

9 Correlated Matter: DMFT and Beyond

Alexander Lichtenstein

I. Institut für Theoretische Physik

Universität Hamburg

Contents

1	Introduction: Reference systems	2
2	Functional approach	4
3	Dual fermion approach with a general reference system	7
4	Superperturbation in dual space	11
5	Numerical examples	13
6	Conclusion: Recent developments	17
A	Path-integrals for fermions	18
B	Exact relations between Green functions	22

1 Introduction: Reference systems

In this lecture we give an introduction to the theoretical description of strongly correlated materials based on non-local extensions of the dynamical mean-field theory (DMFT). This scheme combines the numerically exact DMFT solution of the effective impurity problem with an analytical non-local perturbation scheme. The frequency dependent effective impurity DMFT problem nowadays can be efficiently solved within the continuous time quantum Monte Carlo (CT-QMC) scheme [1]. Therefore the perturbation theory needs to be formulated in the action path-integral formalism. We give a brief introduction to the path integral over fermionic Grassmann fields and formulate a general scheme for the expansion around the DMFT solution using a special dual-space transformation. We discuss here a general way to include nonlocal correlations beyond the DMFT, based on the generalized Hubbard model [2] and describe the dual-fermion formalism [3].

Consider the noninteracting, “kinetic” part H_t of the Hubbard model first [4]. This is fixed by specifying the hopping-matrix elements t_{ij} between sites i and j . In the absence of the local Hubbard-interaction term, H_t is easily diagonalized. For a Hubbard model on a lattice, diagonalization is achieved by Fourier transformation of the hopping parameters to \mathbf{k} -space, and one has the normal “band structure” for a single-orbital model, particularly the simple $\varepsilon_{\mathbf{k}} = t_{\mathbf{k}}$ with band-width W . If, on the other hand, only the local part of the Hamiltonian is kept, i.e., the Hubbard interaction H_U with interaction strength U and the local term of H_t is fixed by the on-site energy ε_0 , the diagonalization of the Hamiltonian is again trivial and reduces to the diagonalization of a single “Hubbard atom”.

The great success of the DMFT approach is related to it numerically interpolating between these two limits [5]. For the Hubbard model on an infinite-dimensional Bethe lattice at half-filling the DMFT gives the exact description of the Mott-transition [6] between the weak-coupling ($U/W \ll 1$) metallic state and the strong-coupling ($U/W \gg 1$) insulating paramagnetic state [7]. In a nutshell, DMFT maps the correlated Hubbard lattice problem onto the self-consistent solution of an effective Anderson impurity problem with a single interacting Hubbard atom (interaction strength U) in a non-interacting fermionic bath (which mimics the rest of the crystal).

Now we can think of how to incorporate nonlocal correlations beyond the DMFT: since the Hubbard and the Anderson-impurity model share the same interaction part, one can think of the Hubbard model as the impurity model plus a residual term $\propto (t_{\mathbf{k}} - \Delta_{\nu})$ and treat this *perturbatively*. Since this term is frequency dependent, we need a novel perturbation theory based on the action formalism. One may view this idea as a generalization of the Kohn-Sham idea in density functional theory (DFT) [8] of an optimal reference system, but with a crucial difference. Here, not an interacting homogeneous electron gas, but an effective impurity model, tailored to the problem of strong correlations, serves as the reference system, see Fig. 1. Since in zeroth order of this perturbative expansion, i.e., on the level of the DMFT problem, we already have an interacting problem and since the perturbation is momentum and frequency dependent, one is forced to replace the Hamiltonians by actions within the path-integral formalism. Note that the fermion path-integral can also be used to formulate the DMFT itself [5, 9]. Now, the separation

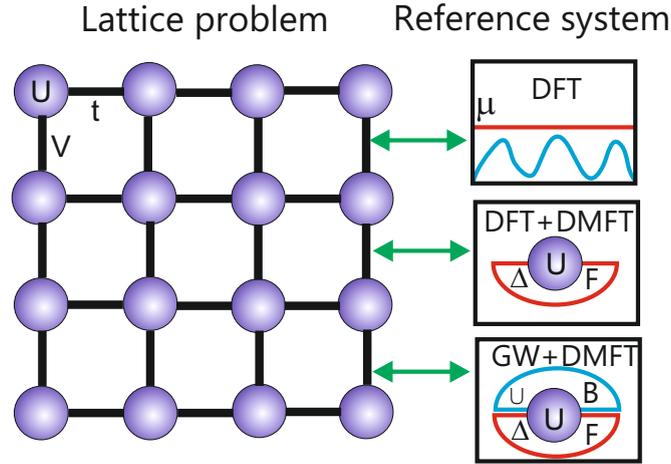


Fig. 1: Schematic representation of the reference systems in many-body approaches to lattice-fermion models: (i) Density-functional theory (DFT) with the interacting homogeneous electron gas as a reference system, defined by a constant external potential μ . (ii) Dynamical mean-field theory (DMFT) with an effective impurity problem as a reference system, defined by fermionic bath, specified by the hybridization function Δ . (iii) GW+DMFT with a correlated atom in a fermionic (Δ) and a bosonic bath (Λ) due to effects of the frequency-dependent screening of long-range Coulomb (V) interactions.

of the local and nonlocal terms is achieved by a Hubbard-Stratonovich transformation applied to the single-particle $(t_{\mathbf{k}} - \Delta_{\nu})$ -term [3]. This provides us with a new action. Moreover, it is formally possible to integrate-out the original local degrees of freedom and in this way generated an effective action in the transformed, so-called dual-fermion representation [3]. Note that integrating out the local degrees of freedom is not only a formal step but can be achieved in practice, by solving the impurity problem within the numerically exact CT-QMC method.

The dual action consists of a bare dual propagator (non-local part of the DMFT Green function) $\tilde{G}_{\mathbf{k},\nu}^0$ and a local but frequency-dependent effective potential related to scattering processes of two, three, and more dual particles on the impurity site. The simplest two-particle dual potential coincides with the fully connected part of the screened impurity interaction vertex $\gamma_{\nu\nu'}^{\omega}$, which can be calculated with the impurity CT-QMC solver as a function of bosonic (ω) and fermionic (ν, ν') Matsubara frequencies. Normally, correlations between three particles on the DMFT impurity site are much weaker than two-particle correlations and can be ignored. The same applies to higher-order terms. One can think of the dual-fermion formalism as an expansion in the order of local multi-particle correlation functions. This means that “bare” interactions between dual fermions are related with the connected part of the screened impurity vertex. Standard diagrammatic techniques can be applied for calculations of the bold dual propagator $\tilde{G}_{\mathbf{k},\nu}$, which allows to obtain the nonlocal self-energy for the original fermions [3] and to describe nonlocal correlations beyond the DMFT.

The dual-fermion approach is not necessarily bound to a specific starting point. However, the DMFT starting point is very efficient. Namely, it corresponds to the elimination of all local diagrams for any n -particle correlation of dual fermions when using the DMFT self-consistency equation. In the dual space, this simply reduces to $\sum_{\mathbf{k}} \tilde{G}_{\mathbf{k},\nu}^0 = 0$ and means that, on average

over the whole Brillouin zone, Δ_ν optimally approximates the electron spectrum $\varepsilon_{\mathbf{k}}$, including its local correlation effects. Therefore, the noninteracting dual fermions correspond to strongly correlated DMFT quasiparticles, and the remaining nonlocal effects can be quite small and reasonably described by perturbative summations of dual diagrams. This also explains the notion “dual fermions”.

