

10 Path Integrals and Dual Fermions

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1 Introduction: DMFT and beyond

In this lecture we give an introduction to the theoretical description of strongly correlated materials based on non-local extensions of dynamical mean-field theory (DMFT). This scheme combines the numerically exact DMFT solution of an effective impurity problem with an analytical non-local perturbation scheme. The frequency-dependent effective-impurity DMFT problem is 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 expansion around the DMFT solution using a special dual space transformation. We discuss a general way to include nonlocal correlations beyond DMFT for generalized Hubbard models, based on the dual-fermion [2] and the dual-boson approach [3].

Consider the noninteracting, “kinetic” part H_t of the Hubbard model first [4]. It is determined 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 transforming the hopping parameters to \mathbf{k} -space, where we obtain the normal “band structure” $\varepsilon_{\mathbf{k}}$ 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 given by an on-site energy ε_0 only, the diagonalization of the Hamiltonian is trivial again and reduces to the diagonalization of a single “Hubbard atom”.

The great success of the DMFT approach is related to its ability to numerically interpolate between these two limits [5]. For the half-filled Hubbard model on an infinite-dimensional Bethe lattice 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. This impurity model, which is fully determined by the local hybridization function Δ_ν on fermionic Matsubara frequencies $i\nu_n$ is solved by the numerically exact CT-QMC scheme and exact the local Green function g_ν is obtained. The DMFT self-consistency condition for the hybridization function equates the local part of the lattice Green function and the impurity Green function

$$\sum_{\mathbf{k}} (g_\nu^{-1} + \Delta_\nu - \varepsilon_{\mathbf{k}})^{-1} = g_\nu,$$

which shows that DMFT minimizes, in local sense, the $|\varepsilon_{\mathbf{k}} - \Delta_\nu|$ distance.

We can now think about how to incorporate nonlocal correlations beyond DMFT: since the Hubbard and the Anderson-impurity model share the same interaction part, we can think of the Hubbard model as the impurity model plus a residual term $\propto \varepsilon_{\mathbf{k}} - \Delta_\nu$ 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,

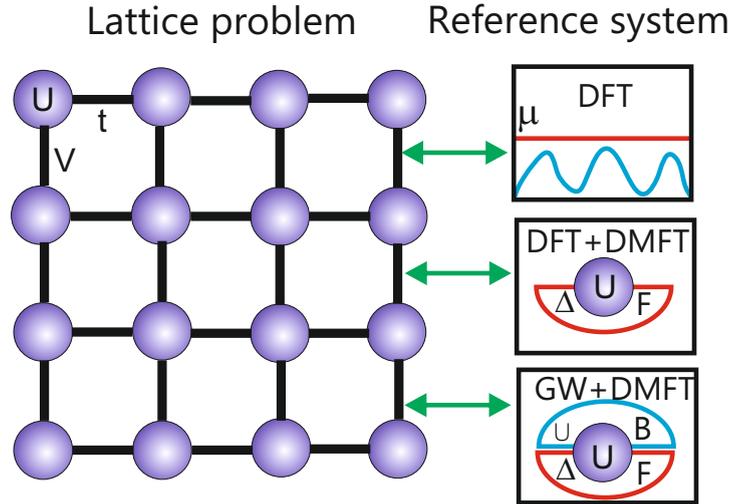


Fig. 1: Schematic representation of the reference systems in many-body approaches to lattice-fermion models: (i) Density-functional theory (DFT) with the interacting homogeneous electron gas as a reference system, defined by a constant external potential μ . (ii) Dynamical mean-field theory (DMFT) with an effective impurity problem as a reference system, defined by a 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.

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 at 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, we are 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 of local and nonlocal terms is achieved by a Hubbard-Stratonovich transformation applied to the single-particle $(\varepsilon_{\mathbf{k}} - \Delta_{\nu})$ -term [2]. 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 generate an effective action in the transformed, so-called dual-fermion representation [2]. Note that integrating out the local degrees of freedom is not just 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 (the non-local part of the DMFT Green function) $\tilde{G}_{\mathbf{k},\nu}^0 = [g_{\nu}^{-1} + \Delta_{\nu} - \varepsilon_{\mathbf{k}}]^{-1} - g_{\nu}$, 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 func-

tions. 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 [2] 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 (1). 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, e.g., ladder summations of dual diagrams. This also explains the notion “dual fermions”.

2 Path-integral for fermions

We first introduce a formalism of path-integration over fermionic fields [10]. Let us consider a simple case of a single quantum state $|i\rangle$ occupied by fermionic particles [11]. Due to the Pauli principle the many-body Hilbert space is spanned only by 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

$$\begin{aligned} \hat{c}_i |1\rangle &= |0\rangle & \hat{c}_i |0\rangle &= 0 \\ \hat{c}_i^\dagger |0\rangle &= |1\rangle & \hat{c}_i^\dagger |1\rangle &= 0. \end{aligned} \quad (1)$$

Moreover, the density operator and the Pauli principle take 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 :

$$\hat{c}_i |c\rangle = c_i |c\rangle. \quad (2)$$

It is worthwhile to note that such a left-eigenbasis has only annihilation operators, due to the fact that they are bounded from below and one can rewrite one of equation from Eq. (1) 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 following multiplication rules [12]:

$$c_i c_j = -c_j c_i \quad \text{and} \quad c_i^2 = 0. \quad (3)$$

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 a Grassmann variable can be represented only by its first two Taylor coefficients

$$f(c) = f_0 + f_1 c. \quad (4)$$

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

$$|c\rangle = e^{-\sum_i c_i \hat{c}_i^\dagger} |0\rangle. \quad (5)$$

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

$$\hat{c} |c\rangle = \hat{c}(1 - c\hat{c}^\dagger) |0\rangle = \hat{c}(|0\rangle - c|1\rangle) = -\hat{c}c|1\rangle = c|0\rangle = c|c\rangle. \quad (6)$$

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

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

Note that new eigenvalues c_i^* is just another Grassmann number and not a complex conjugate of c_i . The left coherent state can be obtained similarly to Eq. (5) as following

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

A general function of two Grassmann variables, analogously to Eq. (4), can be represented by only four Taylor coefficients

$$f(c^*, c) = f_{00} + f_{10}c^* + f_{01}c + f_{11}c^*c. \quad (7)$$

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 the “right-order” in 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 a general two-variable function in Eq. (7) 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 with the following rules [12]:

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

which just show that 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 coherent fermionic states is

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

which is easy to see for the case of one state

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

An important property of coherent states is related to resolution of the unity operator

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

For simplicity we demonstrate this relation only for one fermion state:

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

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

$$\langle c^* | \hat{H}(\hat{c}^\dagger, \hat{c}) |c \rangle = H(c^*, c) \langle c^* |c \rangle = H(c^*, c) e^{\sum_i c_i^* c_i} \quad (8)$$

Within the manifold of coherent states we can map the fermionic operators to functions of 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):

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

The fermionic “minus” sign in the left coherent states comes from the commutation of the (c^*) and (c) coherent states 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 now ready to write a partition function or the grand-canonical quantum ensemble with $H = \hat{H} - \mu \hat{N}$ and inverse temperature β . We have to use the N -slices Trotter decomposition

for the partition function in the interval $[0, \beta)$ with imaginary times $\tau_n = n\Delta\tau = n\beta/N$ ($n = 1, \dots, N$), and insert N -times the resolution of unity as follows

