the following decomposition for the Coulomb interaction in (3.18)

$$\exp\left\{-\int_0^\beta \mathrm{d}\tau\, U \sum_{\mathbf{i}} \bar{\zeta}_{\mathbf{i}\uparrow}(\tau)\,\zeta_{\mathbf{i}\uparrow}(\tau)\,\bar{\zeta}_{\mathbf{i}\downarrow}(\tau)\,\zeta_{\mathbf{i}\downarrow}(\tau)\right\}$$
$$= \frac{1}{\mathcal{W}}\int [\mathcal{D}\varphi]\exp\left\{-\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}\sigma} \sigma\sqrt{U}\varphi_{\mathbf{i},\sigma}(\tau)\,\bar{\zeta}_{\mathbf{i}\sigma}(\tau)\,\zeta_{\mathbf{i}\sigma}(\tau)\right\}\exp\left\{-\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}} \varphi_{\mathbf{i},\uparrow}(\tau)\,\varphi_{\mathbf{i},\downarrow}(\tau)\right\} \tag{3.19c}$$

where

$$\mathcal{W} = \int [\mathcal{D}\varphi]\exp\left\{-\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}} \varphi_{\mathbf{i},\uparrow}(\tau)\,\varphi_{\mathbf{i},\downarrow}(\tau)\right\}. \tag{3.19d}$$

The identity (3.19c) is well-known under the name **Hubbard-Stratonovich transformation**. Physically speaking, the Hubbard-Stratonovich transformation does excellent work converting a two-body interaction, in this case the Coulomb interaction, into an one-body interaction with a time dependent bosonic auxiliary field, which is a boson-fermion interaction.

Applying the Hubbard-Stratonovich transformation (3.19c) to the grand partition function (3.16) leads to a quadratic form of field-operator Grassmann variables $\zeta_{\mathbf{i}\sigma}$ and $\bar{\zeta}_{\mathbf{i}\sigma}$ for the localized electrons, which can be simply and exactly integrated over. This decomposition is called longitudinal because the system is expressed in the terms of response to longitudinal auxiliary fields. The result of this integration is a new functional integral with respect to bosonic auxiliary field variables $\varphi_{\mathbf{i}\sigma}$, corresponding to density and charge fluctuations of the system considered.

Not only density and charge fluctuations are considered by the Hubbard-Stratonovich transformation, but the spin fluctuations can be also included by another decomposition using the Hubbard-Stratonovich transformation, which is transverse decomposition - response to transverse auxiliary fields. In the case, when both decompositions are under consideration to avoid spurious diagrams related to forbidden equal-spin electron interactions violating Pauli's principle, one has to choose right coefficients for corresponding fluctuations.

Taking into account terms up to second order in the bosonic auxiliary fields - the field-quadratic approximation, one can obtain part of the **Hartree-Fock** diagrams (those in which the interaction lines can be linked by just one line) and all bare ring diagrams of the well-known **Random Phase Approximation** (RPA) by using longitudinal decomposition and the bare ladder diagrams of the RPA by using transverse decomposition. However, exploiting higher-order terms, one can understand the two different ways of expressing the same thermodynamical potential Ω. Using the longitudinal decomposition, the ladder diagrams, as well as other types of diagrams, are spread out in the diagrammatic perturbation series of Coulomb interaction U, because the thermodynamical potential Ω is built up of response functions to the longitudinal auxiliary fields [1]. On the other hand, using the transverse decomposition, the **Hartree-Fock** and ring diagrams are spread out in the perturbation series of U because the system are now built up of response functions to transverse auxiliary fields [2]. Therefore, both series are diagrammatically identical.

There are several works on this approach. In this approach one has to face some difficulties for the case of strong coupling limit, i.e. when the Coulomb interaction is very large in comparison with the hopping parameter, $U \longrightarrow \infty$. An attempt to overcome the difficulties in strong coupling limit within

[1] The third order terms of longitudinal auxiliary fields generate the ladder diagrams.

[2] The fourth order terms of transverse auxiliary fields generate the diagrams of **Hartree-Fock** series and of the ring series

longitudinal decomposition was made by Amit and Keiter [2] (1973), who developed an extension of RPA for the Single Impurity Anderson model.

The Strong-Coupling Expansion is another powerful approach to the system considered. This formalism is based on the fact that one treats the local part (3.17b) of $\mathcal{L}\left[\zeta(\tau), \bar{\zeta}(\tau)\right]$ as unperturbed system and the non-local part (3.17c) which is proportional to hopping matrix elements $\varepsilon^{f}_{\mathbf{ii}'}$ for the Hubbard model or to hybridization matrix elements $|V|^2$ for the PAM, as a perturbation to the unperturbed system. This idea goes back to the framework [6] created by Grewe and Keiter in (1981), who found a generalization of Keiter and Kimball approach [7] to the single impurity Anderson model (1970).

The basic ideas of that approach are the following

- If the unperturbed Hamiltonian contains non-quadratic terms, in this case for the localized electrons, clearly Wick's theorem does not hold for the localized electrons. It holds, however, for the band electrons.
- For the localized electrons one exploits the identity $n_{\mathbf{i}}^2 = n_{\mathbf{i}}$ to simplify the number of contributions from n^2 to n in n-th order.

The advantage of this approach is that the Coulomb interaction U will directly enter to all many-particle Green's functions of the unperturbed system. It does not require an extra treatment for the strong coupling limit.

For the Hubbard model, due to the absence of Wick's theorem in the case of a non-quadratic unperturbed part, this approach itself does not satisfy a standard diagrammatic theory. One cannot define one-particle irreducibility for the diagrams, and one has to be very careful in order to avoid multiple counting of certain contributions.

To solve this problem one can define cumulants as in (2.7) and these problems were first solved for the Hubbard model by Metzner [14], who organized the perturbation series as cumulant expansion, and formulated diagrammatic rules with unrestricted sum over momenta for the Hubbard model.

Our formalism allows for an easy extension of these results to the periodic Anderson model, which in context has not been treated in the literature yet and for avoiding to use the identity $n_{\mathbf{i}}^2 = n_{\mathbf{i}}$ for the localized electron operators. Furthermore, in the present formalism these results will be algebraically reproduced and will be extended to find their contributions to thermodynamic quantities of the localized electrons.

For the PAM, one can introduce an effective propagator for the localized electrons and use one of the few available theoretical methods to solve the effective local one-particle Green's function, for example, the well-known **Non-Crossing Approximation** described in detail in [7], [8], [6] and [11]. Next, only the one-particle contributions of the perturbation series are taken into account as in Fig. 3.4, the stationary condition of the thermodynamical potential with respect to the effective propagator introduced is used to get a self-consistent equation for Green's functions of the PAM [13], which is called eXtented Non-Crossing Approximation (XNCA) and can be proved to be equal to Dynamical Mean Field Theory at finite dimensions.

It is also possible to introduce the higher order local cumulants of localized electrons and to sum up some specified diagram families as in Fig. 3.5 to generalize the results of XNCA. The stationary conditions of the resultant thermodynamical potential with respect to all renormalized quantities lead to a self-consistent equation system for themselves. Within this kind of formalism one can include the contributions of non-local processes into the local cumulants and the self-energy of the localized electrons. This was one of the main goals in this thesis.

The results in the next Sections will explain how to determine the many-body local cumulants and which role the non-local processes play in the many-body local cumulants and the self-energy of localized electrons.

SECTION 3.3

The Strong-Coupling expansion

In this Section, we show that by performing a simple transformation - the Grassmannian Hubbard-Stratonovich transformation - for the non-local part $\mathcal{L}^1\left[\zeta(\tau),\bar{\zeta}(\tau)\right]$ of the generic Lagrangian in the grand partition function (3.16) the system considered is converted into the new one of the fermionic auxiliary fields where the many-particle correlation functions of the unperturbed system play the role of the many-particle vertices. It provides the way to recover the diagrammatical results in [14] explicitly and analytically.

SUBSECTION 3.3.1

The Grassmannian Hubbard-Stratonovich transformation

The Grassmannian Hubbard-Stratonovich transformation can be obtained by introducing a fermionic auxiliary functional integral over the auxiliary field-operator Grassmann variables $\psi_{\mathbf{i}\sigma}(\tau)$ and $\bar{\psi}_{\mathbf{i}\sigma}(\tau)$ as follows [3]

$$\mathcal{V}=\int\left[\mathcal{D}\psi\right]\left[\mathcal{D}\bar{\psi}\right]\exp\left\{\int_0^\beta \mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\psi}_{\mathbf{i}'\sigma'}\left(\tau'\right)\left(\Omega^{(0)}\right)^{-1}_{\sigma'\sigma}\left(\mathbf{i}'\;\tau';\mathbf{i}\;\tau\right)\psi_{\mathbf{i}\sigma}(\tau)\right\}, \tag{3.20}$$

and due to the invariance of auxiliary functional integral under the shift transformation

$$\begin{aligned}\psi_{\mathbf{i}\sigma}(\tau)&\longrightarrow\psi_{\mathbf{i}\sigma}(\tau)+\sum_{\mathbf{i}',\sigma'}\int_0^\beta \mathrm{d}\tau'\;\Omega^{(0)}_{\sigma\sigma'}\left(\mathbf{i}\;\tau;\mathbf{i}'\;\tau'\right)\zeta_{\mathbf{i}'\sigma'}\left(\tau'\right)\\ \bar{\psi}_{\mathbf{i}'\sigma'}\left(\tau'\right)&\longrightarrow\bar{\psi}_{\mathbf{i}'\sigma'}\left(\tau'\right)+\sum_{\mathbf{i},\sigma}\int_0^\beta \mathrm{d}\tau\;\bar{\zeta}_{\mathbf{i}\sigma}(\tau)\,\Omega^{(0)}_{\sigma\sigma'}\left(\mathbf{i}\;\tau;\mathbf{i}'\;\tau'\right)\end{aligned} \tag{3.21}$$

one gets the desired transformation - the Grassmannian Hubbard-Stratonovich transformation [4]

$$\begin{aligned}&\mathscr{T}_\tau\exp\left\{-\int_0^\beta \mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\zeta}_{\mathbf{i}\sigma}(\tau)\,\Omega^{(0)}_{\sigma\sigma'}\left(\mathbf{i}\;\tau;\mathbf{i}'\;\tau'\right)\zeta_{\mathbf{i}'\sigma'}\left(\tau'\right)\right\}\\ &\quad=\frac{1}{\mathcal{V}}\int\left[\mathcal{D}\psi\right]\left[\mathcal{D}\bar{\psi}\right]\exp\left\{\int_0^\beta \mathrm{d}\tau\sum_{\mathbf{i}\sigma}\left(\bar{\zeta}_{\mathbf{i}\sigma}(\tau)\,\psi_{\mathbf{i}\sigma}(\tau)+\bar{\psi}_{\mathbf{i}\sigma}(\tau)\,\zeta_{\mathbf{i}\sigma}(\tau)\right)\right\}\\ &\qquad\exp\left\{\int_0^\beta \mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\psi}_{\mathbf{i}'\sigma'}\left(\tau'\right)\left(\Omega^{(0)}\right)^{-1}_{\sigma'\sigma}\left(\mathbf{i}'\;\tau';\mathbf{i}\;\tau\right)\psi_{\mathbf{i}\sigma}(\tau)\right\}.\end{aligned} \tag{3.22}$$

Inserting the Grassmannian Hubbard-Stratonovich transformation into the generic grand partition function (3.16) and integrating over the Grassmann variables of the localized electrons, one gets a

[3] One can easily recognize the convergence of this functional integral due to $\mathrm{Re}\left(\Omega^{(0)}\right)^{-1}<0$. That is the standard condition for convergence of a Gaussian integral.

[4] Without the functional integral, one needs the time-ordering symbol $\mathscr{T}_\tau$ explicitly.

new functional integral representation for the system considered which is now only depending on the fermionic auxiliary fields

$$\mathcal{Z} = \frac{\mathcal{Z}_0 \bar{\mathcal{Z}}_0}{\mathcal{V}} \int [\mathcal{D}\psi] \left[\mathcal{D}\bar{\psi}\right] \bar{\mathcal{Z}} \left[\psi(\tau), \bar{\psi}(\tau)\right] \\ \exp\left\{ \int_0^\beta \mathrm{d}\tau \mathrm{d}\tau' \sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'} \bar{\psi}_{\mathbf{i}'\sigma'}(\tau') \left(\Omega^{(0)}\right)^{-1}_{\sigma'\sigma} \left(\mathbf{i}'\ \tau'; \mathbf{i}\ \tau\right) \psi_{\mathbf{i}\sigma}(\tau) \right\} \tag{3.23}$$

where $\bar{\mathcal{Z}}_0$ is the grand partition function of unperturbed system which is non-quadratic and exactly calculable

$$\begin{aligned} \bar{\mathcal{Z}}_0 &= \int [\mathcal{D}\zeta] \left[\mathcal{D}\bar{\zeta}\right] \exp\left\{ -\int_0^\beta \mathrm{d}\tau\ \mathcal{L}^0 \left[\zeta(\tau), \bar{\zeta}(\tau)\right] \right\} \\ &\equiv \prod_{\mathbf{i}} \int [\mathcal{D}\zeta_{\mathbf{i}}] \left[\mathcal{D}\bar{\zeta}_{\mathbf{i}}\right] \exp\left\{ -\int_0^\beta \mathrm{d}\tau\ \mathcal{L}^0_{\mathbf{i}} \left[\zeta(\tau), \bar{\zeta}(\tau); \varepsilon\right] \right\} \\ &\equiv \prod_{\mathbf{i}} \bar{\mathcal{Z}}_{\mathbf{i},0}. \end{aligned} \tag{3.24}$$

As can be seen in (3.24) the grand partition function of the unperturbed system $\bar{\mathcal{Z}}_0$ is also written as a product of the local, unperturbed grand partition functions which are called the atomic limits of the Hubbard model.

The grand partition function $\bar{\mathcal{Z}}_{\mathbf{i},0}$ with the appearance of a uniform magnetic field h is explicitly calculated as

$$\bar{\mathcal{Z}}_{\mathbf{i},0} = 1 + \mathrm{e}^{-\left(\varepsilon-\mu_\uparrow\right)\beta} + \mathrm{e}^{-\left(\varepsilon-\mu_\downarrow\right)\beta} + \mathrm{e}^{-(2(\varepsilon-\mu)+U)\beta}. \tag{3.25}$$

Analogously, the term $\bar{\mathcal{Z}}\left[\psi(\tau), \bar{\psi}(\tau)\right]$ could be treated in the same way, so it can be also written as a the product of the local contributions. This fact is a consequence of the Grassmannian Hubbard-Stratonovich transformation and locality of the unperturbed system and is simply proved in the expressions below

$$\begin{aligned}
\bar{\mathcal{Z}}\left[\psi(\tau),\bar{\psi}(\tau)\right] &= \left\langle \mathscr{T}_\tau \exp\left\{\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}\sigma}\left(\bar{\zeta}_{\mathbf{i}\sigma}(\tau)\,\psi_{\mathbf{i}\sigma}(\tau)+\bar{\psi}_{\mathbf{i}\sigma}(\tau)\,\zeta_{\mathbf{i}\sigma}(\tau)\right)\right\}\right\rangle_{\bar{\mathcal{Z}}_0} \\
&\equiv \frac{1}{\bar{\mathcal{Z}}_0}\int[\mathcal{D}\zeta]\,[\mathcal{D}\bar{\zeta}]\exp\left\{\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}\sigma}\left(\bar{\zeta}_{\mathbf{i}\sigma}(\tau)\,\psi_{\mathbf{i}\sigma}(\tau)+\bar{\psi}_{\mathbf{i}\sigma}(\tau)\,\zeta_{\mathbf{i}\sigma}(\tau)\right)\right\} \\
&\qquad \exp\left\{-\int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}} \mathcal{L}_i^0\left[\zeta(\tau),\bar{\zeta}(\tau);\varepsilon\right]\right\} \\
&\equiv \prod_{\mathbf{i}}\frac{1}{\bar{\mathcal{Z}}_{\mathbf{i},0}}\int[\mathcal{D}\zeta_{\mathbf{i}}]\,[\mathcal{D}\bar{\zeta}_{\mathbf{i}}]\exp\left\{\int_0^\beta \mathrm{d}\tau \sum_{\sigma}\left(\bar{\zeta}_{\mathbf{i}\sigma}(\tau)\,\psi_{\mathbf{i}\sigma}(\tau)+\bar{\psi}_{\mathbf{i}\sigma}(\tau)\,\zeta_{\mathbf{i}\sigma}(\tau)\right)\right\} \\
&\qquad \exp\left\{-\int_0^\beta \mathrm{d}\tau\, \mathcal{L}_i^0\left[\zeta(\tau),\bar{\zeta}(\tau);\varepsilon\right]\right\} \\
&\equiv \prod_{\mathbf{i}}\left\langle \mathscr{T}_\tau \exp\left\{\int_0^\beta \mathrm{d}\tau \sum_{\sigma}\left(\bar{\zeta}_{\mathbf{i}\sigma}(\tau)\,\psi_{\mathbf{i}\sigma}(\tau)+\bar{\psi}_{\mathbf{i}\sigma}(\tau)\,\zeta_{\mathbf{i}\sigma}(\tau)\right)\right\}\right\rangle_{\bar{\mathcal{Z}}_{\mathbf{i},0}} \\
&\equiv \prod_{\mathbf{i}}\bar{\mathcal{Z}}_{\mathbf{i}}\left[\psi(\tau),\bar{\psi}(\tau)\right].
\end{aligned} \tag{3.26}$$

SUBSECTION 3.3.2

Calculation for $\bar{\mathcal{Z}}_{\mathbf{i}}\left[\psi(\tau),\bar{\psi}(\tau)\right]$

In order to go over to the case with non-local interactions we now calculate $\bar{\mathcal{Z}}_{\mathbf{i}}\left[\psi(\tau),\bar{\psi}(\tau)\right]$ by expanding the exponent functional $\exp\{\ldots\}$ into a series

$$\begin{aligned}
&\mathscr{T}_\tau \exp\left\{\int_0^\beta \mathrm{d}\tau \sum_{\sigma}\left(\bar{\zeta}_{\mathbf{i}\sigma}(\tau)\,\psi_{\mathbf{i}\sigma}(\tau)+\bar{\psi}_{\mathbf{i}\sigma}(\tau)\,\zeta_{\mathbf{i}\sigma}(\tau)\right)\right\} \\
&\quad = 1+\sum_{n=1}^{\infty}\frac{1}{n!}\sum_{\sigma_1,\ldots,\sigma_n}\int_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau_n\ \mathscr{T}_\tau\left(\bar{\zeta}_{\mathbf{i}\sigma_1}(\tau_1)\,\psi_{\mathbf{i}\sigma_1}(\tau_1)+\bar{\psi}_{\mathbf{i}\sigma_1}(\tau_1)\,\zeta_{\mathbf{i}\sigma_1}(\tau_1)\right)\cdots \\
&\qquad\qquad \left(\bar{\zeta}_{\mathbf{i}\sigma_n}(\tau_n)\,\psi_{\mathbf{i}\sigma_n}(\tau_n)+\bar{\psi}_{\mathbf{i}\sigma_n}(\tau_n)\,\zeta_{\mathbf{i}\sigma_n}(\tau_n)\right).
\end{aligned} \tag{3.27}$$

It is not difficult to realize that in all above products only the terms where the numbers of field-operator Grassmann variables $\zeta_{\mathbf{i}\sigma}(\tau)$ and $\bar{\zeta}_{\mathbf{i}\sigma}(\tau)$ are equal have non-zero expectation value even with an $\mathcal{L}^0$ from (3.10), so that $\bar{\mathcal{Z}}_{\mathbf{i}}\left[\psi(\tau),\bar{\psi}(\tau)\right]$ is rewritten as follows

$$\begin{aligned}\bar{\mathcal{Z}}_{\mathbf{i}}\left[\psi(\tau),\bar{\psi}(\tau)\right] &= \left\langle \mathscr{T}_\tau \exp\left\{\int_0^\beta \mathrm{d}\tau \sum_\sigma \left(\bar{\zeta}_{\mathbf{i}\sigma}(\tau)\,\psi_{\mathbf{i}\sigma}(\tau)+\bar{\psi}_{\mathbf{i}\sigma}(\tau)\,\zeta_{\mathbf{i}\sigma}(\tau)\right)\right\}\right\rangle_{\bar{\mathcal{Z}}_{\mathbf{i},0}} \\ &= 1+\sum_{n=1}^{\infty}\frac{(-1)^n}{(n!)^2}\int_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau_n\mathrm{d}\tau_1'\cdots\mathrm{d}\tau_n' \sum_{\substack{\sigma_1,\cdots,\sigma_n\\ \sigma_1',\cdots,\sigma_n'}} \mathscr{T}_\tau\psi_{\mathbf{i}\sigma_1}(\tau_1)\cdots\psi_{\mathbf{i}\sigma_n}(\tau_n) \\ &\quad \bar{\psi}_{\mathbf{i}\sigma_n'}(\tau_n')\cdots\bar{\psi}_{\mathbf{i}\sigma_1'}(\tau_1')\left\langle\mathscr{T}_\tau\left(\zeta_{\mathbf{i}\sigma_1'}(\tau_1')\cdots\zeta_{\mathbf{i}\sigma_n'}(\tau_n')\,\bar{\zeta}_{\mathbf{i}\sigma_n}(\tau_n)\cdots\bar{\zeta}_{\mathbf{i}\sigma_1}(\tau_1)\right)\right\rangle_{\bar{\mathcal{Z}}_{\mathbf{i},0}}.\end{aligned} \tag{3.28}$$

In the original product (3.27) only terms with an even n are non-zero. Since one can take $\frac{n}{2}$ fields ζ and $\bar{\zeta}$, and ψ, $\bar{\psi}$ out of this n, in exactly $\binom{n}{\frac{n}{2}}=\frac{n!}{\left(\frac{n}{2}!\right)^2}$ ways, the factor is $\frac{1}{\left(\frac{n}{2}!\right)^2}$ in (3.27) and the sum runs over on even n. In (3.28) the sum on even $\frac{n}{2}$ was replaced by sum over n and the times in the field operators were relabeled into $\tau_1,\ldots,\tau_n$ and $\tau_1',\ldots,\tau_n'$ for operators ψ and $\bar{\psi}$, resp.. Putting the operators into the standard sequence as in (3.28) yields another factor $(-1)^n$.

We recall the definition of the n-particle Green's function (2.3) and denote $\bar{G}^{(n)}_{\sigma_1',\ldots,\sigma_n';\sigma_1,\ldots,\sigma_n}\Big(\mathbf{i}|\tau_1',\ldots,\tau_n';$ $\tau_1,\ldots,\tau_n\Big)$ for the n-particle Green's function with respect to the grand canonical ensemble of the atomic limit Hubbard model $\bar{\mathcal{Z}}_{\mathbf{i},0}$

$$\begin{aligned}&\bar{G}^{(n)}_{\sigma_1',\ldots,\sigma_n';\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}|\tau_1',\ldots,\tau_n';\tau_1,\ldots,\tau_n\right) \\ &\quad=(-1)^n\left\langle\mathscr{T}_\tau\left(\zeta_{\mathbf{i}\sigma_1'}(\tau_1')\cdots\zeta_{\mathbf{i}\sigma_n'}(\tau_n')\,\bar{\zeta}_{\mathbf{i}\sigma_n}(\tau_n)\cdots\bar{\zeta}_{\mathbf{i}\sigma_1}(\tau_1)\right)\right\rangle_{\bar{\mathcal{Z}}_{\mathbf{i},0}}.\end{aligned} \tag{3.29}$$

Replacing (3.29) into (3.28) then the functional $\bar{\mathcal{Z}}_{\mathbf{i}}\left[\psi(\tau),\bar{\psi}(\tau)\right]$ reaches an immediate result

$$\begin{aligned}\bar{\mathcal{Z}}_{\mathbf{i}}\left[\psi(\tau),\bar{\psi}(\tau)\right] &= 1+\sum_{n=1}^{\infty}\frac{1}{(n!)^2}\int_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau_n\mathrm{d}\tau_1'\cdots\mathrm{d}\tau_n' \sum_{\substack{\sigma_1,\cdots,\sigma_n\\ \sigma_1',\cdots,\sigma_n'}} \mathscr{T}_\tau\psi_{\mathbf{i}\sigma_1}(\tau_1)\cdots\psi_{\mathbf{i}\sigma_n}(\tau_n) \\ &\quad \bar{\psi}_{\mathbf{i}\sigma_n'}(\tau_n')\cdots\bar{\psi}_{\mathbf{i}\sigma_1'}(\tau_1')\,\bar{G}^{(n)}_{\sigma_1',\ldots,\sigma_n';\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}|\tau_1',\ldots,\tau_n';\tau_1,\ldots,\tau_n\right).\end{aligned} \tag{3.30}$$

Because the n-particle Green's function $\bar{G}^{(n)}_{\sigma_1',\ldots,\sigma_n';\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}|\tau_1',\ldots,\tau_n';\tau_1,\ldots,\tau_n\right)$ can be expressed as the sum of products of cumulants $\bar{\mathcal{G}}^{(m)}_{\sigma_1',\ldots,\sigma_n';\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}|\tau_1',\ldots,\tau_n';\tau_1,\ldots,\tau_n\right)$ with the lower order as it was shown in (2.7), one can sum up all terms in this infinite series and gets the final result of $\bar{\mathcal{Z}}_{\mathbf{i}}\left[\psi(\tau),\bar{\psi}(\tau)\right]$ in the form of exponential function as

$$\begin{aligned}\bar{\mathcal{Z}}_{\mathbf{i}}\left[\psi(\tau),\bar{\psi}(\tau)\right] &= \exp\left\{\sum_{n=1}^{\infty}\bar{\mathcal{S}}^{(n)}_{\mathbf{i}}\left[\psi(\tau),\bar{\psi}(\tau)\right]\right\} \\ \bar{\mathcal{S}}^{(n)}_{\mathbf{i}}\left[\psi(\tau),\bar{\psi}(\tau)\right] &= \frac{1}{(n!)^2}\int_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau_n\mathrm{d}\tau_1'\cdots\mathrm{d}\tau_n' \sum_{\substack{\sigma_1,\cdots,\sigma_n\\ \sigma_1',\cdots,\sigma_n'}} \psi_{\mathbf{i}\sigma_1}(\tau_1)\cdots\psi_{\mathbf{i}\sigma_n}(\tau_n) \\ &\quad \bar{\psi}_{\mathbf{i}\sigma_n'}(\tau_n')\cdots\bar{\psi}_{\mathbf{i}\sigma_1'}(\tau_1')\,\bar{\mathcal{G}}^{(n)}_{\sigma_1',\ldots,\sigma_n';\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}|\tau_1',\ldots,\tau_n';\tau_1,\ldots,\tau_n\right)\end{aligned} \tag{3.31}$$

The cumulant $\bar{\mathcal{G}}^{(n)}_{\sigma'_1,\ldots,\sigma'_n;\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}|\tau'_1,\ldots,\tau'_n;\tau_1,\ldots,\tau_n\right)$ is generally determined by the formula (2.19b). It would be helpful to write it down again

$$\begin{aligned}&\bar{\mathcal{G}}^{(n)}_{\sigma'_1,\ldots,\sigma'_n;\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}|\tau'_1,\ldots,\tau'_n;\tau_1,\ldots,\tau_n\right)\\&\qquad=(-1)^n\frac{\delta}{\delta\xi_{\mathbf{i}\sigma_1}\left(\tau_1\right)}\cdots\frac{\delta}{\delta\xi_{\mathbf{i}\sigma_n}\left(\tau_n\right)}\frac{\delta}{\delta\bar{\xi}_{\mathbf{i}\sigma'_n}\left(\tau'_n\right)}\cdots\frac{\delta}{\delta\bar{\xi}_{\mathbf{i}\sigma'_1}\left(\tau'_1\right)}\,\bar{\mathcal{G}}^{(0)}_{\mathbf{i}}\left[\xi,\bar{\xi}\right]\Bigg|_{\xi_{\mathbf{i}}=\bar{\xi}_{\mathbf{i}}=0}\end{aligned}\tag{3.32a}$$

where

$$\bar{\mathcal{G}}^{(0)}_{\mathbf{i}}\left[\xi,\bar{\xi}\right]=\ln\left\langle\mathscr{T}_\tau\exp\left\{-\int_0^\beta\mathrm{d}\tau\,\left[\sum_\sigma\left(\bar{\xi}_{\mathbf{i}\sigma}\left(\tau\right)\zeta_{\mathbf{i}\sigma}\left(\tau\right)+\bar{\zeta}_{\mathbf{i}\sigma}\left(\tau\right)\xi_{\mathbf{i}\sigma}\left(\tau\right)\right)\right]\right\}\right\rangle_{\bar{\mathcal{Z}}_{\mathbf{i},0}}.\tag{3.32b}$$

Returning to the grand partition function (3.23) and replacing $\bar{\mathcal{Z}}\left[\psi\left(\tau\right),\bar{\psi}\left(\tau\right)\right]$ by equations (3.26) and (3.31), the grand partition function of the systems considered now takes the form

$$\mathcal{Z}=\frac{\mathcal{Z}_0\bar{\mathcal{Z}}_0}{\mathcal{V}}\int\left[\mathcal{D}\psi\right]\left[\mathcal{D}\bar{\psi}\right]\exp\left\{-\mathcal{S}_0\left[\psi\left(\tau\right),\bar{\psi}\left(\tau\right)\right]-\sum_{n=1}^{\infty}\mathcal{S}^{(n)}_{\text{int}}\left[\psi\left(\tau\right),\bar{\psi}\left(\tau\right)\right]\right\}\tag{3.33}$$

where the total action has a free (Gaussian) part

$$\mathcal{S}_0\left[\psi\left(\tau\right),\bar{\psi}\left(\tau\right)\right]=-\int_0^\beta\mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\psi}_{\mathbf{i}'\sigma'}\left(\tau'\right)\left(\Omega^{(0)}\right)^{-1}_{\sigma'\sigma}\left(\mathbf{i}'\;\tau';\mathbf{i}\;\tau\right)\psi_{\mathbf{i}\sigma}\left(\tau\right),\tag{3.34a}$$

and an infinite number of interaction terms

$$\mathcal{S}^{(n)}_{\text{int}}\left[\psi\left(\tau\right),\bar{\psi}\left(\tau\right)\right]=-\sum_{\mathbf{i}}\bar{\mathcal{S}}^{(n)}_{\mathbf{i}}\left[\psi\left(\tau\right),\bar{\psi}\left(\tau\right)\right],\tag{3.34b}$$

with $\bar{\mathcal{S}}^{(n)}_{\mathbf{i}}\left[\psi\left(\tau\right),\bar{\psi}\left(\tau\right)\right]$ determined by second equation in (3.31).

The first term of the interaction action also has a quadratic form but that is not included in the free part of the action due to the results of perturbation series of $\Omega^{(0)}_{\sigma\sigma'}\left(\mathbf{i}\;\tau;\mathbf{i}'\;\tau'\right)$.

In this Section with the help of the Grassmannian Hubbard-Stratonovich transformation and the atomic limit of the single band Hubbard model we have converted the system considered into a new fermion system of the auxiliary fields. The newly obtained system does not contain only the two-body interaction but also the many-body interactions of the auxiliary fields. Those many-body interactions are characterized by the many-particle correlation functions of the localized electrons with respect to the atomic limit of the Hubbard model. That apparently shows that the unnegligible role of many-particle contributions in the thermodynamic properties of the system considered. Based on the free (Gaussian) part of the total action where the Wick's theorem is valid one can develop a perturbation theory without carefulness of multiple counting of some contributions. Additionally, that is not difficult to formulate the diagrammatical rules for the thermodynamical potential and the Green's function.