2 Functional approach

We introduce a general functional approach which will cover the density functional (DFT), dynamical mean-field, (DMFT) and Baym-Kadanoff (BK) theories [9]. Let us start from the full many-body Hamiltonian describing electrons moving in the periodic external potential of ions $V(\mathbf{r})$ with chemical potential μ and interacting via Coulomb law: $U(\mathbf{r} - \mathbf{r}') = 1/|\mathbf{r} - \mathbf{r}'|$. We use the atomic units $\hbar = m = e = 1$. In the field-operator representation the Hamiltonian has the form

$$H = \sum_{\sigma} \int d\mathbf{r} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \left(-\frac{\nabla^2}{2} + V(\mathbf{r}) - \mu \right) \hat{\psi}_{\sigma}(\mathbf{r}) + \frac{1}{2} \sum_{\sigma\sigma'} \int d\mathbf{r} \int d\mathbf{r}' \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \hat{\psi}_{\sigma'}^{\dagger}(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \hat{\psi}_{\sigma'}(\mathbf{r}') \hat{\psi}_{\sigma}(\mathbf{r}) \quad (1)$$

We can always use a single-particle orthonormal basis set in solids $\varphi_n(\mathbf{r})$, for example Wannier orbitals with full set of quantum numbers, e.g., site, orbital and spin index: $n = (i, m, \sigma)$ and expand the fields in creation and annihilation operators

$$\hat{\psi}(\mathbf{r}) = \sum_n \varphi_n(\mathbf{r}) \hat{c}_n \quad \hat{\psi}^{\dagger}(\mathbf{r}) = \sum_n \varphi_n^*(\mathbf{r}) \hat{c}_n^{\dagger}. \quad (2)$$

Going from fermionic operators to the Grassmann variables $\{c_n^*, c_n\}$ we can write the functional integral representation for partition function of the many-body Hamiltonian in the imaginary time domain using the Euclidean action S

$$Z = \int \mathcal{D}[c^*, c] e^{-S}, \quad S = \sum_{12} c_1^* (\partial_{\tau} + t_{12}) c_2 + \frac{1}{2} \sum_{1234} c_1^* c_2^* U_{1234} c_4 c_3, \quad (3)$$

where the one- and two-electron matrix elements are defined as

$$t_{12} = \int d\mathbf{r} \varphi_1^*(\mathbf{r}) \left(-\frac{1}{2} \nabla^2 + V(\mathbf{r}) - \mu \right) \varphi_2(\mathbf{r}) \quad (4)$$

$$U_{1234} = \int d\mathbf{r} \int d\mathbf{r}' \varphi_1^*(\mathbf{r}) \varphi_2^*(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \varphi_3(\mathbf{r}) \varphi_4(\mathbf{r}').$$

and we use the following short definition of the sum

$$\sum_1 \dots \equiv \sum_{im} \int d\tau \dots \quad (5)$$

The one-electron Green function is defined via a simple non-zero correlation function for fermions

$$G_{12} = -\langle c_1 c_2^* \rangle_S = -\frac{1}{Z} \int \mathcal{D}[c^*, c] c_1 c_2^* \exp(-S). \quad (6)$$

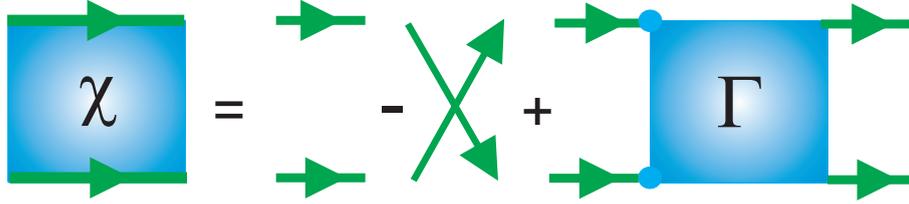


Fig. 2: Representation of the full two-particle Green function in terms of trivial products of single-particle Green function and the full vertex function Γ .

The main problem of strongly interacting electronic systems are related to the fact that the higher-order correlation functions do not separate into products of lower order correlation function. For example the two-particle Green function or generalized susceptibility (X) is defined in the following form [10]

$$X_{1234} = \langle c_1 c_2 c_3^* c_4^* \rangle_S = \frac{1}{Z} \int \mathcal{D}[c^*, c] c_1 c_2 c_3^* c_4^* \exp(-S), \quad (7)$$

and can be expressed graphically through the Green functions and the full vertex function Γ_{1234} [10, 11] (see Fig. 2)

$$X_{1234} = G_{14}G_{23} - G_{13}G_{24} + \sum_{1'2'3'4'} G_{11'}G_{22'}\Gamma_{1'2'3'4'}G_{3'3}G_{4'4} \quad (8)$$

In the case of non-interacting electron systems, the high-order correlations X are reduced to the antisymmetrized product of lower-order correlations G , which correspond to the first two terms (Hartree- and Fock-like) with the vertex function Γ in Eq. (8) equal to zero. In strongly correlated electron systems the last part with the vertex is dominant and even diverges close to the electronic phase transitions.

The Baym-Kadanoff functional [12] gives the one-particle Green function and the total free energy at its stationary point. In order to construct the exact functional of the Green function (Baym-Kadanoff) we modify the action by introducing the source term J

$$S[J] = S + \sum_{12} c_1^* J_{12} c_2. \quad (9)$$

The partition function Z , or equivalently the free energy of the system, F , becomes a functional of the auxiliary source field

$$Z[J] = e^{-F[J]} = \int \mathcal{D}[c^*, c] e^{-S'[J]}. \quad (10)$$

Variation of this source function gives all correlation functions, for example the Green function

$$G_{12} = \left. \frac{\delta F[J]}{\delta J_{21}} \right|_{J=0}. \quad (11)$$

If we use the definition of the generalized susceptibility as a second variation of the $F[J]$ functional instead of $Z[J]$ we will get only the connected part of the X -function, which is represented by the last term in Eq. (8).

The Baym-Kadanoff functional can be obtained by the Legendre transform from variable J to G

$$F[G] = F[J] - \text{Tr}(JG), \quad (12)$$

We can use the standard decomposition of the free energy F into the single-particle part and the correlated part

$$F[G] = \text{Tr} \ln G - \text{Tr}(\Sigma G) + \Phi[G], \quad (13)$$

where Σ_{12} is the single particle self-energy and $\Phi[G]$ is the correlated part of the Baym-Kadanoff functional and is equal to the sum of all two-particle irreducible diagrams. At the stationary point this functional gives the free energy of the system. In practice, $\Phi[G]$ is not known for interacting electron systems, which is similar to the problem in density functional theory. Moreover, this general functional approach reduces to DFT, if one uses only the diagonal part in space-time of the Green function, which corresponds to the one-electron density

$$n_1 = G_{12} \delta_{12} = \langle c_1^* c_1 \rangle_S, \quad (14)$$

with the Kohn-Sham potential $V_{KS} = V_{ext} + V_H + V_{xc}$ playing the role of the ‘‘constrained field’’. Here V_{ext} is the external potential and V_H the Hartree potential. In principle the exchange-correlation potential V_{xc} is known only for the homogeneous electron gas, therefore in all practical applications one uses a so-called local density approximation to DFT. In this case the DFT functional defined as

$$F_{DFT}[n] = T_0[n] + V_{ext}[n] + V_H[n] + V_{xc}[n] \quad (15)$$

where T_0 is kinetic energy of non-interacting systems. Finally, if we define the total electron density as

$$n(\mathbf{r}) = \sum_i \varphi_i^*(\mathbf{r}) \varphi_i(\mathbf{r})$$

the local density approximation to the DFT reads

$$T_0[n] + V_{ext}[n] = \sum_i \int d\mathbf{r} \varphi_i^*(\mathbf{r}) \left(-\frac{1}{2} \nabla^2 + V_{ext}(\mathbf{r}) - \mu \right) \varphi_i(\mathbf{r}) \quad (16)$$

$$V_H[n] = \frac{1}{2} \int d\mathbf{r} n(\mathbf{r}) U(\mathbf{r}-\mathbf{r}') n(\mathbf{r}') \quad (17)$$

$$V_{xc}[n] = \int d\mathbf{r} n(\mathbf{r}) \varepsilon(n(\mathbf{r})) \quad (18)$$

where $\varepsilon(n)$ is the exchange-correlation density for the homogeneous electron gas, which can be calculated within a QMC-scheme [13].

In the DFT scheme we lose information about the non-equal time Green function, which gives the single particle excitation spectrum as well as the k -dependence of the spectral function, and restrict ourselves to only the ground state energy of the many-electron system. Moreover, we also lose also information about all collective excitations in solids, such as plasmons or

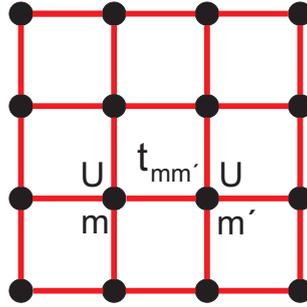


Fig. 3: Generic Hubbard lattice for correlated lattice fermions with the local Coulomb interaction U and hopping parameters t : m can label different orbitals or lattice sites.

magnons, which can be obtained from a generalized susceptibility or from the second variation of the free-energy.