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

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

$$\begin{aligned} \Delta\tau \sum_{n=1}^N \dots &\mapsto \int_0^\beta d\tau \dots \\ \frac{c_n - c_{n-1}}{\Delta\tau} &\mapsto \partial_\tau \\ \prod_{n=0}^{N-1} dc_n^* dc_n &\mapsto D[c^*, c] \end{aligned}$$

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

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

we end up with the standard path integral formulation of the quantum partition function

$$Z = \int D[c^*, c] \exp\left(-\int_0^\beta d\tau [c^*(\tau) \partial_\tau c(\tau) + H(c^*(\tau), c(\tau))]\right). \quad (9)$$

For later discussion we mention the Gaussian path integral for a non-interacting ‘‘quadratic’’ fermionic action. For an arbitrary matrix M_{ij} and Grassmann vectors J_i^* and J_i one can calculate analytically the following integral

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

To prove this relation one needs first to complete the square in order to eliminate J_i^* and J_i and expand the exponential function (only the 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 the Grassmann variables gives the $\det M$ -answer. As a small exercise we will check such an integral for first two many-particle dimensions. For $N = 1$ it is trivial:

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

and for $N = 2$ we have

$$\int D[c^*c] e^{-c_1^* M_{11} c_1 - c_1^* M_{12} c_1 - c_2^* M_{21} c_1 - c_2^* M_{22} c_2} =$$

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

For the shift (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 of a non-interaction action (Wick-theorem):

$$\langle c_i c_j^* \rangle_0 = -\frac{1}{Z_0} \left. \frac{\delta^2 Z_0 [J^*, J]}{\delta J_i^* \delta J_j} \right|_{J=0} = M_{ij}^{-1}$$

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

Corresponding bosonic path-integrals can be formulated in a similar way with complex variables and periodic boundary conditions in imaginary time. The Gaussian path integral over bosonic fields is equal to inverse of the M -matrix determinant [10].

3 Functional approach

We introduce a general functional approach which will cover the Density-Functional Theory (DFT), Dynamical Mean-Field Theory (DMFT), and Baym-Kadanoff (BK) theories [9, 13]. Let us start from the full many-body Hamiltonian describing electrons moving in the periodic external potential of ions $V(\mathbf{r})$ with the chemical potential μ and interacting via the Coulomb repulsion $U(\mathbf{r} - \mathbf{r}') = 1/|\mathbf{r} - \mathbf{r}'|$. We use the atomic units $\hbar = m = e = 1$. In the field-operator representation the Hamiltonian has the form

$$H = \sum_{\sigma} \int d\mathbf{r} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \left(-\frac{1}{2} \nabla^2 + V(\mathbf{r}) - \mu \right) \hat{\psi}_{\sigma}(\mathbf{r}) \quad (10)$$

$$+ \frac{1}{2} \sum_{\sigma\sigma'} \int d\mathbf{r} \int d\mathbf{r}' \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \hat{\psi}_{\sigma'}^{\dagger}(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \hat{\psi}_{\sigma'}(\mathbf{r}') \hat{\psi}_{\sigma}(\mathbf{r}).$$

We can always use the single-particle orthonormal basis set in solids $\phi_n(\mathbf{r})$ for example Wannier orbitals with a 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

$$\hat{\psi}(\mathbf{r}) = \sum_n \phi_n(\mathbf{r}) \hat{c}_n \quad (11)$$

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

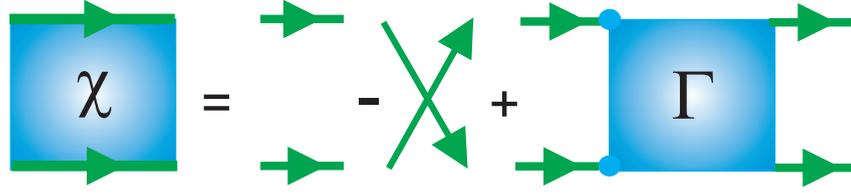


Fig. 2: Representation of the full two-particle Green function in terms trivial products of single-particle Green functions and the full vertex function Γ .

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

$$Z = \int \mathcal{D}[c^*, c] e^{-S} \quad (12)$$

$$S = \sum_{12} c_1^* (\partial_\tau + t_{12}) c_2 + \frac{1}{2} \sum_{1234} c_1^* c_2^* U_{1234} c_4 c_3, \quad (13)$$

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

$$t_{12} = \int d\mathbf{r} \phi_1^*(\mathbf{r}) \left(-\frac{1}{2} \nabla^2 + V(\mathbf{r}) - \mu \right) \phi_2(\mathbf{r}) \quad (14)$$

$$U_{1234} = \int d\mathbf{r} \int d\mathbf{r}' \phi_1^*(\mathbf{r}) \phi_2^*(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \phi_3(\mathbf{r}) \phi_4(\mathbf{r}')$$

and we use the following short definition of the sum:

$$\sum_1 \dots \equiv \sum_{im} \int d\tau \dots \quad (15)$$

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

$$G_{12} = -\langle c_1 c_2^* \rangle_S = -\frac{1}{Z} \int \mathcal{D}[c^*, c] c_1 c_2^* \exp(-S). \quad (16)$$

The main problem of strongly interacting electronic systems is related to the fact that the higher order correlation functions do not separate into a product of lower order correlation functions. For example the two-particle Green function or generalized susceptibility (X) is defined in the following form [14]

$$X_{1234} = \langle c_1 c_2 c_3^* c_4^* \rangle_S = \frac{1}{Z} \int \mathcal{D}[c^*, c] c_1 c_2 c_3^* c_4^* \exp(-S), \quad (17)$$

and can be expressed graphically through the Green functions and the full vertex function Γ_{1234} [15] (see Fig. (2))

$$X_{1234} = G_{14} G_{23} - G_{13} G_{24} + \sum_{1'2'3'4'} G_{11'} G_{22'} \Gamma_{1'2'3'4'} G_{3'3} G_{4'4}. \quad (18)$$

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 would correspond to the first two

terms (Hartree and Fock like), with the vertex function Γ in Eq. (18) equal to zero. In strongly correlated electron systems the last part with the vertex is dominant and even diverges close to electronic phase transitions.

The Baym–Kadanoff functional [13] 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 a source term J in the following form

$$S[J] = S + \sum_{12} c_1^* J_{12} c_2. \quad (19)$$

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

$$Z[J] = e^{-F[J]} = \int \mathcal{D}[c^*, c] e^{-S'[J]}. \quad (20)$$

Variation with respect to this source function gives all correlation functions, for example the Green function

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

If we use the definition of the generalized susceptibility as the second variation of the $F[J]$ functional instead of $Z[J]$ we will get only the connected part of correlation the X -function which is represented by the last term in Eq. (18).

