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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 the cluster DMFT and nonlocal effects in realistic calculations of multiorbital systems. We show that the simplest approximation exactly corresponds to the free-cluster DMFT. We apply this approach to the one-dimensional Hubbard model. Already the first dual-fermion correction to the free cluster leads to a drastic improvement of the calculated Green function.

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One of the successful routes to the description of strongly correlated systems is the Dynamical Mean Field Theory (DMFT) [1, 2]. It is commonly accepted now that this approach typically catches the most essential correlation effects, e.g., the physics of the Mott-Hubbard transition [1, 2]. The method was implemented successfully into realistic electronic structure calculations [3, 4], which now is a standard tool in the microscopic theory of strongly correlated systems [5]. In the DMFT, the many-body problem for the crystal is split into a single-particle lattice problem and the many-body problem for an atom in a self-consistently determined Gaussian fermionic 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 the relevant correlations are even long-ranged. The examples are Luttinger-Liquid formation in low-dimensional systems [6, 7], non-Fermi-Liquid behavior due to van-Hove singularities in two dimensions [8], the physics near quantum critical points [9] or d-wave pairing in high-T_c superconductors [10]. Obviously, the DMFT is not sufficient for the description of such systems. To treat these non-local correlations it is desirable to combine local inter-site many-body phenomena, like the formation of RVB singlets [7], and long-range correlations. The former can be taken into account within various cluster approaches. They include the so-called Dynamical Cluster approximation (DCA) [11], real space periodic [12] and free cluster approaches [13], as well as the Cellular-DMFT [14](CDMFT) and the variational cluster approach [15].

Recently, steps have been taken to go beyond DMFT and to treat long-range correlations. One of them is the Dynamical Vertex approximation [16] and similar approaches [17, 18], where a diagrammatic expansion around the DMFT solution is made. A principally new scheme with a fully renormalized expansion called Dual Fermion Approach has been proposed[19]. It is based on the introduction of new variables in the path integral representation. This approach yields very satisfactory results already for the lowest-order corrections, while the schemes proposed in Refs. [16 – 18] operate with infinite diagrammatic series and require the solution of complicated integral equations. A scheme similar to the Dual Fermion approach has been discussed earlier in terms of Hubbard operators [20], but without attempts to use it in a practical calculation.

In this letter we formulate a general cluster (or multi-orbital) Dual Fermion scheme for non-local correlations. Similar to known cluster methods we consider a system with local interaction and assume that most of the correlations are located within the cluster. We point out however that the remaining long-range part of the correlations is physically important, and take it into account within a diagrammatic expansion of a special kind. By transforming the original interacting problem to so-called dual fermion variables we are able to include the local contribution to the self-energy into a bare propagator of the dual fermions and achieve much faster convergence of the perturbation expansion. An outcome of the scheme is the Green function of the original variables restored from a certain exact relation. Our method allows the treatment of clusters or multiorbital atoms within the Dual Fermion framework and can describe long-range

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correlations in real systems. We test the scheme for the half-filled one-dimensional Hubbard chain and demonstrate its superiority over short-range cluster methods.

Our goal is to find an (approximate) solution to a general multiband problem described by the imaginary time action

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

Here $h_{\mathbf{k}\sigma}$ is the one-electron part of the Hamiltonian, $\omega=(2n+1)\pi/\beta, n=0,\pm1,...$ are the Matsubara frequencies, β and μ are the inverse temperature and chemical potential, respectively, $\sigma=\uparrow,\downarrow$ labels the spin projection, m,m' are orbital indices and c^*,c are Grassmannian variables. The index i labels the lattice sites and the $\mathbf{k}$-vectors are quasimomenta. It is important to note that can be *any* type of interaction inside the multiorbital H_{int} atom. The only requirement and our main assumption is that it is local:

$$H_{\text{int}}[c_i^*,c_i]=\frac{1}{4}\sum_i\int_0^\beta d\tau\, U_{1234}c^*_{i1}c^*_{i2}c_{i4}c_{i3}\ , \quad (2)$$

where U is the general symmetrized Coulomb vertex and e.g. $1\equiv\{\omega_1 m_1\sigma_1\}$ comprehends frequency-, orbital- and spin degrees of freedom and summation over these states is implied.