One can probably find the Baym-Kadanoff interacting potential $\Phi[G]$ for simple lattice models using quantum Monte Carlo (QMC). Unfortunately due to the sign problem in lattice simulations this numerically exact solution of the electronic correlations is not feasible. On the other hand, one can obtain the solution of a local interacting quantum problem in a general fermionic bath, using the QMC scheme, which has no sign problem if it is diagonal in spin and orbital space. Therefore, a reasonable approach to strongly correlated systems is to keep only the local part of the many-body fluctuations. In such a Dynamical Mean-Field Theory (DMFT) one can obtain numerically the correlated part of the local functional. In this scheme we only use the local part of many electron vertex and obtain, in a self-consistent way, an effective functional of the local Green function. In the following section we discuss the general dual fermion (DF) transformations [3] which help us to separate the local fluctuations in many-body system and show a perturbative way to go beyond the DMFT approximations.

3 Dual fermion approach with a general reference system

We start with a general lattice fermion model with the local Hubbard-like interaction vertex U . Generalization to the multi-orbital case is straightforward [14]. All equations will be written in matrix form, giving an idea of how to rewrite the dual fermion (DF) formula to the multi-orbital or multi-site case. The general strategy is related with the formally exact separation of the local and non-local correlation effects. We introduce auxiliary dual fermionic fields which will couple local correlated impurities or clusters back to the original lattice [3].

Using the path-integral formalism (Appendix A) the partition function of a general fermionic lattice system (Fig. 3) can be written in following form as a functional integral over Grassmann variables $[c^*, c]$

$$Z = \int \mathcal{D}[c^*, c] \exp(-S_L[c^*, c]).$$

The original lattice action of interacting lattice fermions, similar to Eq. (3), can be written in Matsubara space as a sum of the lattice one-electron contributions with the Fourier transformed

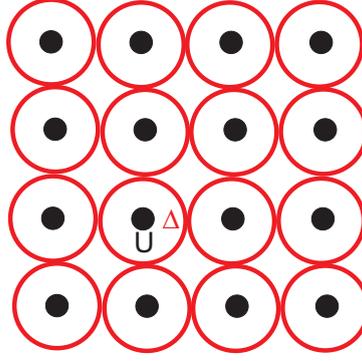


Fig. 4: Schematic view on the real-space DMFT reference system.

hopping $t_{\mathbf{k}}$ (or energy spectrum in the single-orbital case) and the local interaction part U

$$S_L[c^*, c] = - \sum_{\mathbf{k}\nu\sigma} c_{\mathbf{k}\nu\sigma}^* (i\nu + \mu - t_{\mathbf{k}}) c_{\mathbf{k}\nu\sigma} + \sum_i \int_0^\beta d\tau U n_{i\tau\uparrow}^* n_{i\tau\downarrow}. \quad (19)$$

In the following, $\nu = (2n+1)\pi/\beta$, ($\omega = 2n\pi/\beta$), $n = 0, \pm 1, \dots$ are the fermionic (bosonic) Matsubara frequencies, β is the inverse temperature, $\tau \in [0, \beta)$ the imaginary time, and μ the chemical potential. The index i labels the lattice sites, m refers to different orbitals, σ is the spin projection and the \mathbf{k} -vectors are quasimomenta. In order to keep the notation simple, it is useful to introduce the combined index $|1\rangle \equiv |i, m, \sigma, \tau\rangle$ and assume summation over repeated indices. Translational invariance is assumed for simplicity in the following, although a real space formulation is straightforward. The local part of the action, S_U , may contain any type of local multi orbital interaction.

In order to formulate an expansion around the best possible reference action, Fig. 4, a quantum impurity (cluster) problem is introduced by a general frequency-dependent hybridization function Δ_ν and the same local interaction

$$S_\Delta[c_i^*, c_i] = - \sum_{\nu, \sigma} c_{i\nu\sigma}^* (i\nu + \mu - \Delta_\nu) c_{i\nu\sigma} + \sum_\nu U n_{i\nu\uparrow}^* n_{i\nu\downarrow}, \quad (20)$$

where Δ_ν is the effective hybridization matrix describing the coupling of the impurity to an auxiliary fermionic bath. The main motivation for rewriting the lattice action in terms of a quantum impurity model is that such a reference system can be solved numerically exactly for an arbitrary hybridization function using the CT-QMC methods [1]. Using the locality of the hybridization function Δ_ν , the lattice action Eq. (19) can be rewritten exactly in terms of individual impurity models and the effective one-electron coupling ($\Delta_\nu - t_{\mathbf{k}}$) between different impurities, Fig. 5,

$$S_L[c^*, c] = \sum_i S_\Delta[c_i^*, c_i] - \sum_{\mathbf{k}\nu\sigma} c_{\mathbf{k}\nu\sigma}^* (\Delta_\nu - t_{\mathbf{k}}) c_{\mathbf{k}\nu\sigma}. \quad (21)$$

We will find the condition for the optimal choice of the hybridization function later. Although we can solve the individual impurity model exactly, the effect of spatial correlations due to

where Z_Δ is the partition function of the impurity action Eq. (20) and g_ν is the exact impurity Green function

$$g_{12} = -\langle c_1 c_2^* \rangle_\Delta = \frac{1}{Z_\Delta} \int \mathcal{D}[c^*, c] c_1 c_2^* e^{-S_\Delta[c^*, c]}. \quad (27)$$

The above equation may be viewed as the defining equation for the dual potential $V[d^*, d]$. The choice of matrices in Eq. (22) ensures a particularly simple form of this potential. An explicit expression is found by expanding both sides of Eq. (26) and equating the resulting expressions by order. Formally this can be done up to all orders and in this sense the transformation to the dual fermions is exact. For most applications, the dual potential is approximated by the first non-trivial interaction vertex

$$V[d^*, d] = \frac{1}{4} \sum_{1234} \gamma_{1234} d_1^* d_2^* d_4 d_3, \quad (28)$$

where for the local vertex the combined index $1 \equiv \{m\nu\sigma\}$ comprises orbital degrees of freedom (or cluster sites), frequency, and spin. γ is the exact, fully antisymmetric, reducible two-particle vertex of the local quantum impurity problem. With the present choice of normalization in the HS-transformation we did not “amputate” the impurity “legs” or g_{12} Greens function which will be very useful choice for CT-QMC calculations of local vertex for multi-orbital case. It is given then by connected part of the local two-particle correlations function

$$\gamma_{1234} = \chi_{1234} - \chi_{1234}^0 \quad (29)$$

with the two-particle Green function of the local impurity (reference system) being defined as

$$\chi_{1234} = \langle c_1 c_2 c_3^* c_4^* \rangle_\Delta = \frac{1}{Z_\Delta} \int \mathcal{D}[c^*, c] c_1 c_2 c_3^* c_4^* e^{-S_\Delta[c^*, c]}. \quad (30)$$

The disconnected part of a generalized susceptibility reads

$$\chi_{1234}^0 = g_{14} g_{23} - g_{13} g_{24}. \quad (31)$$

The single- and two-particle Green functions can be calculated using the CT-QMC Monte Carlo algorithms [1]. After integrating-out the lattice fermions, the dual action depends on the new variables only and for the one-orbital paramagnetic case reads

$$\tilde{S}[d^*, d] = - \sum_{\mathbf{k}\nu\sigma} d_{\mathbf{k}\nu\sigma}^* \tilde{G}_{0\mathbf{k}\nu}^{-1} d_{\mathbf{k}\nu\sigma} + \sum_i V_i[d_i^*, d_i] \quad (32)$$

while the bare dual Green function is has the form

$$\tilde{G}_{\mathbf{k}\nu}^0 = \left((t_{\mathbf{k}} - \Delta_\nu)^{-1} - g_\nu \right)^{-1}. \quad (33)$$

This formula involves only the local Green function g_ν of the impurity model. It is important to note, that the HS-transformation to dual fermion variables, allows us to “perform the analytical amputation” of impurity “legs” which causes enormous problems in the multi-orbital CT-QMC

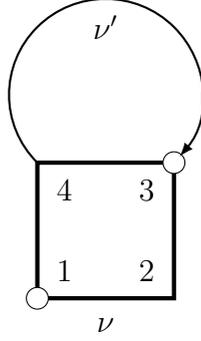


Fig. 6: Feynman diagram for the 1st-order dual fermion perturbation for the self-energy $\tilde{\Sigma}$: a line represents the non-local \tilde{G}_{43} and a box is the local γ_{1234} .

formalism. Transformation to the original DF-normalization where both dual G_d and real Green function have the same dimension unit reads

$$G_d = g \tilde{G} g = G_{DMFT} - g \quad G_{DMFT} = (g_\nu + \Delta_\nu - t_{\mathbf{k}})^{-1}. \quad (34)$$

The Dual Fermion transformation allows us to use arbitrary reference systems and transform the strongly correlated lattice fermion problem to an effective action of weakly coupled dual quasiparticles. This is related with the fact that the bare dual Green function Eq. (34) related with the small non-local part of the DMFT lattice Green function and the main two-particle part of the bare interaction among dual fermions Eq. (28) is exactly equal to the fully screened impurity vertex of the reference system. The rest of the dual fermion problem is related with an optimal perturbation scheme for such an effective action Eq. (32).