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

$$F[G] = F[J] - \text{Tr}(JG). \quad (22)$$

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

$$F[G] = \text{Tr} \ln G - \text{Tr}(\Sigma G) + \Phi[G], \quad (23)$$

where Σ is single particle self-energy and $\Phi[G]$ is the correlated part of the Baym–Kadanoff functional that is equal to the sum of all two-particle irreducible diagrams. In 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 the density functional theory. Moreover, this general functional approach reduces to density-functional theory, if one only uses the diagonal part in space-time of the Green function, which corresponds to the one-electron density

$$n_1 = G_{12} \delta_{12} = \langle c_1^* c_1 \rangle_S, \quad (24)$$

with the Kohn-Sham potential $V_{KS} = V_{ext} + V_H + V_{xc}$ playing the role of the “constrained field” J . Here V_{ext} is external potential and V_H is a 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 in the following way

$$F_{DFT}[n] = T_0[n] + V_{ext}[n] + V_H[n] + V_{xc}[n], \quad (25)$$

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

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

the local density approximation to DFT reads

$$T_0[n] + V_{ext}[n] = \sum_i \int d\mathbf{r} \phi_i^*(\mathbf{r}) \left(-\frac{1}{2}\nabla^2 + V_{ext}(\mathbf{r}) - \mu \right) \phi_i(\mathbf{r}) \quad (26)$$

$$V_H[n] = \frac{1}{2} \int d\mathbf{r} n(\mathbf{r}) U(\mathbf{r} - \mathbf{r}') n(\mathbf{r}') \quad (27)$$

$$V_{xc}[n] = \int d\mathbf{r} n(\mathbf{r}) \varepsilon[n(\mathbf{r})], \quad (28)$$

where $\varepsilon(n)$ is the exchange-correlation energy density for homogeneous electron gas, which can be calculated with quantum Monte Carlo [16].

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 ourself only to 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 magnons, which can be obtained from the 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 the quantum Monte Carlo (QMC). Unfortunately, due to the sign problem in lattice simulations this numerically exact solution of electronic correlations is not possible. On the other hand, one can obtain the solution of local interacting quantum problems 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 the 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 [2] which help us to separate the local fluctuations in a many-body system and show a perturbative way to go beyond the DMFT approximations.

4 Dual Fermion approach for non-local correlations

We will consider here the simplest local Hubbard-like interaction vertex U . A generalization to the multi-orbital case is straightforward [17]. All equations will be written in matrix form, giving the idea of how to generalize a DF scheme to the multiorbital case. The general strategy for separating the local and non-local correlation effects is associated with the introduction of auxiliary fermionic fields that couple separated local correlated impurities models back to the lattice [2].

We rewrite corresponding original action from Eq. (12) in Matsubara space as a sum of the non-local one-electron contribution with energy spectrum $\varepsilon_{\mathbf{k}}$ and the local interaction part U :

$$S[c^*, c] = - \sum_{\mathbf{k}\nu\sigma} c_{\mathbf{k}\nu\sigma}^* (i\nu + \mu - \varepsilon_{\mathbf{k}}) c_{\mathbf{k}\nu\sigma} + \sum_i U n_{i\uparrow}^* n_{i\downarrow}, \quad (29)$$

where $\nu = (2n + 1)\pi/\beta$, ($\omega = 2n\pi/\beta$), $n = 0, \pm 1, \dots$ are the fermionic (bosonic) Matsubara frequencies, β is inverse temperature, and μ is a 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 quasi-momenta. In order to keep the notation simple, it is useful to introduce the combined index $\alpha \equiv \{m, \sigma\}$. In the following, translational invariance is assumed for simplicity, 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 auxiliary local action, a quantum impurity problem is introduced

$$S_{\text{loc}}[c^*, c] = - \sum_{\nu, \sigma} c_{\nu\sigma}^* (i\nu + \mu - \Delta_\nu) c_{\nu\sigma} + U n_{\uparrow}^* n_{\downarrow}, \quad (30)$$

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 with CT-QMC methods [1]. Using the locality of the hybridization function Δ_ν , the lattice action Eq. (29) can be rewritten exactly in terms of individual impurity models and the effective one-electron coupling ($\varepsilon_{\mathbf{k}} - \Delta_\nu$) between different impurities

$$S[c^*, c] = \sum_i S_{\text{loc}}[c_i^*, c_i] + \sum_{\mathbf{k}\nu\sigma} c_{\mathbf{k}\nu\sigma}^* (\varepsilon_{\mathbf{k}} - \Delta_\nu) c_{\mathbf{k}\nu\sigma}. \quad (31)$$

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 the second term in Eq. (31) is very hard to treat, even perturbatively, since the impurity action is non-Gaussian and one cannot use Wick's theorem. The main idea of a dual fermion transformation is the change of variables from (c^*, c) to weakly correlated Grassmann fields (f^*, f) in the path integral representation of the partition function, Eq. (12), followed by a simple perturbation treatment. The new variables are introduced through the following Hubbard-Stratonovich transformation

$$\exp(c_\alpha^* b_\alpha (M^{-1})_{\alpha\beta} b_\beta c_\beta) = \frac{1}{\det M} \int \mathcal{D}[f^*, f] \exp(-f_\alpha^* M_{\alpha\beta} f_\beta - c_\alpha^* b_\alpha f_\alpha - f_\beta^* b_\beta c_\beta). \quad (32)$$

In order to transform the exponential of the bilinear term in Eq. (31), we choose the matrix $M_{\alpha\beta}$ and scaling function b_α in the following way [2]

$$M = g_\nu^{-1} (\Delta_\nu - \varepsilon_{\mathbf{k}})^{-1} g_\nu^{-1}, \quad \text{and} \quad b = g_\nu^{-1}, \quad (33)$$

where g_ν is the local, interacting Green function of the impurity problem:

$$g_\nu = -\langle c_\nu c_\nu^* \rangle_{\text{loc}} = -\frac{1}{\mathcal{Z}_{\text{loc}}} \int \mathcal{D}[c^*, c] c c^* \exp(-S_{\text{loc}}[c^*, c]). \quad (34)$$

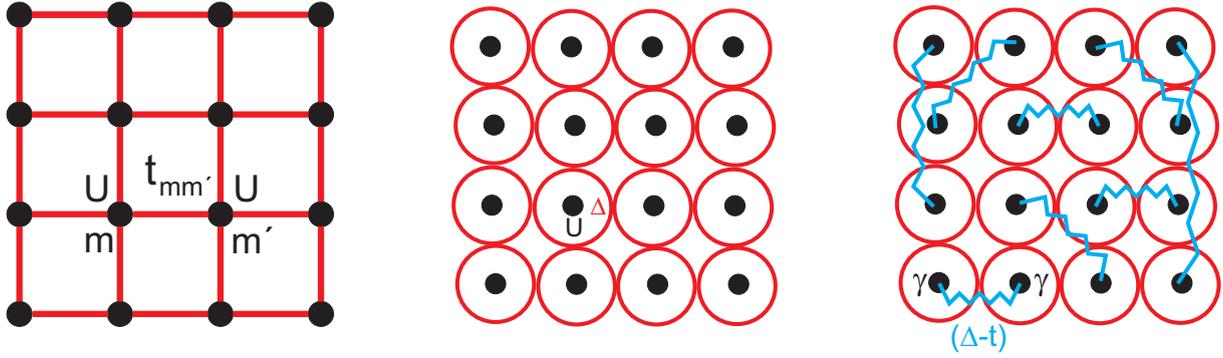


Fig. 3: From the lattice model (left) to the real-space DMFT (middle) and following up with the non-local DF perturbation (right)