SECTION 3.4

The Green's functions and Self-Energy

The calculations in this Section are independent on the models, so it will be potentially applicable for other models which are not listed in this present thesis. The one-particle Green's function and its self-energy of the auxiliary fields are calculated by the standard technique of generating functional within functional integral formalism. The relationships between the Green's functions of the auxiliary fields and those of the localized electrons are also established.

We show now which relationships between the Green's functions of original electrons $f_{\mathbf{i}\sigma}$, $f^{\dagger}_{\mathbf{i}\sigma}$ (their field-operator Grassmann variables - $\zeta_{\mathbf{i}\sigma}$, $\bar{\zeta}_{\mathbf{i}\sigma}$, resp.) and those of auxiliary field-operator Grassmann variables $\psi_{\mathbf{i}\sigma}$, $\bar{\psi}_{\mathbf{i}\sigma}$ to which perturbation theory applies, exists. To do so, we investigate the generating functional for original electrons where the field-operators $\psi(\tau)$ and $\bar{\psi}(\tau)$ in $\bar{\mathcal{Z}}\left[\psi(\tau),\bar{\psi}(\tau)\right]$ are replaced by shift transformations $\psi(\tau)\to\psi(\tau)+\pi(\tau)$ and $\bar{\psi}(\tau)\to\bar{\psi}(\tau)+\bar{\pi}(\tau)$

$$\mathcal{Z}[\pi,\bar{\pi}] = \frac{\mathcal{Z}_0\bar{\mathcal{Z}}_0}{\mathcal{V}}\int[\mathcal{D}\psi]\left[\mathcal{D}\bar{\psi}\right]\bar{\mathcal{Z}}\left[\psi(\tau)+\pi(\tau),\bar{\psi}(\tau)+\bar{\pi}(\tau)\right] \exp\left\{\int\limits_0^{\beta}\mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\psi}_{\mathbf{i}'\sigma'}(\tau')\left(\Omega^{(0)}\right)^{-1}_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right)\psi_{\mathbf{i}\sigma}(\tau)\right\}. \tag{3.35}$$

By definition, the n-particle Green's functions of localized electrons read

$$\begin{aligned}
&G^{(n)}_{\sigma_1'\ldots\sigma_n';\sigma_1\ldots\sigma_n}\left(\mathbf{i}_1'\ \tau_1',\ldots,\mathbf{i}_n'\ \tau_n';\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n\right)\\
&\quad=(-1)^n\left\langle\mathscr{T}_\tau\left(\zeta_{\mathbf{i}_1'\sigma_1'}(\tau_1')\cdots\zeta_{\mathbf{i}_n'\sigma_n'}(\tau_n')\bar{\zeta}_{\mathbf{i}_n\sigma_n}(\tau_n)\cdots\bar{\zeta}_{\mathbf{i}_1\sigma_1}(\tau_1)\right)\right\rangle\\
&\quad\equiv\frac{1}{\mathcal{Z}}\frac{\mathcal{Z}_0\bar{\mathcal{Z}}_0}{\mathcal{V}}\int[\mathcal{D}\psi]\left[\mathcal{D}\bar{\psi}\right]\left[(-1)^n\frac{\delta}{\delta\pi_{\mathbf{i}_1\sigma_1}(\tau_1)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}_n\sigma_n}(\tau_n)}\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_n'\sigma_n'}(\tau_n')}\right.\\
&\qquad\left.\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_1'\sigma_1'}(\tau_1')}\bar{\mathcal{Z}}\left[\psi(\tau)+\pi(\tau),\bar{\psi}(\tau)+\bar{\pi}(\tau)\right]\right|_{\pi=\bar{\pi}=0}\Bigg]\\
&\qquad\exp\left\{\int\limits_0^{\beta}\mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\psi}_{\mathbf{i}'\sigma'}(\tau')\left(\Omega^{(0)}\right)^{-1}_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right)\psi_{\mathbf{i}\sigma}(\tau)\right\}.
\end{aligned}\tag{3.36}$$

Knowing following identity

$$\begin{aligned}
&(-1)^n\frac{\delta}{\delta\pi_{\mathbf{i}_1\sigma_1}(\tau_1)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}_n\sigma_n}(\tau_n)}\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_n'\sigma_n'}(\tau_n')}\\
&\qquad\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_1'\sigma_1'}(\tau_1')}\bar{\mathcal{Z}}\left[\psi(\tau)+\pi(\tau),\bar{\psi}(\tau)+\bar{\pi}(\tau)\right]\right|_{\pi=\bar{\pi}=0}\\
&\quad=(-1)^n\frac{\delta}{\delta\psi_{\mathbf{i}_1\sigma_1}(\tau_1)}\cdots\frac{\delta}{\delta\psi_{\mathbf{i}_n\sigma_n}(\tau_n)}\frac{\delta}{\delta\bar{\psi}_{\mathbf{i}_n'\sigma_n'}(\tau_n')}\cdots\frac{\delta}{\delta\bar{\psi}_{\mathbf{i}_1'\sigma_1'}(\tau_1')}\bar{\mathcal{Z}}\left[\psi(\tau),\bar{\psi}(\tau)\right],
\end{aligned}\tag{3.37}$$

one can insert (3.37) into (3.36); then the n-particle Green's function $G^{(n)}_{\sigma_1'\ldots\sigma_n';\sigma_1\ldots\sigma_n}\Big(\mathbf{i}_1'\ \tau_1',\ldots,\mathbf{i}_n'\ \tau_n';$ $\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n\Big)$ is represented via functional derivatives with respect to the auxiliary fields as

$$
\begin{aligned}
&G^{(n)}_{\sigma_1'\ldots\sigma_n';\sigma_1\ldots\sigma_n}\left(\mathbf{i}_1'\ \tau_1',\ldots,\mathbf{i}_n'\ \tau_n';\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n\right)\\
&\quad=\frac{1}{\mathcal{Z}}\ \frac{\mathcal{Z}_0\bar{\mathcal{Z}}_0}{\mathcal{V}}\int\left[\mathcal{D}\psi\right]\left[\mathcal{D}\bar{\psi}\right]\Bigg[(-1)^n\ \frac{\delta}{\delta\psi_{\mathbf{i}_1\sigma_1}\left(\tau_1\right)}\cdots\frac{\delta}{\delta\psi_{\mathbf{i}_n\sigma_n}\left(\tau_n\right)}\frac{\delta}{\delta\bar{\psi}_{\mathbf{i}_n'\sigma_n'}\left(\tau_n'\right)}\\
&\qquad\cdots\frac{\delta}{\delta\bar{\psi}_{\mathbf{i}_1'\sigma_1'}\left(\tau_1'\right)}\ \bar{\mathcal{Z}}\left[\psi\left(\tau\right),\bar{\psi}\left(\tau\right)\right]\Bigg]\\
&\qquad\qquad\exp\left\{\int_0^\beta\mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\psi}_{\mathbf{i}'\sigma'}\left(\tau'\right)\left(\Omega^{(0)}\right)^{-1}_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right)\psi_{\mathbf{i}\sigma}\left(\tau\right)\right\},
\end{aligned}
\tag{3.38a}
$$

in which one can perform $2n$ integrations by part, and obtains

$$
\begin{aligned}
&G^{(n)}_{\sigma_1'\ldots\sigma_n';\sigma_1\ldots\sigma_n}\left(\mathbf{i}_1'\ \tau_1',\ldots,\mathbf{i}_n'\ \tau_n';\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n\right)\\
&\quad=\frac{1}{\mathcal{Z}}\ \frac{\mathcal{Z}_0\bar{\mathcal{Z}}_0}{\mathcal{V}}\int\left[\mathcal{D}\psi\right]\left[\mathcal{D}\bar{\psi}\right]\Bigg[(-1)^n\ \frac{\delta}{\delta\bar{\psi}_{\mathbf{i}_1'\sigma_1'}\left(\tau_1'\right)}\cdots\frac{\delta}{\delta\bar{\psi}_{\mathbf{i}_n'\sigma_n'}\left(\tau_n'\right)}\frac{\delta}{\delta\psi_{\mathbf{i}_n\sigma_n}\left(\tau_n\right)}\\
&\qquad\cdots\frac{\delta}{\delta\psi_{\mathbf{i}_1\sigma_1}\left(\tau_1\right)}\ \exp\left\{\int_0^\beta\mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\psi}_{\mathbf{i}'\sigma'}\left(\tau'\right)\left(\Omega^{(0)}\right)^{-1}_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right)\psi_{\mathbf{i}\sigma}\left(\tau\right)\right\}\Bigg]\\
&\qquad\quad\bar{\mathcal{Z}}\left[\psi\left(\tau\right),\bar{\psi}\left(\tau\right)\right].
\end{aligned}
\tag{3.38b}
$$

The equation (3.38b) leads to the relationships between the Green's functions of the localized electrons and those of the auxiliary fields, which we want to find.
Direct differential manipulations based on (3.38b) give explicit relations, for $n=1$

$$
\begin{aligned}
&G^{(1)}_{\sigma_1';\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right)=-\left(\Omega^{(0)}\right)^{-1}_{\sigma_1'\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right)\\
&\quad+\sum_{\mathbf{j}_1\mathbf{j}_1',\varsigma_1\varsigma_1'}\int_0^\beta\mathrm{d}\theta_1\mathrm{d}\theta_1'\left(\Omega^{(0)}\right)^{-1}_{\sigma_1'\varsigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{j}_1\ \theta_1\right)\ \Omega^{(1)}_{\varsigma_1\varsigma_1'}\left(\mathbf{j}_1\ \theta_1;\mathbf{j}_1'\ \theta_1'\right)\ \left(\Omega^{(0)}\right)^{-1}_{\varsigma_1'\sigma_1}\left(\mathbf{j}_1'\ \theta_1';\mathbf{i}_1\ \tau_1\right)
\end{aligned}
\tag{3.39a}
$$

and for $n\geq 2$

$$
\begin{aligned}
&\hat{G}^{(n)}_{\sigma_1'\ldots\sigma_n';\sigma_1\ldots\sigma_1}\left(\mathbf{i}_1'\ \tau_1',\ldots,\mathbf{i}_n'\ \tau_n';\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_1\ \tau_1\right)\\
&\quad=\sum_{\substack{\mathbf{j}_1\mathbf{j}_1'\cdots\mathbf{j}_n\mathbf{j}_n'\\ \varsigma_1\varsigma_1'\cdots\varsigma_n\varsigma_n'}}\int_0^\beta\mathrm{d}\theta_1\mathrm{d}\theta_1'\cdots\mathrm{d}\theta_n\mathrm{d}\theta_n'\left(\Omega^{(0)}\right)^{-1}_{\sigma_1'\varsigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{j}_1\ \theta_1\right)\cdots\left(\Omega^{(0)}\right)^{-1}_{\sigma_n'\varsigma_n}\left(\mathbf{i}_n'\ \tau_n';\mathbf{j}_n\ \theta_n\right)\\
&\qquad\hat{\Omega}^{(n)}_{\varsigma_1\ldots\varsigma_n;\varsigma_1'\ldots\varsigma_n'}\left(\mathbf{j}_1\ \theta_1,\ldots,\mathbf{j}_n\ \theta_n;\mathbf{j}_1'\ \theta_1',\ldots,\mathbf{j}_n'\ \theta_n'\right)\\
&\qquad\quad\left(\Omega^{(0)}\right)^{-1}_{\varsigma_n'\sigma_n}\left(\mathbf{j}_n'\ \theta_n';\mathbf{i}_n\ \tau_n\right)\cdots\left(\Omega^{(0)}\right)^{-1}_{\varsigma_1'\sigma_1}\left(\mathbf{j}_1'\ \theta_1';\mathbf{i}_1\ \tau_1\right)
\end{aligned}
\tag{3.39b}
$$

where $\hat{G}^{(n)}_{\sigma_1'\ldots\sigma_n';\sigma_1\ldots\sigma_1}\left(\mathbf{i}_1'\ \tau_1',\ldots,\mathbf{i}_n'\ \tau_n';\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_1\ \tau_1\right)$ and $\hat{\Omega}^{(n)}_{\varsigma_1\ldots\varsigma_n;\varsigma_1'\ldots\varsigma_n'}\left(\mathbf{j}_1\ \theta_1,\ldots,\mathbf{j}_n\ \theta_n;\mathbf{j}_1'\ \theta_1',\ldots,\mathbf{j}_n'\ \theta_n'\right)$ are n-particle cumulants or in other words, connected Green's functions of the localized electrons and of the auxiliary fields, resp.. In the standard many-body theory the one-particle Green's function of localized electrons $G^{(1)}_{\sigma_1';\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right)$ is called scattering matrix or T-matrix for the auxiliary fields and in the view of foregoing we may view the n-particle cumulant of localized electrons $\hat{G}^{(n)}_{\sigma'_1\ldots\sigma'_n;\sigma_1\ldots\sigma_1}\left(\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n;\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_1\ \tau_1\right)$ as n-particle scattering matrix for the auxiliary fields. The relations (3.39a) and (3.39b) can be written in matrix form as

$$\begin{aligned} G^{(1)} &= -\left(\Omega^{(0)}\right)^{-1} + \left(\Omega^{(0)}\right)^{-1}\ \Omega^{(1)}\ \left(\Omega^{(0)}\right)^{-1} \\ \hat{G}^{(n)} &= \left(\Omega^{(0)}\right)^{-1}\cdots\left(\Omega^{(0)}\right)^{-1}\ \hat{\Omega}^{(n)}\ \left(\Omega^{(0)}\right)^{-1}\cdots\ \left(\Omega^{(0)}\right)^{-1} \end{aligned} \tag{3.39c}$$

If the symbol Γ denotes the self-energy of the auxiliary fields then one can find out the relation of the one-particle Green's function of localized electrons $G^{(1)}$ with the self-energy Γ as

$$\begin{aligned} \Omega^{(1)} &= \left(\left(\Omega^{(0)}\right)^{-1} - \Gamma\right)^{-1} \\ G^{(1)} &= \left(\Gamma^{-1} - \Omega^{(0)}\right)^{-1} . \end{aligned} \tag{3.39d}$$

In standard theory, the one-particle Green's function of the localized electrons can be also written in the terms of its self-energy as follows

$$G^{(1)} = \left(i\omega - \varepsilon^f - \Sigma - \Omega^{(0)}\right)^{-1} \tag{3.39e}$$

where the symbol Σ denotes the self-energy of the localized electrons.

Comparing the equations (3.39d) and (3.39e) one can easily point out that the self-energy of the auxiliary fields and thus of the localized electrons are related by the following identity

$$\Gamma^{-1} = i\omega - \varepsilon^f - \Sigma\ . \tag{3.39f}$$

One can interpret that the self-energy of the auxiliary fields is an inverse of the self-energy of the localized electrons.

The self-energy Γ can be determined with the help of the generating functional for the auxiliary fields, which is represented as a functional integral

$$\begin{aligned} \mathcal{Z}\left[\pi,\bar{\pi}\right] = \frac{\mathcal{Z}_0\bar{\mathcal{Z}}_0}{\mathcal{V}}\int\left[\mathcal{D}\psi\right]\left[\mathcal{D}\bar{\psi}\right]\ \bar{\mathcal{Z}}\left[\psi\left(\tau\right),\bar{\psi}\left(\tau\right)\right]\exp\left\{\int_0^\beta \mathrm{d}\tau\sum_{\mathbf{i},\sigma}\left(\bar{\pi}_{\mathbf{i}\sigma}\left(\tau\right)\psi_{\mathbf{i}\sigma}\left(\tau\right) + \bar{\psi}_{\mathbf{i}\sigma}\left(\tau\right)\pi_{\mathbf{i}\sigma}\left(\tau\right)\right)\right\} \\ \exp\left\{\int_0^\beta \mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\psi}_{\mathbf{i}'\sigma'}\left(\tau'\right)\left(\Omega^{(0)}\right)^{-1}_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right)\psi_{\mathbf{i}\sigma}\left(\tau\right)\right\} . \end{aligned} \tag{3.40}$$

Since the auxiliary operators $\psi_{\mathbf{i}\sigma}$ and $\bar{\psi}_{\mathbf{i}\sigma}$ could be generated by functional differentiation

$$\begin{aligned} \psi_{\mathbf{i}\sigma}\left(\tau\right) &= \frac{\delta}{\bar{\pi}_{\mathbf{i}\sigma}\left(\tau\right)} \\ \bar{\psi}_{\mathbf{i}'\sigma'}\left(\tau'\right) &= -\frac{\delta}{\pi_{\mathbf{i}'\sigma'}\left(\tau'\right)} \end{aligned} \tag{3.41}$$

applied to the term

$$\exp\left\{\int_0^\beta \mathrm{d}\tau\sum_{\mathbf{i},\sigma}\left(\bar{\pi}_{\mathbf{i}\sigma}\left(\tau\right)\psi_{\mathbf{i}\sigma}\left(\tau\right) + \bar{\psi}_{\mathbf{i}\sigma}\left(\tau\right)\pi_{\mathbf{i}\sigma}\left(\tau\right)\right)\right\} ,$$

the functional $\bar{\mathcal{Z}}\left[\psi(\tau), \bar{\psi}(\tau)\right]$ can be expressed as a functional of functional-differential operators $\dfrac{\delta}{\bar{\pi}_{\mathbf{i}\sigma}(\tau)}$ and $\dfrac{\delta}{\pi_{\mathbf{i}'\sigma'}(\tau')}$. The generating functional (3.40) reads

$$\begin{aligned}\mathcal{Z}[\pi,\bar{\pi}] = \frac{\mathcal{Z}_0\bar{\mathcal{Z}}_0}{\mathcal{V}}\int [\mathcal{D}\psi]\,[\mathcal{D}\bar{\psi}]\,\bar{\mathcal{Z}}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right]\exp\left\{\int_0^\beta \mathrm{d}\tau\sum_{\mathbf{i},\sigma}\left(\bar{\pi}_{\mathbf{i}\sigma}(\tau)\,\psi_{\mathbf{i}\sigma}(\tau)+\bar{\psi}_{\mathbf{i}\sigma}(\tau)\,\pi_{\mathbf{i}\sigma}(\tau)\right)\right\}\\ \exp\left\{\int_0^\beta \mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\psi}_{\mathbf{i}'\sigma'}(\tau')\left(\Omega^{(0)}\right)^{-1}_{\sigma'\sigma}\left(\mathbf{i}'\,\tau';\mathbf{i}\,\tau\right)\psi_{\mathbf{i}\sigma}(\tau)\right\}.\end{aligned} \tag{3.42}$$

Bringing the functional $\bar{\mathcal{Z}}\left[\dfrac{\delta}{\bar{\pi}(\tau)},\dfrac{\delta}{\pi(\tau)}\right]$ out of integration and using the identity

$$\begin{aligned}&\mathscr{T}_\tau\exp\left\{-\int_0^\beta \mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\pi}_{\mathbf{i}\sigma}(\tau)\,\Omega^{(0)}_{\sigma\sigma'}\left(\mathbf{i}\,\tau;\mathbf{i}'\,\tau'\right)\pi_{\mathbf{i}'\sigma'}(\tau')\right\}\\ &=\frac{1}{\mathcal{V}}\int [\mathcal{D}\psi]\,[\mathcal{D}\bar{\psi}]\exp\left\{\int_0^\beta \mathrm{d}\tau\sum_{\mathbf{i},\sigma}\left(\bar{\pi}_{\mathbf{i}\sigma}(\tau)\,\psi_{\mathbf{i}\sigma}(\tau)+\bar{\psi}_{\mathbf{i}\sigma}(\tau)\,\pi_{\mathbf{i}\sigma}(\tau)\right)\right\}\\ &\qquad\exp\left\{\int_0^\beta \mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\psi}_{\mathbf{i}'\sigma'}(\tau')\left(\Omega^{(0)}\right)^{-1}_{\sigma'\sigma}\left(\mathbf{i}'\,\tau';\mathbf{i}\,\tau\right)\psi_{\mathbf{i}\sigma}(\tau)\right\},\end{aligned} \tag{3.43}$$

one may rewrite the generating functional (3.42) in a form of differential operation applied on the external source field-operators $\bar{\pi}$ and π

$$\begin{aligned}\mathcal{Z}[\pi,\bar{\pi}] = \mathcal{Z}_0\bar{\mathcal{Z}}_0\;\bar{\mathcal{Z}}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right]\\ \mathscr{T}_\tau\exp\left\{-\int_0^\beta \mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\pi}_{\mathbf{i}\sigma}(\tau)\,\Omega^{(0)}_{\sigma\sigma'}\left(\mathbf{i}\,\tau;\mathbf{i}'\,\tau'\right)\pi_{\mathbf{i}'\sigma'}(\tau')\right\}.\end{aligned} \tag{3.44}$$

The expression (3.44) would be used as a starting point for any further calculations of the many-particle Green's functions, it reduces the complexity of mathematical manipulations.

The functional of differential operators $\bar{\mathcal{Z}}\left[\dfrac{\delta}{\bar{\pi}(\tau)},\dfrac{\delta}{\pi(\tau)}\right]$ is determined by (3.31)

$$\begin{aligned}\bar{\mathcal{Z}}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right] &= \exp\left\{-\,\mathcal{S}_{\mathrm{int}}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right]\right\}\\ &\equiv \exp\left\{\sum_{\mathbf{i}}\sum_{n=1}^{\infty}\bar{\mathcal{S}}^{(n)}_{\mathbf{i}}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right]\right\}\end{aligned} \tag{3.45a}$$

where

$$\begin{aligned}\bar{\mathcal{S}}^{(n)}_{\mathbf{i}}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right] = \frac{1}{(n!)^2}\int_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau_n\mathrm{d}\tau'_1\cdots\mathrm{d}\tau'_n\sum_{\substack{\sigma_1\ldots\sigma_n\\ \sigma'_1\ldots\sigma'_n}}\bar{\mathcal{G}}^{(n)}_{\sigma'_1,\ldots,\sigma'_n;\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}|\tau'_1,\ldots,\tau'_n;\tau_1,\ldots,\tau_n\right)\\ \frac{\delta}{\delta\pi_{\mathbf{i}\sigma'_1}(\tau'_1)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}\sigma'_n}(\tau'_n)}\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}\sigma_n}(\tau_n)}\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}\sigma_1}(\tau_1)}\end{aligned} \tag{3.45b}$$

The n-particle Green's function of auxiliary fields reads

$$\begin{aligned}
&\Omega^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n\right)\\
&\quad=(-1)^n\left\langle \mathscr{T}_\tau\left(\psi_{\mathbf{i}_1\sigma_1}(\tau_1)\ldots\psi_{\mathbf{i}_n\sigma_n}(\tau_n)\,\bar{\psi}_{\mathbf{i}'_n\sigma'_n}\left(\tau'_n\right)\ldots\bar{\psi}_{\mathbf{i}'_1\sigma'_1}\left(\tau'_1\right)\right)\right\rangle\\
&\quad\equiv(-1)^n\,\frac{1}{\mathcal{Z}}\,\frac{\delta}{\delta\pi_{\mathbf{i}'_1\sigma'_1}\left(\tau'_1\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}'_n\sigma'_n}\left(\tau'_n\right)}\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_n\sigma_n}(\tau_n)}\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_1\sigma_1}(\tau_1)}\;\mathcal{Z}\left[\pi,\bar{\pi}\right]\Bigg|_{\pi=\bar{\pi}=0}.
\end{aligned}\tag{3.46}$$

For one-particles Green's function i.e. $n=1$, that is

$$\Omega^{(1)}_{\sigma_1\sigma'_1}\left(\mathbf{i}_1\ \tau_1;\mathbf{i}'_1\ \tau'_1\right)=(-1)\,\frac{1}{\mathcal{Z}}\,\frac{\delta}{\delta\pi_{\mathbf{i}'_1\sigma'_1}\left(\tau'_1\right)}\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_1\sigma_1}(\tau_1)}\;\mathcal{Z}\left[\pi,\bar{\pi}\right]\Bigg|_{\pi=\bar{\pi}=0}.\tag{3.47a}$$

Performing the operation $\dfrac{\delta}{\delta\bar{\pi}_{\mathbf{i}_1\sigma_1}(\tau_1)}$ on $\mathcal{Z}\left[\pi,\bar{\pi}\right]$ one gets

$$\begin{aligned}
\Omega^{(1)}_{\sigma_1\sigma'_1}\left(\mathbf{i}_1\ \tau_1;\mathbf{i}'_1\ \tau'_1\right)=\frac{1}{\mathcal{Z}}\,&\frac{\delta}{\delta\pi_{\mathbf{i}'_1\sigma'_1}\left(\tau'_1\right)}\;\mathcal{Z}_0\bar{\mathcal{Z}}_0\;\exp\left\{-\;\mathcal{S}_{\mathrm{int}}\left[\frac{\delta}{\delta\bar{\pi}(\tau)},\frac{\delta}{\delta\pi(\tau)}\right]\right\}\\
&\left(\int_0^\beta \mathrm{d}\theta'\sum_{\mathbf{j}',\varsigma'}\Omega^{(0)}_{\sigma_1\varsigma'}\left(\mathbf{i}_1\ \tau_1;\mathbf{j}'\ \theta'\right)\pi_{\mathbf{j}'\varsigma'}\left(\theta'\right)\right)\\
&\quad\exp\left\{-\int_0^\beta \mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\pi}_{\mathbf{i}\sigma}(\tau)\,\Omega^{(0)}_{\sigma\sigma'}\left(\mathbf{i}\ \tau;\mathbf{i}'\ \tau'\right)\pi_{\mathbf{i}'\sigma'}\left(\tau'\right)\right\}\Bigg|_{\pi=\bar{\pi}=0}.
\end{aligned}\tag{3.47b}$$

In order to bring the operator $\pi_{\mathbf{j}'\varsigma'}(\theta')$ from the right side of $\exp\left\{-\;\mathcal{S}_{\mathrm{int}}\left[\dfrac{\delta}{\delta\bar{\pi}(\tau)},\dfrac{\delta}{\delta\pi(\tau)}\right]\right\}$ to the left side of it one should remind oneself about the commutators (A.6)

$$\begin{aligned}
\bar{\mathcal{S}}_{\mathrm{int}}\left[\frac{\delta}{\delta\bar{\pi}(\tau)},\frac{\delta}{\delta\pi(\tau)}\right]\bar{\pi}_{\mathbf{i}\sigma}(\tau)&=\bar{\pi}_{\mathbf{i}\sigma}(\tau)\,\bar{\mathcal{S}}_{\mathrm{int}}\left[\frac{\delta}{\delta\bar{\pi}(\tau)},\frac{\delta}{\delta\pi(\tau)}\right]\\
&\qquad+\bar{\mathcal{S}}^{(0;1)}_{\mathrm{int}[\cdot;\mathbf{i}\sigma]}\left[\frac{\delta}{\delta\bar{\pi}(\tau)},\frac{\delta}{\delta\pi(\tau)}\right](\tau)\\
\bar{\mathcal{S}}_{\mathrm{int}}\left[\frac{\delta}{\delta\bar{\pi}(\tau)},\frac{\delta}{\delta\pi(\tau)}\right]\pi_{\mathbf{i}'\sigma'}\left(\tau'\right)&=\pi_{\mathbf{i}'\sigma'}\left(\tau'\right)\bar{\mathcal{S}}_{\mathrm{int}}\left[\frac{\delta}{\delta\bar{\pi}(\tau)},\frac{\delta}{\delta\pi(\tau)}\right]\\
&\qquad-\bar{\mathcal{S}}^{(1;0)}_{\mathrm{int}[\mathbf{i}'\sigma';\cdot]}\left[\frac{\delta}{\delta\bar{\pi}(\tau)},\frac{\delta}{\delta\pi(\tau)}\right]\left(\tau'\right)
\end{aligned}\tag{3.47c}$$

where

$$\bar{\mathcal{S}}^{(0;1)}_{\mathrm{int}[\cdot;\mathbf{i}\sigma]}\left[\frac{\delta}{\delta\bar{\pi}\left(\tau\right)},\frac{\delta}{\delta\pi\left(\tau\right)}\right]\left(\tau\right)=\sum_{n=1}^{\infty}\frac{n}{(n!)^2}\int\limits_0^\beta \mathrm{d}\tau_2\cdots\mathrm{d}\tau_n\mathrm{d}\tau'_1\cdots\mathrm{d}\tau'_n$$
$$\sum_{\substack{\sigma_2\cdots\sigma_n\\ \sigma'_1\cdots\sigma'_n}}\bar{\mathcal{G}}^{(n)}_{\sigma'_1,\ldots,\sigma'_n;\sigma,\ldots,\sigma_n}\left(\mathbf{i}|\tau'_1,\ldots,\tau'_n;\tau,\ldots,\tau_n\right)$$
$$\frac{\delta}{\delta\pi_{\mathbf{i}\sigma'_1}\left(\tau'_1\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}\sigma'_n}\left(\tau'_n\right)}\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}\sigma_n}\left(\tau_n\right)}\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}\sigma_2}\left(\tau_2\right)}\tag{3.47d}$$
$$\bar{\mathcal{S}}^{(1;0)}_{\mathrm{int}[\mathbf{i}'\sigma';\cdot]}\left[\frac{\delta}{\delta\bar{\pi}\left(\tau\right)},\frac{\delta}{\delta\pi\left(\tau\right)}\right]\left(\tau'\right)=\sum_{n=1}^{\infty}\frac{n}{(n!)^2}\int\limits_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau_n\mathrm{d}\tau'_2\cdots\mathrm{d}\tau'_n$$
$$\sum_{\substack{\sigma_1\cdots\sigma_n\\ \sigma'_2\cdots\sigma'_n}}\bar{\mathcal{G}}^{(n)}_{\sigma',\ldots,\sigma'_n;\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}'|\tau',\ldots,\tau'_n;\tau_1,\ldots,\tau_n\right)$$
$$\frac{\delta}{\delta\pi_{\mathbf{i}'\sigma'_2}\left(\tau'_2\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}'\sigma'_n}\left(\tau'_n\right)}\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}'\sigma_n}\left(\tau_n\right)}\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}'\sigma_1}\left(\tau_1\right)}.$$

as they were determined in (A.6a) and (A.6b).