4 Superperturbation in dual space

For the general multi-orbital multi-site dual fermion perturbation technique we use the particle-hole notation for local vertex and write the exact spin and imaginary-time structure of generalized connected susceptibility [3, 15]

$$\gamma_{1234}^{\sigma\sigma'}(\tau_1, \tau_2, \tau_3, \tau_4) = -\langle c_{1\sigma} c_{2\sigma}^* c_{3\sigma'} c_{4\sigma'}^* \rangle_\Delta + g_{12}^\sigma g_{34}^{\sigma'} - g_{14}^\sigma g_{32}^\sigma \delta_{\sigma\sigma'}.$$

Then the bare vertex of the dual-fermion perturbation is related with the full impurity vertex, which in Matsubara space depends on two fermionic, (ν, ν') , and one bosonic, (ω) , frequencies. We also symmetrize the vertex for the charge density d - and spin s -channels

$$\gamma_{1234}^{d/m}(\nu, \nu', \omega) = \gamma_{1234}^{\uparrow\uparrow}(\nu, \nu', \omega) \pm \gamma_{1234}^{\uparrow\downarrow}(\nu, \nu', \omega).$$

Now we can write the first-order, local in site (i), DF-correction to the dual self-energy (Fig. 6)

$$\tilde{\Sigma}_{12}^{(1)i}(\nu) = \sum_{\nu', 3, 4} \gamma_{1234}^d(\nu, \nu', 0) \tilde{G}_{43}^{ii}(\nu') \quad (35)$$

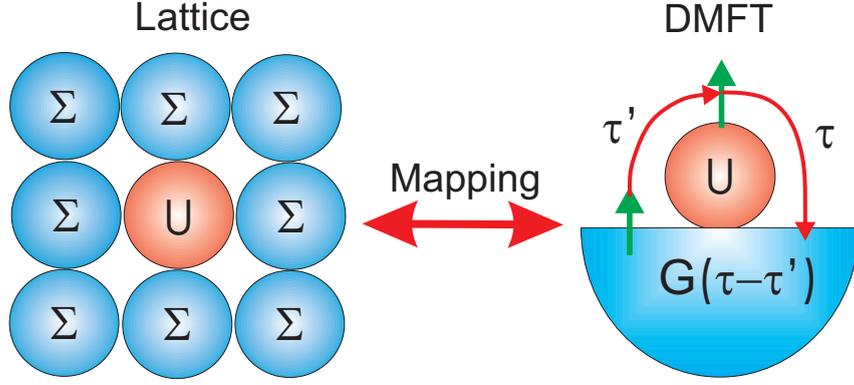


Fig. 7: Schematic representation of the DMFT reference system for correlated lattice models.

We now can use the freedom to choose the hybridization function Δ_ν in order to eliminate the main first-order dual fermion correction Eq. (35). Since the vertex function γ_{1234} is purely local, it is enough to ensure that the local part of dual Green function vanishes $\tilde{G}_{loc}=0$. This is exactly equivalent to the DMFT self-consistency condition for the hybridization function Δ_ν (Fig. 7)

$$\sum_{\mathbf{k}} (g_\nu^{-1} + \Delta_\nu - t_{\mathbf{k}})^{-1} = g_\nu. \quad (36)$$

The effective impurity model, Eq. (20), which is fully determined by the local hybridization function Δ_ν on the fermionic Matsubara frequencies $i\nu_n$ is solved using the numerically exact CT-QMC scheme [1] from which the exact local Green function g_ν is obtained. The self-consistency DMFT condition for the hybridization function equates the local part of the lattice Green function and with that of the impurity, which shows that DMFT minimizes, in local sense, the distance $|t_{\mathbf{k}} - \Delta_\nu|$. It is worthwhile to point here that the “free” or non-interacting dual fermions are equivalent to the full solution of the DMFT problem. This is why dual fermions are only “weakly interacting” so that this perturbation scheme can be very efficient, provided a good reference system.

The second order Feynman diagram for DF-perturbation (Fig. 8) in real space (\mathbf{R}_{ij}) has density- and spin-channel contributions with corresponding constants ($c_d = -1/4$ and $c_m = -3/4$)

$$\tilde{\Sigma}_{12}^{(2)ij}(\nu) = \sum_{\nu'\omega} \sum_{3-8} \sum_{\alpha=d,m} c_\alpha \gamma_{1345}^{\alpha,i}(\nu, \nu', \omega) \tilde{G}_{36}^{ij}(\nu + \omega) \tilde{G}_{74}^{ji}(\nu' + \omega) \tilde{G}_{58}^{ij}(\nu') \gamma_{8762}^{\alpha,j}(\nu', \nu, \omega).$$

Using the exact relation between dual Green function and real Green function (Appendix B), we can express the total lattice self-energy as the sum of the reference contribution Σ^0 (e.g. the impurity) and corrections Σ' , which are related with the dual self-energy $\tilde{\Sigma}$

$$\Sigma_{\mathbf{k}\nu} = \Sigma_\nu^0 + \Sigma'_{\mathbf{k}\nu} \quad (37)$$

$$\Sigma'_{\mathbf{k}\nu} = g_\nu^{-1} - (g_\nu + \tilde{\Sigma}_{\mathbf{k}\nu})^{-1}. \quad (38)$$

We point out that this expression is related with the exact transformation between dual- and real-space and has nothing to do with a correction for missing tree-particle vertices [2].

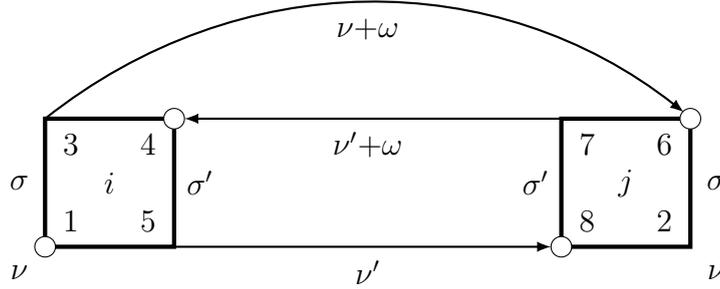


Fig. 8: Feynman diagram for the 2nd-order dual fermion perturbation for the self-energy $\tilde{\Sigma}$.

What is much more important for numerical calculations, is that starting from the full DF-Green function, $\tilde{G}_{\mathbf{k}\nu}^{-1} = \tilde{G}_{0\mathbf{k}\nu}^{-1} - \tilde{\Sigma}_{\mathbf{k}\nu}$, and exact the relation of Appendix B, Eq. (55), we can directly write an expression for the lattice Green function including only the reference impurity Green function and the dual self-energy [2]

$$G_{\mathbf{k}\nu} = \left((g_{\nu} + \tilde{\Sigma}_{\mathbf{k}\nu})^{-1} - \tilde{\Delta}_{\mathbf{k}\nu} \right)^{-1}. \quad (39)$$

This formula is perfectly suitable for the CT-QMC calculations for realistic multi-orbital correlated matter, where from the noisy Monte-Carlo data one needs only local one- and two-particle Green functions, without knowledge of a local self-energy and an “amputated” vertex function. In principle, one can go beyond second-order perturbation theory and include dual ladder diagrams [15], dual parquet diagrams [16], or even try to sum up all dual diagrams with the two-particle vertex γ_{1234} stochastically, using a diagrammatic Monte Carlo in dual space [17, 18]. We can also make the diagrammatic series self-consistent, using the “bold” line and update the bare dual Green function with the dual self-energy. Finally, one can also “upgrade” the reference system, which is not anymore “best” for dual fermion theory, but only for the DMFT approach with non-interacting dual fermions.