With this choice, the lattice action transforms to

$$S[c^*, c, f^*, f] = \sum_i S_{\text{site}}^i + \sum_{\nu\mathbf{k}\sigma} f_{\nu\mathbf{k}\sigma}^* [g_\nu^{-1} (\Delta_\nu - \varepsilon_{\mathbf{k}})^{-1} g_\nu^{-1}] f_{\nu\mathbf{k}\sigma}. \quad (35)$$

Hence the coupling between sites is transferred to a local coupling to the auxiliary fermions

$$S_{\text{site}}^i[c_i^*, c_i, f_i^*, f_i] = S_{\text{loc}}[c_i^*, c_i] + \sum_\sigma f_{i\nu\sigma}^* g_\nu^{-1} c_{i\nu\sigma} + c_{i\nu\sigma}^* g_\nu^{-1} f_{i\nu\sigma}. \quad (36)$$

Since g_ω is local, the sum over all states labeled by \mathbf{k} could be replaced by the equivalent summation over all sites by a change of basis in the second term. The crucial point is that the coupling to the auxiliary fermions is purely local and S_{site} decomposes into a sum of local terms. The lattice fermions can therefore be integrated out from S_{site} for each site i separately. This completes the change of variables:

$$\int \mathcal{D}[c^*, c] \exp(-S_{\text{site}}[c_i^*, c_i, f_i^*, f_i]) = \mathcal{Z}_{\text{loc}} \exp\left(-\sum_{\nu\sigma} f_{i\nu\sigma}^* g_\nu^{-1} f_{i\nu\sigma} - V_i[f_i^*, f_i]\right). \quad (37)$$

The above equation may be viewed as the defining equation for the dual potential $V[f^*, f]$. The choice (33) ensures a particularly simple form of this potential. An explicit expression is found by expanding both sides of Eq. (37) and equating the resulting expressions order 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:

$$V[f^*, f] = \frac{1}{4} \sum_{\{\nu\sigma\}} \gamma_{1234} f_1^* f_2^* f_4 f_3, \quad (38)$$

where the combined index $1 \equiv \{\nu\sigma\}$ comprises frequency, spin, and orbital degrees of freedom. γ is the exact, fully antisymmetric, reducible two-particle vertex of the local quantum impurity problem. It is given by

$$\gamma_{1234} = g_1^{-1} g_2^{-1} [\chi_{1234} - \chi_{1234}^0] g_3^{-1} g_4^{-1}, \quad (39)$$

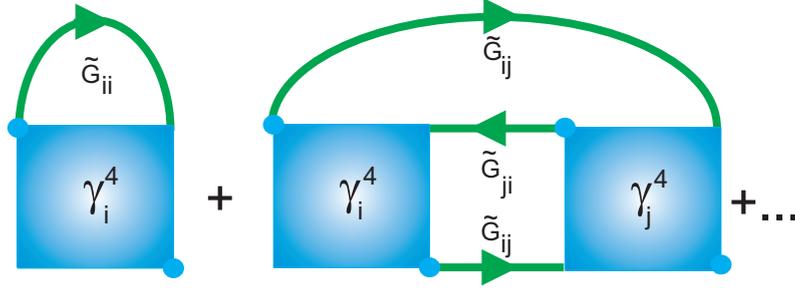


Fig. 4: Diagrams contributing to the dual self-energy $\tilde{\Sigma}$

with the two-particle Green function of the impurity being defined as

$$\chi_{1234} = \langle c_1 c_2 c_3^* c_4^* \rangle_{\text{loc}} = \frac{1}{\mathcal{Z}_{\text{loc}}} \int \mathcal{D}[c^*, c] c_1 c_2 c_3^* c_4^* \exp(-S_{\text{loc}}[c^*, c]). \quad (40)$$

The disconnected part reads

$$\chi_{1234}^0 = g_1 g_2 (\delta_{14} \delta_{23} - \delta_{13} \delta_{24}). \quad (41)$$

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

$$\tilde{S}[f^*, f] = - \sum_{\nu \mathbf{k} \sigma} f_{\nu \mathbf{k} \sigma}^* [\tilde{G}_{\omega}^0(\mathbf{k})]^{-1} f_{\nu \mathbf{k} \sigma} + \sum_i V_i [f_i^*, f_i] \quad (42)$$

and the bare dual Green function is found to be

$$\tilde{G}_{\nu}^0(\mathbf{k}) = (g_{\nu}^{-1} + \Delta_{\nu} - \varepsilon_{\mathbf{k}})^{-1} - g_{\nu}, \quad (43)$$

which involves the local Green function g_{ν} of the impurity model.

Up to now, Eqs. (42) and (43) are merely a reformulation of the original problem. In practice, approximate solutions are constructed by treating the dual problem perturbatively. Several diagrams that contribute to the dual self-energy are shown in Fig. 4. These are constructed from the impurity vertices and the dual Green functions as lines. The first diagram is purely local, while higher orders contain nonlocal contributions, e.g. the second diagram in Fig. 4. In practice, approximations to the self-energy are constructed in terms of skeleton diagrams. The lines shown in Fig. 4 are therefore understood to be fully dressed propagators. The use of skeleton diagrams is necessary to ensure the resulting theory to be conserving in the Baym-Kadanoff sense [13], i.e., to fulfill the basic conservation laws for energy, momentum, spin, and particle number. Finally, we can understand the general dual fermion scheme (Fig. 5) as a two-step process for the k -dependent self-energy. First we need to find an optimal hybridization function Δ_{ν} which defines an effective impurity model. Using the numerically exact Monte-Carlo impurity solver we can obtain the local Green function g_{ν} which, together with the hopping parameters, defines the non-local dual Green function $\tilde{G}_{\nu}^0(\mathbf{k})$ and interaction vertex $\gamma_{\nu, \nu'}^{\omega}$, which can be used in renormalized dual perturbation theory [2]. The hybridization function Δ , which so far has not been specified, allows to optimize the starting point of the perturbation theory and

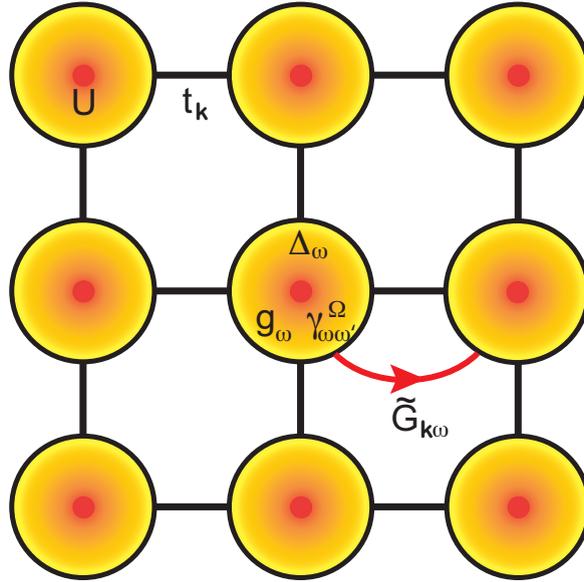


Fig. 5: General view of the dual-fermion approach: An effective impurity model is defined by the hybridization function Δ_ν . It can be exactly solved within the CT-QMC scheme, resulting in a single particle Green function g_ν and a full connected vertex $\gamma_{\nu,\nu'}^\omega$ with two fermionic (ν) and one bosonic (ω) Matsubara frequencies. Based on this local information one can perform an efficient lattice perturbation expansion for the dual Green function $\tilde{G}_\nu^0(\mathbf{k})$.