Inserting the second equation of (3.47c) into (3.47b) and performing differential operation $\frac{\delta}{\delta\pi_{\mathbf{i}'_1\sigma'_1}\left(\tau'_1\right)}$ on the term where external source field operator appears yields

$$\Omega^{(1)}_{\sigma_1\sigma'_1}\left(\mathbf{i}_1\ \tau_1;\mathbf{i}'_1\ \tau'_1\right)=\frac{1}{\mathcal{Z}}\frac{\delta}{\delta\pi_{\mathbf{i}'_1\sigma'_1}\left(\tau'_1\right)}\left(\int\limits_0^\beta \mathrm{d}\theta'\sum_{\mathbf{j}',\varsigma'}\Omega^{(0)}_{\sigma_1\varsigma'}\left(\mathbf{i}_1\ \tau_1;\mathbf{j}'\ \theta'\right)\right.$$
$$\left.\left(\pi_{\mathbf{j}'\varsigma'}\left(\theta'\right)-\bar{\mathcal{S}}^{(1;0)}_{\mathrm{int}[\mathbf{j}'\varsigma';\cdot]}\left[\frac{\delta}{\delta\bar{\pi}\left(\tau\right)},\frac{\delta}{\delta\pi\left(\tau\right)}\right]\left(\theta'\right)\right)\right)\mathcal{Z}\left[\pi,\bar{\pi}\right]\Bigg|_{\pi=\bar{\pi}=0}$$
$$=\Omega^{(0)}_{\sigma_1\sigma'_1}\left(\mathbf{i}_1\ \tau_1;\mathbf{i}'_1\ \tau'_1\right)\tag{3.47e}$$
$$-\int\limits_0^\beta \mathrm{d}\theta'\sum_{\mathbf{j}',\varsigma'}\Omega^{(0)}_{\sigma_1\varsigma'}\left(\mathbf{i}_1\ \tau_1;\mathbf{j}'\ \theta'\right)$$
$$\frac{1}{\mathcal{Z}}\frac{\delta}{\delta\pi_{\mathbf{i}'_1\sigma'_1}\left(\tau'_1\right)}\bar{\mathcal{S}}^{(1;0)}_{\mathrm{int}[\mathbf{j}'\varsigma';\cdot]}\left[\frac{\delta}{\delta\bar{\pi}\left(\tau\right)},\frac{\delta}{\delta\pi\left(\tau\right)}\right]\left(\theta'\right)\mathcal{Z}\left[\pi,\bar{\pi}\right]\Bigg|_{\pi=\bar{\pi}=0}.$$

Using the explicit expression of $\mathcal{S}^{(1;0)}_{\mathrm{int}[\mathbf{j}'\varsigma';\cdot]}\left[\frac{\delta}{\delta\bar{\pi}\left(\tau\right)},\frac{\delta}{\delta\pi\left(\tau\right)}\right]\left(\theta'\right)$ from (3.47d) to write the second term in (3.47e) as a functional of Green's functions of localized electrons and those of the auxiliary fields leads to

$$
\begin{aligned}
&-\frac{1}{\mathcal{Z}}\,\frac{\delta}{\delta\pi_{\mathbf{i}_1'\sigma_1'}\left(\tau_1'\right)}\,\mathcal{S}^{(1;0)}_{\mathrm{int}[\mathbf{j}'\varsigma';\cdot]}\left[\frac{\delta}{\delta\bar{\pi}\left(\tau\right)},\frac{\delta}{\delta\pi\left(\tau\right)}\right]\left(\theta'\right)\mathcal{Z}\left[\pi,\bar{\pi}\right]\Bigg|_{\pi=\bar{\pi}=0} \\
&=\sum_{n=1}^{\infty}\left(-1\right)^{n+1}\frac{n}{\left(n!\right)^2}\int_0^\beta \mathrm{d}\theta'\sum_{\mathbf{j}',\varsigma'}\Omega^{(0)}_{\sigma_1\varsigma'}\left(\mathbf{i}_1\;\tau_1;\mathbf{j}'\;\theta'\right)\int_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau\mathrm{d}\tau_2'\cdots\mathrm{d}\tau_n' \\
&\qquad\sum_{\substack{\sigma_1\cdots\sigma_n\\ \sigma_2'\cdots\sigma_n'}}\bar{\mathcal{G}}^{(n)}_{\varsigma',\ldots,\sigma_n';\sigma_1,\ldots,\sigma_n}\left(\mathbf{j}'|\theta',\ldots,\tau_n';\tau_1,\ldots,\tau_n\right) \\
&\qquad\Omega^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma_1',\ldots,\sigma_n'}\left(\mathbf{j}'\;\tau_1,\ldots,\mathbf{j}'\;\tau_n;\mathbf{i}_1'\;\tau_1',\ldots,\mathbf{j}'\;\tau_n'\right).
\end{aligned}
\tag{3.47f}
$$

Substituting (3.47f) into (3.47e), the self-energy of the auxiliary fields is found and expressed as

$$
\begin{aligned}
\Gamma_{\sigma'\sigma}\left(\mathbf{i}'\;\tau';\mathbf{i}\;\tau\right)&=\sum_{n=1}^{\infty}\left(-1\right)^{n+1}\frac{n}{\left(n!\right)^2}\int_0^\beta \mathrm{d}\theta'\sum_{\mathbf{j}',\varsigma'}\int_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau\mathrm{d}\tau_2'\cdots\mathrm{d}\tau_n' \\
&\sum_{\substack{\sigma_1\cdots\sigma_n\\ \sigma_2'\cdots\sigma_n'}}\bar{\mathcal{G}}^{(n)}_{\sigma',\ldots,\sigma_n';\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}'|\tau',\tau_2',\ldots,\tau_n';\tau_1,\ldots,\tau_n\right) \\
&\Omega^{(n)}_{\sigma_1,\ldots,\sigma_n;\varsigma',\ldots,\sigma_n'}\left(\mathbf{i}'\;\tau_1,\ldots,\mathbf{i}'\;\tau_n;\mathbf{j}'\;\theta',\mathbf{i}'\;\tau_2',\ldots,\mathbf{i}'\;\tau_n'\right)\Omega^{-1}_{\varsigma'\sigma}\left(\mathbf{j}'\;\theta';\mathbf{i}\;\tau\right).
\end{aligned}
\tag{3.47g}
$$

The equation (3.47g) is the exact expression of the self-energy for the auxiliary fields and its inverse is directly appearing in the Green's function of localized electrons (3.39d) in the role of the self-energy. It shows the full dependence of the self-energy of the auxiliary fields on their many-body interactions and Green's functions.

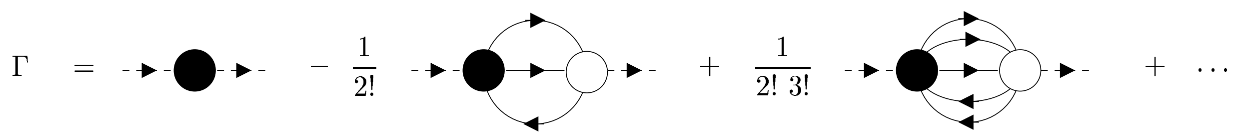


Figure 3.1: Diagram representation for self-energy of auxiliary field operators; black circles indicate $\bar{G}$; white circles - $\hat{\Omega}$; dashed arrows - single input and output lines for localized electrons; solid lines - single input and output lines for auxiliary field operators.

Writing the n-particle Green's function $\Omega^{(n)}_{\sigma_1,\ldots,\sigma_n;\varsigma',\ldots,\sigma_n'}\left(\mathbf{i}'\;\tau_1,\ldots,\mathbf{i}'\;\tau_n;\mathbf{j}'\;\theta',\mathbf{i}'\;\tau_2',\ldots,\mathbf{i}'\;\tau_n'\right)$ as the sum of products of cumulants and collecting all the cumulants with the site variable $\mathbf{i}'$ into the renormalized local many-particle Green's functions, the equation (3.47g) now can be rewritten in the new form as a functional of n-particle cumulants $\hat{\Omega}^{(n)}_{\sigma_1,\ldots,\sigma_n;\varsigma',\ldots,\sigma_n'}\left(\mathbf{i}'\;\tau_1,\ldots,\mathbf{i}'\;\tau_n;\mathbf{j}'\;\theta',\mathbf{i}'\;\tau_2',\ldots,\mathbf{i}'\;\tau_n'\right)$ of the auxiliary fields and renormalized local n-particle Green's functions $\bar{G}^{(n)}_{\sigma',\ldots,\sigma_n';\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}'|\tau',\tau_2',\ldots,\tau_n';\tau_1,\ldots,\tau_n\right)$ of localized electrons

$$
\begin{aligned}
\Gamma_{\sigma'\sigma}\left(\mathbf{i}'\;\tau';\mathbf{i}\;\tau\right)&=\sum_{n=1}^{\infty}\left(-1\right)^{n+1}\frac{n}{\left(n!\right)^2}\int_0^\beta \mathrm{d}\theta'\sum_{\mathbf{j}',\varsigma'}\int_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau\mathrm{d}\tau_2'\cdots\mathrm{d}\tau_n' \\
&\sum_{\substack{\sigma_1\cdots\sigma_n\\ \sigma_2'\cdots\sigma_n'}}\bar{G}^{(n)}_{\sigma',\ldots,\sigma_n';\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}'|\tau',\tau_2',\ldots,\tau_n';\tau_1,\ldots,\tau_n\right) \\
&\hat{\Omega}^{(n)}_{\sigma_1,\ldots,\sigma_n;\varsigma',\ldots,\sigma_n'}\left(\mathbf{i}'\;\tau_1,\ldots,\mathbf{i}'\;\tau_n;\mathbf{j}'\;\theta',\mathbf{i}'\;\tau_2',\ldots,\mathbf{i}'\;\tau_n'\right)\left(\Omega^{(1)}\right)^{-1}_{\varsigma'\sigma}\left(\mathbf{j}'\;\theta';\mathbf{i}\;\tau\right),
\end{aligned}
\tag{3.48}
$$

where the newly introduced renormalized local n-particle Green's function $\bar{G}^{(n)}_{\sigma'_1,\dots,\sigma'_n;\sigma_1,\dots,\sigma_n}(\mathbf{i}'|\tau'_1,\dots,\tau'_n;\tau_1,\dots,\tau_n)$ could be also called renormalized local n-particle vertex and is diagrammatically represented as in Fig. 3.2 and algebraically determined by the following form

$$
\begin{aligned}
\bar{G}^{(n)}_{\boldsymbol{\sigma}'_n;\boldsymbol{\sigma}_n}\left(\mathbf{i}|\boldsymbol{\tau}'_n;\boldsymbol{\tau}_n\right) &= \bar{\mathcal{G}}^{(n)}_{\boldsymbol{\sigma}'_n;\boldsymbol{\sigma}_n}\left(\mathbf{i}|\boldsymbol{\tau}'_n;\boldsymbol{\tau}_n\right) \\
&\quad + \int\limits_0^\beta \mathrm{d}\boldsymbol{\tau}_{m_1}\mathrm{d}\boldsymbol{\tau}'_{m_1} \sum_{\boldsymbol{\sigma}'_{m_1};\boldsymbol{\sigma}_{m_1}} \bar{\mathcal{G}}^{(n+m_1)}_{\boldsymbol{\sigma}'_{n+m_1};\boldsymbol{\sigma}_{n+m_1}}\left(\mathbf{i}|\boldsymbol{\tau}'_{n+m_1};\boldsymbol{\tau}_{n+m_1}\right)\bar{\mathcal{O}}^{(m_1)}_{\boldsymbol{\sigma}'_{m_1};\boldsymbol{\sigma}_{m_1}}\left(\mathbf{i}|\boldsymbol{\tau}'_{m_1};\boldsymbol{\tau}_{m_1}\right) \\
&\quad + \frac{1}{2!}\int\limits_0^\beta \mathrm{d}\boldsymbol{\tau}_{m_1}\mathrm{d}\boldsymbol{\tau}_{m_2}\mathrm{d}\boldsymbol{\tau}'_{m_1}\mathrm{d}\boldsymbol{\tau}'_{m_2} \\
&\qquad \sum_{\substack{\boldsymbol{\sigma}'_{m_1},\boldsymbol{\sigma}'_{m_2}\\ \boldsymbol{\sigma}_{m_1},\boldsymbol{\sigma}_{m_1}}} \bar{\mathcal{G}}^{(n+m_1+m_2)}_{\boldsymbol{\sigma}'_{n+m_1+m_2};\boldsymbol{\sigma}_{n+m_1+m_2}}\left(\mathbf{i}|\boldsymbol{\tau}'_{n+m_1+m_2};\boldsymbol{\tau}_{n+m_1+m_2}\right) \\
&\qquad\qquad \bar{\mathcal{O}}^{(m_1)}_{\boldsymbol{\sigma}'_{m_1};\boldsymbol{\sigma}_{m_1}}\left(\mathbf{i}|\boldsymbol{\tau}'_{m_1};\boldsymbol{\tau}_{m_1}\right)\bar{\mathcal{O}}^{(m_2)}_{\boldsymbol{\sigma}'_{m_2};\boldsymbol{\sigma}_{m_2}}\left(\mathbf{i}|\boldsymbol{\tau}'_{m_2};\boldsymbol{\tau}_{m_2}\right) \\
&\quad \dots \\
&\equiv \bar{\mathcal{G}}^{(n)}_{\boldsymbol{\sigma}'_n;\boldsymbol{\sigma}_n}\left(\mathbf{i}|\boldsymbol{\tau}'_n;\boldsymbol{\tau}_n\right) \\
&\quad + \sum_{p=1}^{\infty}\frac{1}{p!}\int\limits_0^\beta \mathrm{d}\boldsymbol{\tau}_{m_1}\cdots\mathrm{d}\boldsymbol{\tau}_{m_p}\mathrm{d}\boldsymbol{\tau}'_{m_1}\cdots\mathrm{d}\boldsymbol{\tau}'_{m_p} \\
&\qquad \sum_{\substack{\boldsymbol{\sigma}'_{m_1},\boldsymbol{\sigma}'_{m_2}\\ \boldsymbol{\sigma}_{m_1},\boldsymbol{\sigma}_{m_1}}} \bar{\mathcal{G}}^{(n+m_1+\dots+m_p)}_{\boldsymbol{\sigma}'_{n+m_1+\dots+m_p};\boldsymbol{\sigma}_{n+m_1+\dots+m_p}}\left(\mathbf{i}|\boldsymbol{\tau}'_{n+m_1+\dots+m_p};\boldsymbol{\tau}_{n+m_1+\dots+m_p}\right) \\
&\qquad\qquad \bar{\mathcal{O}}^{(m_1)}_{\boldsymbol{\sigma}'_{m_1};\boldsymbol{\sigma}_{m_1}}\left(\mathbf{i}|\boldsymbol{\tau}'_{m_1};\boldsymbol{\tau}_{m_1}\right)\cdots\bar{\mathcal{O}}^{(m_p)}_{\boldsymbol{\sigma}'_{m_p};\boldsymbol{\sigma}_{m_p}}\left(\mathbf{i}|\boldsymbol{\tau}'_{m_p};\boldsymbol{\tau}_{m_p}\right)
\end{aligned}
\tag{3.49}
$$

in which the primed and unprimed bold greek symbols with index n are condensed variables for the corresponding primed and unprimed multiple greek variables form 1 to n, resp..

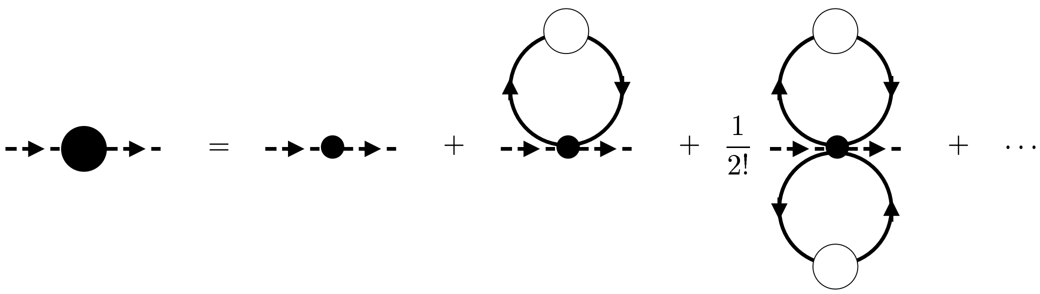


Figure 3.2: Diagram representation for local renormalized n-particle vertex of localized electrons $\bar{G}$: black circles indicate $\bar{G}$; small black circles - $\bar{\mathcal{G}}$; white circles - $\bar{\mathcal{O}}$; bold dashed arrows - multiple input and output lines for localized electrons; bold arrows - multiple input and output lines corresponding to the primed and unprimed bold greek symbols for auxiliary field operators

Additionally, the renormalized local n-particle Green's function $\bar{G}^{(n)}_{\sigma'_1,\dots,\sigma'_n;\sigma_1,\dots,\sigma_n}(\mathbf{i}'|\tau'_1,\dots,\tau'_n;\tau_1,\dots,\tau_n)$

can be also directly determined by functional

$$\begin{aligned}
&\bar{G}^{(n)}_{\sigma'_1,\ldots,\sigma'_n;\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}'|\tau'_1,\ldots,\tau'_n;\tau_1,\ldots,\tau_n\right)\\
&\quad=\frac{1}{\mathcal{Z}}\,\mathcal{S}^{(n;n)}_{\mathbf{i}'[\sigma'_1,\ldots,\sigma'_n;\sigma_1,\ldots,\sigma_n]}\left[\frac{\delta}{\delta\bar{\pi}\left(\tau\right)},\frac{\delta}{\delta\pi\left(\tau\right)}\right]\left(\tau'_1,\ldots,\tau'_n;\tau_1,\ldots,\tau_n\right)\mathcal{Z}\left[\pi,\bar{\pi}\right]\Bigg|_{\pi=\bar{\pi}=0}
\end{aligned}\tag{3.50}$$

where functional differential operator $\bar{\mathcal{S}}^{(n;n)}_{\mathbf{i}'[\sigma'_1,\ldots,\sigma'_n;\sigma_1,\ldots,\sigma_n]}\left[\frac{\delta}{\delta\bar{\pi}\left(\tau\right)},\frac{\delta}{\delta\pi\left(\tau\right)}\right]\left(\tau'_1,\ldots,\tau'_n;\tau_1,\ldots,\tau_n\right)$ can be found as in expression (A.6c).

The quantity $\bar{\mathcal{O}}^{(n)}_{\sigma'_1,\ldots,\sigma'_n;\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}|\tau'_1,\ldots,\tau'_n;\tau_1,\ldots,\tau_n\right)$ is nothing but the n-particle cumulant of the auxiliary fields with site variable $\mathbf{i}$

$$\begin{aligned}
\bar{\mathcal{O}}^{(n)}_{\boldsymbol{\sigma}'_n;\boldsymbol{\sigma}_n}\left(\mathbf{i}|\boldsymbol{\tau}'_n;\boldsymbol{\tau}_n\right)&=\bar{\mathcal{O}}^{(n)}_{\sigma'_1,\ldots,\sigma'_n;\sigma_1,\ldots\sigma_n}\left(\mathbf{i}|\tau'_1,\ldots,\tau'_n;\tau_1,\ldots,\tau_n\right)\\
&=(-1)^n\,\frac{1}{(n!)^2}\,\hat{\Omega}^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{i}|\tau_1,\ldots,\tau_n;\tau'_1,\ldots,\tau'_n\right)
\end{aligned}\tag{3.51}$$

The above equation can be formally written in the form of an exponential functional

$$\bar{G}=\bar{\mathcal{G}}\ \mathrm{e}^{\ \bar{\mathcal{O}}}.\tag{3.52}$$

It provides an inversion which is formally read

$$\bar{\mathcal{G}}=\bar{G}\ \mathrm{e}^{\ -\bar{\mathcal{O}}}\tag{3.53}$$

where the series expansion of the exponential functional is already supplied by the second equation of (3.49) and the prefactor $\frac{1}{p!}$ changes to $\frac{(-1)^p}{p!}$.

Other useful identities that one can obtain from the equation (3.49) and its inversion (3.53) are

$$\begin{aligned}
\frac{\delta}{\delta\bar{\mathcal{O}}^{(m)}_{\boldsymbol{\sigma}'_m;\boldsymbol{\sigma}_m}\left(\mathbf{i}|\boldsymbol{\tau}'_m;\boldsymbol{\tau}_m\right)}\,\bar{G}^{(n)}_{\boldsymbol{\sigma}'_n;\boldsymbol{\sigma}_n}\left(\mathbf{i}|\boldsymbol{\tau}'_n;\boldsymbol{\tau}_n\right)&=\bar{G}^{(n+m)}_{\boldsymbol{\sigma}'_n,\boldsymbol{\sigma}'_m;\boldsymbol{\sigma}_n,\boldsymbol{\sigma}_m}\left(\mathbf{i}|\boldsymbol{\tau}'_n,\boldsymbol{\tau}'_m;\boldsymbol{\tau}_n,\boldsymbol{\tau}_m\right)\\
&\equiv\bar{G}^{(n+m)}_{\boldsymbol{\sigma}'_{n+m};\boldsymbol{\sigma}_{n+m}}\left(\mathbf{i}|\boldsymbol{\tau}'_{n+m};\boldsymbol{\tau}_{n+m}\right)\\
\frac{\delta}{\delta\bar{\mathcal{O}}^{(m)}_{\boldsymbol{\sigma}'_m;\boldsymbol{\sigma}_m}\left(\mathbf{i}|\boldsymbol{\tau}'_m;\boldsymbol{\tau}_m\right)}\,\bar{\mathcal{G}}^{(n)}_{\boldsymbol{\sigma}'_n;\boldsymbol{\sigma}_n}\left(\mathbf{i}|\boldsymbol{\tau}'_n;\boldsymbol{\tau}_n\right)&=-\bar{\mathcal{G}}^{(n+m)}_{\boldsymbol{\sigma}'_n,\boldsymbol{\sigma}'_m;\boldsymbol{\sigma}_n,\boldsymbol{\sigma}_m}\left(\mathbf{i}|\boldsymbol{\tau}'_n,\boldsymbol{\tau}'_m;\boldsymbol{\tau}_n,\boldsymbol{\tau}_m\right)\\
&\equiv-\bar{\mathcal{G}}^{(n+m)}_{\boldsymbol{\sigma}'_{n+m};\boldsymbol{\sigma}_{n+m}}\left(\mathbf{i}|\boldsymbol{\tau}'_{n+m};\boldsymbol{\tau}_{n+m}\right)
\end{aligned}\tag{3.54}$$

The equation (3.49) can be also obtained by the diagram technique used by Metzner in [14]. This work did not point out a concrete equation or an argument determining the "self-energy" $\bar{\mathcal{O}}^{(n)}_{\boldsymbol{\sigma}'_n;\boldsymbol{\sigma}_n}\left(\mathbf{i}|\boldsymbol{\tau}'_n;\boldsymbol{\tau}_n\right)$, but in present thesis we did. The advantage of the current functional integral formalism is that that equation is mathematically and automatically kept in context, and the explicit form of $\bar{\mathcal{O}}^{(n)}_{\sigma'_1,\ldots,\sigma'_n;\sigma_1,\ldots,\sigma_n}$ $\left(\mathbf{i}|\tau'_1,\ldots,\tau'_n;\tau_1,\ldots,\tau_n\right)$ and their related coefficients can be found as in (3.51).

The renormalized vertex $\bar{G}^{(n)}_{\sigma'_1,\ldots,\sigma'_n;\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}'|\tau'_1,\ldots,\tau'_n;\tau_1,\ldots,\tau_n\right)$ contains in itself different collective modes of the system reflected by the appearance of the many-particle cumulants of the auxiliary fields with site variable $\mathbf{i}$, which are contributions of processes where electrons leaving from a certain site $\mathbf{i}$ go the conduction band and after some many-body processes in the "effective" conduction band which are caused by the hoppings, the hybridizations and also the local many-body interactions of the rest of the system, they return to the site $\mathbf{i}$. The high order terms of $\bar{\mathcal{O}}^{(n)}_{\sigma'_1,\ldots,\sigma'_n;\sigma_1,\ldots\sigma_n}\left(\mathbf{i}|\tau'_1\ldots\tau'_n;\tau_1\ldots\tau_n\right)$

in (3.49) indicate the multiple-visit processes of the electrons at the site $\mathbf{i}$. The multiple returns of the electrons at the site $\mathbf{i}$ cause the contributions of high order cumulants in (3.49).

To completely determine the self-energy of the auxiliary fields one has to find out a way to obtain their many-particle Green's functions.

One can perform $2n$ differentiations over the external sources $\pi_{\mathbf{i}\sigma}(\tau)$ and $\bar{\pi}_{\mathbf{i}\sigma}(\tau)$ to get an explicit but extremely complicated form of the n-particle Green's functions of auxiliary fields. To do that do not forget the commutation relationship (A.6c) when moving the field-operators $\pi_{\mathbf{i}\sigma}(\tau)$ or $\bar{\pi}_{\mathbf{i}\sigma}(\tau)$ from the right side to the left side of any functional-differential expression. The results of those manipulations, once again, confirm the correctness of the relationships between the Green's functions of the localized electrons and those of the auxiliary fields obtained in (3.39). Looking deeply into the graph structure of $\hat{G}^{(n)}_{\sigma'_1,\ldots,\sigma'_n;\sigma_1,\ldots,\sigma_n}(\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n;\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n)$, one can recognize that it contains from 1 to $2n$ renormalized vertices $\bar{G}^{(n)}_{\sigma'_1,\ldots,\sigma'_n;\sigma_1,\ldots,\sigma_n}(\mathbf{i}|\tau'_1,\ldots,\tau'_n;\tau_1,\ldots,\tau_n)$ where $\mathbf{i}$ can be one of $\{\mathbf{i}'_1,\ldots,\mathbf{i}'_n,\mathbf{i}_1,\ldots,\mathbf{i}_n\}$. We leave this task to next Section where an analytical structure of the many-particle cumulants will be found.

SECTION 3.5

The structure of the many-particle Green's functions

To obtain one-particle Green's function one uses Dyson's equation abling the explicit consideration of only one-particle irreducible diagrams contributing to the self-energy as it was in last Section 3.4.

The situation is much more complicated at the level of many-particle Green's functions. For two-particle Green's functions and two-particle cumulants one has the well-known Bethe-Salpeter equation of motion to determine two-particle irreducible diagrams but for higher order of many-particle Green's functions there are no previous works pointing out how determine them. In this Section an attempt to find an equation system for many-particle functions like Dyson's equation for one-particle function or Bethe-Salpeter integral equations for two-particle functions are represented.

The following calculations are the generalization of the calculation for one-particle Green's function of the auxiliary fields in (3.47). First we calculate the following differentiation of the generating functional for the auxiliary fields (3.44)

$$\begin{aligned}
&\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_n\sigma_n}(\tau_n)}\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_1\sigma_1}(\tau_1)}\ \mathcal{Z}[\pi,\bar{\pi}]\\
&=\mathcal{Z}_0\bar{\mathcal{Z}}_0\ \bar{\mathcal{Z}}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right]\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_n\sigma_n}(\tau_n)}\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_1\sigma_1}(\tau_1)}\\
&\qquad\mathscr{T}_\tau\exp\left\{-\int_0^\beta \mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\pi}_{\mathbf{i}\sigma}(\tau)\,\Omega^{(0)}_{\sigma\sigma'}\left(\mathbf{i}\ \tau;\mathbf{i}'\ \tau'\right)\pi_{\mathbf{i}'\sigma'}\left(\tau'\right)\right\}\\
&=(-1)^{\frac{n(n+1)}{2}}\mathcal{Z}_0\bar{\mathcal{Z}}_0\ \bar{\mathcal{Z}}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right]\prod_{k=1}^{n}\left(\int_0^\beta \mathrm{d}\theta'_k\sum_{\mathbf{j}'_k,\varsigma'_k}\Omega^{(0)}_{\sigma_k\varsigma'_k}\left(\mathbf{i}_k\ \tau_k;\mathbf{j}'_k\ \theta'_k\right)\pi_{\mathbf{j}'_k\varsigma'_k}\left(\theta'_k\right)\right)\\
&\qquad\mathscr{T}_\tau\exp\left\{-\int_0^\beta \mathrm{d}\tau\mathrm{d}\tau'\sum_{\mathbf{i}\mathbf{i}',\sigma\sigma'}\bar{\pi}_{\mathbf{i}\sigma}(\tau)\,\Omega^{(0)}_{\sigma\sigma'}\left(\mathbf{i}\ \tau;\mathbf{i}'\ \tau'\right)\pi_{\mathbf{i}'\sigma'}\left(\tau'\right)\right\}
\end{aligned}\tag{3.55a}$$

where the factor $(-1)^{\frac{n(n+1)}{2}}$ is the result of applying n differential operators $\dfrac{\delta}{\delta\bar{\pi}}$ on the exponential function and of anticommutation between the differential operator $\dfrac{\delta}{\delta\bar{\pi}}$ and the auxiliary field-operator

π, then bring the $\bar{\mathcal{Z}}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right] = \exp\left\{\sum_{\mathbf{i}} \bar{\mathcal{S}}_{\mathbf{i}}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right]\right\}$ to right side of the product of the external source field operators $\pi_{\mathbf{j}'\varsigma'}(\theta')$. For each permutation it gets an extra term which does not contain the external source field operators

$$\begin{aligned}
&\left[\pi_{\mathbf{j}'\varsigma'}(\theta'), \exp\left\{\sum_{\mathbf{i}} \bar{\mathcal{S}}_{\mathbf{i}}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right]\right\}\right] \\
&= \left[\pi_{\mathbf{j}'\varsigma'}(\theta'), \sum_{\mathbf{i}} \bar{\mathcal{S}}_{\mathbf{i}}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right]\right] \exp\left\{\sum_{\mathbf{i}} \bar{\mathcal{S}}_{\mathbf{i}}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right]\right\} \\
&= \bar{\mathcal{S}}^{(1;0)}_{\mathbf{j}'[\varsigma';\cdot]}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right](\theta') \ \exp\left\{\sum_{\mathbf{i}} \bar{\mathcal{S}}_{\mathbf{i}}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right]\right\}
\end{aligned} \tag{3.55b}$$

then the equation (3.55a) becomes

$$= (-1)^{\frac{n(n+1)}{2}} \prod_{k=1}^{n}\left(\int_0^\beta \mathrm{d}\theta'_k \sum_{\mathbf{j}'_k,\varsigma'_k} \Omega^{(0)}_{\sigma_k\varsigma'_k}\left(\mathbf{i}_k\ \tau_k; \mathbf{j}'_k\ \theta'_k\right)\left(\pi_{\mathbf{j}'_k\varsigma'_k}(\theta'_k) - \bar{\mathcal{S}}^{(1;0)}_{\mathbf{j}'_k[\varsigma'_k;\cdot]}(\theta'_k)\right)\right) \mathcal{Z}[\pi,\bar{\pi}]\,. \tag{3.55c}$$

For $n=1$, this corresponds to the first line of (3.47e). The steps to surmounted in the following, are similar to the ones for the case $n=1$. They are much more complicated and the formulae are clumsy. In the further writing the dependence on differential variables in $\bar{\mathcal{S}}^{(p,0)}$ will not be written down for short. Let's consider the product

$$\prod_{k=1}^{n}\left(\int_0^\beta \mathrm{d}\theta'_k \sum_{\mathbf{j}'_k,\varsigma'_k} \Omega^{(0)}_{\sigma_k\varsigma'_k}\left(\mathbf{i}_k\ \tau_k; \mathbf{j}'_k\ \theta'_k\right)\left(\pi_{\mathbf{j}'_k\varsigma'_k}(\theta'_k) - \bar{\mathcal{S}}^{(1;0)}_{\mathbf{j}'_k[\varsigma'_k;\cdot]}(\theta'_k)\right)\right).$$

Expanding this product as usual without changing the order of the terms in each product and moving the external source field operators $\pi_{\mathbf{j}'\varsigma'}(\theta')$ in these products from right side to left side of all differential expressions yields

$$\begin{aligned}
&\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_n\sigma_n}(\tau_n)} \cdots \frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_1\sigma_1}(\tau_1)}\ \mathcal{Z}[\pi,\bar{\pi}] = (-1)^{\frac{n(n+1)}{2}} \int_0^\beta \mathrm{d}\vartheta_1\cdots\mathrm{d}\vartheta_n \sum_{\substack{\varrho_1\cdots\varrho_n \\ \mathbf{l}_1\ldots\mathbf{l}_n}} \int_0^\beta \mathrm{d}\theta'_1\cdots\mathrm{d}\theta'_n \sum_{\substack{\varsigma'_1\cdots\varsigma'_n \\ \mathbf{j}'_1\cdots\mathbf{j}'_n}} \\
&\Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varrho_1,\ldots,\varrho_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n; \mathbf{l}_1\ \vartheta_1,\ldots,\mathbf{l}_n\ \vartheta_n\right)\Omega^{(0)}_{\varrho_1\varsigma'_1}\left(\mathbf{l}_1\ \vartheta_1;\mathbf{j}'_1\ \theta'_1\right)\ldots\Omega^{(0)}_{\varrho_n\varsigma'_n}\left(\mathbf{l}_n\ \vartheta_n;\mathbf{j}'_n\ \theta'_n\right) \\
&\left(\sum_{k=0}^{n}\frac{1}{k!}\,\pi_{\varsigma'_1}\left(\mathbf{j}'_1\ \theta'_1\right)\ldots\pi_{\varsigma'_k}\left(\mathbf{j}'_k\ \theta'_k\right)\left(\mathrm{e}^{\tilde{\mathcal{S}}}\right)^{(n-k)}_{\varsigma'_{k+1},\ldots,\varsigma'_n}\left(\mathbf{j}'_{k+1}\ \theta'_{k+1},\ldots,\mathbf{j}'_n\ \theta'_n\right)\right)\ \mathcal{Z}[\pi,\bar{\pi}]
\end{aligned} \tag{3.56a}$$

where

$$\tilde{\mathcal{S}}^{(n)}_{\varsigma'_1,\ldots,\varsigma'_n}\left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n\right) = (-1)^{\frac{n(n+1)}{2}}\ \delta_{\mathbf{j}'_1\mathbf{j}'_n}\ldots\delta_{\mathbf{j}'_{n-1}\mathbf{j}'_n}\frac{1}{n!}\,\bar{\mathcal{S}}^{(n;0)}_{\mathbf{j}'_n[\varsigma'_1,\ldots,\varsigma'_n;\cdot]}\left(\theta'_1,\ldots,\theta'_n\right). \tag{3.56b}$$

Here, for short, the exponential function notations (A.3e) are used for the sum of products of differential expressions $\tilde{\mathcal{S}}^{(n)}_{\varsigma'_1,\ldots,\varsigma'_n}\left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n\right)$ appearing in each k-order terms of the external source operators. The function $\Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varrho_1,\ldots,\varrho_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{l}_1\ \vartheta_1,\ldots,\mathbf{l}_n\ \vartheta_n\right)$ ensures the possible permutations of all indices and the sign of each permutation in the expression.