5 Numerical examples

As the first example of the DF-perturbation, we discuss the simple, but non-trivial case of a “two-site” model (Fig. 9) with one correlated site with Hubbard interaction U and one single electron site or a “bath” with the energy level ε coupled by the hybridization V . The reference system is described by the following parameters: $U=2$, $\varepsilon_0=0$ and $V_0=0.5$. The system, calculated by first-order DF-perturbation, has the same interaction U and ε , but 50% larger hybridization $V=1.5V_0$. We use an exact-diagonalization solver and find not only the local Green function at the correlated site G_0 for the reference system, but also the exact G for the target system with an effective broadening corresponding to the first Matsubara frequency. One can also use the Lehmann representation not only for the single-particle Green function, but also for two-particle correlators [19] and moreover integrated over the Matsubara frequency for simplest diagram Eq. (35) analytically [20]. For the dual-fermion calculation we use the Matsubara superperturbation first-order correction for inverse temperature $\beta=5$ and the Padé analytical

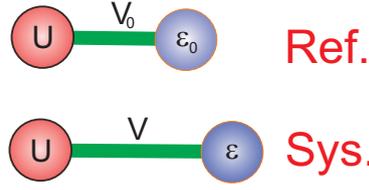


Fig. 9: Schematic representation of dual-fermion superperturbation test for a two-site model.

continuation to the real axes [5]. Results of the first-order DF superperturbation are shown in Fig. 10 together with reference and target DOS. We can conclude that even the first-order DF-correction gives the Green function in very good agreement with the exact one.

The real test for correlated fermions corresponds to a half-filled two-dimensional Hubbard model on the square lattice with a 2×2 plaquette as the reference system (Fig. 11). We used the 2×2 supercell scheme with 4 atoms in the unit cell in order to describe the lattice on the left-hand side of Fig. 11 with the following 4×4 hopping matrix with the nearest neighbor hopping t and next nearest neighbor hopping p

$$t_{\mathbf{k}} = \begin{pmatrix} \varepsilon & tK^{0+} & pL^{-+} & tK^{-0} \\ tK^{0-} & \varepsilon & tK^{-0} & pL^{--} \\ pL^{+-} & tK^{+0} & \varepsilon & tK^{0-} \\ tK^{+0} & pL^{++} & tK^{0+} & \varepsilon \end{pmatrix}$$

where the functions $K_{\mathbf{k}}^{mn}$ and $L_{\mathbf{k}}^{mn}$ with $[m(n)] = -(1), 0, +(1)$ are defined as

$$\begin{aligned} K_{\mathbf{k}}^{mn} &= 1 + e^{i(mk_x + nk_y)} \\ L_{\mathbf{k}}^{mn} &= 1 + e^{i(mk_x + nk_y)} + e^{imk_x} + e^{ink_y} \end{aligned}$$

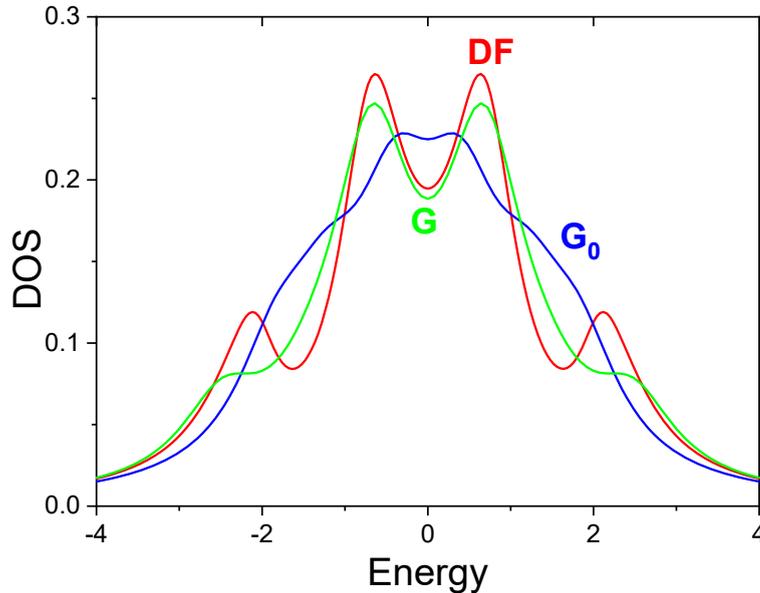


Fig. 10: Density of states for the dual-fermion first-order scheme together with the reference and target Green function for the two-site model.

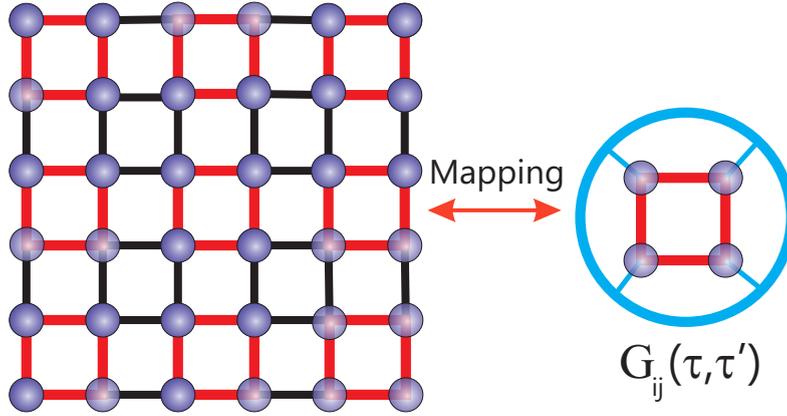


Fig. 11: Schematic representation of a plaquette cluster-reference system for the square lattice.

The standard reference system (Fig. 11) corresponds to the Green function, averaged over the supercell Brillouin zone, which is equivalent to the self-consistent cluster-DMFT scheme [21]. Another possibility for the reference system is related with the $\mathbf{k} = 0$ Green function, which corresponds to the decoupled lattice of plaquettes with periodic boundary condition

$$\Delta_0 = t_{\mathbf{k}=0} = \begin{pmatrix} \varepsilon & 2t & 4p & 2t \\ 2t & \varepsilon & 2t & 4p \\ 4p & 2t & \varepsilon & 2t \\ 2t & 4p & 2t & \varepsilon \end{pmatrix}. \quad (40)$$

Note that the spectrum of this hopping Hamiltonian Eq. (40) is equal to the original cubic tight-binding model

$$\varepsilon_{\mathbf{k}} = 2t(\cos k_x + \cos k_y) + 4p \cos k_x \cos k_y$$

in the 4 \mathbf{k} -points: $\Gamma=(0,0)$, $X=(\pi,0)$, $Y=(0,\pi)$ and $M=(\pi,\pi)$ which corresponds to the 2×2 grid in the original Brillouin zone. In this sense, we can view the dual fermion perturbation from the plaquette reference system [21] as a DF-multigrid interpolation from the 2×2 \mathbf{k} -mesh in the original cubic lattice to, e.g., 64×64 \mathbf{k} -points (for this case one needs to use the 32×32 mesh in our supercell). This is exactly the task for the present numerical test.

In order to calculate the bare dual Green function we use a slightly modified version of Eq. (33) (since $\Delta_{\mathbf{k}} = \Delta_0 - t_{\mathbf{k}} = 0$, for some \mathbf{k} -points, e.g. for $\mathbf{k} = 0$)

$$\tilde{G}_{\mathbf{k},\nu}^0 = \Delta_{\mathbf{k}}(1 - g_{\nu}\Delta_{\mathbf{k}})^{-1}.$$

With this choice of reference system, one can again stay only with the exact diagonalization scheme to calculate the dual Green function and the plaquette vertex function. We choose the strong-coupling parameters with $U=W=8$, $t = -1$, $p=0$ and the temperature $T=1/3$ for which there is a diagrammatic QMC results [18]. In the Fig. 12 we plot the density of states (DOS) for three different Green functions: ED for the reference plaquette, cluster perturbation (CP) which corresponds to Eq. (39) with $\tilde{\Sigma}_{\mathbf{k}\nu}=0$, and the results for the second-order plaquette dual-fermion. We use Padé-analytical continuation from the Matsubara to the real energy axis [5].

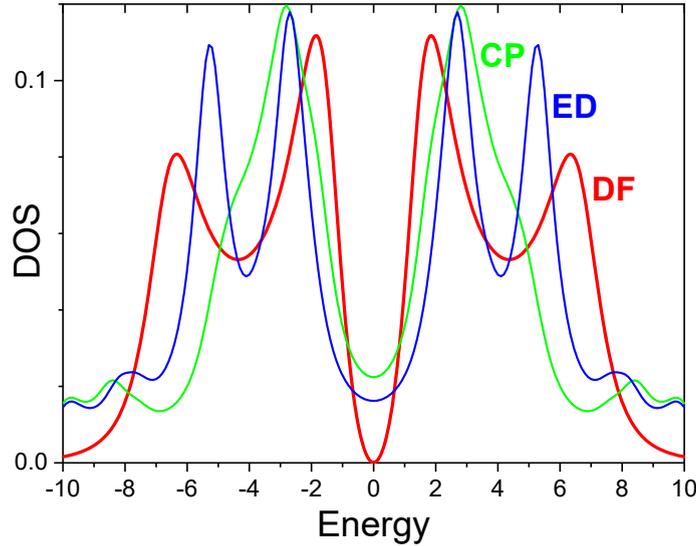


Fig. 12: Density of states for dual fermion perturbation from plaquette for $U=W=8$ (DF-red) in comparison with exact diagonalization for periodic plaquette (ED-blue) and cluster perturbation theory (CP-green).