should be chosen in an optimal way. The condition of the first diagram (Fig. 4) as well as all local diagrams with higher order correlation functions in the expansion of the dual self-energy to be equal to zero at all frequencies, fixes the hybridization. This eliminates the leading order diagrammatic correction to the self-energy and establishes a connection to DMFT, which can be seen as follows: Since the γ vertex is local, this condition amounts to demanding that the local part of the dual Green function be zero

$$\sum_{\mathbf{k}} \tilde{G}_\nu(\mathbf{k}) = 0. \quad (44)$$

The simplest nontrivial approximation is obtained by taking the leading-order correction, the first diagram in Fig. 4, evaluated with the bare dual propagator (43). Using the expression for the DMFT Green function [5]

$$G_\nu^{\text{DMFT}}(\mathbf{k}) = (g_\nu^{-1} + \Delta_\nu - \varepsilon_{\mathbf{k}})^{-1}, \quad (45)$$

it immediately follows that (44) evaluated with the bare dual Green function is exactly equivalent to the DMFT self-consistency condition for Δ_ω

$$\sum_{\mathbf{k}} G_\nu^{\text{DMFT}}(\mathbf{k}) = g_\nu. \quad (46)$$

In the limit of infinitely large lattice connectivity the DMFT scheme becomes exact with the local self-energy [5]. The DMFT approximation for real lattice models appears to be one of the most successful many body schemes for realistic multi orbital systems [9]. Since it involves

the exact solution of the many-body multi-orbital impurity model Eq. (34) all local quantum fluctuations of different orbitals, spins, and charges are included in this scheme.

When diagrammatic corrections are taken into account and the first diagram is evaluated with the dressed propagator \tilde{G} , the condition (44) will in general be violated. It can be enforced by adjusting the hybridization function iteratively. This corresponds to eliminating an infinite partial series of all local diagrams starting from the first term in Fig. 4. These contributions are effectively absorbed into the impurity problem. Note that such an expansion is not one around DMFT, but rather around an optimized impurity problem.

The only difference between a DMFT and a DF calculation are the diagrammatic corrections which are included into the dual Green function. To this end, the local impurity vertex γ has to be calculated in addition to the Green function in the impurity solver step. Numerically, the self-energy is obtained in terms of skeleton diagrams by performing a self-consistent renormalization as described below. Once an approximate dual self-energy is found, the result may be transformed back to a physical result in terms of lattice fermions using exact relations.

The action (42) allows for a Feynman-type diagrammatic expansion in powers of the dual potential V . The rules are similar to those of the antisymmetrized diagrammatic technique [14]. An extension of these rules to include generic n -particle interaction vertices is straightforward. Due to the use of an antisymmetrized interaction, the diagrams acquire a combinatorial prefactor. For a tuple of n equivalent lines, the expression has to be multiplied by a factor $1/n!$. As simplest example we can write schematically the first self-energy correction of the diagram in Fig. 4 which contains a single closed loop

$$\tilde{\Sigma}_{12}^{(1)} = -T \sum_{34} \gamma_{1324} \tilde{G}_{43}^{\text{loc}}, \quad (47)$$

where $\tilde{G}^{\text{loc}} = (1/N_k) \sum_{\mathbf{k}} \tilde{G}(\mathbf{k})$ denotes the local part of the dual Green function. The second-order contribution represented in Fig. 4 contains two equivalent lines and one closed loop and hence is \mathbf{k} -dependent

$$\tilde{\Sigma}_{12}^{(2)}(\mathbf{k}) = -\frac{1}{2} \left(\frac{T}{N_k} \right)^2 \sum_{\mathbf{k}_1 \mathbf{k}_2} \sum_{345678} \gamma_{1345} \tilde{G}_{57}(\mathbf{k}_1) \tilde{G}_{83}(\mathbf{k}_2) \tilde{G}_{46}(\mathbf{k} + \mathbf{k}_2 - \mathbf{k}_1) \gamma_{6728}. \quad (48)$$

In practice, it is more efficient to evaluate the lowest order diagrams in real space and transform back to reciprocal space using the fast Fourier transform. After calculating the best possible series for the self-energy $\tilde{\Sigma}$ in the dual space one can calculate the renormalized Green function matrix for the original fermions using the following simple transformation [3]

$$G_{\nu}(\mathbf{k}) = \left[\left(g_{\nu} + g_{\nu} \tilde{\Sigma}_{\nu}(\mathbf{k}) g_{\nu} \right)^{-1} + \Delta_{\nu} - \varepsilon_{\mathbf{k}} \right]^{-1}, \quad (49)$$

which is a useful generalization of the DMFT Green function (see Eq. (45)) to include the non-local correlation effects. One can see that the dual self-energy plays the role of an effective T -matrix for the exactly solvable local problem.

5 Dual Boson approach for non-local interactions

Many important effects in the physics of correlated systems based on non-local interactions in solids are related with the consistent description of collective excitation (plasmons, magnons, orbitons etc.) which can strongly affect the original electronic degrees of freedom. Using the first-principles constrained-RPA scheme [18] one can obtain non-local interaction parameters for the correlated subspace screened by broad-bands of conducting electrons. The simplest effective Hamiltonian for such an extended Hubbard model reads

$$S = - \sum_{\mathbf{k}\nu\sigma} c_{\mathbf{k}\nu\sigma}^\dagger (i\nu + \mu - \varepsilon_{\mathbf{k}}) c_{\mathbf{k}\nu\sigma} + \frac{1}{2} \sum_{\mathbf{q}\omega} U_{\mathbf{q}} n_{\mathbf{q}\omega}^* n_{\mathbf{q}\omega}. \quad (50)$$

where the Grassmann variables $c_{\mathbf{q}\nu}^\dagger$ ($c_{\mathbf{q}\nu}$) correspond to creation (annihilation) of an electron with momentum \mathbf{k} and fermionic Matsubara frequency ν , and we skip the spin-indices for simplicity. The interaction $U_{\mathbf{q}} = U + V_{\mathbf{q}}$ consists of the on-site (Hubbard term) and non-local long-range Coulomb interactions, respectively. The screened Coulomb interaction can be a frequency dependent $U_{\mathbf{q}\omega}$ as in c-RPA, which does not produce any problems as one can see later. For simplicity we include only charge fluctuations which are given by the complex bosonic variable $n_{\mathbf{q}\omega} = \sum_{\mathbf{k}\nu\sigma} (c_{\mathbf{k}\nu}^* c_{\mathbf{k}+\mathbf{q},\nu+\omega} - \langle c_{\mathbf{k}\nu}^* c_{\mathbf{k}\nu} \rangle \delta_{\mathbf{q}\omega})$. We do not include exchange interactions in the Hamiltonian as well as local spin degrees of freedom, which can be done with some caution for vector spin boson case [19]. Moreover we will consider only a one-band model but keep the matrix form of all equations for simple generalization to cases of few orbitals (bands). The chemical potential μ defines the average number of electrons per site. Finally, $\varepsilon_{\mathbf{k}}$ is the Fourier transform of the hopping integral t_{ij} between different sites.

