Cluster Dual Fermion Approach to Nonlocal Correlations

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We formulate a general cluster Dual Fermion Approach to nonlocal correlations in crystals. The scheme allows the treatment of long-range correlations beyond cluster DMFT and nonlocal effects in realistic calculations of multiorbital systems. We show that the the simplest approximation exactly corresponds to free cluster DMFT. We further consider the relation between the two-particle Green functions in real and dual variables. We apply this approach by calculating the Green function of the Hubbard model in one dimension starting from the two-site cluster DMFT solution. The result agrees well with the Green function obtained from a DMRG calculation.

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I. INTRODUCTION

One of the successful routes to the description of strongly correlated systems is related to the Dynamical Mean Field Theory (DMFT). In this scheme the system is mapped onto an effective local quantum impurity problem in a self-consistently determined bath. The self-energy in the DMFT approach is local in space but frequency dependent. However, there are many phenomena for which non-local correlations are important and often correlations are long-ranged. Among these are Luttinger-Liquid formation in low-dimensional systems, non-Fermi-Liquid behavior due to van-Hove singularities in two dimensions or d-wave pairing in high-$T_c$ superconductors. Obviously, DMFT is not suitable for the description of such systems and there are cases in which DMFT even fails qualitatively, as is for example the case for the one-dimensional Hubbard model. For the description of these non-local correlations it is desirable to combine short-range cluster many-body physics, like formation of singlets, and long-range correlations. Recently the novel Dual Fermion approach for the treatment of nonlocal correlations has been developed. Here we formulate a general cluster (or multi-orbital) scheme for non-local correlations.

Frequently used approaches to account for non-local correlations beyond DMFT comprise the cluster approaches or the so-called Dynamical Cluster approximation (DCA) in k-space, real space periodicity and free cluster approaches, as well as the Cellular DMFT (CDMFT). In the latter approach, the single-site impurity of the DMFT is replaced by a cluster of impurities. The CDMFT scheme however is restricted to relatively small cluster sizes due to computational feasibility and only short-range correlations can be treated within this approach.

Recently, steps have been taken to go beyond DMFT and to treat long-range correlations. One of them is the Dynamical Vertex Approximation and similar approaches, where a diagrammatic expansion around DMFT is made. A principally new scheme with a fully renormalized expansion called Dual Fermion Approach has been proposed, which is based on the introduction of new variables in the path integral representation. Similar schemes for the strong coupling expansion have been discussed in terms of Hubbard operators.

Here we present a cluster generalization of the Dual Fermion approach. This allows the treatment of clusters or multiorbital atoms within the Dual Fermion framework and can describe long-range correlations in realistic systems. The paper is organized as follows: first, we present the formalism and then show that for the case of non-interacting dual fermions one exactly obtains the self-consistency equation of the CDMFT. In the next section we consider the relationship between the two-particle Green functions in real and dual variables. Then we describe the calculation procedure. We finally apply our approach to the Hubbard model in one dimension starting from a two-site CDMFT solution.

II. FORMALISM

Our goal is to find an (approximate) solution to the cluster lattice problem described by the imaginary time action which in cluster or multiband notation reads

$$S[c^*, c] = \sum_{\omega k\sigma m\sigma'} e^{\omega k\sigma m} \left( (i\omega + \mu) 1 - H_\sigma(k) \right)_{mm'} c^*_{\omega k\sigma m} c_{\omega k\sigma' m'} + \sum_{i} H_{\text{int}}[c_i^*, c_i] .$$

Here $H_\sigma(k)$ is the one-electron part of the Hamiltonian, $\omega = (2n + 1)\pi/\beta, n = 0, \pm 1, ...$ are the Matsubara frequencies, $\beta$ and $\mu$ are the inverse temperature and chemical potential, respectively, $\sigma = \uparrow, \downarrow$ labels the spin projection and $c^*, c$ are Grassmannian variables. The indices $i$ label the translations of the super-cell and the $k$-vectors span the reciprocal lattice in the reduced super-cell Brillouin zone. Here we take into account a general type of interaction, $H_{\text{int}}$. It is important to note that it can be any type of interaction inside the multiorbital atom or
We introduce spinors \( c_i^\sigma \) via these quantities.

\[
S_\text{imp}[c^\ast, c] = \sum_{\omega\sigma} c^\ast_{\omega\sigma m}(i\omega + \mu)1 - \Delta_{\omega\sigma} c_{\omega\sigma m} + H_{\text{int}}[c^\ast, c],
\]

where \( \Delta \) is an as yet unspecified hybridization function describing the interaction of the impurity with an electronic bath. We suppose that all properties of the impurity problem are in principle known, i.e. the single-particle Green function \( g_{\omega\sigma} \) and the irreducible vertices \( \gamma^{(4)}, \gamma^{(6)}, \) etc. are known. Our goal is to express the Green function \( G_{\omega k} \) and vertices \( \gamma \) of the original lattice problem via these quantities.