The formalism is equally applied within the cluster (super-site) formalism. In this case, i and m label clusters and atoms within the cluster, repectively, while $\mathbf{k}$ runs over the reduced supercell Brillouin zone. In order to capture the local physics, we introduce a cluster impurity problem just in the spirit of CDMFT[12, 14, 13] in the form

$$S_{\text{imp}}[c^*,c]=-\sum_{\omega\sigma} c^*_{\omega\sigma m}\left((i\omega+\mu)\mathbf{1}-\Delta_{\omega\sigma}\right)_{mm'} c_{\omega\sigma m'} + \\ + H_{\text{int}}[c^*,c]\ , \quad (3)$$

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

Since Δ is local, one may formally rewrite the original lattice problem in the following form:

$$S[c^*,c]=\sum_i S_{\text{imp}}[c^*_{\omega i\sigma},c_{\omega i\sigma}] - \\ -\sum_{\omega\mathbf{k}\sigma mm'} c^*_{\omega\mathbf{k}\sigma m}\left(\Delta_{\omega\sigma}-h_{\mathbf{k}\sigma}\right)_{mm'} c_{\omega\mathbf{k}\sigma m'}\ . \quad (4)$$

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

$$\int\exp\left(-\mathbf{f}^*\hat{A}\mathbf{f}-\mathbf{f}^*\hat{B}\mathbf{c}-\mathbf{c}^*\hat{B}\mathbf{f}\right)\mathcal{D}[\mathbf{f},\mathbf{f}^*]= \\ =\det(\hat{A})\ \exp\left(\mathbf{c}^*\hat{B}\hat{A}^{-1}\hat{B}\mathbf{c}\right), \quad (5)$$

which is valid for arbitrary complex matrices $\hat{A}$ and $\hat{B}$. In order to decouple the non-local term in Eq. (4), we choose

$$A=g^{-1}_{\omega\sigma}\left(\Delta_{\omega\sigma}-h_{\mathbf{k}\sigma}\right)^{-1}g^{-1}_{\omega\sigma}\ , \\ B=g^{-1}_{\omega\sigma}\ , \quad (6)$$

where $g_{\omega\sigma}$ is the Green function matrix of the local impurity problem in orbital space (m,m'). Using this identity, the lattice action can be rewritten in the form

$$S[\mathbf{c}^*,\mathbf{c},\mathbf{f}^*,\mathbf{f}]=\sum_i S_{\text{site},i} + \\ +\sum_{\omega\mathbf{k}\sigma}\left[\mathbf{f}^*_{\omega\mathbf{k}\sigma}\ g^{-1}_{\omega\sigma}\ \left(\Delta_{\omega\sigma}-h_{\mathbf{k}\sigma}\right)^{-1}\ g^{-1}_{\omega\sigma}\ \mathbf{f}_{\omega\mathbf{k}\sigma}\right]\ , \quad (7)$$

where

$$\sum_i S_{\text{site},i}=\sum_i S_{\text{imp}}[\mathbf{c}_i^*,\mathbf{c}_i]+ \\ +\mathbf{f}^*_{\omega i\sigma}\ g^{-1}_{\omega\sigma}\mathbf{c}_{\omega i\sigma}+\mathbf{c}^*_{\omega i\sigma}\ g^{-1}_{\omega\sigma}\mathbf{f}_{\omega i\sigma}.\ * \quad (8)$$

Here the summation in the last term over states labeled by $\mathbf{k}$ 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

$$Z=\int\exp\left(-S[\mathbf{c}^*,\mathbf{c}]\right)\mathcal{D}[\mathbf{c},\mathbf{c}^*]= \\ =Z_f\int\int\exp\left(-S[\mathbf{c}^*,\mathbf{c},\mathbf{f}^*,\mathbf{f}]\right)\mathcal{D}[\mathbf{f},\mathbf{f}^*]\mathcal{D}[\mathbf{c},\mathbf{c}^*], \quad (9)$$

where

$$Z_f=\prod_{\omega\mathbf{k}\sigma}\det\left[g_{\omega\sigma}\left(\Delta_{\omega\sigma}-h_{\mathbf{k}\sigma}\right)g_{\omega\sigma}\right]. \quad (10)$$