The dual boson scheme [3] aims to treat the action (50) in a way, similar to the dual-fermion approach. In addition to the dual fermionic degrees of freedom, the bosonic fields are treated in a similar manner. This allows for the consideration of strongly correlated systems beyond the Hubbard model. Also, it can be employed for an explicit treatment of the collective excitations in the Hubbard model. Here we present the basic idea of this approach (Fig. 6).

First we split the lattice action (50) into a sum of effective single-site local impurity reference actions $S_{\text{ref}}^{(i)}$ defined by hybridization function Δ_ν with screened local interaction \mathcal{U}_ω and a non-local remaining part \tilde{S}

$$S = \sum_i S_{\text{ref}}^{(i)} + \Delta S, \quad (51)$$

which are given by the following explicit relations

$$\begin{aligned} S_{\text{ref}} &= - \sum_{\nu\sigma} c_{\nu\sigma}^\dagger (i\nu + \mu - \Delta_\nu) c_{\nu\sigma} + \frac{1}{2} \sum_{\omega} \mathcal{U}_\omega \rho_\omega^* \rho_\omega, \\ \Delta S &= \sum_{\nu\mathbf{k}\sigma} c_{\nu\mathbf{k}\sigma}^\dagger (\varepsilon_{\mathbf{k}} - \Delta_\nu) c_{\nu\mathbf{k}\sigma} + \frac{1}{2} \sum_{\mathbf{q}\omega} (U_{\mathbf{q}} - \mathcal{U}_\omega) \rho_{\mathbf{q}\omega}^* \rho_{\mathbf{q}\omega}. \end{aligned} \quad (52)$$

The local bare interaction of the impurity model is then equal to $\mathcal{U}_\omega = U_\omega + \Lambda_\omega$ and it is easy to see that $U_{\mathbf{q}} - \mathcal{U}_\omega = V_{\mathbf{q}} - \Lambda_\omega$ which makes the method independent of the U - V separation. The

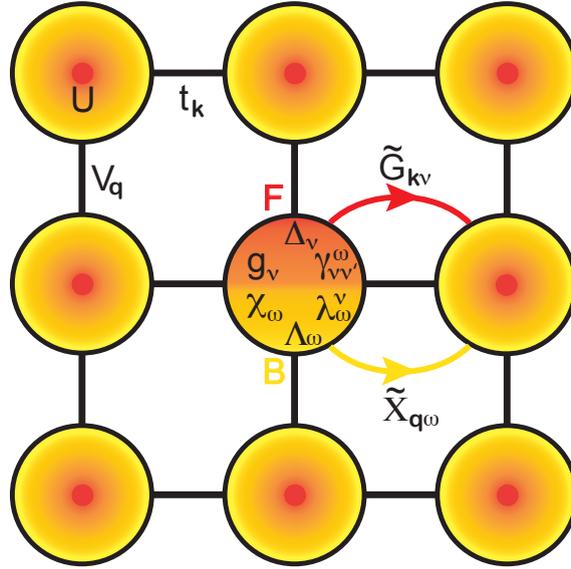


Fig. 6: General view on dual-fermion approach: effective impurity model defined by fermionic hybridization function Δ_ν and bosonic screened interactions Λ_ω . It can be exactly solved within CT-QMC scheme, resulting in electronic local Green function g_ν and bosonic local susceptibility χ_ω as well as full connected vertex $\gamma_{\nu\nu'}^\omega$ and electron-boson vertex λ_ω^ν . Based on this local information one can performed an efficient lattice perturbation expansion for the dual Green function $\tilde{G}_{\mathbf{k}\nu}$ and dual boson propagator $\tilde{W}_{\mathbf{q}\omega}$.

impurity problem with frequency dependent interactions (as well as spin-dependent exchange) can be solved using, e.g., continuous-time quantum Monte Carlo solvers [1], and one can obtain the local impurity Green function g_ν , susceptibility χ_ω , and renormalized interaction \mathcal{W}_ω as

$$\begin{aligned} g_\nu &= -\langle c_\nu c_\nu^* \rangle_{\text{imp}}, \\ \chi_\omega &= -\langle \rho_\omega \rho_\omega^* \rangle_{\text{imp}}, \\ \mathcal{W}_\omega &= \mathcal{U}_\omega + \mathcal{U}_\omega \chi_\omega \mathcal{U}_\omega, \end{aligned} \quad (53)$$

where the average is taken with respect to the impurity action (52). The strategy here is similar to the dual fermion scheme and consists of an efficient perturbation scheme for ΔS in the action formalism. In addition to the fermionic Hubbard-Stratonovich transformation Eq. (32) on the first term $(\varepsilon_{\mathbf{k}} - \Delta_\nu) c_{\nu\mathbf{k}\sigma}^\dagger c_{\nu\mathbf{k}\sigma}$, which give the dual fermion variables $f_{\nu\mathbf{k}\sigma}^\dagger, f_{\nu\mathbf{k}\sigma}$, we perform a bosonic transformation

$$\sqrt{\det[\Lambda_\omega - V_{\mathbf{q}}]} e^{\frac{1}{2} \sum_{\mathbf{q}\omega} \rho_{\mathbf{q}\omega}^* [\Lambda_\omega - V_{\mathbf{q}}] \rho_{\mathbf{q}\omega}} = \int D[\phi] e^{-\frac{1}{2} \sum_{\mathbf{q}\omega} \{ \phi_{\mathbf{q}\omega}^* [\Lambda_\omega - V_{\mathbf{q}}]^{-1} \phi_{\mathbf{q}\omega} + \rho_\omega^* \phi_\omega + \phi_\omega^* \rho_\omega \}}, \quad (54)$$

and we use that $\mathcal{U}_\omega - U_{\mathbf{q}} = \Lambda_\omega - V_{\mathbf{q}}$. Note that caution should be taken for convergence problem of the integral over the new dual variable $\tilde{\phi}$ which does not affect the final equations [3]. Rescaling the bosonic fields $\phi_{\mathbf{q}\omega}$ as $\phi_{\mathbf{q}\omega} \alpha_\omega^{-1}$ and integrating out the original degrees of freedom c^\dagger and c we arrive at the dual action

$$\tilde{S} = - \sum_{\mathbf{k}\nu} f_{\mathbf{k}\nu}^* \tilde{G}_0^{-1} f_{\mathbf{k}\nu} - \frac{1}{2} \sum_{\mathbf{q}\omega} \phi_{\mathbf{q}\omega}^* \tilde{W}_0^{-1} \phi_{\mathbf{q}\omega} + \tilde{V} \quad (55)$$

with the bare dual fermion-boson propagators

$$\tilde{G}_0 = (G_{\text{ref},\nu}^{-1} + \Delta_\nu - \varepsilon_{\mathbf{k}})^{-1} - g_\nu = G_{\text{E}} - g_\nu, \quad (56)$$

$$\tilde{W}_0 = \alpha_\omega^{-1} ([U_{\mathbf{q}} - \mathcal{U}_\omega)^{-1} - \chi_\omega]^{-1} \alpha_\omega^{-1} = W_{\text{E}} - \mathcal{W}_\omega, \quad (57)$$

and the dual interaction term \tilde{V} . The explicit form of the dual interaction can be obtained by expanding the c^\dagger and c dependent part of partition function in an infinite series and integrating out these degrees of freedom. The two first terms in \tilde{V} are given by

$$\tilde{V} = \frac{1}{4} \sum_{\nu\nu'\omega} \gamma_{\nu\nu'\omega} f_\nu^* f_{\nu'}^* f_{\nu+\omega} f_{\nu'-\omega} + \sum_{\nu\omega} (\lambda_{\nu\omega} f_\nu^* f_{\nu+\omega} \phi_\omega^* + h.c.). \quad (58)$$

