The effect of six-point one-particle reducible local interactions in the dual fermion approach

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Abstract.   We formulate the dual fermion approach for strongly correlated electronic systems in terms of the lattice and dual effective interactions, obtained by using the covariation splitting formula. This allows us to consider the effect of six-point one-particle reducible interactions, which are usually neglected by the dual fermion approach. We show that the consideration of one-particle reducible six-point (as well as higher order) vertices is crucially important for the diagrammatic consistency of this approach. In particular, the relation between the dual and lattice self-energy, derived in the dual fermion approach, implicitly accounts for the effect of the diagrams, containing 6-point and higher order local one-particle reducible vertices, and should be applied with caution, if these vertices are neglected. Apart from that, the treatment of the self-energy feedback is also modified by 6-point and higher order vertices; these vertices are also important to account for some non-local corrections to the lattice self-energy, which have the same order in the local 4-point vertices, as the diagrams usually considered in the approach. These observations enlighten an importance of 6-point and higher order vertices in the dual fermion approach, and call for development of new schemes of treatment of non-local fluctuations, which are based on one-particle irreducible quantities.

1. Introduction

Strongly correlated electron systems became one of the touchstone of modern physics. They demonstrate a variety of phenomena: magnetism, (unconventional) superconductivity, "colossal" magnetoresistance, and quantum critical behavior. The dynamical mean-field theory (DMFT)[1, 2] allowed to describe accurately the Mott-Hubbard metal-insulator transition.[3]. DMFT becomes exact in the limit of high spatial dimensions $(d \rightarrow \infty)$ and accounts for an important local part of electronic correlations. Real physical systems are however one-, two-, or three-dimensional. Therefore, nonlocal correlations, which are neglected in DMFT, may be important. Recently, a progress to go beyond DMFT through cluster extensions[4, 5, 6, 7, 8] was achieved. These correlations are however necessarily short-range in nature due to numerical limitations of the cluster size[9].

This limitation motivated developing the diagrammatic extensions of the dynamical mean-field theory. The dynamical vertex approximation (DΓA) was introduced in Refs. [10, 11, 12, 13, 14, 15]. Starting from the local particle-hole irreducible vertex, this approximation sums ladder diagrams for the vertex in the particle-hole channel, where particle-hole irreducible vertices assumed to be local, but the effect of the non-locality of the Green functions is considered. Alternative dual fermion (DF) approach was proposed in Refs. [16, 17, 18, 19], which splits the degrees of freedom into the local ones, treated within DMFT, and the non-local (dual) degrees, considered perturbatively, with a possibility of summation of infinite series of diagrams for dual fermions [19, 20].

Although both abovementioned approaches use 4-point local vertex as an effective interaction between fermionic degrees of freedom (lattice fermions in case of DΓA and dual fermions in the DF approach), they make in fact very different assumptions on the neglect of higher-order local vertices. Indeed, DΓA operates with one-particle irreducible (1PI) vertices, and neglects six-point and higher order 1PI local vertices. At the same time, DF representation does not use the assumption of the one-particle irreducibility; in particular its formulation in Refs. [16, 17, 18, 19] neglects one-particle *reducible* six-point and higher vertices.

This difference appears to be important for analysing diagrammatic consistency of the abovediscussed approaches. While the dynamic vertex approximation is based on the diagrammatic approach, formulated in terms of the original lattice degrees of freedom, the diagrammatic consistency of the dual fermion approach (in terms of the same lattice degrees of freedom) has to be verified. In the present paper we show that the inculision of the one-particle reducible six-point (and more generally, higher vertices) into the DF approach appears to be necessary to make it diagrammatically consistent.

2. The model, dynamical mean-field theory, and the dual fermion approach

2.1. The model and dynamical mean-field theory

We consider general one-band model of fermions, interacting via local interaction $H_{\text{int}}[\widehat{c}_{i\sigma}, \widehat{c}_{i\sigma}^+]$

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k},\sigma} \widehat{c}_{\mathbf{k},\sigma}^+ \widehat{c}_{\mathbf{k},\sigma} + \sum_{i,\sigma} H_{\text{int}}[\widehat{c}_{i\sigma}, \widehat{c}_{i\sigma}^+], \tag{1}$$

where $\widehat{c}_{i\sigma}, \widehat{c}_{i\sigma}^+$ are the fermionic operators, and $\widehat{c}_{\mathbf{k},\sigma}, \widehat{c}_{\mathbf{k},\sigma}^+$ are the corresponding Fourier transformed objects, $\sigma = \uparrow, \downarrow$ corresponds to a spin index. The model is characterized by the generating functional

$$Z[\eta, \eta^+] = \int d[c, c^+] \exp\left\{-\mathcal{S}[c, c^+] + \eta^+ c + c^+ \eta\right\} \tag{2}$$

$$\mathcal{S}[c, c^+] = \int d\tau \left\{\sum_{i,\sigma} c_{i\sigma}^\dagger(\tau) \frac{\partial}{\partial \tau} c_{i\sigma}(\tau) + H[c, c^+]\right\} \tag{3}$$