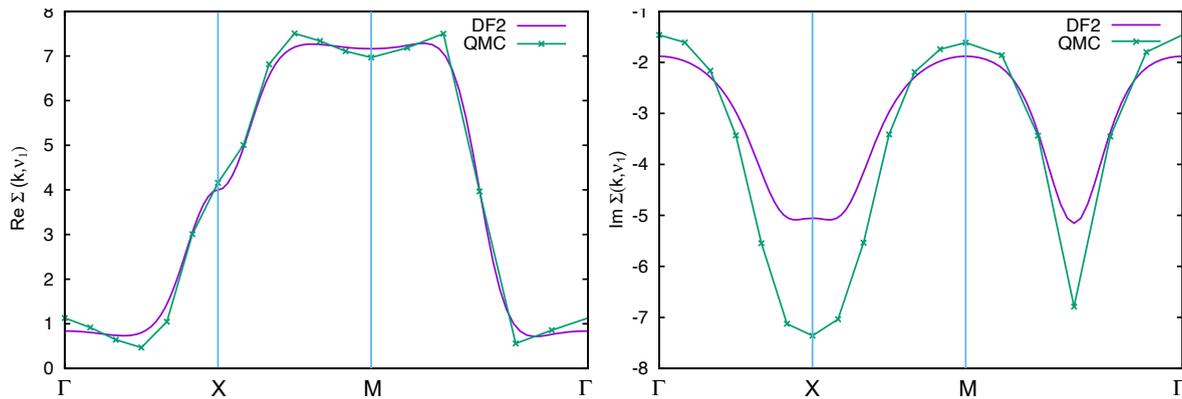


Fig. 13: Real (left) and imaginary (right) part of the self-energy for the DF plaquette scheme in comparison with diagrammatic-QMC results [18] at the first Matsubara frequency.

We conclude that the DOS for dual fermion theory differs strongly from the results of the simple perturbation (CP) and the original reference system (ED), and has a broad four-peaks structure, characteristic for the lattice QMC results [22].

Fig. 13 shows the DF-plaquette second-order lattice self-energy Eq. (38) for the standard \mathbf{k} -dependent path Γ - X - M - Γ in the two-dimensional Brillouin zone, together with numerically exact lattice diagrammatic QMC [18]. The almost perfect agreement for the real-part of the self-energy $\Sigma(\mathbf{k}, \nu=\pi T)$ underlines the strength of the dual-fermion superperturbation technique starting from a “reasonable” plaquette reference system.

Finally, we plot in Fig. 14 the full Brillouin zone 64×64 \mathbf{k} -mesh of the real and imaginary part of DF-plaquette self-energy periodize to original square lattice, in order to have an impression of the complex behavior for strongly correlated lattice fermion systems.

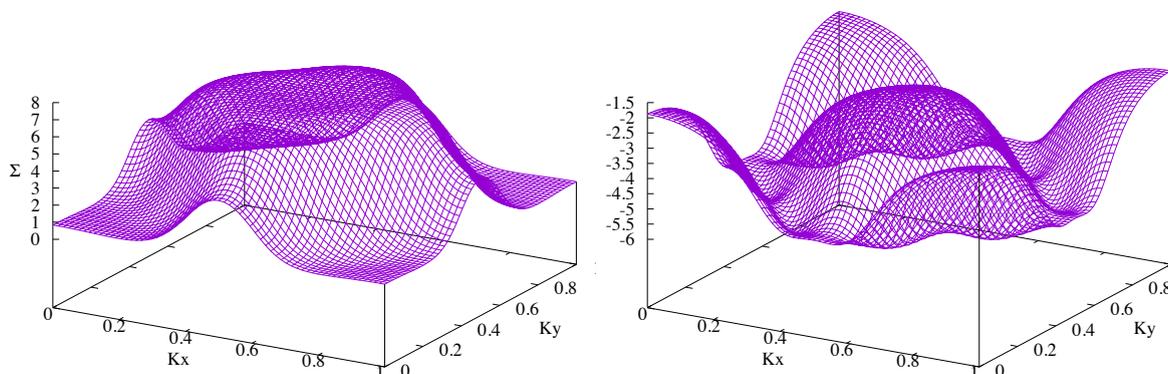


Fig. 14: Full Brillouin zone 64×64 \mathbf{k} -mesh for the real (left) and imaginary (right) part of the DF plaquette self-energy at the first Matsubara frequency.

6 Conclusion: Recent developments

We discussed the path-integral expansion for correlated lattice systems beyond the local DMFT approximation using transformations to dual variables. We would like to mention other recent developments in this field. Very important generalization of the dual variable approach are related with the dual-boson approach [23, 2], which properly includes effects of non-local interactions. This scheme allows the very efficient treatment of charge [24] and spin [25] collective fluctuations, and their effects on electronic spectrum and vice versa. Careful analyses of the two-particle divergence using dual variables [26] and fast calculations of the polarization function in correlated solids [27] show the strength of proper path-integral perturbation starting from the best local approximation. The efficient version of dual perturbation based on partial bosonization [28] has a strong potential for development of the realistic GW-like scheme with proper charge- and spin-fluctuations.

Acknowledgments

The author would like to thank for very fruitful discussions with Mikhail Katsnelson, Alexey Rubtsov, Sergey Brener, Evgeny Stepanov, Friedrich Krien, Erik van Loon, Sergey Isakov, and George Rohringer. Supports by the Cluster of Excellence “Advanced Imaging of Matter” (EXC 2056) of the Deutsche Forschungsgemeinschaft, Project No. ID390715994 and by the European Research Council via Synergy Grant 854843 - FASTCORR are greatly acknowledged.

Appendices

A Path-integrals for fermions

We first introduce a formalism of the path integral over fermionic fields [11]. Let us consider a simple case of a single quantum state $|i\rangle$ occupied by fermionic particles [29]. Due to the Pauli principle the many-body Hilbert space is spanned by only two orthonormal states $|0\rangle$ and $|1\rangle$. In the second quantization scheme for fermions with annihilation \hat{c}_i and creations \hat{c}_i^\dagger operators with anticommutation relations $\{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij}$ we have the following simple rules

$$\hat{c}_i |1\rangle = |0\rangle \quad \hat{c}_i |0\rangle = 0 \quad \text{and} \quad \hat{c}_i^\dagger |0\rangle = |1\rangle \quad \hat{c}_i^\dagger |1\rangle = 0. \quad (41)$$

Moreover, the density operator and the Pauli principle have the form

$$\hat{c}_i^\dagger \hat{c}_i |n\rangle = n_i |n\rangle \quad \text{and} \quad \hat{c}_i^2 = (\hat{c}_i^\dagger)^2 = 0.$$

The central object here are the so-called fermionic coherent states $|c\rangle$, which are eigenstates of annihilation operator \hat{c}_i with eigenvalue c_i

$$\hat{c}_i |c\rangle = c_i |c\rangle. \quad (42)$$

It is worthwhile to note that such a left-eigenbasis has only annihilation operators, due to the fact that they are bounded from the below and one can rewrite one of equations from Eq. (41) in the following ‘‘eigenvalue’’ form

$$\hat{c}_i |0\rangle = 0 |0\rangle.$$

Due to the anti-commutation relations for the fermionic operators the eigenvalues of coherent states c_i are so-called Grassmann numbers with the multiplication rules [30]

$$c_i c_j = -c_j c_i \quad \text{and} \quad c_i^2 = 0. \quad (43)$$

It is convenient to assume that the Grassmann numbers also anti-commute with the fermionic operators

$$\{c, \hat{c}\} = \{c, \hat{c}^\dagger\} = 0.$$

An arbitrary function of one Grassmann variable can be represented by only the first two Taylor coefficients

$$f(c) = f_0 + f_1 c. \quad (44)$$

One can prove the following general many-body representation of coherent states

$$|c\rangle = e^{-\sum_i c_i \hat{c}_i^\dagger} |0\rangle. \quad (45)$$

Let us show this for the simple case of one fermionic state

$$\hat{c} |c\rangle = \hat{c}(1 - c\hat{c}^\dagger) |0\rangle = \hat{c}(|0\rangle - c|1\rangle) = -\hat{c}c|1\rangle = c|0\rangle = c|c\rangle. \quad (46)$$