We define the three-point electron-boson vertex $\lambda_{\nu\omega}$ in the following way

$$\lambda_{\nu\omega} = g_\nu^{-1} g_{\nu+\omega}^{-1} \alpha_\omega^{-1} \langle c_\nu c_{\nu+\omega}^* \rho_\omega \rangle_{\text{loc}}, \quad (59)$$

where $\alpha_\omega = \mathcal{W}_\omega / \mathcal{U}_\omega = (1 + \mathcal{U}_\omega \chi_\omega)$ is the local renormalization factor. The four-point vertex function $\gamma_{\nu\nu'\omega}$ can be determined similarly to the dual fermion section. Then, the dual Green function $\tilde{G}_{\mathbf{k}\nu} = -\langle f_{\mathbf{k}\nu} f_{\mathbf{k}\nu}^* \rangle$ and renormalized dual interaction $\tilde{W}_{\mathbf{q}\omega} = -\langle \phi_{\mathbf{q}\omega} \phi_{\mathbf{q}\omega}^* \rangle$, as well as dual self-energy $\tilde{\Sigma}_{\mathbf{k}\nu}$ and polarization operator $\tilde{\Pi}_{\mathbf{q}\omega}$, can be obtained diagrammatically [20]. These dual Green function have the following relation

$$\tilde{G}_{\mathbf{k}\nu}^{-1} = \tilde{G}_0^{-1} - \tilde{\Sigma}_{\mathbf{k}\nu}, \quad (60)$$

$$\tilde{W}_{\mathbf{q}\omega}^{-1} = \tilde{W}_0^{-1} - \tilde{\Pi}_{\mathbf{q}\omega}. \quad (61)$$

Finally, the Green function $G_{\mathbf{k}\nu}$ and renormalized interaction $W_{\mathbf{q}\omega}$ of the original model can be exactly expressed in terms of dual quantities as

$$G_{\mathbf{k}\nu}^{-1} = G_{\text{E}}^{-1} - \Sigma'_{\mathbf{k}\nu}, \quad (62)$$

$$W_{\mathbf{q}\omega}^{-1} = W_{\text{E}}^{-1} - \Pi'_{\mathbf{q}\omega}, \quad (63)$$

where the non-local self-energy and polarization operator introduced beyond EDMFT are

$$\Sigma'_{\mathbf{k}\nu} = \frac{\tilde{\Sigma}_{\mathbf{k}\nu}}{1 + g_\nu \tilde{\Sigma}_{\mathbf{k}\nu}}, \quad (64)$$

$$\Pi'_{\mathbf{q}\omega} = \frac{\tilde{\Pi}_{\mathbf{q}\omega}}{1 + \mathcal{W}_\omega \tilde{\Pi}_{\mathbf{q}\omega}}. \quad (65)$$

The dual-boson self-consistency conditions reads [3]

$$\sum_{\mathbf{k}} G_{\mathbf{k}\nu} = g_\nu, \quad (66)$$

$$\sum_{\mathbf{q}} W_{\mathbf{q}\omega} = \mathcal{W}_\omega. \quad (67)$$

The DB relations up to this point are exact and derived without any approximations. It is

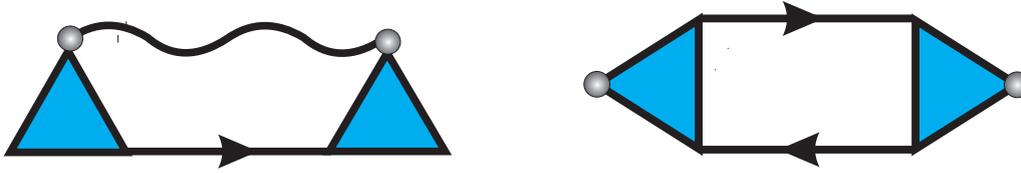


Fig. 7: Second order approximation for dual-boson scheme with triangular electron-boson vertex ($\lambda_{\nu\omega}$), dual-boson wavy line ($\tilde{W}_{\mathbf{q}\omega}$) and dual-fermion directed line ($\tilde{G}_{\mathbf{k}\nu}$): (Left) Electron self-energy ($\tilde{\Sigma}_{\mathbf{k}\nu}$), (Right) Boson self-energy ($\tilde{\Pi}_{\mathbf{q}\omega}$).

worth mentioning, that the non-interacting dual theory ($\tilde{V} = 0$) is equivalent to EDMFT. However, even in the weakly-interacting limit of the original model, $U \rightarrow 0$, the fermion-boson vertex $\lambda_{\nu\omega}$ is non-zero. Thus, the Dual Boson formalism explicitly shows, that corrections to EDMFT are not negligible. Therefore, the dynamical mean-field level is insufficient for describing non-local bosonic excitations, because the interactions between the non-local fermionic and bosonic degrees of freedom are always relevant. The simplest approximation for $\tilde{\Sigma}_{\mathbf{k}\nu}$ and $\tilde{\Pi}_{\mathbf{q}\omega}$ related with second order perturbation theory are presented in (Fig. 7). In principle one can use so-called bold diagrammatic Monte Carlo method to perform the summation of the most important contributions to the dual fermion and boson self-energy, similar to first attempts for dual-fermion action [21].

6 Numerical results

We present now two examples of recent calculations using dual-fermion and dual-boson methods. First, we are able to conduct a realistic dual-fermion study of the interaction of electrons and paramagnons in the strongly correlated sodium cobaltate Na_xCoO_2 close to the in-plane ferromagnetic order at $x = 0.7$ [22]. Sodium cobaltate consists of triangular CoO_2 planes, subject to strong electronic correlations, that are held together by Na ions in between. Using a tailored one-band description of the low-energy cobaltate physics, we derived a realistic DFT-based dispersion, applied a proper Hubbard $U = 5 \text{ eV}$ and solved for the local and nonlocal correlations by the dual-fermion framework (see [22] for details). And indeed, for $x = 0.7$ an additional anti-bound state is detected close to Γ , split off from the renormalized quasiparticle dispersion (Fig. 8a). In terms of physics, it corresponds to the interaction of renormalized electrons with strong ferromagnetic fluctuations. The resulting emerging excitation is a so-called spin polaron [22]. Hence besides refinements of the DMFT-determined electronic spectrum, the inclusion of nonlocal correlations may be important to reveal more complex excitations with possible relevance for future materials science.