By taking the functional derivative of the partition function, Eq. (9), one can obtain the following exact relationship between the dual and lattice Green functions:

$$G_{\omega\mathbf{k}\sigma} = (\Delta_{\omega\sigma} - h_{\mathbf{k}\sigma})^{-1} + \\ + (g_{\omega\sigma}(\Delta_{\omega\sigma} - h_{\mathbf{k}\sigma}))^{-1} G^{\mathrm{d}}_{\omega\mathbf{k}\sigma}((\Delta_{\omega\sigma} - h_{\mathbf{k}\sigma}) g_{\omega\sigma})^{-1}, \quad (11)$$

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

$$G_{12} = -\frac{1}{Z}\int c_1 c_2^* \exp(-S[\mathbf{c}^*, \mathbf{c}])\, \mathcal{D}[\mathbf{c}, \mathbf{c}^*] \qquad (12)$$

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 $\mathbf{c}$,$\mathbf{c}^*$. The crucial point is that this can be done for each site separately:

$$\int \exp(-S_{\mathrm{site}}[\mathbf{c}_i^*, \mathbf{c}_i, \mathbf{f}_i^*, \mathbf{f}_i])\, \mathcal{D}[\mathbf{c}_i, \mathbf{c}_i^*] = \\ = Z_{\mathrm{imp}} e^{-\left(\sum_{\omega\sigma} \mathbf{f}^*_{\omega i\sigma}\, g^{-1}_{\omega\sigma}\, \mathbf{f}_{\omega i\sigma} + V_i[\mathbf{f}_i^*, \mathbf{f}_i]\right)}. \qquad (13)$$

This equation can be seen as the defining equation for the dual potential $V[\mathbf{f}^*, \mathbf{f}]$. Since S_{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 the resulting expressions by order, one finds that the dual potential in the lowest order approximation is given by

$$V[\mathbf{f}^*, \mathbf{f}] = \frac{1}{4}\sum_i \gamma^{(4)}_{1234} \mathbf{f}^*_{i1}\mathbf{f}^*_{i2}\mathbf{f}_{i4}\mathbf{f}_{i3} + \ldots \qquad (14)$$

where

$$\gamma^{(4)}_{1234} = g^{-1}_{11'} g^{-1}_{22'} \left[\chi^{\mathrm{imp}}_{1'2'3'4'} - \chi^{\mathrm{imp},0}_{1'2'3'4'}\right] g^{-1}_{3'3} g^{-1}_{4'4}\,, \\ \chi^{\mathrm{imp},0}_{1234} = g_{14}g_{23} - g_{13}g_{24} \qquad (15)$$

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

$$\chi^{\mathrm{imp}}_{1234} = \frac{1}{Z_{\mathrm{imp}}}\int c_1 c_2 c_3^* c_4^* \exp(-S_{\mathrm{imp}}[\mathbf{c}^*, \mathbf{c}])\, \mathcal{D}[\mathbf{c}, \mathbf{c}^*]\,. \qquad (16)$$

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

$$S_{\mathrm{d}}[\mathbf{f}^*, \mathbf{f}] = -\sum_{\omega\mathbf{k}\sigma} \mathbf{f}^*_{\omega\mathbf{k}\sigma} (G^{\mathrm{d},0}_{\omega\mathbf{k}\sigma})^{-1} \mathbf{f}_{\omega\mathbf{k}\sigma} + \sum_i V[\mathbf{f}_i^*, \mathbf{f}_i]\,. \qquad (17)$$

The bare dual Green function is given by

$$G^{\mathrm{d},0}_{\omega\mathbf{k}\sigma} = -g_{\omega\sigma}\left[g_{\omega\sigma} + (\Delta_{\omega\sigma} - h_{\mathbf{k}\sigma})^{-1}\right]^{-1} g_{\omega\sigma}\,. \qquad (18)$$

and the dual self energy reads

$$\Sigma^{\mathrm{d}}_{\omega\mathbf{k}\sigma} = (G^{\mathrm{d},0}_{\omega\mathbf{k}\sigma})^{-1} - (G^{\mathrm{d}}_{\omega\mathbf{k}\sigma})^{-1}. \qquad (19)$$

Let us introduce non-local part $\widetilde{\Sigma}$ as the difference between the self-energy Σ of the lattice problem and it's DMFT value, i.e. $\widetilde{\Sigma} = g^{-1} + \Delta - h - G^{-1}$. For this quantity, there is a simple matrix relation with the dual self-energy:

$$\widetilde{\Sigma}^{-1} = \Sigma_{\mathrm{d}}^{-1} + g\,, \qquad (20)$$

as one can obtain from the previous formulas.