Inserting (3.56a) into (3.46) and using the symmetric form

$$\frac{\delta}{\delta\pi_{\mathbf{i}'_1\sigma'_1}(\tau'_1)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}'_n\sigma'_n}(\tau'_n)}=(-1)^{\frac{n(n-1)}{2}}\frac{1}{n!}\int_0^\beta \mathrm{d}\vartheta'_1\cdots\mathrm{d}\vartheta'_n\sum_{\substack{\varrho'_1\cdots\varrho'_n\\ \mathbf{l}'_1\cdots\mathbf{l}'_n}} \frac{\delta}{\delta\pi_{\mathbf{l}'_n\varrho'_n}(\vartheta'_n)}\cdots\frac{\delta}{\delta\pi_{\mathbf{l}'_1\varrho'_1}(\vartheta'_1)}\,\Delta^{(n)}_{\varrho'_1,\ldots,\varrho'_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{l}'_1\ \vartheta'_1,\ldots,\mathbf{l}'_n\ \vartheta'_n;\mathbf{i}'_1\ \tau_1,\ldots,\mathbf{i}'_n\ \tau'_n\right) \tag{3.57}$$

the many-particle Green's functions of the auxiliary fields defined in (3.46) now can be rewritten as follows

$$\begin{aligned}
&\Omega^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n\right)\\
&\quad\equiv(-1)^n\frac{1}{\mathcal{Z}}\frac{\delta}{\delta\pi_{\mathbf{i}'_1\sigma'_1}(\tau'_1)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}'_n\sigma'_n}(\tau'_n)}\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_n\sigma_n}(\tau_n)}\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}_1\sigma_1}(\tau_1)}\,\mathcal{Z}[\pi,\bar{\pi}]\Bigg|_{\pi=\bar{\pi}=0}\\
&\quad\equiv\frac{1}{\mathcal{Z}}\int_0^\beta \mathrm{d}\vartheta_1\cdots\mathrm{d}\vartheta_n\sum_{\substack{\varrho_1\cdots\varrho_n\\ \mathbf{l}_1\cdots\mathbf{l}_n}}\frac{1}{n!}\int_0^\beta \mathrm{d}\vartheta'_1\cdots\mathrm{d}\vartheta'_n\sum_{\substack{\varrho'_1\cdots\varrho'_n\\ \mathbf{l}'_1\cdots\mathbf{l}'_n}}\int_0^\beta \mathrm{d}\theta'_1\cdots\mathrm{d}\theta'_n\sum_{\substack{\varsigma'_1\cdots\varsigma'_n\\ \mathbf{j}'_1\cdots\mathbf{j}'_n}}\\
&\quad\Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varrho_1,\ldots,\varrho_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{l}_1\ \vartheta_1,\ldots,\mathbf{l}_n\ \vartheta_n\right)\Omega^{(0)}_{\varrho_1\varsigma'_1}\left(\mathbf{l}_1\ \vartheta_1;\mathbf{j}'_1\ \theta'_1\right)\ldots\Omega^{(0)}_{\varrho_n\varsigma'_n}\left(\mathbf{l}_n\ \vartheta_n;\mathbf{j}'_n\ \theta'_n\right)\\
&\quad\frac{\delta}{\delta\pi_{\mathbf{l}'_n\varrho'_n}(\vartheta'_n)}\cdots\frac{\delta}{\delta\pi_{\mathbf{l}'_1\varrho'_1}(\vartheta'_1)}\\
&\qquad\left(\sum_{k=0}^n\frac{1}{k!}\pi_{\varsigma'_1}\left(\mathbf{j}'_1\ \theta'_1\right)\ldots\pi_{\varsigma'_k}\left(\mathbf{j}'_k\ \theta'_k\right)\left(\mathrm{e}^{\tilde{\mathcal{S}}}\right)^{(n-k)}_{\varsigma'_{k+1},\ldots,\varsigma'_n}\left(\mathbf{j}'_{k+1}\ \theta'_{k+1},\ldots,\mathbf{j}'_n\ \theta'_n\right)\right)\mathcal{Z}[\pi,\bar{\pi}]\Bigg|_{\pi=\bar{\pi}=0}\\
&\qquad\quad\Delta^{(n)}_{\varrho'_1,\ldots,\varrho'_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{l}'_1\ \vartheta'_1,\ldots,\mathbf{l}'_n\ \vartheta'_n;\mathbf{i}'_1\ \tau_1,\ldots,\mathbf{i}'_n\ \tau'_n\right).
\end{aligned} \tag{3.58}$$

Inserting the results provided in (A.7) into the functional differentiation

$$\begin{aligned}
&\frac{1}{\mathcal{Z}}\frac{\delta}{\delta\pi_{\mathbf{l}'_n\varrho'_n}(\vartheta'_n)}\cdots\frac{\delta}{\delta\pi_{\mathbf{l}'_1\varrho'_1}(\vartheta'_1)}\\
&\quad\left(\sum_{k=0}^n\frac{1}{k!}\pi_{\varsigma'_1}\left(\mathbf{j}'_1\ \theta'_1\right)\ldots\pi_{\varsigma'_k}\left(\mathbf{j}'_k\ \theta'_k\right)\left(\mathrm{e}^{\tilde{\mathcal{S}}}\right)^{(n-k)}_{\varsigma'_{k+1},\ldots,\varsigma'_n}\left(\mathbf{j}'_{k+1}\ \theta'_{k+1},\ldots,\mathbf{j}'_n\ \theta'_n\right)\right)\mathcal{Z}[\pi,\bar{\pi}]\Bigg|_{\pi=\bar{\pi}=0}
\end{aligned} \tag{3.59}$$

and summing up one gets the "explicit" expression for the n-particle Green's function containing only the π-free terms

$$\begin{aligned}
&\Omega^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n\right)\\
&\quad\equiv\int_0^\beta \mathrm{d}\vartheta_1\cdots\mathrm{d}\vartheta_n\sum_{\substack{\varrho_1\cdots\varrho_n\\ \mathbf{l}_1\cdots\mathbf{l}_n}}\int_0^\beta \mathrm{d}\vartheta'_1\cdots\mathrm{d}\vartheta'_n\sum_{\substack{\varrho'_1\cdots\varrho'_n\\ \mathbf{l}'_1\cdots\mathbf{l}'_n}}\int_0^\beta \mathrm{d}\theta'_1\cdots\mathrm{d}\theta'_n\sum_{\substack{\varsigma'_1\cdots\varsigma'_n\\ \mathbf{j}'_1\cdots\mathbf{j}'_n}}\\
&\quad\Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varrho_1,\ldots,\varrho_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{l}_1\ \vartheta_1,\ldots,\mathbf{l}_n\ \vartheta_n\right)\Omega^{(0)}_{\varrho_1\varsigma'_1}\left(\mathbf{l}_1\ \vartheta_1;\mathbf{j}'_1\ \theta'_1\right)\ldots\Omega^{(0)}_{\varrho_n\varsigma'_n}\left(\mathbf{l}_n\ \vartheta_n;\mathbf{j}'_n\ \theta'_n\right)\\
&\quad\Bigg(\sum_{k=0}^n\frac{1}{(k!)^2}\Delta^{(k)}_{\varsigma'_1,\ldots,\varsigma'_k;\varrho'_1,\ldots,\varrho'_k}\left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_k\ \theta'_k;\mathbf{l}'_1\ \vartheta'_1,\ldots,\mathbf{l}'_k\ \vartheta'_k\right)\\
&\qquad\frac{1}{(n-k)!}\frac{1}{\mathcal{Z}}\frac{\delta}{\delta\pi_{\mathbf{l}'_n\varrho'_n}(\vartheta'_n)}\cdots\frac{\delta}{\delta\pi_{\mathbf{l}'_{k+1}\varrho'_{k+1}}(\vartheta'_{k+1})}\left(\mathrm{e}^{\tilde{\mathcal{S}}}\right)^{(n-k)}_{\varsigma'_{k+1},\ldots,\varsigma'_n}\left(\mathbf{j}'_{k+1}\ \theta'_{k+1},\ldots,\mathbf{j}'_n\ \theta'_n\right)\mathcal{Z}[\pi,\bar{\pi}]\Bigg|_{\pi=\bar{\pi}=0}\Bigg)\\
&\qquad\Delta^{(n)}_{\varrho'_1,\ldots,\varrho'_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{l}'_1\ \vartheta'_1,\ldots,\mathbf{l}'_n\ \vartheta'_n;\mathbf{i}'_1\ \tau_1,\ldots,\mathbf{i}'_n\ \tau'_n\right).
\end{aligned} \tag{3.60a}$$

The appearance of the functions $\Delta^{(k)}_{\varsigma'_1,\ldots,\varsigma'_k;\varrho'_1,\ldots,\varrho'_k}\left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_k\ \theta'_k;\mathbf{l}'_1\ \vartheta'_1,\ldots,\mathbf{j}'_k\ \vartheta'_k\right)$ is the result of performing k times of differential operations on the k-order terms of the external source field operators. This function contains also the sign of each term resulted by anticommunication relation of the field-operator π and its differential operator $\dfrac{\delta}{\delta\pi}$.

Applying the expansion theorem for determinants (A.2) to (3.60a) then it can be rewritten as

$$
\begin{aligned}
&\Omega^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n\right)\\
&\quad\equiv\int_0^\beta \mathrm{d}\vartheta_1\cdots\mathrm{d}\vartheta_n\mathrm{d}\vartheta'_1\cdots\mathrm{d}\vartheta'_n\sum_{\substack{\varrho_1\cdots\varrho_n\\ \mathbf{l}_1\cdots\mathbf{l}_n}}\ \sum_{\substack{\varrho'_1\cdots\varrho'_n\\ \mathbf{l}'_1\cdots\mathbf{l}'_n}}\Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varrho_1,\ldots,\varrho_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{l}_1\ \vartheta_1,\ldots,\mathbf{l}_n\ \vartheta_n\right)\\
&\qquad\Bigg(\int_0^\beta \mathrm{d}\theta_1\cdots\mathrm{d}\theta_n\mathrm{d}\theta'_1\cdots\mathrm{d}\theta'_n\sum_{\substack{\varsigma_1\cdots\varsigma_n\\ \mathbf{j}_1\cdots\mathbf{j}_n}}\ \sum_{\substack{\varsigma'_1\cdots\varsigma'_n\\ \mathbf{j}'_1\cdots\mathbf{j}'_n}}\\
&\qquad\Bigg(\sum_{k=0}^n\frac{1}{(k!)^2}\ \Delta^{(k)}_{\varrho_1,\ldots,\varrho_k;\varsigma_1,\ldots,\varsigma_k}\left(\mathbf{l}_1\ \theta_1,\ldots,\mathbf{l}_k\ \theta_k;\mathbf{j}_1\ \theta_1,\ldots,\mathbf{j}_k\ \theta_k\right)\\
&\qquad\frac{1}{k!}\ \Omega^{(0)}_{\varsigma_1\varsigma'_1}\left(\mathbf{j}_1\ \theta_1;\mathbf{j}'_1\ \theta'_1\right)\ldots\Omega^{(0)}_{\varsigma_k\varsigma'_k}\left(\mathbf{j}_k\ \theta_k;\mathbf{j}'_k\ \theta'_k\right)\Delta^{(k)}_{\varsigma'_1,\ldots,\varsigma'_k;\varrho'_1,\ldots,\varrho'_k}\left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_k\ \theta'_k;\mathbf{l}'_1\ \vartheta'_1,\ldots,\mathbf{l}'_k\ \vartheta'_k\right)\\
&\qquad\frac{1}{(n-k)!}\ \Delta^{(n-k)}_{\varrho_{k+1},\ldots,\varrho_n;\varsigma_{k+1},\ldots,\varsigma_n}\left(\mathbf{l}_{k+1}\ \theta_{k+1},\ldots,\mathbf{l}_n\ \theta_n;\mathbf{j}_{k+1}\ \theta_{k+1},\ldots,\mathbf{j}_n\ \theta_n\right)\\
&\qquad\qquad\Omega^{(0)}_{\varsigma_{k+1}\varsigma'_{k+1}}\left(\mathbf{j}_{k+1}\ \theta_{k+1};\mathbf{j}'_{k+1}\ \theta'_{k+1}\right)\ldots\Omega^{(0)}_{\varsigma_n\varsigma'_n}\left(\mathbf{j}_n\ \theta_n;\mathbf{j}'_n\ \theta'_n\right)\\
&\qquad\frac{1}{(n-k)!}\ \frac{1}{\mathcal{Z}}\ \frac{\delta}{\delta\pi_{\mathbf{l}'_n\varrho'_n}\left(\vartheta'_n\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{l}'_{k+1}\varrho'_{k+1}}\left(\vartheta'_{k+1}\right)}\\
&\qquad\qquad\left(\mathrm{e}^{\tilde{S}}\right)^{(n-k)}_{\varsigma'_{k+1},\ldots,\varsigma'_n}\left(\mathbf{j}'_{k+1}\ \theta'_{k+1},\ldots,\mathbf{j}'_n\ \theta'_n\right)\ \mathcal{Z}\left[\pi,\bar{\pi}\right]\Bigg|_{\pi=\bar{\pi}=0}\Bigg)\Bigg)\\
&\qquad\qquad\qquad\Delta^{(n)}_{\varrho'_1,\ldots,\varrho'_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{l}'_1\ \vartheta'_1,\ldots,\mathbf{l}'_n\ \vartheta'_n;\mathbf{i}'_1\ \tau_1,\ldots,\mathbf{i}'_n\ \tau'_n\right).
\end{aligned}
\tag{3.60b}
$$

Integrating and summing over possible indices the equation (3.60b) is simplified as follows

$$
\begin{aligned}
&\Omega^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n\right)\\
&\quad\equiv\int_0^\beta \mathrm{d}\vartheta_1\cdots\mathrm{d}\vartheta_n\mathrm{d}\vartheta'_1\cdots\mathrm{d}\vartheta'_n\sum_{\substack{\varrho_1\cdots\varrho_n\\ \mathbf{l}_1\cdots\mathbf{l}_n}}\ \sum_{\substack{\varrho'_1\cdots\varrho'_n\\ \mathbf{l}'_1\cdots\mathbf{l}'_n}}\Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varrho_1,\ldots,\varrho_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{l}_1\ \vartheta_1,\ldots,\mathbf{l}_n\ \vartheta_n\right)\\
&\Bigg(\sum_{k=0}^n\frac{1}{k!}\ \Omega^{(0)}_{\varrho_1\varrho'_1}\left(\mathbf{l}_1\ \vartheta_1;\mathbf{l}'_1\ \vartheta'_1\right)\ldots\Omega^{(0)}_{\varrho_k\varrho'_k}\left(\mathbf{l}_k\ \vartheta_k;\mathbf{l}'_k\ \vartheta'_k\right)\ \frac{1}{(n-k)!}\int_0^\beta \mathrm{d}\theta'_{k+1}\cdots\mathrm{d}\theta'_n\sum_{\substack{\varsigma'_{k+1}\cdots\varsigma'_n\\ \mathbf{j}'_{k+1}\cdots\mathbf{j}'_n}}\\
&\quad\Omega^{(0)}_{\varrho_{k+1}\varsigma'_{k+1}}\left(\mathbf{l}_{k+1}\ \vartheta_{k+1};\mathbf{j}'_{k+1}\ \theta'_{k+1}\right)\ldots\Omega^{(0)}_{\varrho_n\varsigma'_n}\left(\mathbf{l}_n\ \vartheta_n;\mathbf{j}'_n\ \theta'_n\right)\\
&\quad\frac{1}{\mathcal{Z}}\ \frac{\delta}{\delta\pi_{\mathbf{l}'_n\varrho'_n}\left(\vartheta'_n\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{l}'_{k+1}\varrho'_{k+1}}\left(\vartheta'_{k+1}\right)}\left(\mathrm{e}^{\tilde{S}}\right)^{(n-k)}_{\varsigma'_{k+1},\ldots,\varsigma'_n}\left(\mathbf{j}'_{k+1}\ \theta'_{k+1},\ldots,\mathbf{j}'_n\ \theta'_n\right)\ \mathcal{Z}\left[\pi,\bar{\pi}\right]\Bigg|_{\pi=\bar{\pi}=0}\Bigg)\\
&\qquad\qquad\Delta^{(n)}_{\varrho'_1,\ldots,\varrho'_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{l}'_1\ \vartheta'_1,\ldots,\mathbf{l}'_n\ \vartheta'_n;\mathbf{i}'_1\ \tau_1,\ldots,\mathbf{i}'_n\ \tau'_n\right).
\end{aligned}
\tag{3.60c}
$$

The identity (3.60c) has the following form when all indices are omitted

$$\Omega^{(n)} = \Delta^{(n)} \left(\sum_{k=0}^{n} \frac{1}{k!} \, \Omega^{(0)} \dots \Omega^{(0)} \, \frac{1}{(n-k)!} \, \Omega^{(0)} \dots \Omega^{(0)} \left(\frac{1}{\mathcal{Z}} \frac{\delta}{\delta \pi} \cdots \frac{\delta}{\delta \pi} \left(\mathrm{e}^{\tilde{\mathcal{S}}} \right)^{(n-k)} \mathcal{Z}\left[\pi, \bar{\pi}\right] \Bigg|_{\pi=\bar{\pi}=0} \right) \right) \Delta^{(n)}. \tag{3.60d}$$

Inserting (A.8a) into (3.60c) and comparing it with the expressions for the n-particle Green's function (2.7b) one can find what was expected.
It was found that with $n = 1$

$$\bar{\Omega}^{(1)}_{\sigma_1;\sigma'_1} \left(\mathbf{i}_1 \ \tau_1 ; \mathbf{i}'_1 \ \tau'_1 \right) = \bar{\Omega}^{(0)}_{\sigma_1;\sigma'_1} \left(\mathbf{i}_1 \ \tau_1 ; \mathbf{i}'_1 \ \tau'_1 \right) + \bar{\mathcal{L}}^{(1)}_{\sigma_1;\sigma'_1} \left(\mathbf{i}_1 \ \tau_1 ; \mathbf{i}'_1 \ \tau'_1 \right) \tag{3.61a}$$

and with $n \geq 2$

$$\begin{aligned} &\bar{\Omega}^{(n)}_{\sigma_1,\dots,\sigma_n;\sigma'_1,\dots,\sigma'_n} \left(\mathbf{i}_1 \ \tau_1, \dots, \mathbf{i}_n \ \tau_n ; \mathbf{i}'_1 \ \tau'_1, \dots, \mathbf{i}'_n \ \tau'_n \right) \\ &= \int_0^\beta \mathrm{d}\theta_1 \cdots \mathrm{d}\theta_n \mathrm{d}\theta'_1 \cdots \mathrm{d}\theta'_n \sum_{\substack{\varsigma_1,\dots,\varsigma_n \\ \mathbf{j}_1,\dots,\mathbf{j}_n}} \sum_{\substack{\varsigma'_1,\dots,\varsigma'_n \\ \mathbf{j}'_1,\dots,\mathbf{j}'_n}} \Delta^{(n)}_{\sigma_1,\dots,\sigma_n;\varsigma_1,\dots,\varsigma_n} \left(\mathbf{i}_1 \ \tau_1, \dots, \mathbf{i}_n \ \tau_n ; \mathbf{j}_1 \ \theta_1, \dots, \mathbf{j}_n \ \theta_n \right) \\ &\quad \bar{\mathcal{L}}^{(n)}_{\varsigma_1,\dots,\varsigma_n;\varsigma'_1,\dots,\varsigma'_n} \left(\mathbf{j}_1 \ \theta_1, \dots, \mathbf{j}_n \ \theta_n ; \mathbf{j}'_1 \ \theta'_1, \dots, \mathbf{j}'_n \ \theta'_n \right) \\ &\quad \Delta^{(n)}_{\varsigma'_1,\dots,\varsigma'_n;\sigma'_1,\dots,\sigma'_n} \left(\mathbf{j}'_1 \ \theta'_1, \dots, \mathbf{j}'_n \ \theta'_n ; \mathbf{i}'_1 \ \tau'_1, \dots, \mathbf{i}'_n \ \tau'_n \right) \end{aligned} \tag{3.61b}$$

As it was mentioned in expression (A.8), the functional $\bar{\mathcal{L}}^{(n)}_{\sigma_1,\dots,\sigma_n;\sigma'_1,\dots,\sigma'_n} \left(\mathbf{i}_1 \ \tau_1, \dots, \mathbf{i}_n \ \tau_n ; \mathbf{i}'_1 \ \tau'_1, \dots, \mathbf{i}'_n \ \tau'_n \right)$ is the connected part of the diagrams generated from the expression

$$\begin{aligned} &\frac{1}{n!} \int_0^\beta \mathrm{d}\theta'_1 \cdots \mathrm{d}\theta'_n \sum_{\substack{\varsigma'_1 \cdots \varsigma'_n \\ \mathbf{j}'_1 \cdots \mathbf{j}'_n}} \Omega^{(0)}_{\sigma_1 \varsigma'_1} \left(\mathbf{i}_1 \ \tau_1 ; \mathbf{j}'_1 \ \theta'_1 \right) \dots \Omega^{(0)}_{\sigma_n \varsigma'_n} \left(\mathbf{i}_n \ \tau_n ; \mathbf{j}'_n \ \theta'_n \right) \\ &\quad \frac{1}{\mathcal{Z}} \frac{\delta}{\delta \pi_{\mathbf{i}'_n \sigma'_n} \left(\tau'_n \right)} \cdots \frac{\delta}{\delta \pi_{\mathbf{i}'_1 \sigma'_1} \left(\tau'_1 \right)} \left(\mathrm{e}^{\tilde{\mathcal{S}}} \right)^{(n)}_{\varsigma'_1,\dots,\varsigma'_n} \left(\mathbf{j}'_1 \ \theta'_1, \dots, \mathbf{j}'_n \ \theta'_n \right) \ \mathcal{Z}\left[\pi, \bar{\pi}\right] \Bigg|_{\pi=\bar{\pi}=0} . \end{aligned} \tag{3.62}$$

They show the dependence of the many-particle cumulant of the auxiliary fields on the derivatives of the interaction Lagrangian i.e. the explicit dependence on many-body interaction characterized by local many-body correlation functions of the localized electrons.

In order to determine how this dependence looks like, one must consider the generating expression of the many-particle cumulants (3.62) in detail.

The functional $\left(\mathrm{e}^{\tilde{\mathcal{S}}} \right)^{(n)}_{\varsigma'_1,\dots,\varsigma'_n} \left(\mathbf{j}'_1 \ \theta'_1, \dots, \mathbf{j}'_n \ \theta'_n \right)$ containing several combinations of differential operators $\frac{\delta}{\delta \pi \left(\tau \right)}, \frac{\delta}{\delta \bar{\pi} \left(\tau \right)}$ at the sites $\mathbf{j}'_1, \dots, \mathbf{j}'_n$ generates internal diagrams connecting between internal sites $\mathbf{j}'_1, \dots, \mathbf{j}'_n$ and provides many possible combinations of "waiting lines", at least there are n "waiting lines" for each term, to establish connections to the given external sites $\mathbf{i}'_1, \dots, \mathbf{i}'_n$. These "waiting lines" will not return to the internal sites by any many-particle Green's function of the auxiliary field operators without appearance of external sites. As in Fig. 3.3, the "waiting lines" will wait for connecting to the external sites and the internal sites are connected by many-particle Green's functions of the auxiliary fields.

Since the internal diagrams consist of the renormalized local many-particle cumulants of the localized electrons and non-local many-particle Green's functions of the auxiliary fields connecting between internal sites $\mathbf{j}'_1, \ldots, \mathbf{j}'_n$, they require mathematically the balance of the numbers of differential operators $\dfrac{\delta}{\delta\pi(\tau)}$ and $\dfrac{\delta}{\delta\bar{\pi}(\tau)}$. They can be described by the expression

$$\left(\mathrm{e}^{\tilde{\mathcal{S}}}\right)^{(n,q)}_{\varsigma'_1,\ldots,\varsigma'_n,\varrho'_1,\ldots,\varrho'_q;\varrho_1,\ldots,\varrho_{n+q}} \left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n \middle|\ \vartheta'_1,\ldots,\ \vartheta'_q;\ \vartheta_1,\ldots,\ \vartheta_{n+q}\right)\ \mathcal{Z}\left[\pi,\bar{\pi}\right]\Bigg|_{\pi=\bar{\pi}=0} \tag{3.63a}$$

where

$$\begin{aligned}
&\left(\mathrm{e}^{\tilde{\mathcal{S}}}\right)^{(n,q)}_{\varsigma'_1,\ldots,\varsigma'_n,\varrho'_1,\ldots,\varrho'_q;\varrho_1,\ldots,\varrho_{n+q}} \left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n \middle|\ \vartheta'_1,\ldots,\ \vartheta'_q;\ \vartheta_1,\ldots,\ \vartheta_{n+q}\right) \\
&\quad= \sum_{k=1}^{n} \frac{1}{k!} \sum_{\substack{p_1+\cdots+p_k=n \\ m_1+\cdots+m_k=q \\ l_1+\cdots+l_k=n+q}} \prod_{r=1}^{k} (-1)^{(p_r+m_r+l_r)\ m_r} \\
&\qquad \tilde{\mathcal{S}}^{(p_r+m_r,l_r)}_{\varsigma'_{p_1+\cdots+p_{r-1}+1},\ldots,\varsigma'_{p_1+\cdots+p_r},\varrho'_{m_1+\cdots+m_{r-1}+1},\ldots,\varrho'_{m_1+\cdots+m_r};\varrho_{l_1+\cdots+l_{r-1}+1},\ldots,\varrho_{l_1+\cdots+l_r}} \\
&\qquad\quad \Big(\mathbf{j}'_{p_1+\cdots+p_{r-1}+1}\ \theta'_{p_1+\cdots+p_{r-1}+1},\ldots,\mathbf{j}'_{p_1+\cdots+p_r}\ \theta'_{p_1+\cdots+p_r} \Big|\ \vartheta'_{m_1+\cdots+m_{r-1}+1},\ldots,\ \vartheta'_{m_1+\cdots+m_r}; \\
&\qquad\qquad\qquad\qquad \vartheta_{l_1+\cdots+l_{r-1}+1},\ldots,\ \vartheta'_{l_1+\cdots+l_r}\Big)
\end{aligned} \tag{3.63b}$$

and

$$\begin{aligned}
&\tilde{\mathcal{S}}^{(p+m,l)}_{\varsigma'_1,\ldots,\varsigma'_p,\varrho'_1,\ldots,\varrho'_m;\varrho_1,\ldots,\varrho_l} \left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_p\ \theta'_p \middle|\ \vartheta'_1,\ldots,\ \vartheta'_m;\ \vartheta_1,\ldots,\ \vartheta'_l\right) \\
&\quad= (-1)^{\frac{p(p+1)}{2}}\ \frac{1}{p!}\ \frac{1}{m!}\ \frac{1}{l!}\ \delta_{\mathbf{j}'_1\mathbf{j}'_p} \cdots\ \delta_{\mathbf{j}'_{p-1}\mathbf{j}'_p} \\
&\qquad\qquad \bar{\mathcal{S}}^{(p+m,l)}_{\mathbf{j}'_p[\varsigma'_1,\ldots,\varsigma'_p,\varrho'_1,\ldots,\varrho'_m;\varrho_1,\ldots,\varrho_l]} \left(\theta'_1,\ldots,\ \theta'_p,\ \vartheta'_1,\ldots,\ \vartheta'_m;\ \vartheta_1,\ldots,\ \vartheta_l\right).
\end{aligned} \tag{3.63c}$$

For every fixed order n the index q is an integer number running from 0 to ∞. Once again, the exponential function notation is used for certain sum of products of differential operators $\tilde{\mathcal{S}}^{(p+m,l)}$. The factors in each term of the expression are the consequence of putting "extra" differential operators in right side of $\tilde{\mathcal{S}}^{(p+m,l)}$.

The "extra" differential operators which do not appear in the above sum provide the "waiting lines". They will couple with differential operators of external sites $\mathbf{i}'_1, \ldots, \mathbf{i}'_n$ to generate the external diagrams. The permutation of those differential operators causes the factorial factors in each term of the products.

The notation $\Sigma^{(n,q)}_{\varsigma'_1,\ldots,\varsigma'_n,\varrho'_1,\ldots,\varrho'_q;\varrho_1,\ldots,\varrho_{n+q}} \left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n \middle|\ \vartheta'_1,\ldots,\ \vartheta'_q;\ \vartheta_1,\ldots,\ \vartheta_{n+q}\right)$ will be used for the resultant functional of the expression (3.63a).