One can also define a “left” coherent state $\langle c|$ as the left-eigenstates of creation operators \hat{c}_i^\dagger

$$\langle c| \hat{c}_i^\dagger = \langle c| c_i^*.$$

Note that new eigenvalue c_i^* is just another Grassmann number, not the complex conjugate of c_i . The left coherent state can be obtained similar to Eq. (45)

$$\langle c| = \langle 0| e^{-\sum_i \hat{c}_i c_i^*}.$$

A general function of two Grassmann variables can, analogously to Eq. (44), be represented by only four Taylor coefficients

$$f(c^*, c) = f_{00} + f_{10}c^* + f_{01}c + f_{11}c^*c. \quad (47)$$

Using this expansion we can define a derivative of Grassmann variables in the natural way

$$\frac{\partial c_i}{\partial c_j} = \delta_{ij}.$$

One needs to be careful with “right-order” of such a derivative and remember the anti-commutation rules, i.e.,

$$\frac{\partial}{\partial c_2} c_1 c_2 = -c_1.$$

For the case of the general two-variable function in Eq. (47) we have

$$\frac{\partial}{\partial c^*} \frac{\partial}{\partial c} f(c^*, c) = \frac{\partial}{\partial c^*} (f_{01} - f_{11}c^*) = -f_{11} = -\frac{\partial}{\partial c} \frac{\partial}{\partial c^*} f(c^*, c).$$

One also needs a formal definition of the integration over Grassmann variables, and the natural way consists of the following rules [30]

$$\int 1 dc = 0 \quad \text{and} \quad \int c dc = 1,$$

which just shows that the integration over a Grassmann variable is equivalent to differentiation

$$\int \dots dc \rightarrow \frac{\partial}{\partial c} \dots$$

The coherent states are not orthonormal and the overlap of any two such states is equal to

$$\langle c|c \rangle = e^{\sum_i c_i^* c_i}$$

which is easy to see for the case of one particle

$$\langle c|c \rangle = (\langle 0| - \langle 1| c^*) (|0 \rangle - c|1 \rangle) = 1 + c^*c = e^{c^*c}.$$

An important property of coherent states is the resolution of unity

$$\int dc^* \int dc e^{-\sum_i c_i^* c_i} |c \rangle \langle c| = \hat{1} = \iint dc^* dc \frac{|c \rangle \langle c|}{\langle c|c \rangle}.$$

For simplicity we demonstrate this relation only for one fermion state

$$\begin{aligned} \iint dc^* dc e^{-c^*c} |c\rangle\langle c| &= \iint dc^* dc (1 - c^*c) (|0\rangle - c|1\rangle) (\langle 0| - \langle 1| c^*) = \\ &= - \iint dc^* dc c^*c (|0\rangle\langle 0| + |1\rangle\langle 1|) = \sum_n |n\rangle\langle n| = \hat{1}. \end{aligned}$$

Matrix elements of normally ordered operators are very easy to calculate in the coherent basis by operating with \hat{c}^\dagger on the states to the right and \hat{c} to the left:

$$\langle c^* | \hat{H}(\hat{c}^\dagger, \hat{c}) |c\rangle = H(c^*, c) \langle c^* |c\rangle = H(c^*, c) e^{\sum_i c_i^* c_i} \quad (48)$$

Within the manifold of coherent states we can map the fermionic operators to the Grassmann variables $(\hat{c}_i^\dagger, \hat{c}_i) \rightarrow (c_i^*, c_i)$.

Finally, we prove the so-called “trace-formula” for arbitrary fermionic operators in normal order (in one-fermion notation)

$$\begin{aligned} \text{Tr } \hat{O} &= \sum_{n=0,1} \langle n | \hat{O} |n\rangle = \sum_{n=0,1} \iint dc^* dc e^{-c^*c} \langle n |c\rangle \langle c | \hat{O} |n\rangle = \\ &= \iint dc^* dc e^{-c^*c} \sum_{n=0,1} \langle -c | \hat{O} |n\rangle \langle n |c\rangle = \iint dc^* dc e^{-c^*c} \langle -c | \hat{O} |c\rangle. \end{aligned}$$

The fermionic “minus” sign in the left coherent states come from the commutation of the (c^*) and (c) coherent state in such a transformation: $\langle n |c\rangle \langle c |n\rangle = \langle -c |n\rangle \langle n |c\rangle$. One has to use the standard Grassmann rules: $c_i^* c_j = -c_j c_i^*$ and $|-c\rangle = |0\rangle + c|1\rangle$.

We are ready now to write the partition function for the grand-canonical quantum ensemble with $H = \hat{H} - \mu \hat{N}$ and inverse temperature β . One has to use the N -slices Trotter decomposition for the partition function in $[0, \beta)$ with imaginary time $\tau_n = n\Delta\tau = n\beta/N$ ($n = 1, \dots, N$), and insert N times the resolution of unity as follows

$$\begin{aligned} Z &= \text{Tr } e^{-\beta H} = \iint dc^* dc e^{-c^*c} \langle -c | e^{-\beta H} |c\rangle \\ &= \int \prod_{n=1}^N dc_n^* dc_n e^{-\sum_n c_n^* c_n} \langle c_N | e^{-\Delta\tau H} |c_{N-1}\rangle \langle c_{N-1} | e^{-\Delta\tau H} |c_{N-2}\rangle \dots \langle c_1 | e^{-\Delta\tau H} |c_0\rangle \\ &= \int \prod_{n=1}^N dc_n^* dc_n e^{-\Delta\tau \sum_{n=1}^N [c_n^* (c_n - c_{n-1}) / \Delta\tau + H(c_n^*, c_{n-1})]} \end{aligned}$$

In the continuum limit ($N \rightarrow \infty$)

$$\Delta\tau \sum_{n=1}^N \dots \rightarrow \int_0^\beta d\tau \dots, \quad \frac{c_n - c_{n-1}}{\Delta\tau} \rightarrow \partial_\tau \quad \text{and} \quad \prod_{n=0}^{N-1} dc_n^* dc_n \rightarrow \mathcal{D}[c^*, c]$$

with antiperiodic boundary conditions for fermionic Grassmann variables in imaginary time $c(\tau)$ and $c^*(\tau)$

$$c(\beta) = -c(0), \quad c^*(\beta) = -c^*(0)$$

we end up in the standard path-integral formulation of the partition function

$$Z = \int \mathcal{D}[c^*, c] e^{-\int_0^\beta d\tau [c^*(\tau) \partial_\tau c(\tau) + H(c^*(\tau), c(\tau))]} . \quad (49)$$

It is useful to mention the general form of the Gaussian path-integral for a non-interacting “quadratic” fermionic action, which is equivalent to the Hubbard-Stratonovich transformation used in the dual-fermion derivation Eq. (22). For an arbitrary matrix M_{ij} and Grassmann vectors J_i^* and J_i one can calculate analytically the following integral

$$Z_0[J^*, J] = \int \mathcal{D}[c^* c] e^{-\sum_{i,j=1}^N c_i^* M_{ij} c_j - \sum_{i=1}^N (c_i^* J_i + J_i^* c_i)} = \det M e^{\sum_{i,j=1}^N J_i^* (M^{-1})_{ij} J_j} . \quad (50)$$

To prove this relation one need first to change variables in order to eliminate J_i^* and J_i and expand the exponential function (only N -th order is non-zero)

$$e^{-\sum_{i,j=1}^N c_i^* M_{ij} c_j} = \frac{1}{N!} \left(- \sum_{i,j=1}^N c_i^* M_{ij} c_j \right)^N .$$

Finally, different permutations of c_i^* and c_j and integration over Grassmann variables will give $\det M$. As a small exercise we will check such integrals for the first two many-particle dimensions. For $N=1$ it is trivial

$$\int \mathcal{D}[c^* c] e^{-c_1^* M_{11} c_1} = \int \mathcal{D}[c^* c] (-c_1^* M_{11} c_1) = M_{11} = \det M$$

and for $N=2$ we have

$$\begin{aligned} & \int \mathcal{D}[c^* c] e^{-c_1^* M_{11} c_1 - c_1^* M_{12} c_2 - c_2^* M_{21} c_1 - c_2^* M_{22} c_2} = \\ & = \frac{1}{2!} \int \mathcal{D}[c^* c] (-c_1^* M_{11} c_1 - c_1^* M_{12} c_2 - c_2^* M_{21} c_1 - c_2^* M_{22} c_2)^2 = M_{11} M_{22} - M_{12} M_{21} = \det M . \end{aligned}$$

For a change of variables in the path integral one uses the following transformation with unit Jacobian: $c \rightarrow c + M^{-1} J$ and

$$c^* M c + c^* J + J^* c = (c^* + J^* M^{-1}) M (c + M^{-1} J) - J^* M^{-1} J .$$

Using the Gaussian path-integral it is very easy to calculate any correlation function for a non-interaction action (Wick-theorem)

$$\begin{aligned} \langle c_i c_j^* \rangle_0 &= - \frac{1}{Z_0} \frac{\delta^2 Z_0[J^*, J]}{\delta J_i^* \delta J_j} \Bigg|_{J=0} = M_{ij}^{-1} \\ \langle c_i c_j c_k^* c_l^* \rangle_0 &= \frac{1}{Z_0} \frac{\delta^4 Z_0[J^*, J]}{\delta J_i^* \delta J_j^* \delta J_l \delta J_k} \Bigg|_{J=0} = M_{il}^{-1} M_{jk}^{-1} - M_{ik}^{-1} M_{jl}^{-1} . \end{aligned}$$

Corresponding bosonic path-integrals can be formulated in a similar way with complex variables and periodic boundary conditions on imaginary time. The Gaussian path-integral over bosonic fields is equal to inverse of the M -matrix determinant [11].