It immediately follows that $\widetilde{\Sigma} = 0$ for $\Sigma^{\mathrm{d}} = 0$, which corresponds to neglecting the nonlinear dual potential V, i.e. non-interacting dual fermions. In this case the DMFT result is restored, for a properly chosen Δ (for details, see below). In order to obtain the nonlocal correction to the DMFT, we thus need to calculate the dual self-energy with higher order in V. This is achieved by performing a regular diagrammatic series expansion of the dual action, Eq. (17) and considering the lowest order skeleton diagrams for Σ_{d}, constructed from the irreducible vertices and the dual Green function as lines. The use of skeleton diagrams ensures that the resulting theory is conserving according to the Baym-Kadanoff criterion [21, 19]. The diagrams considered here are shown in Fig. 1. The lowest order diagram is local while the next diagram already gives a nonlocal contribution to the self energy.

So far we have not established a condition for Δ. We require that the first diagram in the expansion of the dual self-energy should be equal to zero at all frequencies. Since $\gamma^{(4)}$ is local, we can use the condition $\sum_{\mathbf{k}} G^d_{\mathbf{k}\omega} = 0$. 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

$$\sum_{\mathbf{k}}\left[g_{\omega\sigma} + (\Delta_{\omega\sigma} - h_{\mathbf{k}\sigma})^{-1}\right]^{-1} = 0 \qquad (21)$$

which is equivalent to the self-consistency condition for the hybridization function in free-cluster CDMFT [12, 14, 13]. Usually, this equation is solved iteratively, with a repeated substitution

$$\Delta \to \Delta + g^{-1} G^{\mathrm{d}}_{\mathrm{loc}} G^{-1}_{\mathrm{loc}}. \qquad (22)$$

Finally the resulting scheme is as follows: in order to include non-local correlations beyond the cluster approximation, one should take into account two-particle vertex, which plays the role of the effective interactions between the dual fermions, and perform the standard perturbation expansion. In our calculations, we take into account the first non-vanishing diagram for the dual self energy (the right diagram in Fig.1), and use the same substitution rule (22). The calculation procedure

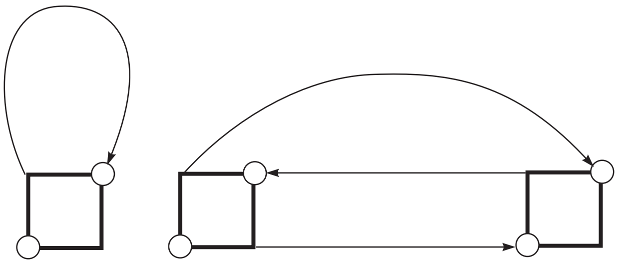

Fig.1. The first two lowest order diagrams for the dual self energy Σ^d

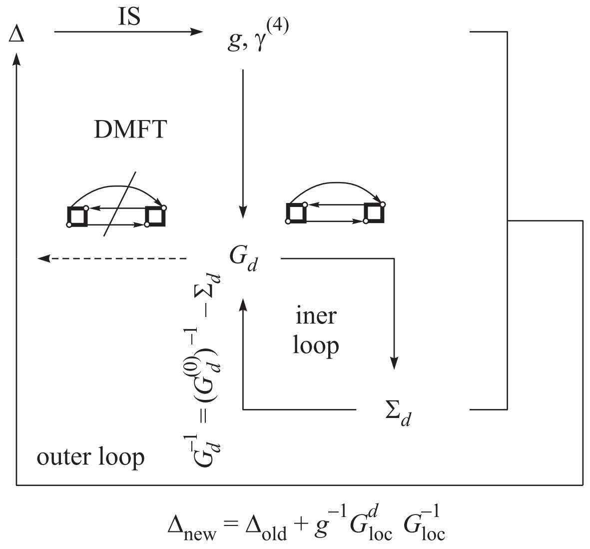

Fig.2. The scheme of the calculation procedure. The outer loop corresponds to the an iterative calculation of the hybridization function δ; it requires a solution of the impurity problem at each step. The inner loop describes the iterative calculation of the skeleton diagrams for dual self-energy, given the properties of the impurity problem. DMFT implies $\widetilde{\Sigma} = 0$ and therefore does not require the inner loop, as indicated by the dashed line