After inserting (3.63) into expression $\left(\mathrm{e}^{\tilde{\mathcal{S}}}\right)^{(n)}_{\varsigma'_1,\ldots,\varsigma'_n}(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n)$ it can be read as follows

$$\begin{aligned}
&\left(\mathrm{e}^{\tilde{\mathcal{S}}}\right)^{(n)}_{\varsigma'_1,\ldots,\varsigma'_n}\left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n\right)\\
&\quad\propto\sum_{q=0}^{\infty}\sum_{\substack{\varrho_1,\ldots,\varrho_{n+q}\\ \varrho'_1,\ldots,\varrho'_q}}\int_0^\beta \mathrm{d}\vartheta_1\ldots\mathrm{d}\vartheta_{n+q}\mathrm{d}\vartheta'_1\ldots\mathrm{d}\vartheta_q\sum_{k=1}^{n}\frac{1}{k!}\sum_{\substack{p_1+\cdots+p_k=n\\ m_1+\cdots+m_k=q\\ l_1+\cdots+l_k=n+q}}\prod_{r=1}^{k}(-1)^{(p_r+m_r+l_r)\ m_r}\\
&\qquad\tilde{\mathcal{S}}^{(p_r+m_r,l_r)}_{\varsigma'_{p_1+\cdots+p_{r-1}+1},\ldots,\varsigma'_{p_1+\cdots+p_r},\varrho'_{m_1+\cdots+m_{r-1}+1},\ldots,\varrho'_{m_1+\cdots+m_r};\varrho_{l_1+\cdots+l_{r-1}+1},\ldots,\varrho_{l_1+\cdots+l_r}}\\
&\qquad\Big(\mathbf{j}'_{p_1+\cdots+p_{r-1}+1}\ \theta'_{p_1+\cdots+p_{r-1}+1},\ldots,\mathbf{j}'_{p_1+\cdots+p_r}\ \theta'_{p_1+\cdots+p_r}|\ \vartheta'_{m_1+\cdots+m_{r-1}+1},\ldots,\ \vartheta'_{m_1+\cdots+m_r};\\
&\qquad\qquad\vartheta_{l_1+\cdots+l_{r-1}+1},\ldots,\ \vartheta'_{l_1+\cdots+l_r}\Big)\\
&\qquad\frac{\delta}{\delta\pi_{\mathbf{j}'_{p_r}\varrho'_{m_1+\cdots+m_{r-1}+1}}\left(\vartheta'_{m_1+\cdots+m_{r-1}+1}\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{j}'_{p_r}\varrho'_{m_1+\cdots+m_r}}\left(\vartheta'_{m_1+\cdots+m_r}\right)}\\
&\qquad\frac{\delta}{\delta\bar{\pi}_{\mathbf{j}'_{p_r}\varrho_{l_1+\cdots+l_r}}\left(\vartheta_{l_1+\cdots+l_r}\right)}\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{j}'_{p_r}\varrho_{l_1+\cdots+l_{r-1}+1}}\left(\vartheta_{l_1+\cdots+l_{r-1}+1}\right)}.
\end{aligned}\tag{3.64}$$

Substituting the above expression (3.64) in (3.62) one gets

$$\begin{aligned}
&\frac{1}{n!}\int_0^\beta\mathrm{d}\theta'_1\cdots\mathrm{d}\theta'_n\sum_{\substack{\varsigma'_1\cdots\varsigma'_n\\ \mathbf{j}'_1\cdots\mathbf{j}'_n}}\Omega^{(0)}_{\sigma_1\varsigma'_1}\left(\mathbf{i}_1\ \tau_1;\mathbf{j}'_1\ \theta'_1\right)\ldots\Omega^{(0)}_{\sigma_n\varsigma'_n}\left(\mathbf{i}_n\ \tau_n;\mathbf{j}'_n\ \theta'_n\right)\\
&\qquad\frac{1}{\mathcal{Z}}\ \frac{\delta}{\delta\pi_{\mathbf{i}'_n\sigma'_n}\left(\tau'_n\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}'_1\sigma'_1}\left(\tau'_1\right)}\left(\mathrm{e}^{\tilde{\mathcal{S}}}\right)^{(n)}_{\varsigma'_1,\ldots,\varsigma'_n}\left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n\right)\ \mathcal{Z}\left[\pi,\bar{\pi}\right]\Big|_{\pi=\bar{\pi}=0}\\
&\quad=\frac{1}{n!}\int_0^\beta\mathrm{d}\theta'_1\cdots\mathrm{d}\theta'_n\sum_{\substack{\varsigma'_1\cdots\varsigma'_n\\ \mathbf{j}'_1\cdots\mathbf{j}'_n}}\Omega^{(0)}_{\sigma_1\varsigma'_1}\left(\mathbf{i}_1\ \tau_1;\mathbf{j}'_1\ \theta'_1\right)\ldots\Omega^{(0)}_{\sigma_n\varsigma'_n}\left(\mathbf{i}_n\ \tau_n;\mathbf{j}'_n\ \theta'_n\right)\\
&\qquad\sum_{q=0}^{\infty}\sum_{\substack{\varrho_1,\ldots,\varrho_{n+q}\\ \varrho'_1,\ldots,\varrho'_q}}\int_0^\beta\mathrm{d}\vartheta_1\ldots\mathrm{d}\vartheta_{n+q}\mathrm{d}\vartheta'_1\ldots\mathrm{d}\vartheta_q\sum_{k=1}^{n}\frac{1}{k!}\sum_{\substack{p_1+\cdots+p_k=n\\ m_1+\cdots+m_k=q\\ l_1+\cdots+l_k=n+q}}\frac{1}{\mathcal{Z}}\ \frac{\delta}{\delta\pi_{\mathbf{i}'_n\sigma'_n}\left(\tau'_n\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}'_1\sigma'_1}\left(\tau'_1\right)}\\
&\qquad\prod_{r=1}^{k}(-1)^{(p_r+m_r+l_r)\ m_r}\ \tilde{\mathcal{S}}^{(p_r+m_r,l_r)}_{\varsigma'_{p_1+\cdots+p_{r-1}+1},\ldots,\varsigma'_{p_1+\cdots+p_r},\varrho'_{m_1+\cdots+m_{r-1}+1},\ldots,\varrho'_{m_1+\cdots+m_r};\varrho_{l_1+\cdots+l_{r-1}+1},\ldots,\varrho_{l_1+\cdots+l_r}}\\
&\qquad\Big(\mathbf{j}'_{p_1+\cdots+p_{r-1}+1}\ \theta'_{p_1+\cdots+p_{r-1}+1},\ldots,\mathbf{j}'_{p_1+\cdots+p_r}\ \theta'_{p_1+\cdots+p_r}|\ \vartheta'_{m_1+\cdots+m_{r-1}+1},\ldots,\ \vartheta'_{m_1+\cdots+m_r};\\
&\qquad\qquad\vartheta_{l_1+\cdots+l_{r-1}+1},\ldots,\ \vartheta'_{l_1+\cdots+l_r}\Big)\\
&\qquad\frac{\delta}{\delta\pi_{\mathbf{j}'_{p_r}\varrho'_{m_1+\cdots+m_{r-1}+1}}\left(\vartheta'_{m_1+\cdots+m_{r-1}+1}\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{j}'_{p_r}\varrho'_{m_1+\cdots+m_r}}\left(\vartheta'_{m_1+\cdots+m_r}\right)}\\
&\qquad\frac{\delta}{\delta\bar{\pi}_{\mathbf{j}'_{p_r}\varrho_{l_1+\cdots+l_r}}\left(\vartheta_{l_1+\cdots+l_r}\right)}\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{j}'_{p_r}\varrho_{l_1+\cdots+l_{r-1}+1}}\left(\vartheta_{l_1+\cdots+l_{r-1}+1}\right)}\ \mathcal{Z}\left[\pi,\bar{\pi}\right]\Big|_{\pi=\bar{\pi}=0}
\end{aligned}\tag{3.65}$$

The expression (3.65) generates two classes of diagrams. The first class contains the diagrams connecting a subset of internal sites with a subset of external sites and is called unconnected. This

class of diagrams contributes to the lower order Green's functions. The second class of diagrams contains all diagrams connecting between all internal sites $\mathbf{j}'_1, \ldots, \mathbf{j}'_n$ and from these sites to the given external sites $\mathbf{i}'_1, \ldots, \mathbf{i}'_n$ and is called connected.
As it was discussed in (3.63), summation of the connected diagrams generated by the equation (3.65) can be rewritten as follows

$$
\begin{aligned}
&\frac{1}{n!}\int_0^\beta \mathrm{d}\theta'_1 \cdots \mathrm{d}\theta'_n \sum_{\substack{\varsigma'_1\cdots\varsigma'_n \\ \mathbf{j}'_1\cdots\mathbf{j}'_n}} \Omega^{(0)}_{\sigma_1\varsigma'_1}\left(\mathbf{i}_1\ \tau_1;\mathbf{j}'_1\ \theta'_1\right)\ldots\Omega^{(0)}_{\sigma_n\varsigma'_n}\left(\mathbf{i}_n\ \tau_n;\mathbf{j}'_n\ \theta'_n\right) \\
&\sum_{q=0}^{\infty}\sum_{\substack{\varrho_1,\ldots,\varrho_{n+q}\\ \varrho'_1,\ldots,\varrho'_q}}\int_0^\beta \mathrm{d}\vartheta_1\ldots\mathrm{d}\vartheta_{n+q}\mathrm{d}\vartheta'_1\ldots\mathrm{d}\vartheta_q \sum_{k=1}^{n}\frac{1}{k!}\sum_{\substack{p_1+\cdots+p_k=n\\ m_1+\cdots+m_k=q\\ l_1+\cdots+l_k=n+q}} \\
&\quad(-1)^\eta\,\Sigma^{k;(n,q)}_{\varsigma'_1,\ldots,\varsigma'_n,\varrho'_1,\ldots,\varrho'_q;\varrho_1,\ldots,\varrho_{n+q}}\left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n|\ \vartheta'_1,\ldots,\ \vartheta'_q;\ \vartheta_1,\ldots,\ \vartheta_{n+q}\right) \\
&\quad\frac{1}{\mathcal{Z}}\ \frac{\delta}{\delta\pi_{\mathbf{i}'_n\sigma'_n}\left(\tau'_n\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}'_1\sigma'_1}\left(\tau'_1\right)} \\
&\qquad\prod_{r=1}^{k}\frac{\delta}{\delta\pi_{\mathbf{j}'_{p_r}\varrho'_{m_1+\cdots+m_{r-1}+1}}\left(\vartheta'_{m_1+\cdots+m_{r-1}+1}\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{j}'_{p_r}\varrho'_{m_1+\cdots+m_r}}\left(\vartheta'_{m_1+\cdots+m_r}\right)} \\
&\qquad\quad\frac{\delta}{\delta\bar{\pi}_{\mathbf{j}'_{p_r}\varrho_{l_1+\cdots+l_r}}\left(\vartheta_{l_1+\cdots+l_r}\right)}\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{j}'_{p_r}\varrho_{l_1+\cdots+l_{r-1}+1}}\left(\vartheta_{l_1+\cdots+l_{r-1}+1}\right)}\ \mathcal{Z}\left[\pi,\bar{\pi}\right]\Bigg|^{c}_{\pi=\bar{\pi}=0}
\end{aligned}
\tag{3.66a}
$$

where

$$
\begin{aligned}
&\Sigma^{k;(n,q)}_{\varsigma'_1,\ldots,\varsigma'_n,\varrho'_1,\ldots,\varrho'_q;\varrho_1,\ldots,\varrho_{n+q}}\left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n|\ \vartheta'_1,\ldots,\ \vartheta'_q;\ \vartheta_1,\ldots,\ \vartheta_{n+q}\right) \\
&\quad=\prod_{r=1}^{k}(-1)^{(p_r+m_r+l_r)\ m_r}\ \tilde{\mathcal{S}}^{(p_r+m_r,l_r)}_{\varsigma'_{p_1+\cdots+p_{r-1}+1},\ldots,\varsigma'_{p_1+\cdots+p_r},\varrho'_{m_1+\cdots+m_{r-1}+1},\ldots,\varrho'_{m_1+\cdots+m_r};\varrho_{l_1+\cdots+l_{r-1}+1},\ldots,\varrho_{l_1+\cdots+l_r}} \\
&\qquad\Big(\mathbf{j}'_{p_1+\cdots+p_{r-1}+1}\ \theta'_{p_1+\cdots+p_{r-1}+1},\ldots,\mathbf{j}'_{p_1+\cdots+p_r}\ \theta'_{p_1+\cdots+p_r}|\ \vartheta'_{m_1+\cdots+m_{r-1}+1},\ldots,\ \vartheta'_{m_1+\cdots+m_r}; \\
&\qquad\qquad\vartheta_{l_1+\cdots+l_{r-1}+1},\ldots,\ \vartheta'_{l_1+\cdots+l_r}\Big)\ \mathcal{Z}\left[\pi,\bar{\pi}\right]\Bigg|_{\pi=\bar{\pi}=0}\ ,
\end{aligned}
\tag{3.66b}
$$

the superscript c indicates that only the connected diagrams are taken into account, and moving all differential operators to the right hand side of the operator $\left(\mathrm{e}^{\tilde{\mathcal{S}}}\right)^{(n,q)}_{\varsigma'_1,\ldots,\varsigma'_n,\varrho'_1,\ldots,\varrho'_q;\varrho_1,\ldots,\varrho_{n+q}}\Big(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n|$ $\vartheta'_1,\ldots,\ \vartheta'_q;\ \vartheta_1,\ldots,\ \vartheta_{n+q}\Big)$ yields a factor $(-1)^\eta$ with $\eta=\sum_{r=k-1}^{1}(m_r+l_r)\left(\sum_{s=r+1}^{k}(p_s+m_s+l_s)\right)+$ $n\left(\sum_{s=1}^{k}(p_s+m_s+l_s)\right)$. Furthermore, one can represent the differential operation in last three lines of the expression (3.66a) as many-particle Green's functions

$$\frac{1}{\mathcal{Z}}\frac{\delta}{\delta\pi_{\mathbf{i}'_n\sigma'_n}\left(\tau'_n\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}'_1\sigma'_1}\left(\tau'_1\right)}$$
$$\prod_{r=1}^{k}\frac{\delta}{\delta\pi_{\mathbf{j}'_{p_r}\varrho'_{m_1+\cdots+m_{r-1}+1}}\left(\vartheta'_{m_1+\cdots+m_{r-1}+1}\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{j}'_{p_r}\varrho'_{m_1+\cdots+m_r}}\left(\vartheta'_{m_1+\cdots+m_r}\right)}$$
$$\frac{\delta}{\delta\bar{\pi}_{\mathbf{j}'_{p_r}\varrho_{l_1+\cdots+l_r}}\left(\vartheta_{l_1+\cdots+l_r}\right)}\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{j}'_{p_r}\varrho_{l_1+\cdots+l_{r-1}+1}}\left(\vartheta_{l_1+\cdots+l_{r-1}+1}\right)}\,\mathcal{Z}\left[\pi,\bar{\pi}\right]\Big|^{c}_{\pi=\bar{\pi}=0} \tag{3.66c}$$
$$=(-1)^{\nu}\,\tilde{\Omega}^{(n+q);k}_{\varrho_1,\ldots,\varrho_{n+q};\alpha'_1,\ldots,\alpha'_n,\varrho'_1,\ldots,\varrho'_q}\Big(\mathbf{j}'_{p_1}\ \vartheta_1,\ldots,\mathbf{j}'_{p_1}\ \vartheta_{l_1},\ldots,\mathbf{j}'_{p_k}\ \vartheta_{l_1+\ldots l_{k-1}+1},\ldots,\mathbf{j}'_{p_k}\ \vartheta_{l_1+\cdots+l_k};$$
$$\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n,\mathbf{j}'_{p_1}\ \vartheta'_1,\ldots,\mathbf{j}'_{p_1}\ \vartheta'_{m_1},\ldots,\mathbf{j}'_{p_k}\ \vartheta'_{m_1+\ldots m_{k-1}+1},\ldots,\mathbf{j}'_{p_k}\ \vartheta'_{m_1+\cdots+m_k}\Big)$$

where $\nu=\frac{1}{2}n\left(n-1\right)+\left(n+q\right)+\sum_{r=2}^{k}\left(m_r+l_r\right)\left(\sum_{s=1}^{r-1}l_s\right)$. One should keep in mind that these many-particle Green's functions $\tilde{\Omega}^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n\right)$ do not contain terms which depend only on parameters of internal sites. All terms of these many-particle Green's functions must first connect to the external sites and then in some probability return to the internal sites when $q>0$. Finally one obtains an equation for the part of connected diagrams of n-particle Green's functions $\bar{\mathcal{L}}^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n\right)$ as

$$\bar{\mathcal{L}}^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n\right)$$
$$=\frac{1}{n!}\int_0^{\beta}\mathrm{d}\theta'_1\cdots\mathrm{d}\theta'_n\sum_{\substack{\varsigma'_1\cdots\varsigma'_n\\ \mathbf{j}'_1\cdots\mathbf{j}'_n}}\Omega^{(0)}_{\sigma_1\varsigma'_1}\left(\mathbf{i}_1\ \tau_1;\mathbf{j}'_1\ \theta'_1\right)\ldots\Omega^{(0)}_{\sigma_n\varsigma'_n}\left(\mathbf{i}_n\ \tau_n;\mathbf{j}'_n\ \theta'_n\right)$$
$$\sum_{q=0}^{\infty}\sum_{\substack{\varrho_1,\cdots,\varrho_{n+q}\\ \varrho'_1,\cdots,\varrho'_q}}\int_0^{\beta}\mathrm{d}\vartheta_1\ldots\mathrm{d}\vartheta_{n+q}\mathrm{d}\vartheta'_1\ldots\mathrm{d}\vartheta_q\sum_{k=1}^{n}\frac{1}{k!}\sum_{\substack{p_1+\cdots+p_k=n\\ m_1+\cdots+m_k=q\\ l_1+\cdots+l_k=n+q}}(-1)^{\eta+\nu} \tag{3.67a}$$
$$\Sigma^{k;(n,q)}_{\varsigma'_1,\ldots,\varsigma'_n,\varrho'_1,\ldots,\varrho'_q;\varrho_1,\ldots,\varrho_{n+q}}\left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n|\ \vartheta'_1,\ldots,\ \vartheta'_q;\ \vartheta_1,\ldots,\ \vartheta_{n+q}\right)$$
$$\tilde{\Omega}^{(n+q);k}_{\varrho_1,\ldots,\varrho_{n+q};\alpha'_1,\ldots,\alpha'_n,\varrho'_1,\ldots,\varrho'_q}\Big(\mathbf{j}'_{p_1}\ \vartheta_1,\ldots,\mathbf{j}'_{p_1}\ \vartheta_{l_1},\ldots,\mathbf{j}'_{p_k}\ \vartheta_{l_1+\ldots l_{k-1}+1},\ldots,\mathbf{j}'_{p_k}\ \vartheta_{l_1+\cdots+l_k};$$
$$\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n,\mathbf{j}'_{p_1}\ \vartheta'_1,\ldots,\mathbf{j}'_{p_1}\ \vartheta'_{m_1},\ldots,\mathbf{j}'_{p_k}\ \vartheta'_{m_1+\ldots m_{k-1}+1},\ldots,\mathbf{j}'_{p_k}\ \vartheta'_{m_1+\cdots+m_k}\Big).$$

Recalling the relation between $\bar{\mathcal{L}}^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n\right)$ and $\bar{\Omega}^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}$

$(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n)$ (3.61b) one can easily verify that

$$\begin{aligned}
&\bar{\Omega}^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n\right)\\
&\quad=\int_0^\beta \mathrm{d}\theta_1\cdots\mathrm{d}\theta_n \sum_{\substack{\varsigma_1,\ldots,\varsigma_n\\ \mathbf{j}_1,\ldots,\mathbf{j}_n}} \Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varsigma_1,\ldots,\varsigma_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{j}_1\ \theta_1,\ldots,\mathbf{j}_n\ \theta_n\right)\\
&\qquad\int_0^\beta \mathrm{d}\theta'_1\cdots\mathrm{d}\theta'_n \sum_{\substack{\varsigma'_1\cdots\varsigma'_n\\ \mathbf{j}'_1\cdots\mathbf{j}'_n}} \Omega^{(0)}_{\varsigma_1\varsigma'_1}\left(\mathbf{j}_1\ \theta_1;\mathbf{j}'_1\ \theta'_1\right)\ldots\Omega^{(0)}_{\varsigma_n\varsigma'_n}\left(\mathbf{j}_n\ \theta_n;\mathbf{j}'_n\ \theta'_n\right)\\
&\qquad\sum_{q=0}^{\infty}\sum_{\substack{\varrho_1,\ldots,\varrho_{n+q}\\ \varrho'_1,\ldots,\varrho'_q}}\int_0^\beta \mathrm{d}\vartheta_1\ldots\mathrm{d}\vartheta_{n+q}\mathrm{d}\vartheta'_1\ldots\mathrm{d}\vartheta_q\sum_{k=1}^{n}\frac{1}{k!}\sum_{\substack{p_1+\cdots+p_k=n\\ m_1+\cdots+m_k=q\\ l_1+\cdots+l_k=n+q}}(-1)^{\eta+\nu}\\
&\qquad\Sigma^{k;(n,q)}_{\varsigma'_1,\ldots,\varsigma'_n,\varrho'_1,\ldots,\varrho'_q;\varrho_1,\ldots,\varrho_{n+q}}\left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n|\ \vartheta'_1,\ldots,\ \vartheta'_q;\ \vartheta_1,\ldots,\ \vartheta_{n+q}\right)\\
&\qquad\tilde{\Omega}^{(n+q);k}_{\varrho_1,\ldots,\varrho_{n+q};\alpha'_1,\ldots,\alpha'_n,\varrho'_1,\ldots,\varrho'_q}\Big(\mathbf{j}'_{p_1}\ \vartheta_1,\ldots,\mathbf{j}'_{p_1}\ \vartheta_{l_1},\ldots,\mathbf{j}'_{p_k}\ \vartheta_{l_1+\ldots l_{k-1}+1},\ldots,\mathbf{j}'_{p_k}\ \vartheta_{l_1+\cdots+l_k};\\
&\qquad\qquad\mathbf{i}'_1\ \tau'_1,\ldots,\mathbf{i}'_n\ \tau'_n,\mathbf{j}'_{p_1}\ \vartheta'_1,\ldots,\mathbf{j}'_{p_1}\ \vartheta'_{m_1},\ldots,\mathbf{j}'_{p_k}\ \vartheta'_{m_1+\ldots m_{k-1}+1},\ldots,\mathbf{j}'_{p_k}\ \vartheta'_{m_1+\cdots+m_k}\Big)
\end{aligned}\tag{3.67b}$$

or in short format where all indices are omitted the equation (3.67b) will be read

$$\begin{aligned}
\bar{\Omega}^{(n)} &= \Delta^{(n)}\ \Omega^{(0)}\ldots\Omega^{(0)}\ \left(\frac{1}{k!}\ \Sigma^{k;(n,q)}\ \tilde{\Omega}^{(n+q);k}\right)\\
&= \left(\Delta^{(n)}\ \Omega^{(0)}\ldots\Omega^{(0)}\ \Sigma^{(n,q)}\right)\ \tilde{\Omega}^{(n+q)}
\end{aligned}\tag{3.67c}$$

Making an ansatz

$$\tilde{\Omega}^{(n+q)} = \hat{\Omega}^{(n+q)} + \bar{\Omega}^{(n+q)}\tag{3.68a}$$

then equation (3.67c) can be divided into two parts as follows

$$\bar{\Omega}^{(n)}\ = \left(\Delta^{(n)}\ \Omega^{(0)}\ldots\Omega^{(0)}\ \Sigma^{(n,q)}\right)\ \hat{\Omega}^{(n+q)} + \left(\Delta^{(n)}\ \Omega^{(0)}\ldots\Omega^{(0)}\ \Sigma^{(n,q)}\right)\ \bar{\Omega}^{(n+q)}.\tag{3.68b}$$

The ansatz (3.68a) separates the many-particle Green's functions $\tilde{\Omega}^{(n+q)}$ into two terms; the first is the sum of products of lower order many-particle Green's functions which describe the connections from internal sites to a subset of external sites and the latter is only one $(n+q)$-particle cumulant, i.e. all internal sites connect to all external sites via this many-particle cumulant.

It is more convenient to rewrite the system of equations (3.68b) with $n > 2$ in matrix form

$$\bar{\boldsymbol{\Omega}} = \boldsymbol{\Sigma}\ \hat{\boldsymbol{\Omega}} + \boldsymbol{\Sigma}\ \bar{\boldsymbol{\Omega}}\tag{3.69a}$$

where the matrices are defined as follows

$$\bar{\boldsymbol{\Omega}} = \begin{pmatrix}\bar{\Omega}^{(2)}\\ \bar{\Omega}^{(3)}\\ \bar{\Omega}^{(4)}\\ \vdots\end{pmatrix},\qquad \hat{\boldsymbol{\Omega}} = \begin{pmatrix}\hat{\Omega}^{(2)}\\ \hat{\Omega}^{(3)}\\ \hat{\Omega}^{(4)}\\ \vdots\end{pmatrix},\tag{3.69b}$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \Delta^{(2)}\ \Omega^{(0)}\Omega^{(0)}\ \Sigma^{(2,0)} & \Delta^{(2)}\ \Omega^{(0)}\Omega^{(0)}\ \Sigma^{(2,1)} & \Delta^{(2)}\ \Omega^{(0)}\Omega^{(0)}\ \Sigma^{(2,2)} & \dots \\ 0 & \Delta^{(3)}\ \Omega^{(0)}\Omega^{(0)}\ \Omega^{(0)}\ \Sigma^{(3,0)} & \Delta^{(3)}\ \Omega^{(0)}\Omega^{(0)}\Omega^{(0)}\ \Sigma^{(3,1)} & \dots \\ 0 & 0 & \Delta^{(4)}\ \Omega^{(0)}\Omega^{(0)}\Omega^{(0)}\Omega^{(0)}\ \Sigma^{(4,0)} & \dots \\ \vdots & \vdots & \vdots & \end{pmatrix} \tag{3.69c}$$

Formally solving the matrix equation (3.69a) one gets a formal solution for all many-particle cumulants $\bar{\Omega}^{(n)}$ of auxiliary field operator

$$\bar{\boldsymbol{\Omega}} = (\mathbf{I} - \boldsymbol{\Sigma})^{-1}\ \boldsymbol{\Sigma}\ \hat{\boldsymbol{\Omega}} \tag{3.69d}$$

which can be explicitly written as in following series

$$\begin{aligned} \bar{\Omega}^{(n)} = & \sum_{k=1}^{\infty}\sum_{q_1=1}^{\infty} \Delta^{(n)} \underbrace{\Omega^{(0)}\dots\Omega^{(0)}}_{n} \Sigma^{(n,q_1)} \\ & \sum_{q_2=1}^{\infty} \Delta^{(n+q_1)} \underbrace{\Omega^{(0)}\dots\Omega^{(0)}}_{n+q_1} \Sigma^{((n+q_1),q_2)} \dots \hat{\Omega}^{(n+q_1+\dots+q_k)}, \end{aligned} \tag{3.69e}$$

where the quantity $\Sigma^{(n,q)}$ is fully determined in expressions (3.63) and (3.66b).

The solutions (3.69e) describe the processes done by n particles of auxiliary field operators which from the n given input sites $\mathbf{i}_1, \dots, \mathbf{i}_n$ move to intermediate sites $\mathbf{j}'_1, \dots, \mathbf{j}'_k$ $(k \le n)$ where some many-particle processes should happen and then they leave those immediate sites to given output sites $\mathbf{i}'_1, \dots, \mathbf{i}'_n$ or to other intermediate sites.

Because of structural symmetry of the many-body Green's functions with respect to the parameters of their external sites one can rewrite the quantity $\Sigma^{(n,q)}$ in symmetric form

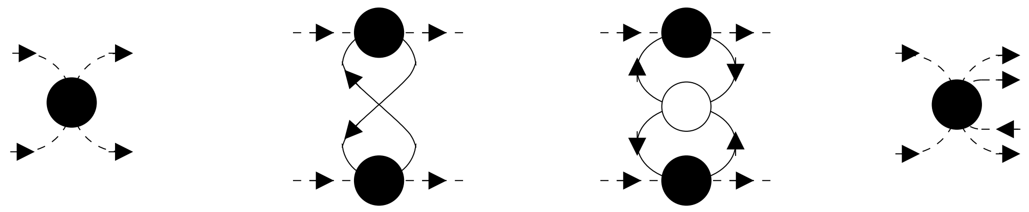
$$\Delta^{(n)} \underbrace{\Omega^{(0)}\dots\Omega^{(0)}}_{n} \Sigma^{(n,q_1)} = \sum_{p_1=1}^{\infty} \hat{\Omega}^{(n+p_1)} \Lambda^{(n,p_1,q_1)}. \tag{3.70}$$

Inserting the symmetric form of Σ in (3.70) into (3.69e) one will get a system of equations for the renormalized many-particle cumulants of the auxiliary fields, on which one can base to determine other quantities of the system considered self-consistently

$$\begin{aligned} \bar{\Omega}^{(n)} = & \sum_{k=1}^{\infty}\sum_{q_1=1}^{\infty}\sum_{p_1=1}^{\infty} \hat{\Omega}^{(n+p_1)} \Lambda^{(n,p_1,q_1)} \\ & \sum_{q_2=1}^{\infty}\sum_{p_2=1}^{\infty} \hat{\Omega}^{(n+q_1+p_2)} \Lambda^{((n+q_1),p_2,q_2)} \dots \hat{\Omega}^{(n+q_1+\dots+q_k)}. \end{aligned} \tag{3.71}$$

It is easy to realize that the functional Λ is the renormalized irreducible many-body correlation function of the localized electrons.

In the Fig. 3.3, the diagrams (a) – (c) with two incoming particles and also two outgoing, in which the renormalized local vertices are connected by different many-particle Green's functions of the auxiliary fields. Having an approximation with $\Lambda^{(n,q_1,q_2)} = \Lambda^{(n,0,0)} = \frac{1}{n!}\bar{G}^{(n)}$ and $\hat{\Omega}^{(n+q)} = \hat{\Omega}^{(n)}$ - the product on n renormalized one-particle Green's function, i.e. only the simplest many-particle contributions of the equations (3.71) are taken into account, then one gets the expressions of many-particle Green's functions of the auxiliary fields and those of the localized electrons which are generated by the generating functional in the Fig. 3.5.



a) b) c) d)

Figure 3.3: Diagrammatical representation of some lowest order contributions of the correlation function Λ

The final integral equation system (3.71) has the same form as Bethe-Salpeter integral equation of motion for two-particle irreducible Green's function, but it is extended for the many-particle Green's functions or in other words, for many-particle cumulants defined in our case. They will be called Bethe-Salpeter-like equations.

The Bethe-Salpeter-like equations for many-particle cumulants provide a systematic way of summation and renormalization of Feynman diagrams. Instead of concentrating on one-particle contributions and their Dyson's equation, the Bethe-Salpeter-like equation approach sums many-particle diagrams contributing to the many-particle cumulants for which the Bethe-Salpeter-like equations are constructed. Because of the complexity of the Bethe-Salpeter-like equations their corresponding algebra will be very complicated in comparison with that of one-particle. We will leave this problem open for the future investigation.

SECTION 3.6

Calculation for the grand partition function

The grand partition function (3.33) can be calculated within the help of a modification involving a "switch" λ for all interaction terms of the action (3.34b), running form 0 to 1

$$\mathcal{Z}\left[\lambda\right] = \frac{\mathcal{Z}_0 \bar{\mathcal{Z}}_0}{\mathcal{V}} \int \left[\mathcal{D}\psi\right] \left[\mathcal{D}\bar{\psi}\right] \exp\left\{-\mathcal{S}_0\left[\psi\left(\tau\right), \bar{\psi}\left(\tau\right)\right] - \lambda \sum_{n=1}^{\infty} \mathcal{S}_{\text{int}}^{(n)}\left[\psi\left(\tau\right), \bar{\psi}\left(\tau\right)\right]\right\} \tag{3.72}$$

The extremal values $\lambda = 0$ and $\lambda = 1$ correspond to the grand partition functions of the free system where the hybridization is vanished and of the system considered, resp..