Since \( \Delta \) is local, one may formally rewrite the original lattice problem in the following form:

\[
S[c^\ast, c] = \sum_i S_\text{imp}[c^\ast_{i\sigma i\sigma}, c_{i\omega i\omega}] - \sum_{\omega \kappa \kappa m'} c^\ast_{\omega \kappa \kappa m'}(\Delta_{\omega\sigma} - H_\sigma(\kappa))_{m'm}, c_{\omega \kappa \kappa m'}.
\]

We introduce spinors \( c_{\omega \kappa \kappa} = (\ldots, c_{\omega \kappa \kappa m}, \ldots) \), \( c^\ast_{\omega \kappa \kappa} = (\ldots, c^\ast_{\omega \kappa \kappa m}, \ldots) \). Omitting indices, in matrix-vector notation, the Gaussian identity that facilitates the transformation to the dual variables is

\[
\int \exp\left( -\mathbf{f}^\ast \hat{A} \mathbf{f} - \mathbf{f}^\ast \hat{B} \mathbf{c} - \mathbf{c}^\ast \hat{B}^\ast \mathbf{f} \right) \mathcal{D}[\mathbf{f}, \mathbf{f}^\ast] = \det(\hat{A}) \exp\left( \mathbf{c}^\ast \hat{B} \hat{A}^{-1} \hat{B} \mathbf{c} \right),
\]

which is valid for arbitrary complex matrices \( \hat{A} \) and \( \hat{B} \).

In order to decouple the non-local term in Eqn. 4, we introduce a cluster impurity problem just in the spirit of CDMFT in the form

\[
S_\text{imp}[c^\ast, c] = \sum_{i} S_\text{imp}[c^\ast_{i\sigma i\sigma}, c_{i\omega i\omega}] + \sum_{\omega \kappa \kappa m'} \left[ c^\ast_{\omega \kappa \kappa m'}(\Delta_{\omega\sigma} - H_\sigma(\kappa))_{m'm}, c_{\omega \kappa \kappa m'} \right],
\]

where

\[
\sum_i S_{\text{site}, i} = \sum_i S_\text{imp}[c^\ast_{i\sigma i\sigma}, c_{i\omega i\omega}] + \sum_{\omega \kappa \kappa m'} f_{\omega \kappa \kappa}^\ast g_{\omega \sigma}^{-1} f_{\omega \sigma} g_{\omega \sigma}^{-1} f_{\omega \sigma} \mathcal{D}[c, f^\ast].
\]

Here the summation in the last term over states labeled by \( k \) has been replaced by the equivalent summation over all sites. The Gaussian identity can further be used to establish an exact relation between the lattice Green function and the dual Green function. To this end, the partition function of the lattice is written in the two equivalent forms

\[
Z = \int \exp(-S[c^\ast, c]) \mathcal{D}[c, c^\ast] = Z_f \int \int \exp(-S[c^\ast, c, f^\ast, f]) \mathcal{D}[f, f^\ast] \mathcal{D}[c, c^\ast],
\]

where

\[
Z_f = \prod_{\omega k\sigma} \det \left( g_{\omega \sigma} (\Delta_{\omega\sigma} - H_\sigma(\kappa)) \right).
\]

By taking the functional derivative of the partition function, Eqn. 9 with respect to the Hamiltonian, i.e.

\[
G_{\omega k\sigma} = \frac{1}{Z} \frac{\delta Z}{\delta H_{\sigma}(k)_{m'm}},
\]

one can obtain the following exact relationship between the dual and lattice Green functions:

\[
G_{\omega k\sigma} = (g_{\omega \sigma} (\Delta_{\omega\sigma} - H_\sigma(\kappa)))^{-1} G^d_{\omega k\sigma} \times ((\Delta_{\omega\sigma} - H_\sigma(\kappa)) g_{\omega \sigma})^{-1} + (\Delta_{\omega\sigma} - H_\sigma(\kappa))^{-1},
\]

where the lattice Green function is defined via the imaginary time path integral as

\[
G_{12} = -\frac{1}{Z} \int c_1 c^\ast_2 \exp(-S[c^\ast, c]) \mathcal{D}[c, c^\ast]
\]

and similarly for the local Green function \( g \) and dual Green function \( G^d \) with \( Z \) and \( S \) replaced by the corresponding expressions.