where $c_{i\sigma}, c_{i\sigma}^+, \eta_{i\sigma}, \eta_{i\sigma}^+$ are the Grassman fields, the fields $\eta_{i\sigma}, \eta_{i\sigma}^+$ correspond to source terms, $\tau \in [0, \beta = 1/T]$ is the imaginary time. The dynamical mean-field theory corresponds to considering the effective single-site problem with the action

$$\mathcal{S}_{\text{DMFT}}[c, c^+] = \sum_{i,\sigma} \int d\tau \left\{-\frac{1}{\beta^2} \int d\tau' \zeta^{-1}(\tau - \tau') c_{i\sigma}^\dagger(\tau) c_{i\sigma}(\tau') \right. \tag{4}$$

$$\left. + H_{\text{int}}[c_{i\sigma}, c_{i\sigma}^+]\right\},$$

where the "Weiss field" function $\zeta(\tau)$ and its Fourier transform $\zeta(i\nu_n)$ has to be determined self-consistently from the condition

$$G_{\text{loc}}(i\nu_n) \equiv \frac{1}{\zeta^{-1}(i\nu_n) - \Sigma_{\text{loc}}(i\nu_n)} = \sum_{\mathbf{k}} G(\mathbf{k}, i\nu_n) \tag{5}$$

where

$$G(\mathbf{k}, i\nu_n) \equiv G_k = \left[G_{0k}^{-1} - \Sigma_{\text{loc}}(i\nu_n)\right]^{-1} \tag{6}$$

$G_{0k}^{-1} = i\nu_n - \varepsilon_{\mathbf{k}}$ is the lattice noninteracting Green function (we use the 4-vector notation $k = (\mathbf{k}, i\nu_n)$) and $\Sigma_{\text{loc}}(i\nu_n)$ is the self-energy of the impurity problem (4), which is in practice obtained within one of the impurity solvers: exact diagonalization, quantum Monte-Carlo, etc.

2.2. The formulation of the dual fermion approach by means of covariation splitting formula

The dual fermion approach of Refs. [16, 17, 18, 19] can be conveniently formulated in terms of an effective interaction of the lattice theory (see, e.g. Ref. [21])

$$\mathcal{V}[\eta, \eta^+]: \quad = -\ln \int d[c, c^+] \exp\left\{\sum_{k,\sigma} G_{0k}^{-1}\left(c_{k\sigma}^+ + \eta_{k\sigma}^+\right)(c_{k\sigma} + \eta_{k\sigma})\right.$$

$$- \sum_{i,\sigma} \int d\tau \, H_{\mathrm{int}}[c_{i\sigma}, c_{i\sigma}^+] \Bigg\}$$

$$= - \ln Z[G_{0k}^{-1}\eta_{k\sigma}, G_{0k}^{-1}\eta_{k\sigma}^+] - \eta_{k\sigma}^+ G_{0k}^{-1}\eta_{k\sigma}. \tag{7}$$

Expansion of the effective interaction $\mathcal{V}[\eta, \eta^+]$ in source fields generates connected (in general, one-particle reducible) Green functions, amputated by the non-interacting Green functions of the lattice theory G_{0k}. The relation between one-particle reducible and 1PI counterparts of the vertices can be involved. In particular, the (one-particle irreducible) self-energy Σ_k of the lattice problem (i.e. the 1PI 2-point vertex function) can be extracted from the two-point connected vertex function $V^{(2)}$ via the relation $V_k^{(2)} = \Sigma_k/(1 - G_{0k}\Sigma_k)$.

To split the local and non-local degrees of freedom in the effective interaction (7) we use the covariation splitting formula [21], which is based on the identity

$$\sum_{k,\sigma} C_k^{-1} c_{k\sigma}^+ c_{k\sigma} = \ln \int d[\widetilde{c}, \widetilde{c}^+] \exp \Bigg\{ \sum_{k,\sigma} \widetilde{c}_{k,\sigma}^+ B_k^{-1} \widetilde{c}_{k,\sigma} \tag{8}$$

$$+ \sum_{k\sigma} A_k^{-1} \left(\widetilde{c}_{k,\sigma}^+ + c_{k,\sigma}^+ \right) \left(\widetilde{c}_{k,\sigma} + c_{k,\sigma} \right) \Bigg\}$$

with $A_k + B_k = C_k$; Eq. (8) can be proven by integrating over the $\widetilde{c}, \widetilde{c}^+$ fields. For $A_k = \zeta(i\nu_n)$, $C_k = G_{0k}$ this implies

$$\mathcal{V}[\eta, \eta^+] = - \ln \int d[\widetilde{c}, \widetilde{c}^+] \exp \Bigg\{ \sum_{k,\sigma} \widetilde{c}_{k,\sigma}^+ \widetilde{G}_{0k}^{-1} \widetilde{c}_{k,\sigma} - \mathcal{V}_{\mathrm{DMFT}}[\eta^+ + \widetilde{c}^+, \eta + \widetilde{c}] \Bigg\} \tag{9}$$

where $\mathcal{V}_{\mathrm{DMFT}}[\eta, \eta^+]$ is an effective potential of the dynamical mean-field theory, defined by

$$e^{-\mathcal{V}_{\mathrm{DMFT}}[\eta, \eta^+]} = \int d[c, c^+] \exp \Bigg\{ - \sum_{i,\sigma} \int d\tau \, H_{\mathrm{int}}[c_{i\sigma}, c_{i\sigma}^+]$$

$$+ \sum_{k,\sigma} \zeta^{-1}(i\nu_n) \left(c_{k,\sigma}^+ + \eta_{k,\sigma}^+ \right)(c_{k,\sigma} + \eta_{k,\sigma}) \Bigg\}, \tag{10}$$