Performing some algebraic manipulations with λ, starting by differentiating

$$\frac{\partial}{\partial\lambda} \ln \mathcal{Z}\left[\lambda\right] = -\sum_{n=1}^{\infty} \left\langle \mathcal{S}_{\text{int}}^{n}\left[\psi\left(\tau\right), \bar{\psi}\left(\tau\right)\right]\right\rangle_{\mathcal{Z}\left[\lambda\right]}, \tag{3.73a}$$

next, integrating over λ leads to

$$\begin{aligned}\int_0^1 \mathrm{d}\lambda \frac{\partial}{\partial\lambda} \ln \mathcal{Z}\left[\lambda\right] &= \ln \mathcal{Z}\left[1\right] - \ln \mathcal{Z}\left[0\right] \\ &= -\int_0^1 \mathrm{d}\lambda \sum_{n=1}^{\infty} \left\langle \mathcal{S}_{\text{int}}^{n}\left[\psi\left(\tau\right), \bar{\psi}\left(\tau\right)\right]\right\rangle_{\mathcal{Z}\left[\lambda\right]}.\end{aligned} \tag{3.73b}$$

It is clear that

$$\begin{aligned}\mathcal{Z}[1] &= \mathcal{Z}\\ \mathcal{Z}[0] &= \mathcal{Z}_0\bar{\mathcal{Z}}_0,\end{aligned}\tag{3.73c}$$

then we obtain

$$\begin{aligned}\ln\mathcal{Z} &= \ln\mathcal{Z}[1]\\ &= -\sum_{n=1}^{\infty}\int_0^1 \mathrm{d}\lambda \left\langle \mathcal{S}_{\mathrm{int}}^{n}\left[\psi(\tau),\bar{\psi}(\tau)\right]\right\rangle_{\mathcal{Z}[\lambda]} + \ln\mathcal{Z}_0 + \ln\bar{\mathcal{Z}}_0.\end{aligned}\tag{3.73d}$$

As it was known from equation (3.34b) and (3.31)

$$\begin{aligned}\mathcal{S}_{\mathrm{int}}^{n}\left[\psi(\tau),\bar{\psi}(\tau)\right] &= -\sum_{\mathbf{i}}\bar{\mathcal{S}}_{\mathbf{i}}^{(n)}\left[\psi(\tau),\bar{\psi}(\tau)\right]\\ &= -\sum_{\mathbf{i}}\frac{1}{(n!)^2}\int_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau_n\mathrm{d}\tau_1'\cdots\mathrm{d}\tau_n' \sum_{\substack{\sigma_1,\cdots,\sigma_n\\ \sigma_1',\cdots,\sigma_n'}}\psi_{\mathbf{i}\sigma_1}(\tau_1)\cdots\psi_{\mathbf{i}\sigma_n}(\tau_n)\\ &\qquad \bar{\psi}_{\mathbf{i}\sigma_n'}\left(\tau_n'\right)\cdots\bar{\psi}_{\mathbf{i}\sigma_1'}\left(\tau_1'\right)\bar{\mathcal{G}}^{(n)}_{\sigma_1',\ldots,\sigma_n';\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}|\tau_1',\ldots,\tau_n';\tau_1,\ldots,\tau_n\right)\end{aligned}\tag{3.73e}$$

so that the expectation value $\left\langle \mathcal{S}_{\mathrm{int}}^{n}\left[\psi(\tau),\bar{\psi}(\tau)\right]\right\rangle_{\mathcal{Z}[\lambda]}$ has the following form

$$\begin{aligned}&\left\langle \mathcal{S}_{\mathrm{int}}^{n}\left[\psi(\tau),\bar{\psi}(\tau)\right]\right\rangle_{\mathcal{Z}[\lambda]}\\ &= -\sum_{\mathbf{i}}\frac{1}{(n!)^2}\int_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau_n\mathrm{d}\tau_1'\cdots\mathrm{d}\tau_n' \sum_{\substack{\sigma_1,\cdots,\sigma_n\\ \sigma_1',\cdots,\sigma_n'}}\Bigg\langle \mathscr{T}_\tau\Big(\psi_{\mathbf{i}\sigma_1}(\tau_1)\cdots\psi_{\mathbf{i}\sigma_n}(\tau_n)\\ &\qquad \bar{\psi}_{\mathbf{i}\sigma_n'}\left(\tau_n'\right)\cdots\bar{\psi}_{\mathbf{i}\sigma_1'}\left(\tau_1'\right)\Big)\Bigg\rangle_{\mathcal{Z}[\lambda]}\bar{\mathcal{G}}^{(n)}_{\sigma_1',\ldots,\sigma_n';\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}|\tau_1',\ldots,\tau_n';\tau_1,\ldots,\tau_n\right)\\ &\equiv -\sum_{\mathbf{i}}\frac{(-1)^n}{(n!)^2}\int_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau_n\mathrm{d}\tau_1'\cdots\mathrm{d}\tau_n' \sum_{\substack{\sigma_1,\cdots,\sigma_n\\ \sigma_1',\cdots,\sigma_n'}}\bar{\mathcal{G}}^{(n)}_{\sigma_1',\ldots,\sigma_n';\sigma_1,\ldots,\sigma_n}\left(\mathbf{i}|\tau_1',\ldots,\tau_n';\tau_1,\ldots,\tau_n\right)\\ &\qquad \Omega^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma_1',\ldots,\sigma_n'}[\lambda]\left(\mathbf{i}|\tau_1,\ldots,\tau_n;\tau_1',\ldots,\tau_n'\right)\\ &\equiv -\sum_{\mathbf{i}}\frac{(-1)^n}{(n!)^2}\,\mathrm{Tr}\,\bar{\mathcal{G}}^{(n)}(\mathbf{i})\,\Omega^{(n)}(\mathbf{i})[\lambda],\end{aligned}\tag{3.73f}$$

here, the symbol Tr is understood as the summation over all spins and integration over all imaginary-time variables.
Finally, we can rewrite the grand partition function (3.73d) in an explicit form

$$\ln\mathcal{Z} = \ln\mathcal{Z}_0 + \ln\bar{\mathcal{Z}}_0 + \sum_{\mathbf{i}}\left(\sum_{n=1}^{\infty}\frac{(-1)^n}{(n!)^2}\int_0^1 \mathrm{d}\lambda\;\mathrm{Tr}\,\bar{\mathcal{G}}^{(n)}(\mathbf{i})\,\Omega^{(n)}(\mathbf{i})[\lambda]\right)\tag{3.74}$$

which is directly connected to the thermodynamical potential

$$\Omega = -\beta^{-1}\ln\mathcal{Z}.\tag{3.75}$$

The equation (3.74) shows that the solution of the system considered can be reduced to the solution of a effective local one, the non-local contributions are included via the Green's functions of auxiliary fields $\Omega^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma'_1,\ldots,\sigma'_n}(\mathbf{i}|\tau_1,\ldots,\tau_n;\tau'_1,\ldots;\tau'_n)$. This conclusion is the same as the results obtained by diagrammatic techniques in recent work of Keiter [10]. The integral over λ in (3.74) means the permutation of cumulants $\bar{\mathcal{G}}^{(n)}_{\sigma'_1,\ldots,\sigma'_n;\sigma_1,\ldots,\sigma_n}(\mathbf{i}|\tau'_1,\ldots,\tau'_n;\tau_1,\ldots,\tau_n)$ appearing under the operator Tr. The prefactors $\frac{1}{(n!)^2}$ are telling us about permutation of n primed and n unprimed variables under the symbol Tr.

Likewise, from the identity (3.73a) we also get the explicit form for $\mathcal{Z}$

$$\begin{aligned}\int_0^1 \mathrm{d}\lambda\,\frac{\partial}{\partial\lambda}\mathcal{Z}[\lambda] &= \mathcal{Z}[1]-\mathcal{Z}[0]\\ &= -\int_0^1 \mathrm{d}\lambda\sum_{n=1}^{\infty}\left\langle\mathcal{S}^n_{\mathrm{int}}\left[\psi(\tau),\bar{\psi}(\tau)\right]\right\rangle_{\mathcal{Z}[\lambda]}\mathcal{Z}[\lambda] \qquad (3.76)\\ &= \sum_{\mathbf{i}}\left(\sum_{n=1}^{\infty}\frac{(-1)^n}{(n!)^2}\int_0^1\frac{\mathrm{d}\lambda}{\lambda}\,\mathrm{Tr}\left[\left(\lambda\bar{\mathcal{G}}^{(n)}(\mathbf{i})\right)\Omega^{(n)}(\mathbf{i})\left[\lambda\bar{\mathcal{G}}\right]\right]\mathcal{Z}[\lambda]\right),\end{aligned}$$

or

$$\mathcal{Z}[1] = \mathcal{Z}[0]+\sum_{\mathbf{i}}\left(\sum_{n=1}^{\infty}\frac{(-1)^n}{(n!)^2}\int_0^1\frac{\mathrm{d}\lambda}{\lambda}\,\mathrm{Tr}\left[\left(\lambda\bar{\mathcal{G}}^{(n)}(\mathbf{i})\right)\Omega^{(n)}(\mathbf{i})\left[\lambda\bar{\mathcal{G}}\right]\right]\mathcal{Z}[\lambda]\right). \qquad (3.77)$$

The equations (3.74) and (3.77) are rather general and do not depend on certain conditions of physical input parameters such as the hopping matrix element, the Coulomb interaction U or the dimensionality of the system. Because of that we can use them to investigate many different regimes of the system considered and to add corrections to a given approximation such as the non-local corrections to the solution of Dynamical Mean Field Theory (DMFT), which is a powerful approximation for investigation of strongly correlated electron systems, where the dimensionality is assumed infinity.

The auxiliary grand partition function (3.72) can be also written in another form as follows

$$\frac{\mathcal{Z}_0\bar{\mathcal{Z}}_0}{\mathcal{Z}[\lambda]} = 1+\sum_{k=1}^{\infty}\frac{\lambda^k}{k!}\left\langle\left(\sum_{n=1}^{\infty}\mathcal{S}^{(n)}_{\mathrm{int}}\left[\psi(\tau),\bar{\psi}(\tau)\right]\right)^k\right\rangle_{\mathcal{Z}[\lambda]}, \qquad (3.78a)$$

when $\lambda=1$ it returns to the grand partition function as

$$\frac{\mathcal{Z}_0\bar{\mathcal{Z}}_0}{\mathcal{Z}} = 1+\sum_{k=1}^{\infty}\frac{1}{k!}\left\langle\left(\sum_{n=1}^{\infty}\mathcal{S}^{(n)}_{\mathrm{int}}\left[\psi(\tau),\bar{\psi}(\tau)\right]\right)^k\right\rangle_{\mathcal{Z}}. \qquad (3.78b)$$

Next we are now going to compute the expectation values in (3.78b). It is easy to recognize that these expectation values contain generally two kinds of terms, the connected ones and unconnected ones. On the other hand one has to be aware that in every k-order expectation value only k sites will appear in all terms of this order. Additionally, in each term (connected or unconnected) all imaginary time and sigma variables are integrated over and summed over, resp., so that all terms are imaginary time and sigma independent and are only site dependent. We will denote $\mathcal{F}^{(k)}_{\mathbf{i}_1,\ldots,\mathbf{i}_k}$ for the connected term of the kth-order expectation value which is explicitly site-dependent.

In the term of $\mathcal{F}^{(k)}_{\mathbf{i}_1,\ldots,\mathbf{i}_k}$ we can write down the expectation values in (3.78b) as follows [5]

$$\frac{1}{k!}\left\langle\left(\sum_{n=1}^{\infty}\mathcal{S}^{(n)}_{\text{int}}\left[\psi(\tau),\bar{\psi}(\tau)\right]\right)^{k}\right\rangle_{\mathcal{Z}}=\left(\mathrm{e}^{\mathcal{O}}\right)^{(k)} \tag{3.79b}$$

where

$$\mathcal{O}^{n}=\frac{1}{k!}\sum_{\mathbf{i}_1,\ldots,\mathbf{i}_k}\mathcal{F}^{(k)}_{\mathbf{i}_1,\ldots,\mathbf{i}_k}. \tag{3.79c}$$

Inserting expression (3.79b) into (3.78b) and then group all terms in subseries we get the general form of the grand partition function of the system considered

$$\frac{\mathcal{Z}_0\bar{\mathcal{Z}}_0}{\mathcal{Z}}=\exp\left\{\sum_{k=1}^{n}\frac{1}{k!}\left(\sum_{\mathbf{i}_1,\ldots,\mathbf{i}_k}\mathcal{F}^{(k)}_{\mathbf{i}_1,\ldots,\mathbf{i}_k}\right)\right\}, \tag{3.80a}$$

or the general form of thermodynamical potential of the system considered

$$\ln\mathcal{Z}=\ln\mathcal{Z}_0+\ln\bar{\mathcal{Z}}_0-\sum_{k=1}^{n}\frac{1}{k!}\left(\sum_{\mathbf{i}_1,\ldots,\mathbf{i}_k}\mathcal{F}^{(k)}_{\mathbf{i}_1,\ldots,\mathbf{i}_k}\right). \tag{3.80b}$$

Generally speaking one is able to write all quantities $\mathcal{F}^{(k)}_{\mathbf{i}_1,\ldots,\mathbf{i}_k}$ in explicit form depending on renormalized local cumulants of the localized electrons (the number of renormalized local cumulants is the order of this term) and the renormalized many-particle Green's functions of the auxiliary fields. The functionals $\mathcal{F}^{(k)}_{\mathbf{i}_1,\ldots,\mathbf{i}_k}$ depend explicitly and implicitly (through renormalized many-particle Green's functions of the auxiliary fields) on renormalized local cumulants of the localized electrons.

The thermodynamical potential (3.80b) depending only on the fully renormalized many-particle vertices of the localized electrons and many-particle cumulants of the auxiliary fields provides a general starting point to construct a generating Luttinger-Ward functional which guarantees the thermodynamic consistencies of the corresponding approximation.

Choosing some certain diagram family from diagrams of the thermodynamical potential (3.80b) one gets the correspondent approximation. For example, the following diagram families serve as the generating Luttinger-Ward functional for XNCA [13] in Fig. 3.4 and for a possible generalization of XNCA in Fig. 3.5 where the renormalized non-local one-particle contributions of conduction electrons are included.

[5]Here we represent the explicit expressions for $k=1$ and $k=2$

$$\left\langle\left(\sum_{n=1}^{\infty}\mathcal{S}^{(n)}_{\text{int}}\left[\psi(\tau),\bar{\psi}(\tau)\right]\right)^{k}\right\rangle_{\mathcal{Z}}=\begin{cases}\left.\begin{array}{l}\displaystyle\sum_{\mathbf{i}_1}\left\langle\left(\sum_{n_1=1}^{\infty}\bar{\mathcal{S}}^{(n_1)}_{\mathbf{i}_1}\left[\psi(\tau),\bar{\psi}(\tau)\right]\right)\right\rangle_{\mathcal{Z}}\\ \displaystyle=\sum_{\mathbf{i}_1}\mathcal{F}^{(1)}_{\mathbf{i}_1}\end{array}\right\} & \text{for } k=1\\ \left.\begin{array}{l}\displaystyle\sum_{\mathbf{i}_1,\mathbf{i}_2}\frac{1}{2!}\left\langle\left(\sum_{n_1=1}^{\infty}\bar{\mathcal{S}}^{(n_1)}_{\mathbf{i}_1}\left[\psi(\tau),\bar{\psi}(\tau)\right]\right)\left(\sum_{n_2=1}^{\infty}\bar{\mathcal{S}}^{(n_2)}_{\mathbf{i}_2}\left[\psi(\tau),\bar{\psi}(\tau)\right]\right)\right\rangle_{\mathcal{Z}}\\ \displaystyle=\sum_{\mathbf{i}_1,\mathbf{i}_2}\frac{1}{2!}\mathcal{F}^{(2)}_{\mathbf{i}_1,\mathbf{i}_2}+\frac{1}{2!}\sum_{\mathbf{i}_1}\mathcal{F}^{(1)}_{\mathbf{i}_1}\sum_{\mathbf{i}_2}\mathcal{F}^{(1)}_{\mathbf{i}_2}\end{array}\right\} & \text{for } k=2\\ \ldots & \ldots\end{cases} \tag{3.79a}$$

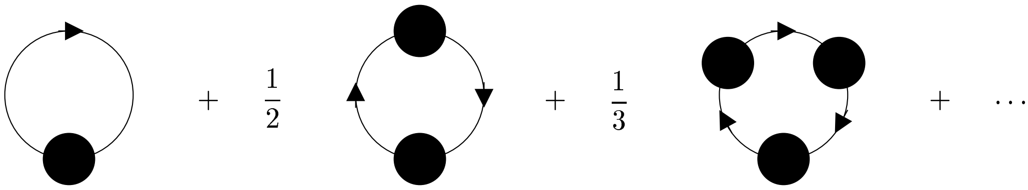


Figure 3.4: Diagram family of generating functional for XNCA

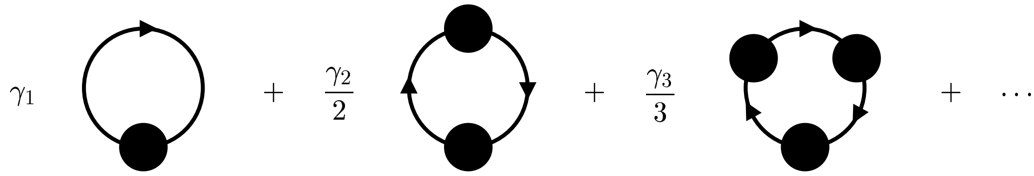


Figure 3.5: A simplest generalization of generating functional for XNCA, where instead of the one-particle Green's function $\Omega^{(1)}$ as in Figure 3.4. one uses the product of n one-particle Green's function $\Omega^{(1)}$. In this case some new coefficient $\gamma_k = \left(\frac{1}{n!}\right)^k$ will be taken into account.

One can also easily prove that when all sites $\mathbf{i}_1, \ldots, \mathbf{i}_k$ are equal the grand partition function of DMFT is automatically obtained from the grand partition function (3.80b).

CHAPTER 4

Applications and Approximations

This Chapter focuses on the derivative results which can be obtained from the very general formulation in previous Chapters.

A generating Luttinger-Ward functional with respect to renormalized one-particle Green's function, many-particle local vertices and their self-energy is constructed. It shows the relationship between the thermodynamical potential and generating functional. The stationary conditions of functional derivatives with respect to the renormalized quantities keeping the thermodynamic consistencies and conserving character of the solution are checked.

The Dynamical Mean Field Theory (DMFT) and its generating functional is obtained in framework of strong coupling expansion. The relations of many-particle functions in DMFT to those of the general ones are discussed.

SECTION 4.1

The Thermodynamical Potential and The Self-Consistent Theory

Recall the general grand partition function which is obtained after performing the Grassmann Hubbard-Stratonovich transformation and the integration over the Grassmann variables $\zeta_{\mathbf{i}\sigma}$ and $\bar{\zeta}_{\mathbf{i}\sigma}$

$$\mathcal{Z} = \frac{\mathcal{Z}_0 \bar{\mathcal{Z}}_0}{\mathcal{V}} \int \left[\mathcal{D}\psi\right] \left[\mathcal{D}\bar{\psi}\right] \exp\left\{ -\mathcal{S}_0 \left[\psi\left(\tau\right), \bar{\psi}\left(\tau\right)\right] - \sum_{n=1}^{\infty} \mathcal{S}_{\text{int}}^{(n)} \left[\psi\left(\tau\right), \bar{\psi}\left(\tau\right)\right] \right\} \tag{4.1}$$

where the action has a free (Gaussian) part

$$\mathcal{S}_0 \left[\psi\left(\tau\right), \bar{\psi}\left(\tau\right)\right] = -\int\limits_0^\beta \mathrm{d}\tau \mathrm{d}\tau' \sum_{\mathbf{i}\mathbf{i}', \sigma\sigma'} \bar{\psi}_{\mathbf{i}'\sigma'}\left(\tau'\right) \left(\Omega^{(0)}\right)^{-1}_{\sigma'\sigma} \left(\mathbf{i}'\ \tau'; \mathbf{i}\ \tau\right) \psi_{\mathbf{i}\sigma}\left(\tau\right), \tag{4.2a}$$

and an infinite number of interaction terms

$$\mathcal{S}_{\text{int}}^{(n)} \left[\psi\left(\tau\right), \bar{\psi}\left(\tau\right)\right] = -\sum_{\mathbf{i}} \bar{\mathcal{S}}_{\mathbf{i}}^{(n)} \left[\psi\left(\tau\right), \bar{\psi}\left(\tau\right)\right], \tag{4.2b}$$

with $\bar{\mathcal{S}}_{\mathbf{i}}^{(n)}\left[\psi\left(\tau\right),\bar{\psi}\left(\tau\right)\right]$ determined by second equation in (3.31) as

$$\begin{aligned}\bar{\mathcal{S}}_{\mathbf{i}}^{(n)}\left[\psi\left(\tau\right),\bar{\psi}\left(\tau\right)\right] = \frac{1}{(n!)^2}\int\limits_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau_n\mathrm{d}\tau_1'\cdots\mathrm{d}\tau_n' \sum_{\substack{\sigma_1,\cdots,\sigma_n\\ \sigma_1',\cdots,\sigma_n'}} \psi_{\mathbf{i}\sigma_1}\left(\tau_1\right)\cdots\psi_{\mathbf{i}\sigma_n}\left(\tau_n\right) \\ \bar{\psi}_{\mathbf{i}\sigma_n'}\left(\tau_n'\right)\cdots\bar{\psi}_{\mathbf{i}\sigma_1'}\left(\tau_1'\right)\bar{\mathcal{G}}^{(n)}_{\sigma_1',\dots,\sigma_n';\sigma_1,\dots,\sigma_n}\left(\mathbf{i}|\tau_1',\dots,\tau_n';\tau_1,\dots,\tau_n\right)\end{aligned} \tag{4.2c}$$

In order to construct a self-consistent theory for the considered system one could follow the idea of Baym [4] to change the functional dependence in the thermodynamical potential functional by a new representation with renormalized Green's functions $\hat{\Omega}$ of auxiliary fields $\psi_{\mathbf{i}\sigma}$ and $\bar{\psi}_{\mathbf{i}\sigma}$ and renormalized vertices (local Green's functions) $\bar{G}^{(n)}$, defined in equations (3.49).
Rewrite the grand partition function as

$$\mathcal{Z}\left[\left(\Omega^{(0)}\right)^{-1};\bar{\mathcal{G}}\right] = \frac{\mathcal{Z}_0\bar{\mathcal{Z}}_0}{\mathcal{V}}\int\left[\mathcal{D}\psi\right]\left[\mathcal{D}\bar{\psi}\right]\exp\left\{-\mathcal{S}\left[\psi,\bar{\psi};\left(\Omega^{(0)}\right)^{-1};\bar{\mathcal{G}}\right]\right\} \tag{4.3}$$

then, the thermodynamical potential functional is given by

$$\begin{aligned}-\beta\,\Omega\left[\left(\Omega^{(0)}\right)^{-1};\bar{\mathcal{G}}\right] &= \ln\mathcal{Z}\left[\left(\Omega^{(0)}\right)^{-1};\bar{\mathcal{G}}\right] \\ &\equiv \ln\mathcal{Z}_0 + \ln\bar{\mathcal{Z}}_0 + \ln\left(\frac{1}{\mathcal{V}}\int\left[\mathcal{D}\psi\right]\left[\mathcal{D}\bar{\psi}\right]\exp\left\{-\mathcal{S}\left[\psi,\bar{\psi};\left(\Omega^{(0)}\right)^{-1};\bar{\mathcal{G}}\right]\right\}\right).\end{aligned} \tag{4.4}$$

As it was mentioned in (3.24), the $\bar{\mathcal{Z}}_0$ is the product of all local $\bar{\mathcal{Z}}_{\mathbf{i},0}$ and we use the notation $\bar{\mathcal{G}}_{\mathbf{i}}^{(0)}$ for the function $\ln\bar{\mathcal{Z}}_{\mathbf{i},0}$, now the thermodynamical potential functional reads

$$-\beta\,\Omega\left[\left(\Omega^{(0)}\right)^{-1};\bar{\mathcal{G}}\right] = \ln\mathcal{Z}_0 + \sum_{\mathbf{i}}\bar{\mathcal{G}}_{\mathbf{i}}^{(0)} + \ln\left(\frac{1}{\mathcal{V}}\int\left[\mathcal{D}\psi\right]\left[\mathcal{D}\bar{\psi}\right]\exp\left\{-\mathcal{S}\left[\psi,\bar{\psi};\left(\Omega^{(0)}\right)^{-1};\bar{\mathcal{G}}\right]\right\}\right) \tag{4.5}$$

Substitute the free Green's function $\Omega^{(0)}$ of auxiliary fields by its renormalized one $\Omega^{(1)}$ and its self-energy Γ which are related by the exact relation

$$\left(\Omega^{(0)}\right)^{-1} = \left(\Omega^{(1)}\right)^{-1} + \Gamma \tag{4.6}$$

The new variables $\Omega^{(1)}$ and Γ enter the thermodynamical potential functional. We can treat those renormalized quantities as independent variables in the thermodynamical potential. The new thermodynamical potential must, however, not depend on the variations of the new variables $\Omega^{(1)}$ and Γ in order to keep the thermodynamical relations fulfilled. To secure vanishing of the variations of the thermodynamical potential with respect to the $\Omega^{(1)}$ and Γ we have to modify the thermodynamical potential functional, since the variations with respect to $\left(\Omega^{(0)}\right)^{-1}$ do not vanish. We should add a contribution being a functional of $\Omega^{(1)}$ and Γ. If we denote it by $\Omega\left[\Omega^{(1)},\Gamma\right]$ we must fulfill the following identities

$$\begin{aligned}\frac{\delta}{\delta\left(\Omega^{(1)}\right)^{-1}_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right)}\ \Omega\left[\Omega^{(1)},\Gamma\right] &= -\frac{\delta}{\delta\left(\Omega^{(0)}\right)^{-1}_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right)}\ \Omega\left[\left(\Omega^{(0)}\right)^{-1};\bar{\mathcal{G}}\right] \\ \frac{\delta}{\delta\Gamma_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right)}\ \Omega\left[\Omega^{(1)},\Gamma\right] &= -\frac{\delta}{\delta\left(\Omega^{(0)}\right)^{-1}_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right)}\ \Omega\left[\left(\Omega^{(0)}\right)^{-1};\bar{\mathcal{G}}\right]\end{aligned} \tag{4.7}$$

to keep the total thermodynamical potential

$$\Omega\left[\Omega^{(1)},\Gamma;\bar{\mathcal{G}}\right]=\Omega\left[\left(\Omega^{(1)}\right)^{-1}+\Gamma;\bar{\mathcal{G}}\right]+\Omega\left[\Omega^{(1)},\Gamma\right] \tag{4.8}$$

independent of $\Omega^{(1)}$ and Γ. It can be easily obtained

$$\begin{aligned}-\beta\Omega\left[\Omega^{(1)},\Gamma;\bar{\mathcal{G}}\right]=-\beta\Omega&\left[\left(\Omega^{(1)}\right)^{-1}+\Gamma;\bar{\mathcal{G}}\right]\\&+\operatorname{Tr}\ln\left(\left(\Omega^{(0)}\right)^{-1}-\Gamma\right)-\operatorname{Tr}\ln\left(\left(\Omega^{(1)}\right)^{-1}\right)\\&-\operatorname{Tr}\ln\left(\left(\Omega^{(0)}\right)^{-1}\right)+\operatorname{Tr}\ln\left(\left(\Omega^{(1)}\right)^{-1}+\Gamma\right).\end{aligned} \tag{4.9}$$

In the next step, we repeat all the above stages for the quantities $\bar{\mathcal{G}}$, which are formulated in the form of functional of renormalized variables $\bar{G}$ and $\bar{\mathcal{O}}$, that we provided in equation (3.53) of the Section 3.4 on page 22. Here we write it down again

$$\bar{\mathcal{G}}=\bar{G}\ \mathrm{e}^{\,-\bar{\mathcal{O}}}. \tag{4.10}$$

The new total thermodynamical potential functional

$$-\beta\Omega\left[\Omega^{(1)},\Gamma;\bar{G},\bar{\mathcal{O}}\right]=-\beta\Omega\left[\Omega^{(1)},\Gamma;\bar{\mathcal{G}}\left[\bar{G},\bar{\mathcal{O}}\right]\right]-\beta\Omega\left[\bar{G},\bar{\mathcal{O}}\right] \tag{4.11}$$

should not depend on the variations of the renormalized variables $\bar{G}$ and $\bar{\mathcal{O}}$, i.e.

$$\begin{aligned}&\frac{\delta}{\delta\bar{G}^{(n)}_{\boldsymbol{\sigma}'_n,\boldsymbol{\sigma}_n}(\mathbf{i}|,\boldsymbol{\tau}'_n;\boldsymbol{\tau}_n)}\ \Omega\left[\Omega^{(1)},\Gamma;\bar{G},\bar{\mathcal{O}}\right]\\&\quad=\frac{\delta}{\delta\bar{G}^{(n)}_{\boldsymbol{\sigma}'_n,\boldsymbol{\sigma}_n}(\mathbf{i}|,\boldsymbol{\tau}'_n;\boldsymbol{\tau}_n)}\ \Omega\left[\Omega^{(1)},\Gamma;\bar{\mathcal{G}}\left[\bar{G},\bar{\mathcal{O}}\right]\right]+\frac{\delta}{\delta\bar{G}^{(n)}_{\boldsymbol{\sigma}'_n,\boldsymbol{\sigma}_n}(\mathbf{i}|,\boldsymbol{\tau}'_n;\boldsymbol{\tau}_n)}\ \Omega\left[\bar{G},\bar{\mathcal{O}}\right]\\&\quad=0\\&\frac{\delta}{\delta\bar{\mathcal{O}}^{(n)}_{\boldsymbol{\sigma}'_n,\boldsymbol{\sigma}_n}(\mathbf{i}|,\boldsymbol{\tau}'_n;\boldsymbol{\tau}_n)}\ \Omega\left[\Omega^{(1)},\Gamma;\bar{G},\bar{\mathcal{O}}\right]\\&\quad=\frac{\delta}{\delta\bar{\mathcal{O}}^{(n)}_{\boldsymbol{\sigma}'_n,\boldsymbol{\sigma}_n}(\mathbf{i}|,\boldsymbol{\tau}'_n;\boldsymbol{\tau}_n)}\ \Omega\left[\Omega^{(1)},\Gamma;\bar{\mathcal{G}}\left[\bar{G},\bar{\mathcal{O}}\right]\right]+\frac{\delta}{\delta\bar{\mathcal{O}}^{(n)}_{\boldsymbol{\sigma}'_n,\boldsymbol{\sigma}_n}(\mathbf{i}|,\boldsymbol{\tau}'_n;\boldsymbol{\tau}_n)}\ \Omega\left[\bar{G},\bar{\mathcal{O}}\right]\\&\quad=0\end{aligned} \tag{4.12}$$

Solving the equation system (4.12), one finds

$$-\beta\Omega\left[\bar{G},\bar{\mathcal{O}}\right]\quad=\sum_{\mathbf{i}}\bar{\mathcal{G}}^{(0)}_{\mathbf{i}}\mathrm{e}^{\,\bar{\mathcal{O}}}. \tag{4.13}$$

We insert equations (4.9) and (4.13) into equation (4.11), then the thermodynamical potential functional is

$$\begin{aligned}-\beta\Omega\left[\Omega^{(1)},\Gamma;\bar{G},\bar{\mathcal{O}}\right]=-\beta\Omega&\left[\left(\Omega^{(0)}\right)^{-1}=\left(\Omega^{(1)}\right)^{-1}+\ \Gamma;\bar{\mathcal{G}}=\bar{G}\mathrm{e}^{\,-\bar{\mathcal{O}}}\right]\\&+\operatorname{Tr}\ln\left(\left(\Omega^{(0)}\right)^{-1}-\Gamma\right)-\operatorname{Tr}\ln\left(\left(\Omega^{(1)}\right)^{-1}\right)\\&-\operatorname{Tr}\ln\left(\left(\Omega^{(0)}\right)^{-1}\right)+\operatorname{Tr}\ln\left(\left(\Omega^{(1)}\right)^{-1}+\Gamma\right)\\&+\sum_{\mathbf{i}}\bar{\mathcal{G}}^{(0)}_{\mathbf{i}}\mathrm{e}^{\,\bar{\mathcal{O}}}.\end{aligned} \tag{4.14}$$

The original thermodynamical potential functional $\Omega\left[\left(\Omega^{(0)}\right)^{-1};\bar{\mathcal{G}}\right]$ is clearly determined by (3.74) in the Section 3.6 on page 44 or (3.80b) on page 46

$$-\beta\Omega\left[\left(\Omega^{(0)}\right)^{-1};\bar{\mathcal{G}}\right]=\ln\mathcal{Z}_0+\sum_{\mathbf{i}}\bar{\mathcal{G}}^{(0)}_{\mathbf{i}}+\sum_{\mathbf{i}}\left(\sum_{n=1}^{\infty}\frac{(-1)^n}{(n!)^2}\int_0^1 \mathrm{d}\lambda\ \mathrm{Tr}\ \bar{\mathcal{G}}^{(n)}\left(\mathbf{i}\right)\Omega^{(n)}\left(\mathbf{i}\right)[\lambda]\right) \tag{4.15}$$

The last two equations give the total thermodynamical potential functional depending on renormalized quantities, on which a self-consistent theory for the system considered can be based. The term $\Omega\left[\left(\Omega^{(0)}\right)^{-1}=\left(\Omega^{(1)}\right)^{-1}+\ \Gamma;\bar{\mathcal{G}}=\bar{G}\mathrm{e}^{\ -\bar{\mathcal{O}}}\right]$ contains only the renormalized one-particle Green's function $\Omega^{(1)}$, its self-energy Γ, renormalized local vertices $\bar{G}$ and its "self-energy" $\bar{\mathcal{O}}$ reflecting contributions of many-body processes. The renormalized variables of the thermodynamical potential functional are treated independently and stationary conditions of it with respect to these variables lead to a self-consistent equation system to determine the relationship between the physical quantities of the system considered.