We now wish to derive an action depending on the dual variables only. This can be achieved by integrating out the original variables \( c, c^\ast \). The crucial point is that this can be done for each site separately:

\[
\int \exp \left( -S_{\text{site}}[c^\ast_{i\sigma i\sigma}, c_{i\omega i\omega}, f^\ast_{i\sigma i\sigma}, f_{i\omega i\omega}] \right) \mathcal{D}[c_{i\omega i\omega}, f_{i\omega i\omega}] = Z_\text{imp} e^{-\left( \sum_{\sigma} \int \left( \omega_{\omega\sigma} f^\ast_{\omega \sigma} g_{\omega \sigma}^{-1} f_{\omega \sigma} + V_{i\sigma i\sigma} f^\ast_{i\sigma i\sigma} f_{i\omega i\omega} \right) \right)}. \]

This equation can be seen as the defining equation for the dual potential \( V[f^\ast, f] \). Since \( S_{\text{site}} \) contains the impurity action, expanding the remaining part of the exponential and integrating out the original variables corresponds to averaging over the impurity degrees of freedom. Equating
FIG. 1: The first two lowest order diagrams for the dual self energy $\Sigma^d$. 

The resulting expressions by order, one finds that the dual potential in lowest order approximation is given by

$$ V[f^*, f] = \frac{1}{4} \sum_i \chi^{(4)}_{1234} f_i^* c_{i2} c_{i4} f_{i3} + \ldots $$

(15)

where

$$ \chi^{(4)}_{1234} = g_{12}^i g_{23}^i \left( \chi^{(0)}_{12} - \chi^{(0)}_{34} \right) g_{34}^i g_{45}^i, \quad \chi^{(0)}_{1234} = g_{14} g_{23} - g_{13} g_{24} $$

(16)

is the fully antisymmetric irreducible vertex and the local two-particle Green function of the impurity model is defined as

$$ \chi^{imp}_{1234} = \frac{1}{Z^{imp}} \int c_{123} c_{4}^* c_{4}^* \exp(-S_{imp}[c^*, c]) D[c, c^*]. $$

(17)

The dual action now depends on dual variables only and can be written as

$$ S_d[f^*, f] = -\sum_{\omega_k \sigma} f_{\omega_k \sigma} \left( c_{\omega_k \sigma}^{(d)} \right)^{-1} f_{\omega_k \sigma} + \sum_i V[f_i, f_i]. $$

(18)

The bare dual Green function is given by

$$ G_{\omega k \sigma}^{d} = -g_{\omega \sigma} \left[ \left( \Delta_{\omega \sigma} - H_{\sigma}(k) \right)^{-1} + g_{\omega \sigma} \right]^{-1} g_{\omega \sigma}. $$

(19)

For the nonlocal part of the self energy defined by $\Sigma_{nonloc} = \Sigma - \Sigma_{loc}$ we find a simple matrix relation to the dual self-energy:

$$ \Sigma_{nonloc}^{-1} = \Sigma_{d}^{-1} + g. $$

(20)

The local part of the self energy is obtained by the solution of the impurity problem. In order to obtain the nonlocal contribution, we thus need to calculate the dual self-energy. This is achieved by performing a regular diagrammatic series expansion of the dual action, Eqn. 18 and considering the lowest order diagrams for $\Sigma_d$, constructed from the irreducible vertices and the dual Green function as lines. The diagrams considered here are shown in Fig. 1. The lowest order diagram is local while the next diagram gives a nonlocal contribution to the self energy.