is as follows (see Fig.2): Starting from a starting guess for Δ, e.g. the DMFT result, we obtain a new local Green function g and the irreducible vertex $\gamma^{(4)}$. The continuous-time quantum Monte Carlo impurity solver [22] is employed for this calculation. Given g, we estimate the bare Green function (18) and calculate the diagram for Σ_d with the lines given by $G^{d,0}$. This guess for Σ_d is used for a new estimate of the dual Green function. A repeated execution of this procedure is illustrated by the inner loop in Fig. 2. After a few iterations it converges to a value for $\widetilde{\Sigma}$, corresponding to a skeleton diagram (a diagram with renormalized lines). The dual Green function and the lattice Green function are then again used to obtain a new hybridization function according to the rule (22). It serves as input for the calculation of a new local Green function and renormalized vertex in the impurity solver step. This 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.

In order to obtain information about the instabilities in the system, one needs to consider the two-particle Green function. The exact relation between the four-point correlation function for original lattice problem and the dual fermions is established by taking the second derivative of Z with respect to $h_{\mathbf{k}}$ using the two equivalent representations of the partition function, Eq. (9). After some straightforward algebra we obtain the following expression for the four-point correlation function:

$$\begin{aligned}\chi_{\lambda\mu\nu\rho} &= \left[(\Delta-h)^{-1}\otimes(\Delta-h)^{-1}\right]_{\lambda\mu\nu\rho} + \\ &+\left[(\Delta-h)^{-1}\otimes\left[(\Delta-h)^{-1}g^{-1}G_d g^{-1}(\Delta-h)^{-1}\right]\right]_{\lambda\mu\nu\rho} + \\ &+\left[\left[(\Delta-h)^{-1}g^{-1}G_d g^{-1}(\Delta-h)^{-1}\right]\otimes(\Delta-h)^{-1}\right]_{\lambda\mu\nu\rho} + \\ &+\left[(\Delta-h)^{-1}g^{-1}\right]_{\lambda l}\left[(\Delta-h)^{-1}g^{-1}\right]_{\mu m}\chi^d_{lmnr}\times \\ &\times\left[g^{-1}(\Delta-h)^{-1}\right]_{n\nu}\left[g^{-1}(\Delta-h)^{-1}\right]_{r\rho}. \end{aligned} \quad (23)$$

Here $\chi^d_{lmnr} \equiv \langle \mathrm{f}_l f_m f^*_n f^*_r \rangle$ is the dual four-point correlation function and $(A\otimes B)_{\lambda\mu\nu\rho} \equiv A_{\lambda\rho}B_{\mu\nu} - A_{\lambda\nu}B_{\mu\rho}$ is the antisymmetrized direct product of two matrices.

As one can see from Eq. (23), the two-particle excitations for dual fermions coincide with those for real fermions so that information about the instabilities can be obtained by considering the dual correlation function. Two different approximations to the four-point correlation function are obtained by summing up the ladders for the two-particle dual fermion Green function:

$$\chi^{d(pp)}_{lmnr} = \chi^{d,0}_{lmnr} + \chi^{d,0}_{lm\nu\rho}\gamma_{\rho\nu\mu\lambda}\chi^{d(pp)}_{\lambda\mu nr} \quad (24)$$

or

$$\chi^{d(ph)}_{lnmr} = \chi^{d,0}_{lnmr} + \chi^{d,0}_{l\nu m\rho}\gamma_{\rho\mu\nu\lambda}\chi^{d(ph)}_{\lambda n\mu\rho}\,, \quad (25)$$

where the first equation is written for the particle-particle channel and the second for the particle-hole channel. Here $\chi^{d0} = G_d \otimes G_d$ is the bare two-particle dual Green function. The particle-particle channel is useful for investigation of superconducting instability, while the particle-hole excitations can give different magnetic behaviors.