Here, we will show how one can get the results obtained in the above chapters directly from the total thermodynamical potential functional.

One of the derivatives of the unmodified grand partition function $\mathcal{Z}$ (3.16) is

$$G^{(1)}_{\sigma_1'\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right)=-\frac{\delta}{\delta\Omega^{(0)}_{\sigma_1\sigma_1'}\left(\mathbf{i}_1\ \tau_1;\mathbf{i}_1'\ \tau_1'\right)}\ \ln\mathcal{Z} \tag{4.16a}$$

which one can also obtain by differentiating the thermodynamical potential functional (4.14)

$$\begin{aligned}&\frac{\delta}{\delta\Omega^{(0)}_{\sigma_1\sigma_1'}\left(\mathbf{i}_1\ \tau_1;\mathbf{i}_1'\ \tau_1'\right)}\left(-\beta\Omega\left[\Omega^{(1)},\Gamma;\bar{G},\bar{\mathcal{O}}\right]\right)\\&\quad=-\sum_{\mathbf{j}_1\mathbf{j}_1',\varsigma_1\varsigma_1'}\int_0^{\beta}\mathrm{d}\theta_1\mathrm{d}\theta_1'\left(\Omega^{(0)}\right)^{-1}_{\sigma_1'\varsigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{j}_1\ \theta_1\right)\left(\left(\Omega^{(0)}\right)^{-1}-\Gamma\right)^{-1}_{\varsigma_1\varsigma_1'}\left(\mathbf{j}_1\ \theta_1;\mathbf{j}_1'\ \theta_1'\right)\\&\qquad\left(\Omega^{(0)}\right)^{-1}_{\varsigma_1'\sigma_1}\left(\mathbf{j}_1'\ \theta_1';\mathbf{i}_1\ \tau_1\right)+\left(\Omega^{(0)}\right)^{-1}_{\sigma_1'\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right).\end{aligned} \tag{4.16b}$$

Inserting the latter into the first equation (4.16a) we get equation (3.39a) with the self-energy for the auxiliary field.

The stationarity of the thermodynamical potential functional $\Omega\left[\Omega^{(1)},\Gamma;\bar{G},\bar{\mathcal{O}}\right]$ with respect to the variation of the renormalized variables $\Omega^{(1)}_{\sigma,\sigma'}\left(\mathbf{i}\ \tau;\mathbf{i}'\ \tau'\right)$ and its self-energy $\Gamma_{\sigma',\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right)$

$$\frac{\delta}{\delta\Gamma_{\sigma_1'\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right)}\left(-\beta\Omega\left[\Omega^{(1)},\Gamma;\bar{G},\bar{\mathcal{O}}\right]\right)=0 \tag{4.17a}$$

$$\frac{\delta}{\delta\left(\Omega^{(1)}\right)^{-1}_{\sigma_1'\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right)}\left(-\beta\Omega\left[\Omega^{(1)},\Gamma;\bar{G},\bar{\mathcal{O}}\right]\right)=0 \tag{4.17b}$$

gives the equations depending on the free Green's function as shown below. Using the equation (4.14) one has

$$\begin{aligned}\left(\Omega^{(1)}\right)^{-1}_{\sigma_1'\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right)&=\left(\Omega^{(0)}\right)^{-1}_{\sigma_1'\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right)-\Gamma_{\sigma_1'\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right)\\\Omega^{(1)}_{\sigma_1\sigma_1'}\left(\mathbf{i}_1\ \tau_1;\mathbf{i}_1'\ \tau_1'\right)&=\frac{1}{\mathcal{Z}_\psi}\int\left[\mathcal{D}\psi\right]\left[\mathcal{D}\bar{\psi}\right]\bar{\psi}_{\mathbf{i}_1'\sigma_1'}\left(\tau_1'\right)\psi_{\mathbf{i}_1\sigma_1}\left(\tau_1\right)\\&\qquad\exp\left\{-\mathcal{S}\left[\psi,\bar{\psi};\left(\Omega^{(1)}\right)^{-1}+\Gamma;\bar{\mathcal{G}}\right]\right\}\end{aligned} \tag{4.18a}$$

where

$$\mathcal{Z}_{\psi} = \int [\mathcal{D}\psi]\,[\mathcal{D}\bar{\psi}]\,\exp\left\{-\mathcal{S}\left[\psi,\bar{\psi};\left(\Omega^{(1)}\right)^{-1}+\Gamma;\bar{\mathcal{G}}\right]\right\}, \tag{4.18b}$$

which is the integral part of (4.3) with the substitution (4.6). On the other hand, using the equation (4.15) one has an equivalent equation system

$$\begin{aligned}
\left(\Omega^{(1)}\right)^{-1}_{\sigma_1'\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right) &= \left(\Omega^{(0)}\right)^{-1}_{\sigma_1'\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right) - \Gamma_{\sigma_1'\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right)\\
\Omega^{(1)}_{\sigma_1\sigma_1'}\left(\mathbf{i}_1\ \tau_1;\mathbf{i}_1'\ \tau_1'\right) &= \left(\left(\Omega^{(1)}\right)^{-1}+\Gamma\right)^{-1}_{\sigma_1\sigma_1'}\left(\mathbf{i}_1\ \tau_1;\mathbf{i}_1'\ \tau_1'\right)\\
&\quad+\sum_{\mathbf{i}}\left(\sum_{n=1}^{\infty}\frac{(-1)^n}{(n!)^2}\frac{\delta}{\delta\Gamma_{\sigma_1'\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right)}\int_0^1 \mathrm{d}\lambda\ \mathrm{Tr}\ \bar{\mathcal{G}}^{(n)}(\mathbf{i})\,\Omega^{(n)}(\mathbf{i})\,[\lambda]\right).
\end{aligned} \tag{4.18c}$$

Performing functional differentiation in last term of the second equation in (4.18c) one gets

$$\begin{aligned}
&\sum_{\mathbf{i}}\left(\sum_{n=1}^{\infty}\frac{(-1)^n}{(n!)^2}\frac{\delta}{\delta\Gamma_{\sigma_1'\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right)}\int_0^1 \mathrm{d}\lambda\ \mathrm{Tr}\ \bar{\mathcal{G}}^{(n)}(\mathbf{i})\,\Omega^{(n)}(\mathbf{i})\,[\lambda]\right)\\
&= \sum_{\mathbf{i}}\sum_{\substack{n=0\\m=0}}^{\infty}\frac{(-1)^{m+n}}{n!\ (n+1)!\ m!\ (m+1)!}\int_0^1 \mathrm{d}\lambda\sum_{\substack{\varsigma_m,\varsigma_{n+1}\\ \varsigma'_{m+1},\varsigma'_n}}\int_0^{\beta}\mathrm{d}\boldsymbol{\theta}_m\mathrm{d}\boldsymbol{\theta}_{n+1}\mathrm{d}\boldsymbol{\theta}'_{m+1}\mathrm{d}\boldsymbol{\theta}'_n\\
&\quad \hat{\Omega}^{(m+1)}_{\sigma_1\varsigma_m,\varsigma'_{m+1}}\left(\mathbf{i}_1\ \tau_1,\mathbf{i}\ \boldsymbol{\theta}_m;\mathbf{i}\ \boldsymbol{\theta}'_{m+1}\right)[\lambda]\ \bar{G}^{(m+n+1)}_{\varsigma'_{m+1},\varsigma'_n;\varsigma_{n+1},\varsigma_m}\left(\mathbf{i}|\boldsymbol{\theta}'_{m+1},\boldsymbol{\theta}'_n;\boldsymbol{\theta}_{n+1},\boldsymbol{\theta}_m\right)[\lambda]\\
&\quad \hat{\Omega}^{(n+1)}_{\varsigma_{n+1};\sigma_1',\varsigma'_n}\left(\mathbf{i}\ \boldsymbol{\theta}_{n+1};\mathbf{i}_1'\ \tau_1',\mathbf{i}\ \boldsymbol{\theta}'_n\right)[\lambda]\\
&+\sum_{\mathbf{i}}\sum_{n=1}^{\infty}\frac{(-1)^n}{(n!)^2}\int_0^1\mathrm{d}\lambda\sum_{\varsigma_n,\varsigma'_n}\int_0^{\beta}\mathrm{d}\boldsymbol{\theta}_n\mathrm{d}\boldsymbol{\theta}'_n\ \bar{G}^{(n)}_{\varsigma'_n,\varsigma_n}\left(\mathbf{i}|\boldsymbol{\theta}'_n;\boldsymbol{\theta}_n\right)[\lambda]\\
&\quad \hat{\Omega}^{(n+1)}_{\sigma_1,\varsigma_n,\sigma_1'\varsigma'_n}\left(\mathbf{i}_1\ \tau_1,\mathbf{i}\ \boldsymbol{\theta}_n;\mathbf{i}_1'\ \tau_1',\mathbf{i}\ \boldsymbol{\theta}'_n\right)[\lambda].
\end{aligned} \tag{4.18d}$$

The n-particle Green's functions $\hat{\Omega}^{(n)}$ are a functional of $\left(\left(\Omega^{(1)}\right)^{-1}+\Gamma\right)$, as it was seen in (3.39b) one may denote

$$\begin{aligned}
&\sum_{\mathbf{i},\mathbf{i}'}\sum_{\sigma,\sigma'}\int_0^{\beta}\mathrm{d}\tau\mathrm{d}\tau'\left(\left(\Omega^{(1)}\right)^{-1}+\Gamma\right)^{-1}_{\sigma_1\sigma'}\left(\mathbf{i}_1\ \tau_1;\mathbf{i}'\ \tau'\right)\ \Lambda_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right)\\
&\qquad\left(\left(\Omega^{(1)}\right)^{-1}+\Gamma\right)^{-1}_{\sigma\sigma_1'}\left(\mathbf{i}\ \tau;\mathbf{i}_1'\ \tau_1'\right)
\end{aligned} \tag{4.18e}$$

for the sum (4.18d).

Inserting (4.18d) in the form of (4.18e) into (4.18c) one finds that the functional $\Lambda_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right)$ is nothing but the one-particle Green's function for localized electrons $G^{(1)}_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right)$.

Once again, we have the equation for the self-energy of the auxiliary fields as

$$\begin{aligned}
\Gamma_{\sigma_1'\sigma_1}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}_1\ \tau_1\right) &= \sum_{\mathbf{i}\mathbf{i}'}\sum_{\sigma\sigma'}\int_0^{\beta}\mathrm{d}\tau\mathrm{d}\tau'\Lambda_{\sigma_1'\sigma}\left(\mathbf{i}_1'\ \tau_1';\mathbf{i}\ \tau\right)\left(\left(\Omega^{(1)}\right)^{-1}+\Gamma\right)^{-1}_{\sigma\sigma'}\left(\mathbf{i}\ \tau;\mathbf{i}'\ \tau'\right)\\
&\qquad\left(\Omega^{(1)}\right)^{-1}_{\sigma'\sigma_1}\left(\mathbf{i}'\ \tau';\mathbf{i}_1\ \tau_1\right).
\end{aligned} \tag{4.19}$$

This equation specifies the relation of the self-energy $\Gamma_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right)$ to the input parameters of system considered and to itself, i.e. it provides consistency for the solutions of the system in the sense of Baym [4]. The equation (4.19) should equal to equation (3.48) determining the relations between n-particle cumulants $\hat{\Omega}^{(n)}$ of auxiliary fields and n-particle cumulants $\hat{\Omega}^{(n)}\left[\lambda\right]$ where the switch λ presents at every appearance of $\bar{\mathcal{G}}^{(n)}$.

The stationarity of the total thermodynamical potential functional $\Omega\left[\Omega^{(1)},\Gamma;\bar{G},\bar{\mathcal{O}}\right]$ in (4.14) with respect to the variations of the renormalized vertices $\bar{G}^{(n)}$ and its "self-energy" $\bar{\mathcal{O}}^{(n)}$ ensures the exactness of formulae (3.49) and (3.51), that are

$$\bar{G} = \bar{\mathcal{G}}\ \mathrm{e}^{\ \bar{\mathcal{O}}} \tag{4.20a}$$

and

$$\bar{\mathcal{O}}^{(n)}_{\boldsymbol{\sigma}'_n;\boldsymbol{\sigma}_n}\left(\mathbf{i}|\boldsymbol{\tau}'_n;\boldsymbol{\tau}_n\right) = (-1)^n\,\frac{1}{(n!)^2}\,\hat{\Omega}^{(n)}_{\boldsymbol{\sigma}_n;\boldsymbol{\sigma}'_n}\left(\mathbf{i}|\boldsymbol{\tau}_n;\boldsymbol{\tau}'_n\right). \tag{4.20b}$$

The thermodynamical potential functional, where the unrenormalized one-particle Green's function $\left(\Omega^{(0)}\right)^{-1}$ is replaced by renormalized one and its self-energy as $\left(\Omega^{(1)}\right)^{-1}+\Gamma$ is suitable for the exact solution and for the cases where the result cannot be generated by a sum of a simple skeleton diagrams. If one has to rely on sums of classes of particular diagrams it is more practical if one defines a new functional

$$\Psi\left[\ldots,\Gamma\right] = -\mathbf{Tr}\ln\left(\Omega^{(1)}\right)^{-1} + \ln\mathcal{Z}\left[\ldots,\left(\Omega^{(1)}\right)^{-1}+\Gamma\right] \tag{4.21}$$

that is, due to the stationary equations with respect to renormalized quantities, independent of the one-particle Green's function $\Omega^{(1)}$. One has no diagrammatic representation for the functional Ψ. But if one perform a Legendre transformation Ψ to a functional of the one-particle Green's function $\Omega^{(1)}$

$$\Phi\left[\ldots,\Omega^{(1)}\right] = \Psi\left[\ldots,\Gamma\right] - \mathbf{Tr}\left(\Gamma\ \Omega^{(1)}\right) \tag{4.22}$$

it will be a sum of all connected diagrams, free of self-insertions, i.e. skeleton diagrams only. Inserting (4.21) and (4.22) into the original generating functional one reveals the Baym thermodynamical potential functional, Baym [4].

Both the thermodynamical potentials, original and newly obtained, are exact. They are connected by a Legendre transformations (4.21) and (4.22). While the original one is applicable without restrictions, the direct application of the Baym's functional is restricted to the cases where one was able to find a diagrammatical representation for the functional Φ. We then speak about Φ-derivable approximations. Of cause, not all approximations are Φ-derivable. The simplest example for a non-Φ-derivable solution is a 0-dimensional lattice (single site or atomic solution).

One of the important features of the Baym's representation for the thermodynamical potential is that the variational variables present sums of classes of Feynman diagrams from perturbation theory.

SECTION 4.2

Dynamical Mean Field Theory (DMFT)

Here, we will demonstrate how to obtain the Dynamical Mean Field Theory in the frame of strong-coupling expansion. It is shown that the forthcoming results are identical with those obtained by DMFT without the strong-coupling expansion that was mentioned in Appendix B. Following the formalism presented in Appendix B, we introduce a local (site-independent) self-energy for auxiliary fields $\psi_{\mathbf{i}\sigma}$ and $\bar{\psi}_{\mathbf{i}'\sigma'}$, that is denoted as $\Gamma_\sigma(\omega_n)$. The thermodynamical potential functional (4.9) is rewritten as

$$\begin{aligned}
-\beta\Omega\left[\Omega^{(1)},\Gamma;\bar{\mathcal{G}}\right] = & -\beta\sum_{\mathbf{i}}\Omega_{\mathbf{i}}\left[\left(\Omega^{(1)}\right)^{-1}+\Gamma;\bar{\mathcal{G}}\right] \\
& +\sum_{\omega_n}\sum_{\mathbf{k}\sigma}\ln\left(\left(\Omega^{(0)}\right)^{-1}-\Gamma\right)_\sigma(\mathbf{k}\ \omega_n)-\sum_{\omega_n}\sum_{\mathbf{i}\sigma}\ln\left(\left(\Omega^{(1)}\right)^{-1}\right)(\omega_n) \\
& -\sum_{\omega_n}\sum_{\mathbf{k}\sigma}\ln\left(\left(\Omega^{(0)}\right)^{-1}\right)_\sigma(\mathbf{k}\ \omega_n)+\sum_{\omega_n}\sum_{\mathbf{k}\sigma}\ln\left(\left(\Omega^{(1)}\right)^{-1}+\Gamma\right)(\omega_n)
\end{aligned} \tag{4.23}$$

where $\Omega_{\mathbf{i}}\left[\left(\Omega^{(1)}\right)^{-1}+\Gamma;\bar{\mathcal{G}}\right]$ is defined as in (4.3) and (4.5) with the replacement (4.6) but the self-energy functional is local. The stationary conditions of the total thermodynamical potential functional $\Omega\left[\Omega^{(1)},\Gamma;\bar{\mathcal{G}}\right]$ with respect to the renormalized local Green's function $\Omega^{(1)}_\sigma(\omega_n)$ of the auxiliary fields and its self-energy $\Gamma_\sigma(\omega_n)$ ensure that the thermodynamical conditions of the system are fulfilled. As in (B.10) we have the equation system for the renormalized Green's function of auxiliary fields

$$\begin{aligned}
\Omega^{(1)}_\sigma(\omega_n) &= \frac{1}{N}\sum_{\mathbf{k}}\left(\left(\Omega^{(0)}\right)^{-1}_\sigma(\mathbf{k}\ \omega_n)-\Gamma_\sigma(\omega_n)\right)^{-1} \\
\Omega^{(1)}_\sigma(\omega_n) &= \frac{1}{N}\sum_{\mathbf{i}}\frac{1}{\mathcal{Z}_{\mathbf{i}}}\int[\mathcal{D}\psi_{\mathbf{i}}]\left[\mathcal{D}\bar{\psi}_{\mathbf{i}}\right]\bar{\psi}_{\mathbf{i}\sigma}(\omega_n)\,\psi_{\mathbf{i}\sigma}(\omega_n)\exp\left\{-\mathcal{S}_{\mathbf{i}}\left[\psi,\bar{\psi}\right]\right\}.
\end{aligned} \tag{4.24}$$

Solving the second equation of (4.24) we have the solution for the DMFT within strong-coupling expansion.

Rereading the Green's function for the localized electrons (3.39a) and (3.39c), the resultant DMFT Green's function for the localized electrons is

$$\begin{aligned}
G^{(1)}_\sigma(\omega_n) &= \frac{1}{N}\sum_{\mathbf{k}}\left(\Gamma^{-1}_\sigma(\omega_n)-\Omega^{(0)}_\sigma(\mathbf{k}\ \omega_n)\right)^{-1} \\
G^{(1)}_\sigma(\omega_n) &= \Gamma_\sigma(\omega_n)+\Gamma_\sigma(\omega_n)\,\Omega^{(1)}_\sigma(\omega_n)\,\Gamma_\sigma(\omega_n)
\end{aligned} \tag{4.25}$$

with

$$\Gamma^{-1}_\sigma(\omega_n) = i\omega_n-\varepsilon^f-\Sigma^f_\sigma(\omega_n)\,. \tag{4.26}$$

The equations (4.25) and (4.26) are nothing but the Green's function of localized electrons directly obtained from (B.10) for the Hubbard model and the periodic Anderson model.

The equation (3.48) rewritten in DMFT form reads

$$\begin{aligned}
\Gamma_\sigma\left(\tau';\tau\right) = & \sum_{n=1}^{\infty}(-1)^{n+1}\frac{n}{(n!)^2}\int_0^\beta \mathrm{d}\theta'\int_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau_n\mathrm{d}\tau'_2\cdots\mathrm{d}\tau'_n \\
& \sum_{\substack{\sigma_1\cdots\sigma_n\\ \sigma'_2\cdots\sigma'_n}}\bar{G}^{(n)}_{\sigma,\ldots,\sigma'_n;\sigma_1,\ldots,\sigma_n}\left(\tau',\tau'_2,\ldots,\tau'_n;\tau_1,\ldots,\tau_n\right) \\
& \hat{\Omega}^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma,\ldots,\sigma'_n}\left(\tau_1,\ldots,\tau_n;\theta',\tau'_2,\ldots,\tau'_n\right)\left(\Omega^{(1)}\right)^{-1}_\sigma\left(\theta';\tau\right),
\end{aligned} \tag{4.27}$$

where the DMFT n-particle Green's function $\hat{\Omega}^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma,\ldots,\sigma'_n}(\tau_1,\ldots,\tau_n;\theta',\tau'_2,\ldots,\tau'_n)$ is defined in (3.39b) where all site variables are omitted

$$\begin{aligned}
&\hat{G}^{(n)}_{\sigma'_1\ldots\sigma'_n;\sigma_1\ldots\sigma_1}\left(\tau'_1,\ldots,\tau'_n;\tau_1,\ldots,\tau_1\right) \\
&= \int\limits_0^\beta \mathrm{d}\theta_1\mathrm{d}\theta'_1\cdots\mathrm{d}\theta_n\mathrm{d}\theta'_n \left(\Omega^{(0)}\right)^{-1}_{\sigma'_1}\left(\tau'_1;\theta_1\right)\cdots\left(\Omega^{(0)}\right)^{-1}_{\sigma'_n}\left(\tau'_n;\ \theta_n\right) \\
&\qquad \hat{\Omega}^{(n)}_{\sigma'_1,\ldots\sigma'_n;\sigma_1\ldots\sigma_n}\left(\theta_1,\ldots,\theta_n;\theta'_1,\ldots,\theta'_n\right)\left(\Omega^{(0)}\right)^{-1}_{\sigma_n}\left(\theta'_n;\tau_n\right)\cdots\left(\Omega^{(0)}\right)^{-1}_{\sigma_1}\left(\theta'_1;\tau_1\right).
\end{aligned} \tag{4.28}$$

It is recognized that the DMFT n-particle cumulant $\hat{\Omega}^{(n)}_{\sigma'_1,\ldots\sigma'_n;\sigma_1\ldots\sigma_n}(\theta_1,\ldots,\theta_n;\theta'_1,\ldots,\theta'_n)$ contains only the one-site contributions.

That is not difficult to see that the last result for the DMFT (4.27) can be approximately obtained by dropping the site-dependence in the generic equation for the self-energy of the auxiliary fields (3.48).

SECTION 4.3

Approximations

In the last Section we have discussed about the DMFT which is obtained in the framework of strong-coupling expansion theory. The results that have been seen are that in the DMFT only one-site Green's function are included. That means that only the first term of following separation

$$\Gamma_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right) = \delta_{\sigma'\sigma}\delta_{\mathbf{i}'\mathbf{i}}\Gamma_\sigma\left(\mathbf{i}|\tau';\ \tau\right) + \left(1-\delta_{\sigma'\sigma}\delta_{\mathbf{i}'\mathbf{i}}\right)\Gamma_{\sigma'\sigma}\left(\mathbf{i}'\ \tau';\mathbf{i}\ \tau\right) \tag{4.29}$$

is appearing in the calculations of the local Green's function $\Omega^{(1)}_\sigma(\omega_n)$ in (4.24). Assume that $\Gamma_\sigma(\mathbf{i}|\tau';\ \tau)$ is site-independent, then in the mixed site-frequency space the first equation of (4.24) has the following form

$$\begin{aligned}
\Omega^{(1)}_\sigma(\omega_n) = \Omega^{(0)}_\sigma(\mathbf{i};\mathbf{i}|\omega_n) + \sum_{n=1}^{\infty}\sum_{\mathbf{i}_1,\ldots\mathbf{i}_n}\Omega^{(0)}_\sigma(\mathbf{i};\mathbf{i}_1|\omega_n)\,\Gamma_\sigma(\omega_n) \\
\cdots\Omega^{(0)}_\sigma(\mathbf{i}_{n-1};\mathbf{i}_n|\omega_n)\,\Gamma_\sigma(\omega_n)\,\Omega^{(0)}_\sigma(\mathbf{i}_n;\mathbf{i}|\omega_n).
\end{aligned} \tag{4.30}$$

Using the self-avoiding walk approximation [10] for the above equation one must perform the following substitution

$$\Omega^{(0)}_\sigma(\mathbf{i}_{l-1};\mathbf{i}_l|\omega_n) = \Omega^{(0)}_\sigma(\mathbf{i}_{l-1};\mathbf{i}_l|\omega_n) - \Omega^{(1)}_\sigma(\omega_n) \tag{4.31}$$

then the self-avoiding walk equation within DMFT reads

$$\Omega^{(1)}_\sigma(\omega_n) = \sum_{\mathbf{k}}\frac{\Omega^{(0)}_\sigma(\mathbf{k}\ \omega_n)}{1-\Gamma_\sigma(\omega_n)\left(\Omega^{(0)}_\sigma(\mathbf{k}\ \omega_n)-\Omega^{(1)}_\sigma(\omega_n)\right)}. \tag{4.32}$$

Up to now in all approximations the self-energy $\Gamma_\sigma(\omega_n)$ is only treated with the first term of general form (4.27), i.e.

$$\Gamma_\sigma(\omega_n) = \bar{G}_\sigma(\omega_n) \tag{4.33}$$

within the NCA of the single-impurity Anderson model.

Actually, the renormalized vertex (3.49) still contains other contributions of many-body collective processes which are can be described as many-impurity processes.

We also know that thus many-body collective processes are contributing to $\bar{G}_\sigma(\omega_n)$ by appearance of the n-particle cumulants $\hat{\Omega}^{(n)}$ defined in (3.39b), containing the n-particle connected Green's function $\hat{G}^{(n)}$. That is, if we take into account only the one-site approximation of the n-particle connected Green's function $\hat{G}^{(n)}$ the results will be equivalent to the treatment of single impurity model. That allows us to explain why DMFT is treated within an approximation for the single impurity Anderson model.

Within the approximation (4.33) all corrections to the DMFT's solution will be local. The non-local corrections to the DMFT's solution require the contributions of the next terms in the expression of the self-energy of the auxiliary fields (3.48) where the site index $\mathbf{i}$ is set equal to site index $\mathbf{i}'$.

We now can conclude that in order to include non-local contributions to the DMFT's solution one has to add many-site cumulants of the auxiliary fields to the newly renormalized local many-particle vertices determined as in equation (3.49) where the DMFT's many-particle correlation functions serve as correspondingly unrenormalized vertices. One has also to go over the local approximation in which only renormalized one-particle vertex of the self-energy of the auxiliary fields is taken into account. The role of higher order terms containing many-particle cumulants of the auxiliary fields in non-local corrections to DMFT's solution is unnegligible.

Our results in (3.49), (3.39b) and (3.71) already show us how to add a correction to DMFT and to control such procedures.