So far we have not established a condition for $\Delta$. We require that the first diagram in the expansion of the dual self-energy should be equal to zero at all frequencies. Since $\chi^{(4)}$ is local, we can use the following condition:

$$ \sum_k G_k^{d} = 0. $$

(21)

In the simplest approximation, which corresponds to non-interacting dual fermions, the full dual Green function is replaced by the corresponding bare Green function and the above condition can be reduced to

$$ \sum_k \left[ \left( \Delta_{\omega \sigma} - H_{\sigma}(k) \right)^{-1} + g_{\omega \sigma} \right]^{-1} = 0 $$

(22)

which is equivalent to the self-consistency condition for the hybridization function in free-cluster CDMFT. The self-consistency condition for $\Delta$ which satisfies this condition is

$$ \Delta_{new} = \Delta_{old} + g^{-1} G_{loc}^{d} G_{loc}^{-1}. $$

(23)

If we restrict the matrix $\Delta_{\omega \sigma}$ to be equivalent for all cluster sites with periodic boundary conditions then this approximation leads to the DCA scheme.

III. TWO-PARTICLE EXCITATIONS

In order to find the exact relation between the four-point correlation function in dual and conventional variables we have to calculate the second derivative of $Z$ with respect to $H_{\sigma}(k) \mu \lambda, H_{\sigma}(k) \nu \rho$, using the two equivalent representations of the partition function, Eqn. 9. Differentiating the partition function in its original form gives us

$$ \frac{1}{Z} \frac{\delta^2 Z}{\delta H_{\mu \lambda} \delta H_{\nu \rho}} = \langle T c_{\lambda} \gamma_{\mu} c_{\nu} c_{\rho} \rangle \equiv \chi_{\lambda \mu \nu \rho}, $$

(24)

while differentiating the second expression for $Z$ using the above relation for Green’s function, Eqn. 12 yields for $\chi_{\lambda \mu \nu \rho}$ after some straightforward algebra:

$$ \frac{1}{Z} \frac{\delta^2 Z}{\delta H_{\mu \lambda} \delta H_{\nu \rho}} = \langle (\Delta - H)^{-1} \otimes (\Delta - H)^{-1} \rangle_{\lambda \mu \nu \rho} + \langle (\Delta - H)^{-1} \otimes (\Delta - H)^{-1} \rangle_{\lambda \mu \nu \rho} + \langle (\Delta - H)^{-1} \otimes (\Delta - H)^{-1} \rangle_{\lambda \mu \nu \rho} \times \langle g^{-1} \otimes g^{-1} \rangle_{\nu \gamma \lambda \mu \nu \rho} \times \langle g^{-1} \otimes g^{-1} \rangle_{\mu \nu \gamma \lambda \mu \nu \rho} \times \langle g^{-1} \otimes g^{-1} \rangle_{\nu \gamma \lambda \mu \nu \rho} \times \langle g^{-1} \otimes g^{-1} \rangle_{\mu \nu \gamma \lambda \mu \nu \rho}. $$

(25)

Here $\chi_{\lambda \mu \nu \rho} \equiv \langle T f_{\mu} f_{\nu} f_{\lambda} f_{\rho} \rangle$ is the dual four-point correlation function and

$$ (A \otimes B)_{\lambda \mu \nu \rho} \equiv A_{\lambda \mu} B_{\nu \rho} - A_{\lambda \rho} B_{\mu \nu} $$

is the antisymmetrized direct product of two matrices.

As one can see from (25), the two-particle excitations for dual fermions coincide with those for real fermions. Thus to get the information about the instabilities in the system under consideration it is sufficient to sum up the ladder for the two-particle dual fermion Green function in the ladder approximation:

$$ \chi_{\lambda \mu \nu \rho} = \chi_{\lambda \mu \nu \rho}^{(0)} + \chi_{\lambda \mu \nu \rho}^{(0)} \gamma_{\mu \lambda \nu} \chi_{\lambda \mu \nu \rho}^{(0)}. $$

(26)
FIG. 2: Calculation procedure

\[ \Delta_{\text{new}} = \Delta_{\text{old}} + g^{-1} G_{\text{loc}}^d G_{\text{loc}}^{-1} \]

or

\[ \chi_{d\text{m}\nu\text{r}\lambda} = \chi_{d\text{m}\nu\text{r}\lambda}^{0} + \chi_{d\text{m}\nu\text{r}\lambda}^{\delta \nu} \chi_{d\text{m}\nu\text{r}\lambda}^{\delta \nu} \]  \tag{27} \]

where the first equation is written for the particle-particle channel and the second for the particle-hole one, and \( \chi_{d\text{m}\nu\text{r}\lambda}^{0} = G_{d\text{m}} \otimes G_{d\text{r}} \) is the bare two-particle dual Green function.