B Exact relations between Green functions

After appropriate diagrammatic results for the dual self-energy and the dual Green function have been obtained, they have to be transformed back to the corresponding physical quantities in terms of real lattice fermions. The fact that dual fermions are introduced through the exact Hubbard-Stratonovich transformation, Eq. (22), allows to establish exact identities between dual and lattice Greens function [3, 15].

The relations between the n -particle cumulants of dual and lattice fermions can be established using the cumulant (linked cluster) technique. To this end one may consider two different, equivalent representations of the following generating functional

$$e^{F[J^*J, L^*L]} = \mathcal{Z}_d \int \mathcal{D}[c^*c, d^*d] e^{-S[c^*c, d^*d] + J_1^*c_1 + c_2^*J_2 + L_1^*d_1 + d_2^*L_2}. \quad (51)$$

Integrating-out the lattice fermions from this functional similar to (26) (this can be done with the sources J and J^* set to zero) yields

$$e^{F[L^*, L]} = \tilde{\mathcal{Z}}_d \int \mathcal{D}[d^*, d] e^{-S_d[d^*, d] + L_1^*d_1 + d_2^*L_2} \quad (52)$$

with $\tilde{\mathcal{Z}}_d = \mathcal{Z}/\tilde{\mathcal{Z}}$. The dual Green function and the two-particle correlator related with non-local susceptibilities are obtained from (52) by suitable functional derivatives, e.g.,

$$\tilde{G}_{12} = - \left. \frac{\delta^2 F}{\delta L_2 \delta L_1^*} \right|_{L^*=L=0} \quad (53)$$

where $G \otimes G$ is the antisymmetrized direct product of Green functions, so that the angular bracket is the connected part of the dual two-particle Green function. Conversely, integrating out the dual fermions from Eq. (51) using the HS-transformation, one obtains an alternative representation, which more clearly reveals the connection of the functional derivatives with respect to the sources J , J^* , and L , L^* . The result is

$$F[J^*J, L^*L] = L_1^*(\Delta - t)_{12}L_2 + \ln \int \mathcal{D}[c^*, c] \exp\left(-S[c^*, c] + J_1^*c_1 + c_2^*J_2 + L_1^*(\Delta - t)_{12}c_2 + c_1^*(\Delta - t)_{12}L_2\right). \quad (54)$$

In analogy to (53), the cumulants in terms of lattice fermions are obviously obtained by functional derivative with respect to the sources J and J^* with L and L^* set to zero. Applying the derivatives with respect to L , L^* to (54) with $J = J^* = 0$ and comparing to (53), e.g., yields the identity

$$\tilde{G}_{12} = -(\Delta - t)_{12} + (\Delta - t)_{11'}G_{1'2'}(\Delta - t)_{2'2}. \quad (55)$$

Solving for G provides the rule how to transform the dual Green function to the physical quantity in terms of lattice fermions.

References

- [1] E. Gull, A. Millis, A. Lichtenstein, A. Rubtsov, M. Troyer, and P. Werner, *Rev. Mod. Phys.* **83**, 349 (2011)
- [2] G. Rohringer, H. Hafermann, A. Toschi, A.A. Katanin, A.E. Antipov, M.I. Katsnelson, A.I. Lichtenstein, A.N. Rubtsov, and K. Held *Rev. Mod. Phys.* **90**, 025003 (2018)
- [3] A.N. Rubtsov, M.I. Katsnelson, and A.I. Lichtenstein, *Phys. Rev. B* **77**, 033101 (2008)
- [4] F. Lechermann, A.I. Lichtenstein, and M. Potthoff, *Eur. Phys. J. Special Topics* **226**, 2591 (2017)
- [5] A. Georges, G. Kotliar, W. Krauth, and M.J. Rozenberg, *Rev. Mod. Phys.* **68**, 13 (1996)
- [6] N.F. Mott: *Metal-Insulator Transitions*, 2nd ed. (Taylor and Francis, 1990)
- [7] A. Georges and G. Kotliar, *Phys. Rev. B* **45**, 6479 (1992)
- [8] P. Hohenberg and W. Kohn, *Phys. Rev.* **136**, 864 (1964)
- [9] G. Kotliar, S.Y. Savrasov, K. Haule, V.S. Oudovenko, O. Parcollet, and C.A. Marianetti, *Rev. Mod. Phys.* **78**, 865 (2006)
- [10] A.A. Abrikosov, L.P. Gorkov, and I.E. Dzyaloshinski: *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, New Jersey, 1964)
- [11] J.W. Negele, and H. Orland: *Quantum Many-Particle Systems* (Addison-Wesley, New York, 1988)
- [12] G. Baym and L.P. Kadanoff, *Phys. Rev.* **124**, 287 (1961)
- [13] D.M. Ceperley and B.J. Alder, *Phys. Rev. Lett.* **45**, 566 (1980)
- [14] H. Hafermann, F. Lechermann, A.N. Rubtsov, M.I. Katsnelson, A. Georges, and A.I. Lichtenstein, *Lecture Notes in Physics* **843**, 145 (2012)
- [15] H. Hafermann: *Numerical Approaches to Spatial Correlations in Strongly Interacting Fermion Systems* (Cuvillier Verlag, Göttingen, Singapore, 2010)
- [16] F. Krien and A. Valli *Phys. Rev. B* **100**, 245147 (2019)
- [17] S. Isakov, A.E. Antipov, and E. Gull, *Phys. Rev. B* **94**, 035102 (2016)
- [18] J. Gukelberger, E. Kozik, and H. Hafermann, *Phys. Rev. B* **96**, 035152 (2017)
- [19] H. Hafermann, Ch. Jung, S. Brener, M.I. Katsnelson, A.N. Rubtsov, and A.I. Lichtenstein, *Europhys. Lett.* **85**, 27007 (2009)

-
- [20] X. Dai, K. Haule, and G. Kotliar, *Phys. Rev. B* **72**, 045111 (2005)
- [21] A.I. Lichtenstein and M.I. Katsnelson, *Phys. Rev. B* **62**, R9283 (2000)
- [22] D. Rost, E.V. Gorelik, F. Assaad, and N. Blümer, *Phys. Rev. B* **86**, 155109 (2012)
- [23] A.N. Rubtsov, M.I. Katsnelson, and A.I. Lichtenstein, *Ann. Phys.* **327**, 1320 (2012)
- [24] E.G.C.P. van Loon, H. Hafermann, A.I. Lichtenstein, A.N Rubtsov, and M.I. Katsnelson, *Phys. Rev. Lett.* **113**, 246407 (2014)
- [25] E.A. Stepanov, L. Peters, I.S. Krivenko, A.I. Lichtenstein, M.I. Katsnelson, and A.N Rubtsov, *npj Quantum Materials* **3**, 54 (2018)
- [26] F. Krien, E.G.C.P. van Loon, M.I. Katsnelson, A.I. Lichtenstein, and M. Capone, *Phys. Rev. B* **99**, 245128 (2019)
- [27] F. Krien, *Phys. Rev. B* **99**, 235106 (2019)
- [28] E.A. Stepanov, V. Harkov, and A.I. Lichtenstein, *Phys. Rev. B* **100**, 205115 (2019)
- [29] A. Kamenev: *Field Theory of Non-Equilibrium Systems* (Cambridge University Press, 2011)
- [30] F.A. Berezin: *Method of Second Quantization* (Academic Press, New York, 1966)