APPENDIX A

Auxiliary Mathematical Relations

SECTION A.1

The product of two n-dimensional totally symmetric tensors

The product of two n-dimensional totally symmetric tensors is denoted by the symbol $\Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varsigma_1,\ldots,\varsigma_n}$ $(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{j}_1\ \theta_1,\ldots,\mathbf{j}_n\ \theta_n)$ and is defined as a n-dimensional determinant

$$
\begin{aligned}
&\Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varsigma_1,\ldots,\varsigma_n}(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{j}_1\ \theta_1,\ldots,\mathbf{j}_n\ \theta_n)\\
&\quad=\varepsilon_{(\sigma_1\mathbf{i}_1\ \tau_1)\ldots(\sigma_n\mathbf{i}_n\ \tau_n)}\ \varepsilon_{(\varsigma_n\mathbf{j}_n\ \theta_n)\ldots(\varsigma_1\mathbf{j}_1\ \theta_1)}\\
&\quad=\det\begin{vmatrix}\delta_{\sigma_1\varsigma_1}\delta_{\mathbf{i}_1\mathbf{j}_1}\delta\left(\tau_1-\theta_1\right) & \ldots & \delta_{\sigma_1\varsigma_n}\delta_{\mathbf{i}_1\mathbf{j}_n}\delta\left(\tau_1-\theta_n\right)\\ \ldots & \ldots & \ldots\\ \delta_{\sigma_n\varsigma_1}\delta_{\mathbf{i}_n\mathbf{j}_1}\delta\left(\tau_n-\theta_1\right) & \ldots & \delta_{\sigma_n\varsigma_n}\delta_{\mathbf{i}_n\mathbf{j}_n}\delta\left(\tau_n-\theta_n\right)\end{vmatrix}
\end{aligned}
\tag{A.1}
$$

and the following identities - expansion theorem for determinants, hold with any integer $k \leq n$

$$
\begin{aligned}
&\Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varsigma_1,\ldots,\varsigma_n}(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{j}_1\ \theta_1,\ldots,\mathbf{j}_n\ \theta_n)\\
&\quad=\frac{1}{k!}\int_0^\beta \mathrm{d}\vartheta_1\ldots\mathrm{d}\vartheta_k\sum_{\substack{\varrho_1,\ldots,\varrho_k\\ \mathbf{l}_1,\ldots,\mathbf{l}_k}}\\
&\qquad\Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varrho_1,\ldots,\varrho_k,\varsigma_{k+1},\ldots,\varsigma_n}(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{l}_1\ \vartheta_1,\ldots,\mathbf{l}_k\ \vartheta_k,\mathbf{j}_{k+1}\ \theta_{k+1},\ldots,\mathbf{j}_n\ \theta_n)\\
&\qquad\qquad\Delta^{(k)}_{\varrho_1,\ldots,\varrho_k;\varsigma_1,\ldots,\varsigma_k}(\mathbf{l}_1\ \vartheta_1,\ldots,\mathbf{l}_k\ \vartheta_k;\mathbf{j}_1\ \theta_1,\ldots,\mathbf{j}_k\ \theta_k)\\
&\quad=\frac{1}{k!}\frac{1}{(n-k)!}\int_0^\beta \mathrm{d}\vartheta_1\ldots\mathrm{d}\vartheta_n\sum_{\substack{\varrho_1,\ldots,\varrho_n\\ \mathbf{l}_1,\ldots,\mathbf{l}_n}}\Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varrho_1,\ldots,\varrho_n}(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{l}_1\ \vartheta_1,\ldots,\mathbf{l}_n\ \vartheta_n)\\
&\qquad\qquad\Delta^{(k)}_{\varrho_1,\ldots,\varrho_k;\varsigma_1,\ldots,\varsigma_k}(\mathbf{l}_1\ \vartheta_1,\ldots,\mathbf{l}_k\ \vartheta_k;\mathbf{j}_1\ \theta_1,\ldots,\mathbf{j}_k\ \theta_k)\\
&\qquad\qquad\Delta^{(n-k)}_{\varrho_{k+1},\ldots,\varrho_n;\varsigma_{k+1},\ldots,\varsigma_n}(\mathbf{l}_{k+1}\ \vartheta_{k+1},\ldots,\mathbf{l}_n\ \vartheta_n;\mathbf{j}_{k+1}\ \theta_{k+1},\ldots,\mathbf{j}_n\ \theta_n)
\end{aligned}
\tag{A.2}
$$

SECTION A.2

Exponential function notation

The exponential function notation is the series of functions which can be formally written in the form like exponential function as

$$\mathrm{e}^{X}=1+\sum_{k=1}^{\infty}\frac{1}{k!}\,X^{(p_1)}\cdots X^{(p_k)}. \tag{A.3a}$$

We also define the n-order term of this exponential function

$$\left(\mathrm{e}^{X}\right)^{(n)}=\begin{cases}1 & \text{for } n=0\\ X^{(1)} & \text{for } n=1\\ X^{(2)}+\dfrac{1}{2!}X^{(1)}X^{(1)} & \text{for } n=2\\ \cdots & \cdots\\ \sum\limits_{k=1}^{n}\sum\limits_{p_1+\cdots+p_k=n}\dfrac{1}{k!}\,X^{(p_1)}\cdots X^{(p_k)} & \text{for any } n \text{ integer}\end{cases} \tag{A.3b}$$

If the variable is chosen as

$$X^{(n)}=\frac{1}{(n!)^2}\,\bar{\mathcal{O}}^{(n)}_{\varsigma_1,\ldots,\varsigma_n;\varsigma'_1,\ldots,\varsigma'_n}\left(\mathbf{j}_1\ \theta_1,\ldots,\mathbf{j}_n\ \theta_n;\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n\right) \tag{A.3c}$$

then $\left(\mathrm{e}^{X}\right)^{(n)}$ will be an n-order function like

$$\begin{aligned}\left(\mathrm{e}^{\bar{\mathcal{O}}}\right)^{(n)}&\longrightarrow\left(\mathrm{e}^{\bar{\mathcal{O}}}\right)^{(n)}_{\varsigma_1,\ldots,\varsigma_n;\varsigma'_1,\ldots,\varsigma'_n}\left(\mathbf{j}_1\ \theta_1,\ldots,\mathbf{j}_n\ \theta_n;\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n\right)\\ &=\begin{cases}\bar{\mathcal{O}}^{(1)}_{\varsigma_1;\varsigma'_1}\left(\mathbf{j}_1\ \theta_1;\mathbf{j}'_1\ \theta'_1\right) & \text{for } n=1\\ \dfrac{1}{(2!)^2}\,\bar{\mathcal{O}}^{(2)}_{\varsigma_1,\varsigma_2;\varsigma'_1,\varsigma'_2}\left(\mathbf{j}_1\ \theta_1,\mathbf{j}_2\ \theta_2;\mathbf{j}'_1\ \theta'_1,\mathbf{j}'_2\ \theta'_2\right)+ & \\ \qquad\dfrac{1}{2!}\,\bar{\mathcal{O}}^{(1)}_{\varsigma_1;\varsigma'_1}\left(\mathbf{j}_1\ \theta_1;\mathbf{j}'_1\ \theta'_1\right)\bar{\mathcal{O}}^{(1)}_{\varsigma_2;\varsigma'_2}\left(\mathbf{j}_2\ \theta_2;\mathbf{j}'_2\ \theta'_2\right) & \text{for } n=2\\ \cdots & \cdots\end{cases}\end{aligned} \tag{A.3d}$$

Another useful case is

$$\begin{aligned}\left(\mathrm{e}^{\bar{\mathcal{O}}}\right)^{(n)}&\longrightarrow\left(\mathrm{e}^{\bar{\mathcal{O}}}\right)^{(n)}_{\varsigma'_1,\ldots,\varsigma'_n}\left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n\right)\\ &=\begin{cases}\bar{\mathcal{O}}^{(1)}_{\varsigma'_1}\left(\mathbf{j}'_1\ \theta'_1\right) & \text{for } n=1\\ \dfrac{1}{2!}\,\bar{\mathcal{O}}^{(2)}_{\varsigma'_1,\varsigma'_2}\left(\mathbf{j}'_1\ \theta'_1,\mathbf{j}'_2\ \theta'_2\right)+\dfrac{1}{2!}\,\bar{\mathcal{O}}^{(1)}_{\varsigma'_1}\left(\mathbf{j}'_1\ \theta'_1\right)\bar{\mathcal{O}}^{(1)}_{\varsigma'_2}\left(\mathbf{j}'_2\ \theta'_2\right) & \text{for } n=2\\ \cdots & \cdots\end{cases}\end{aligned} \tag{A.3e}$$

when the variable is chosen as

$$X^{(n)}=\frac{1}{n!}\,\bar{\mathcal{O}}^{(n)}_{\varsigma'_1,\ldots,\varsigma'_n}\left(\mathbf{j}'_1\ \theta'_1,\ldots,\mathbf{j}'_n\ \theta'_n\right) \tag{A.3f}$$

SECTION A.3

Generalization of commutator and anticommutator

We consider some generalized notations for commutator and anticommutator. Supposed that $\mathcal{A}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right]$ is some product of differential operators $\frac{\delta}{\bar{\pi}(\tau)}$ and $\frac{\delta}{\pi(\tau)}$, in which all operators $\frac{\delta}{\pi(\tau)}$ stay on the left of all operators $\frac{\delta}{\bar{\pi}(\tau)}$. It would be convenient to introduce some notations

$$\begin{aligned}\mathcal{A}^{(0;1)}_{[\cdot;\mathbf{i}\sigma]}(\tau) &= \left[\mathcal{A}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right], \bar{\pi}_{\mathbf{i}\sigma}(\tau)\right] \\ &= \mathcal{A}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right]\bar{\pi}_{\mathbf{i}\sigma}(\tau) - (-1)^{\nu}\,\bar{\pi}_{\mathbf{i}\sigma}(\tau)\,\mathcal{A}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right]\end{aligned} \tag{A.4a}$$

$$\begin{aligned}\mathcal{A}^{(1;0)}_{[\mathbf{i}'\sigma';\cdot]}(\tau') &= \left[\pi_{\mathbf{i}'\sigma'}(\tau'), \mathcal{A}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right]\right] \\ &= \pi_{\mathbf{i}'\sigma'}(\tau')\,\mathcal{A}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right] - (-1)^{\nu}\,\mathcal{A}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right]\pi_{\mathbf{i}'\sigma'}(\tau')\end{aligned} \tag{A.4b}$$

where ν is the number of differential operators $\frac{\delta}{\bar{\pi}(\tau)}$ and $\frac{\delta}{\pi(\tau)}$ in expression $\mathcal{A}$.
For the differential operator

$$\begin{aligned}\bar{\mathcal{S}}_{\text{int}}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right] &= -\,\mathcal{S}_{\text{int}}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right] \\ &= \sum_{\mathbf{i}}\sum_{n=1}^{\infty}\bar{\mathcal{S}}^{(n)}_{\mathbf{i}}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right] \\ &= \sum_{\mathbf{i}}\bar{\mathcal{S}}_{\mathbf{i}}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right]\end{aligned} \tag{A.5}$$

we may have

$$\begin{aligned}\bar{\mathcal{S}}^{(0;1)}_{\text{int}[\cdot;\mathbf{i}\sigma]}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right](\tau) &= \left[\bar{\mathcal{S}}_{\text{int}}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right], \bar{\pi}_{\mathbf{i}\sigma}(\tau)\right] \\ &= \left[\bar{\mathcal{S}}_{\mathbf{i}}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right], \bar{\pi}_{\mathbf{i}\sigma}(\tau)\right] \\ &= \bar{\mathcal{S}}^{(0;1)}_{\mathbf{i}[\cdot;\sigma]}\left[\frac{\delta}{\bar{\pi}(\tau)}, \frac{\delta}{\pi(\tau)}\right](\tau) \\ &= \sum_{n=1}^{\infty}\frac{1}{n!\,(n-1)!}\int_{0}^{\beta} \mathrm{d}\tau_2\cdots\mathrm{d}\tau_n\mathrm{d}\tau'_1\cdots\mathrm{d}\tau'_n \\ &\qquad \sum_{\substack{\sigma_2\ldots\sigma_n\\ \sigma'_1\ldots\sigma'_n}}\bar{\mathcal{G}}^{(n)}_{\sigma'_1,\ldots,\sigma'_n;\sigma,\ldots,\sigma_n}\left(\mathbf{i}|\tau'_1,\ldots,\tau'_n;\tau,\ldots,\tau_n\right) \\ &\qquad\qquad \frac{\delta}{\delta\pi_{\mathbf{i}\sigma'_1}(\tau'_1)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}\sigma'_n}(\tau'_n)}\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}\sigma_n}(\tau_n)}\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}\sigma_2}(\tau_2)}\end{aligned} \tag{A.6a}$$

$$
\begin{aligned}
\bar{\mathcal{S}}^{(1;0)}_{\mathrm{int}[\mathbf{i}'\sigma';\cdot]}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right](\tau') &= \left[\pi_{\mathbf{i}'\sigma'}(\tau'),\bar{\mathcal{S}}_{\mathrm{int}}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right]\right] \\
&= \left[\pi_{\mathbf{i}'\sigma'}(\tau'),\bar{\mathcal{S}}_{\mathbf{i}'}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right]\right] \\
&= \bar{\mathcal{S}}^{(1;0)}_{\mathbf{i}'[\sigma';\cdot]}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right](\tau') \\
&= \sum_{n=1}^{\infty}\frac{1}{(n-1)!n!}\int_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau_n\mathrm{d}\tau_2'\cdots\mathrm{d}\tau_n' \\
&\quad \sum_{\substack{\sigma_1\dots\sigma_n\\ \sigma_2'\dots\sigma_n'}}\bar{\mathcal{G}}^{(n)}_{\sigma',\dots,\sigma_n';\sigma_1,\dots,\sigma_n}\left(\mathbf{i}'|\tau',\dots,\tau_n';\tau_1,\dots,\tau_n\right) \\
&\quad \frac{\delta}{\delta\pi_{\mathbf{i}'\sigma_2'}(\tau_2')}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}'\sigma_n'}(\tau_n')}\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}'\sigma_n}(\tau_n)}\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}'\sigma_1}(\tau_1)}
\end{aligned}
\tag{A.6b}
$$

or more general

$$
\begin{aligned}
&\bar{\mathcal{S}}^{(p+1;q+1)}_{\mathrm{int}[\mathbf{i}_1'\sigma_1',\dots,\mathbf{i}_{p+1}'\sigma_{p+1}';\mathbf{i}_1\sigma_1,\dots,\mathbf{i}_{q+1}\sigma_{q+1}]}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right](\tau_1',\dots\tau_{p+1}';\tau_1,\dots\tau_{q+1}) \\
&= \left[\pi_{\mathbf{i}_{p+1}'\sigma_{p+1}'}(\tau_{p+1}'),\left[\bar{\mathcal{S}}^{(p;q)}_{\mathrm{int}[\mathbf{i}_1'\sigma_1',\dots,\mathbf{i}_p'\sigma_p';\mathbf{i}_1\sigma_1,\dots,\mathbf{i}_q\sigma_q]}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right](\tau_1',\dots\tau_p';\tau_1,\dots\tau_q),\bar{\pi}_{\mathbf{i}_{q+1}\sigma_{q+1}}(\tau_{q+1})\right]\right] \\
&= \left[\left[\pi_{\mathbf{i}_{p+1}'\sigma_{p+1}'}(\tau_{p+1}'),\bar{\mathcal{S}}^{(p;q)}_{\mathrm{int}[\mathbf{i}_1'\sigma_1',\dots,\mathbf{i}_p'\sigma_p';\mathbf{i}_1\sigma_1,\dots,\mathbf{i}_q\sigma_q]}\left[\frac{\delta}{\bar{\pi}(\tau)},\frac{\delta}{\pi(\tau)}\right](\tau_1',\dots\tau_p';\tau_1,\dots\tau_q)\right],\bar{\pi}_{\mathbf{i}_{q+1}\sigma_{q+1}}(\tau_{q+1})\right] \\
&= \delta_{\mathbf{i}\mathbf{i}_1'}\dots\delta_{\mathbf{i}\mathbf{i}_{p+1}'}\delta_{\mathbf{i}\mathbf{i}_1}\dots\delta_{\mathbf{i}\mathbf{i}_{q+1}'}\bar{\mathcal{S}}^{(p+1;q+1)}_{\mathbf{i}[\sigma_1',\dots,\sigma_{p+1}';\sigma_1,\dots,\sigma_{q+1}]}\left[\frac{\delta}{\bar{\pi}(\tau)}\frac{\delta}{\pi(\tau)}\right](\tau_1',\dots\tau_{p+1}';\tau_1,\dots\tau_{q+1}) \\
&= \delta_{\mathbf{i}\mathbf{i}_1'}\dots\delta_{\mathbf{i}\mathbf{i}_{p+1}'}\delta_{\mathbf{i}\mathbf{i}_1}\dots\delta_{\mathbf{i}\mathbf{i}_{q+1}'}\sum_{n=\max(p+1,q+1)}^{\infty}\frac{1}{(n-p-1)!\,(n-q-1)!}\int_0^\beta\mathrm{d}\tau_{q+2}\cdots\mathrm{d}\tau_n\mathrm{d}\tau_{p+2}'\cdots\mathrm{d}\tau_n' \\
&\sum_{\substack{\sigma_{q+2}\dots\sigma_n\\ \sigma_{p+2}'\dots\sigma_n'}}\bar{\mathcal{G}}^{(n)}_{\sigma_1',\dots,\sigma_{p+1}',\sigma_{p+2}',\dots\sigma_n';\sigma_1,\dots,\sigma_{q+1},\sigma_{q+2},\dots,\sigma_n}\left(\mathbf{i}|\tau_1',\dots,\tau_{p+1}',\tau_{p+2}',\dots\tau_n';\tau_1,\dots,\tau_{q+1},\tau_{q+2},\dots,\tau_n\right) \\
&\quad\frac{\delta}{\delta\pi_{\mathbf{i}\sigma_{p+2}'}\left(\tau_{p+2}'\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}\sigma_n'}(\tau_n')}\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}\sigma_n}(\tau_n)}\cdots\frac{\delta}{\delta\bar{\pi}_{\mathbf{i}\sigma_{q+2}}(\tau_{q+2})}.
\end{aligned}
\tag{A.6c}
$$

Useful differential expressions are used in calculations, for example in (3.60a)

$$
\begin{aligned}
&\frac{1}{\mathcal{Z}}\frac{\delta}{\delta\pi_{\mathbf{i}_n'\sigma_n'}(\tau_n')}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}_1'\sigma_1'}(\tau_1')} \\
&\quad\frac{1}{k!}\pi_{\varsigma_1'}(\mathbf{j}_1'\ \theta_1')\dots\pi_{\varsigma_k'}(\mathbf{j}_k'\ \theta_k')\left(\mathrm{e}^{\tilde{\mathcal{S}}}\right)^{(n-k)}_{\varsigma_{k+1}',\dots,\varsigma_n'}(\mathbf{j}_{k+1}'\ \theta_{k+1}',\dots,\mathbf{j}_n'\ \theta_n')\ \mathcal{Z}[\pi,\bar{\pi}]\Big|_{\pi=\bar{\pi}=0} \\
&= \frac{1}{k!}\int_0^\beta\mathrm{d}\vartheta_1'\dots\mathrm{d}\vartheta_n'\sum_{\substack{\varrho_1',\dots,\varrho_1'\\ \mathbf{l}_1',\dots,\mathbf{l}_n'}}\frac{1}{k!}\Delta^{(k)}_{\varsigma_1',\dots,\varsigma_k';\varrho_1',\dots,\varrho_k'}(\mathbf{j}_1'\ \theta_1',\dots,\mathbf{j}_k'\ \theta_k';\mathbf{l}_1'\ \vartheta_1',\dots,\mathbf{l}_k'\ \vartheta_k') \\
&\quad\frac{1}{(n-k)!}\frac{1}{\mathcal{Z}}\frac{\delta}{\delta\pi_{\mathbf{l}_n'\varrho_n'}(\vartheta_n')}\cdots\frac{\delta}{\delta\pi_{\mathbf{l}_{k+1}'\varrho_{k+1}'}(\vartheta_{k+1}')}\left(\mathrm{e}^{\tilde{\mathcal{S}}}\right)^{(n-k)}_{\varsigma_{k+1}',\dots,\varsigma_n'}(\mathbf{j}_{k+1}'\ \theta_{k+1}',\dots,\mathbf{j}_n'\ \theta_n')\ \mathcal{Z}[\pi,\bar{\pi}]\Big|_{\pi=\bar{\pi}=0} \\
&\quad\quad\Delta^{(n)}_{\varrho_1',\dots,\varrho_n';\sigma_1',\dots,\sigma_k'}(\mathbf{l}_1'\ \vartheta_1',\dots,\mathbf{l}_n'\ \vartheta_n';\mathbf{i}_1'\ \tau_1',\dots,\mathbf{i}_n'\ \tau_n')
\end{aligned}
\tag{A.7}
$$

and in (3.60c)

$$\frac{1}{n!}\int_0^\beta \mathrm{d}\theta_1'\cdots\mathrm{d}\theta_n' \sum_{\substack{\varsigma_1'\cdots\varsigma_n'\\ \mathbf{j}_1'\cdots\mathbf{j}_n'}} \Omega^{(0)}_{\sigma_1\varsigma_1'}\left(\mathbf{i}_1\ \tau_1;\mathbf{j}_1'\ \theta_1'\right)\ldots\Omega^{(0)}_{\sigma_n\varsigma_n'}\left(\mathbf{i}_n\ \tau_n;\mathbf{j}_n'\ \theta_n'\right)$$

$$\frac{1}{\mathcal{Z}}\ \frac{\delta}{\delta\pi_{\mathbf{i}_n'\sigma_n'}\left(\tau_n'\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}_1'\sigma_1'}\left(\tau_1'\right)}\left(\mathrm{e}^{\tilde{\mathcal{S}}}\right)^{(n)}_{\varsigma_1',\ldots,\varsigma_n'}\left(\mathbf{j}_1'\ \theta_1',\ldots,\mathbf{j}_n'\ \theta_n'\right)\ \mathcal{Z}\left[\pi,\bar{\pi}\right]\Bigg|_{\pi=\bar{\pi}=0}$$

$$= \frac{1}{(n!)^2}\int_0^\beta \mathrm{d}\theta_1\cdots\mathrm{d}\theta_n\mathrm{d}\theta_1'\cdots\mathrm{d}\theta_n' \sum_{\substack{\varsigma_1,\ldots,\varsigma_n\\ \mathbf{j}_1,\ldots,\mathbf{j}_n}}\ \sum_{\substack{\varsigma_1',\ldots,\varsigma_n'\\ \mathbf{j}_1',\ldots,\mathbf{j}_n'}} \Delta^{(n)}_{\sigma_1,\ldots,\sigma_n;\varsigma_1,\ldots,\varsigma_n}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{j}_1\ \theta_1,\ldots,\mathbf{j}_n\ \theta_n\right) \tag{A.8a}$$

$$\left(\mathrm{e}^{\bar{\mathcal{L}}}\right)^{(n)}_{\varsigma_1,\ldots,\varsigma_n;\varsigma_1',\ldots,\varsigma_n'}\left(\mathbf{j}_1\ \theta_1,\ldots,\mathbf{j}_n\ \theta_n;\mathbf{j}_1'\ \theta_1',\ldots,\mathbf{j}_n'\ \theta_n'\right)$$

$$\Delta^{(n)}_{\varsigma_1',\ldots,\varsigma_n';\sigma_1',\ldots,\sigma_n'}\left(\mathbf{j}_1'\ \theta_1',\ldots,\mathbf{j}_n'\ \theta_n';\mathbf{i}_1'\ \tau_1',\ldots,\mathbf{i}_n'\ \tau_n'\right)$$

where $\bar{\mathcal{L}}^{(n)}_{\sigma_1,\ldots,\sigma_n;\sigma_1',\ldots,\sigma_n'}\left(\mathbf{i}_1\ \tau_1,\ldots,\mathbf{i}_n\ \tau_n;\mathbf{i}_1'\ \tau_1',\ldots,\mathbf{i}_n'\ \tau_n'\right)$ is summation of all connected diagrams generated by equation

$$\frac{1}{n!}\int_0^\beta \mathrm{d}\theta_1'\cdots\mathrm{d}\theta_n' \sum_{\substack{\varsigma_1'\cdots\varsigma_n'\\ \mathbf{j}_1'\cdots\mathbf{j}_n'}} \Omega^{(0)}_{\sigma_1\varsigma_1'}\left(\mathbf{i}_1\ \tau_1;\mathbf{j}_1'\ \theta_1'\right)\ldots\Omega^{(0)}_{\sigma_n\varsigma_n'}\left(\mathbf{i}_n\ \tau_n;\mathbf{j}_n'\ \theta_n'\right)$$

$$\frac{1}{\mathcal{Z}}\ \frac{\delta}{\delta\pi_{\mathbf{i}_n'\sigma_n'}\left(\tau_n'\right)}\cdots\frac{\delta}{\delta\pi_{\mathbf{i}_1'\sigma_1'}\left(\tau_1'\right)}\left(\mathrm{e}^{\tilde{\mathcal{S}}}\right)^{(n)}_{\varsigma_1',\ldots,\varsigma_n'}\left(\mathbf{j}_1'\ \theta_1',\ldots,\mathbf{j}_n'\ \theta_n'\right)\ \mathcal{Z}\left[\pi,\bar{\pi}\right]\Bigg|_{\pi=\bar{\pi}=0}$$

APPENDIX B

Dynamical Mean Field Theory: An Introduction

The Dynamical Mean Field Theory was first established by Metzner, Vollhardt [15], Müller-Hartmann [16] and others. The idea is, in analogy to classical spin models, to use a non-trivial scaling of the kinetic energy (hopping) and to define a mean field as an exact solution of the infinite dimensional model. Such a mean field theory is free of unphysical and spurious poles or singularities. The non-trivial scaling of the kinetic energy is characterized by a collapse of diagrams, i.e. reduces the initial perturbation expansion to a theory with an effective Green's functions and summations over frequencies only. The resultant exact thermodynamical potential in d $\longrightarrow \infty$ does not allow to resolve the d $\longrightarrow \infty$ theory explicitly because it still has the structure of a many-body theory (infinitely many degrees of freedom). And this mean field theory is called Dynamical Mean Field Theory.

Here, we will present how to build the Dynamical Mean Field Theory in the functional integral formalism.

The grand partition function of our interest is represented via a general functional integral as in (2.12)

$$\mathcal{Z} = \int [\mathcal{D}\varphi]\,[\mathcal{D}\bar{\varphi}]\ \exp\Big\{ -\mathcal{S}\,[\varphi;\bar{\varphi}]\Big\}. \tag{B.1}$$

Without lost of generality, we assume that the action $\mathcal{S}\,[\varphi\,(\tau)\,;\bar{\varphi}\,(\tau)]$ can be divided into two parts: the first is free non-local one-body (Gaussian) part which in the frequency representation with Matsubara fermionic frequencies $\omega_n = \beta^{-1}\,(2n+1)\,\pi$ has the form [1]

$$\mathcal{S}_0\,[\varphi;\bar{\varphi}] = -\sum_{\omega_n}\sum_{\mathbf{k},\sigma}\bar{\varphi}_\sigma\,(\mathbf{k}\;\omega_n)\,G^{(0)}_\sigma\,(\mathbf{k}\;\omega_n)\,\varphi_\sigma\,(\mathbf{k}\;\omega_n)\,, \tag{B.2a}$$

and the second part is a local, many-body functional that can be denoted as

$$\mathcal{S}_{\text{int}}\,[\varphi;\bar{\varphi}] = \int_0^\beta \mathrm{d}\tau \sum_{\mathbf{i}} \mathcal{L}_{\text{int};\mathbf{i}}\,[\varphi\,(\tau)\,;\bar{\varphi}\,(\tau)]\,. \tag{B.2b}$$

The representation (B.1) with the action in (B.2) is a compact expression (generating functional) for the sum of the perturbation expansion. This expansion is obtained when the part of the exponential with the time integration is expanded into a series and the integration over the Grassmann variables φ and $\bar{\varphi}$ is performed.

[1] The Fourier transformation of the field operator leads to factor (-1) in the free action part (B.2a)

The symbol $G^{(0)}_{\sigma}(\mathbf{k}\ \omega_n)$ stands for the free Green's function for fermionic field φ and $\bar{\varphi}$; for the Hubbard model

$$\left(G^{(0)}\right)^{-1}_{\sigma}(\mathbf{k}\ \omega_n) = i\omega_n - \varepsilon^f(\mathbf{k}) + \mu_\sigma, \tag{B.3a}$$

and for the PAM

$$\left(G^{(0)}\right)^{-1}_{\sigma}(\mathbf{k}\ \omega_n) = i\omega_n - \varepsilon^f + \mu_\sigma - \frac{\left|V(\mathbf{k})\right|^2}{i\omega_n - \varepsilon^c(\mathbf{k}) + \mu_\sigma}. \tag{B.3b}$$

In the limits of the large spatial dimensions one should rescale the momentum dependent quantities. For instance, for the Hubbard model and for the PAM with momentum independence of hybridization the rescaling of the nearest-neighbor hopping is

$$t \longrightarrow \frac{1}{\sqrt{2\mathrm{d}}}\, t^* \tag{B.4}$$

where d is the dimensionality of our system.

We then have a reduced number of diagrams (terms from the perturbation expansion) contributing to the grand partition function (B.1) or its logarithm, i.e. the thermodynamical potential.

So, the thermodynamical potential in the limit $\mathrm{d} \longrightarrow \infty$ can be written as a variational functional of local (site-independent) self-energies $\Sigma_\sigma(\omega_n)$, just like coherent potentials as in the Coherent Potential Approximation (CPA)

$$-\beta\Omega[G,\Sigma] = -\sum_{\omega_n}\sum_{\mathbf{k}\sigma}\ln\left(\left(G^{(0)}\right)^{-1}_{\sigma}(\mathbf{k}\ \omega_n) - \Sigma_\sigma(\mathbf{k}\ \omega_n)\right)^{-1} - \beta\sum_{\mathbf{i}}\Omega_{\mathbf{i}}[G,\Sigma], \tag{B.5}$$

where $\Omega_{\mathbf{i}}[G,\Sigma]$ is a local functional of $G_\sigma(\omega)$ and $\Sigma_\sigma(\omega_n)$. The $\mathcal{Z}_{\mathbf{i}}$ can be obtained from the original grand partition function by the replacement

$$\left(G^{(0)}\right)^{-1}_{\sigma}(\mathbf{k}\ \omega_n) \longrightarrow G^{-1}_{\sigma}(\omega_n) + \Sigma_\sigma(\omega_n). \tag{B.6}$$

The $\Omega_{\mathbf{i}}[G,\Sigma]$ can be represented by a local functional integral

$$-\beta\Omega_{\mathbf{i}}[G,\Sigma] = \ln\left(\int[\mathcal{D}\varphi_{\mathbf{i}}][\mathcal{D}\bar{\varphi}_{\mathbf{i}}]\ \exp\Big\{-\mathcal{S}_{\mathbf{i}}[\varphi,\bar{\varphi}]\Big\}\right) + \sum_{\sigma}\sum_{\omega_n}\ln G_\sigma(\omega_n) \tag{B.7}$$

with

$$\mathcal{S}_{\mathbf{i}}[\varphi,\bar{\varphi}] = -\sum_{\sigma}\sum_{\omega_n}\bar{\varphi}_{\mathbf{i}\sigma}(\omega_n)\left(G^{-1}_{\sigma}(\omega_n) + \Sigma_\sigma(\omega_n)\right)\varphi_{\mathbf{i}\sigma}(\omega_n) + \int_0^\beta \mathrm{d}\tau\ \mathcal{L}_{\mathrm{int};\mathbf{i}}[\varphi(\tau),\bar{\varphi}(\tau)]. \tag{B.8}$$

The principal aspect of the representation (B.5) - (B.8) is that the thermodynamical potential functional $\Omega[G,\Sigma]$ is stationary with respect to variations of both renormalized variables $\Sigma_\sigma(\omega_n)$ and $G_\sigma(\omega_n)$. The stationarity of $\Omega[G,\Sigma]$ then defines equations of state, i.e. equations for the $\Sigma_\sigma(\omega_n)$ and $G_\sigma(\omega_n)$. We have from (B.5) and (B.7)

$$\frac{\delta}{\delta\Sigma_\sigma(\omega)_n}\,\Omega[G,\Sigma] = 0$$

$$-\sum_{\mathbf{k}}\left(\left(G^{(0)}\right)^{-1}_{\sigma}(\mathbf{k}\ \omega_n) - \Sigma_\sigma(\mathbf{k}\ \omega_n)\right)^{-1} + \sum_{\mathbf{i}}\frac{1}{\mathcal{Z}_{\mathbf{i}}}\int[\mathcal{D}\varphi_{\mathbf{i}}][\mathcal{D}\bar{\varphi}_{\mathbf{i}}]\,\bar{\varphi}_{\mathbf{i}\sigma}(\omega_n)\,\varphi_{\mathbf{i}\sigma}(\omega_n) \tag{B.9a}$$

$$\exp\Big\{-\mathcal{S}_{\mathbf{i}}[\varphi,\bar{\varphi}]\Big\} = 0$$

$$\frac{\delta}{\delta G_\sigma\left(\omega\right)_n}\,\Omega\left[G,\Sigma\right]=0$$

$$NG_\sigma\left(\omega_n\right)-\sum_{\mathbf{i}}\frac{1}{\mathcal{Z}_{\mathbf{i}}}\int\left[\mathcal{D}\varphi_{\mathbf{i}}\right]\left[\mathcal{D}\bar{\varphi}_{\mathbf{i}}\right]\bar{\varphi}_{\mathbf{i}\sigma}\left(\omega_n\right)\varphi_{\mathbf{i}\sigma}\left(\omega_n\right)\exp\Big\{-\mathcal{S}_{\mathbf{i}}\left[\varphi,\bar{\varphi}\right]\Big\}=0 \tag{B.9b}$$

where $\mathcal{Z}_{\mathbf{i}}$ equals

$$\mathcal{Z}_{\mathbf{i}}=\int\left[\mathcal{D}\varphi_{\mathbf{i}}\right]\left[\mathcal{D}\bar{\varphi}_{\mathbf{i}}\right]\exp\Big\{-\mathcal{S}_{\mathbf{i}}\left[\varphi,\bar{\varphi}\right]\Big\} \tag{B.9c}$$

and $\mathcal{S}_{\mathbf{i}}\left[\varphi,\bar{\varphi}\right]$ is defined in (B.8).
The final system of equations for $G_\sigma\left(\omega_n\right)$ and $\Sigma_\sigma\left(\omega_n\right)$ reads

$$\begin{aligned}G_\sigma\left(\omega_n\right)&=\frac{1}{N}\sum_{\mathbf{k}}\left(\left(G^{(0)}\right)^{-1}_\sigma\left(\mathbf{k}\;\omega_n\right)-\Sigma_\sigma\left(\mathbf{k}\;\omega_n\right)\right)^{-1}\\ G_\sigma\left(\omega_n\right)&=\frac{1}{N}\sum_{\mathbf{i}}\frac{1}{\mathcal{Z}_{\mathbf{i}}}\int\left[\mathcal{D}\varphi_{\mathbf{i}}\right]\left[\mathcal{D}\bar{\varphi}_{\mathbf{i}}\right]\bar{\varphi}_{\mathbf{i}\sigma}\left(\omega_n\right)\varphi_{\mathbf{i}\sigma}\left(\omega_n\right)\exp\Big\{-\mathcal{S}_{\mathbf{i}}\left[\varphi,\bar{\varphi}\right]\Big\}\end{aligned} \tag{B.10}$$

Equations (B.10) thus close the expression for the thermodynamical potential functional (B.5) - (B.8), which now depends only on external parameters of our initials. The thermodynamical potential (B.5) - (B.8) generates a self-consistent and conserving theory in the Baym sense [4] and is exact in the limit d $\longrightarrow\infty$.

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