IV. CALCULATION PROCEDURE

The calculation procedure is as follows: Starting from a starting guess for \( \Delta \), e.g. \( \Delta = 0 \), we solve the impurity problem and obtain a new local Green function \( g \). From this we calculate the bare dual \( k \)-dependent Green function via Eqn. 19. In order to reach the self-consistent free-cluster DMFT solution we calculate the local part of the lattice Green function via Eqn. 12 and insert it into Eqn. 23 to obtain a new \( \Delta \) with which we again solve the impurity problem. This loop, which is closed by the dashed arrow in Fig. 2 is repeated until the self-consistent CDMFT solution is reached. With the thus obtained \( \Delta \) we then calculate the irreducible vertex \( \gamma^{(4)} \). Now we do not follow the path indicated by the dashed line but calculate an approximation to the dual self-energy by summing up the first diagram(s) in the perturbation series expansion. From this and the bare dual Green function an approximation for the dual Green function \( G_{d\text{m}\nu\text{r}\lambda} \) is obtained which is subsequently used in the diagrams. This inner loop is executed until self-consistency. The outer loop is also executed until self-consistency. Self-consistency for both loops is usually reached after a few iterations (depending on the system). The computational cost for the calculations aside from DMFT is less than for the DMFT itself, whereby the computation of the vertex is the computationally most expensive part. We use the continuous-time quantum Monte Carlo impurity solver\(^{12} \) for the solution of the impurity problem and for the calculation of the irreducible vertex.

V. APPLICATION TO 1D HUBBARD MODEL

We consider the one-dimensional Hubbard model described by the following Hamiltonian:

\[ H_0 + H_{\text{int}} = t \sum_i c_{i+1}^\dagger c_i + U \sum_i n_{i\uparrow} n_{i\downarrow}. \]  \tag{28} \]

FIG. 3: Schematic representation of the 1D chain as a chain of two-site clusters.

For the half-filled case the main physics is related with the formation of a local singlet pair. Therefore we start from a two-site cluster DMFT solution and then include the long-ranged non-local effects via the Cluster Dual Fermion approach. When this one-dimensional system is treated as a chain of two-site clusters as depicted in Fig. 3 the tight-binding Hamiltonian for this model is readily shown to be

\[ H_0(k) = \begin{pmatrix} 0 & t(1 + e^{-ika}) \\ t(1 + e^{ika}) & 0 \end{pmatrix}. \]

\[ \tag{29} \]

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Due to the absence of a Mott transition in one dimension, the system is an insulator for any finite value of the on-site repulsion \( U \). It is known that single-site DMFT gives a qualitatively wrong answer, i.e. predicts the system to be metallic even for \( U/t = 6 \). Here we compare our results with the one obtained by a Density Matrix Renormalization Group (DMRG) calculation\(^{13} \), since DMRG is known to reproduce the spectral properties of 1D systems quite well. The free cluster DMFT solution obtained in our calculation is qualitatively correct and reproduces the DMRG solution quite well, since short range fluctuations between nearest neighbours are predominant. For our calculations we use the parameters \( U/t = 6 \) and \( \beta = 20 \). The DMRG solution corresponds to \( T = 0 \). For the calculation we considered only the first two lowest order diagrams in the series expansion shown in Fig. 1. The result of our calculation is depicted in Fig. 4 where we show the imaginary part of the on-site Green function as a function of Matsubara frequencies on one of...
FIG. 4: (color online) Local Matsubara Green function on the Matsubara axis obtained from DMRG for $T = 0$ in comparison with the results obtained from DMFT and from fully self-consistent dual fermion calculations. For the 2-site free cluster DMFT the renormalization of the vertex has a small effect since the CDMFT is already a good starting point. For the single site calculation the renormalization is essential since DMFT even gives a qualitatively wrong answer, while the dual fermion result correctly predicts the system to be an insulator.

VI. CONCLUSIONS

We have generalized the recently proposed Dual Fermion Approach to the multiorbital case, facilitating the treatment of multiorbital systems within this framework. We further established the relation between the four-point correlation functions in real and dual variables and found that the two-particle excitations for real fermions and dual fermions coincide. The approach was applied to the one-dimensional Hubbard model starting from the free two-site cluster DMFT solution. Although the CDMFT solution already quite well reproduces the DMRG solution, the cluster dual fermion solution considerably improved this result. The cluster formulation allows to combine this approach with realistic density functional calculations and thus opens a new way to describe long-range correlations in real systems.

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