The density of states at $x = 0.67$ (Fig. 8b), shows a striking difference between DMFT and DF results. In DMFT, the quasiparticle peak is considerably larger and the QP weight Z is significantly enhanced compared to the case of low doping. This is expected, since $Z \approx 1$ should only hold far away from half-filling towards the opposite (band-insulating) endpoint $x = 1$. We further see that the upper Hubbard band has completely dissolved in the DMFT

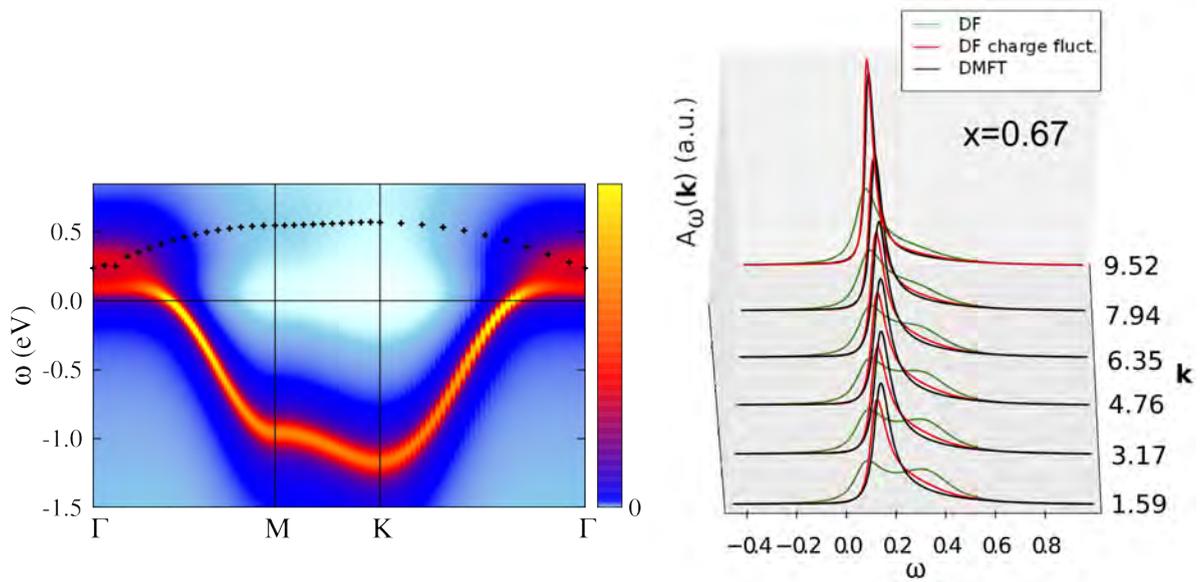


Fig. 8: The Na_xCoO_2 system close to $x = 0.7$ for electron-paramagnon interactions. (Left) Effective one-band dispersion as obtained by the dual-fermion method. (Right) Spectral function in the DMFT and DB scheme. Crosses mark a model spin-polaron dispersion (from [22]).

perspective. In DF, on the contrary, the QP peak close to Γ is strongly renormalized. The spectral function additionally exhibits a broad sideband excitation at $\omega \sim 0.3 - 0.4$ eV. By restricting the DF calculation to the charge channel only, this sideband excitation disappears. This is a strong indication that this excitation is of *magnetic* origin.

Despite the successes of GW +EDMFT [23,24], the method does not provide a completely valid description of plasmons. This is due to an inconsistent treatment of the single and two-particle

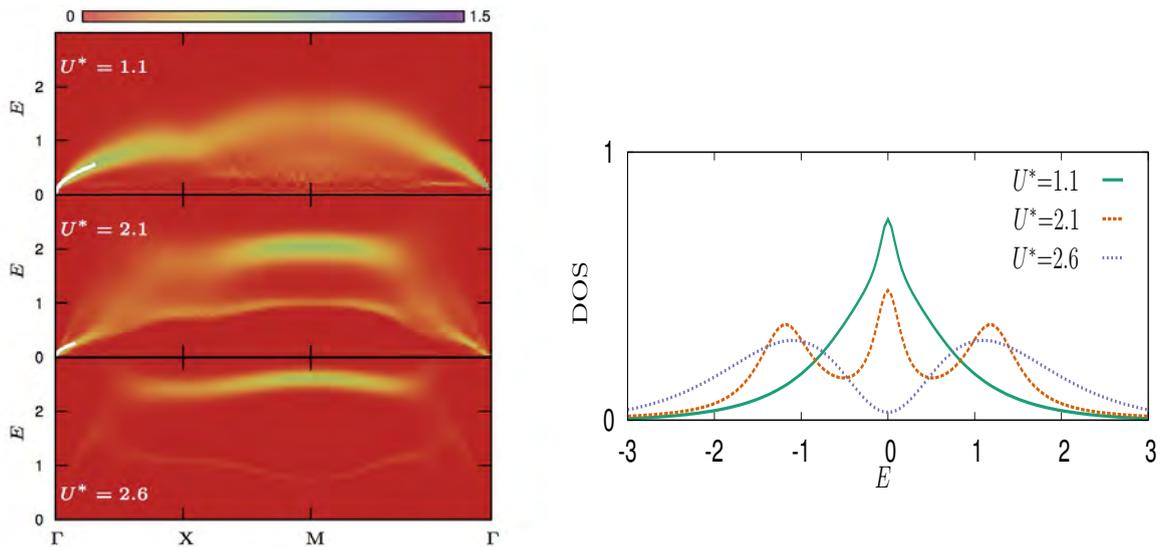


Fig. 9: Inverse dielectric function (Left) and density of states (Right) of the extended 2d Hubbard model with long-range Coulomb interaction as a function of momentum and energy, for three different values of the effective on-site interaction U^* (from [25]).

properties, which breaks local charge conservation and gauge invariance. The problem generally occurs when working with renormalized Green functions [13], but does not include the vertex corrections. In the case of the local, frequency-dependent self-energy of EDMFT, vertex corrections from a local but frequency dependent irreducible vertex are necessary to fulfill the Ward identity. In the dual boson approach, they can be included via non-local polarization corrections, which are constructed diagrammatically. The resulting polarization vanishes in the long wavelength limit at finite frequencies, as required by local charge conservation [3, 20]. It therefore becomes possible to study the effect of strong correlations on the plasmon spectra. We showed that the two-particle excitations exhibit both renormalization of the dispersion and spectral weight transfer [25]. Fig. 9 shows the inverse dielectric function $-\text{Im} \epsilon_{\mathbf{q}}^{-1}(\omega)$ of 2d surface plasmons in the presence of a long-range interaction $U(q) = U + V_{\mathbf{q}}$. For weak interactions one observes a broad particle-hole continuum and the expected \sqrt{q} dependence of the 2d plasmon dispersion at small q . As the interaction increases, the plasmon dispersion $\omega_p^2(q) \approx \alpha V_0 q$ is renormalized (α is decreased). Two branches are clearly visible in the spectrum. The lower branch can be associated with particle-hole excitations between a Hubbard band and the quasiparticle peak, while the upper branch stems from excitations between the Hubbard bands. Spectral weight is transferred from the lower to the upper branch as the interaction increases. Above a critical effective onsite interaction of $U^* \sim 2.4$ the system is a Mott insulator. In this state a two-particle excitation corresponds to the creation of a doublon and a holon. Such an excitation is highly localized, leading to a weakly dispersing band at energy U^* .

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