As an example, we consider the two-site cluster calculation for the half-filled Hubbard chain. This model is described by the following Hamiltonian:

$$H_0 + H_{\text{int}} = t \sum_i (c_{i+1}^\dagger c_i + c_{i-1}^\dagger c_i) + U \sum_i n_{i\uparrow} n_{i\downarrow} \ . \tag{26}$$

When this one-dimensional system is treated as a chain of two-site clusters as depicted in Fig.3, the tight-binding

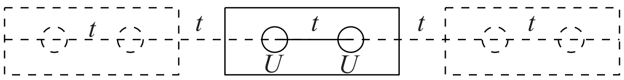

Fig.3. Schematic representation of the 1D chain as a chain of two-site clusters

Hamiltonian for this model is readily shown to be

$$h_k = \begin{pmatrix} 0 & t(1+e^{-2ika}) \\ t(1+e^{2ika}) & 0 \end{pmatrix} . \tag{27}$$

Due to the absence of a Mott transition in one dimension [23], the system is an insulator for any finite value of the on-site repulsion U. For the case of sufficiently large $U/2t$, the basic physics of the model is determined by the tendency of the formation of a spin-singlet between neighboring sites [7], and thus one can expect that the two-site cluster serves as a reasonable starting point, in contrast to the single-site DMFT. There is an obvious note that the translational invariance of the original lattice is broken in such a consideration. However it is not crucial for our purposes, since we will only be interested in the local part of the Green function.

In Fig.4, we compare our results with the one obtained by a Density Matrix Renormalization Group (DMRG) calculation [24], which is known to reproduce the spectral properties of 1D systems quite well. For our calculations we use the parameters $U/t = 6$ and $\beta = 20$. The DMRG solution corresponds to $T = 0$. We also present the results of the single-site DMFT and dual-fermion calculations. The single-site DMFT gives a qualitatively wrong answer, i.e. predicts the system to be metallic even for U as large as $U/t = 6$. The single-site dual-fermion approach fixes this, but is still quantitatively inaccurate. On the other hand, the results of the two-site CDMFT already provide a rather good

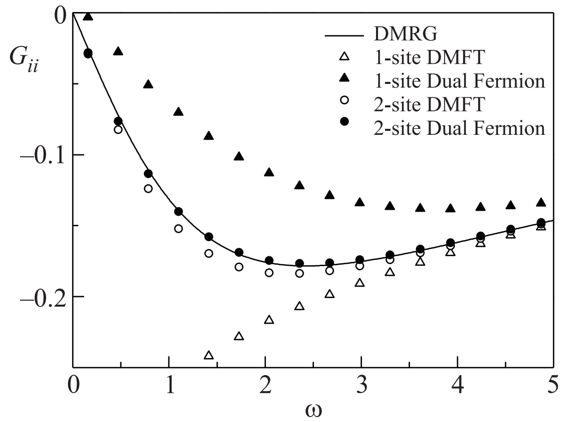

Fig.4. Local Matsubara Green function on the Matsubara axis obtained from DMRG for $T = 0$ in comparison with the results obtained from DMFT and from fully self-consistent dual fermion calculations. For the 2-site calculation the renormalization of the vertex has a small effect since the CDMFT is already 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

description of the local Green function. This underlines the statement that local singlet physics is of pivotal importance. It is known that this result is hardly improvable by the consideration of larger clusters [24], which indicates the relevance of long-range correlations in the model. However, the two-site dual-fermion scheme with just the lowest-order correction taken into account improves the results substantially.

To conclude, we have generalized the recently proposed Dual Fermion Approach to the multiorbital case, facilitating the treatment of multiorbital systems within this framework. The approach was applied to the one-dimensional Hubbard model starting from the free two-site cluster DMFT solution. The cluster dual fermion solution considerably improved the CDMFT 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. The advantage of this multiorbital approach is that it preserves translational invariance. Discussing possible further developments for Hubbard-like lattices, one can restore the translational invariance of the method. This can be achieved if the dual-fermion expansion is built on top of the cluster DCA method.

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