$\widetilde{G}_{0k} = G_{0k} - \zeta(i\nu_n)$ is the bare Green function of the non-local degrees of freedom. Similarly to $\mathcal{V}[\eta, \eta^+]$, the functional $\mathcal{V}_{\mathrm{DMFT}}[\eta, \eta^+]$ generates connected vertices (which are in general one-particle reducible), amputated by the bath Green function $\zeta(i\nu_n)$.

To simplify Eq. (9), we perform a shift $\widetilde{c}_{k\sigma} \to \widetilde{c}_{k\sigma} - \eta_{k\sigma}$, such that

$$\mathcal{V}[\eta, \eta^+] = - \ln \int d[\widetilde{c}, \widetilde{c}^+] e^{\sum_{k,\sigma} \left(\widetilde{c}_{k,\sigma}^+ - \eta_{k,\sigma}^+ \right) \widetilde{G}_{0k}^{-1} \left(\widetilde{c}_{k,\sigma} - \eta_{k,\sigma} \right) - \mathcal{V}_{\mathrm{DMFT}}[\widetilde{c}, \widetilde{c}^+]}. \tag{11}$$

To arrive at the standard dual fermion approach[16, 17, 18, 19] we consider an expansion of $\mathcal{V}_{\mathrm{DMFT}}[\widetilde{c}, \widetilde{c}^+]$ in fields

$$\mathcal{V}_{\mathrm{DMFT}}[\widetilde{c}, \widetilde{c}^+] = \sum_{k,\sigma} \widetilde{c}_{k,\sigma}^+ \frac{\Sigma_{\mathrm{loc}}(i\nu_n)}{1 - \zeta(i\nu_n)\Sigma_{\mathrm{loc}}(i\nu_n)} \widetilde{c}_{k,\sigma} + \widetilde{\mathcal{V}}_{\mathrm{DMFT}}[\widetilde{c}, \widetilde{c}^+]$$

$$\widetilde{\mathcal{V}}_{\text{DMFT}}[\widetilde{c}, \widetilde{c}^+] = \frac{1}{2}\widetilde{\Gamma}_{\text{loc}} \circ (\widetilde{c}^+_{k_{1\sigma}}\widetilde{c}_{k_{2\sigma}})(\widetilde{c}^+_{k_{3\sigma'}}\widetilde{c}_{k_{4\sigma'}}) \tag{12}$$

$$+ \frac{1}{6}\widetilde{\Gamma}^{(6)}_{\text{loc}} \circ (\widetilde{c}^+_{k_{1\sigma}}\widetilde{c}_{k_{2\sigma}})(\widetilde{c}^+_{k_{3\sigma'}}\widetilde{c}_{k_{4\sigma'}})(\widetilde{c}^+_{k_{5\sigma''}}\widetilde{c}_{k_{6\sigma''}}) + ...$$

where $\widetilde{\Gamma}_{\text{loc}}$ and $\widetilde{\Gamma}^{(6)}_{\text{loc}}$ are the connected 4- and 6- point local vertices, amputated with the bare Green functions ζ, e.g.

$$\widetilde{\Gamma}^{\sigma\sigma'}_{\text{loc}}(i\nu_1..i\nu_3) = (1 + \delta_{\sigma\sigma'})^{-1}\prod_{i=1}^{4}\zeta^{-1}(i\nu_i) \tag{13}$$

$$\times \left[G^{(4)}_{\text{loc},\sigma\sigma'}(i\nu_1..i\nu_3) - G_{\text{loc}}(i\nu_1)G_{\text{loc}}(i\nu_2)(\delta_{\nu_1\nu_3} - \delta_{\sigma\sigma'}\delta_{\nu_2\nu_3}) \right],$$

and $\circ$ stands for summation over momenta- frequency- and spin indices fulfilling the conservation laws, $G^{(4)}_{\text{loc}}$ is the two-particle local Green function, which can be obtained via the solution of the impurity problem[10, 22]. We therefore obtain

$$\mathcal{V}[\eta, \eta^+] = -\sum_{k,\sigma}\eta^+_{k,\sigma}\widetilde{G}^{-1}_{0k}\eta_{k,\sigma} \tag{14}$$

$$- \ln \int d[\widetilde{c}, \widetilde{c}^+]e^{\sum_{k,\sigma}\left[\widetilde{c}^+_{k,\sigma}(\widetilde{G}'_k)^{-1}\widetilde{c}_{k,\sigma} - \widetilde{c}^+_{k,\sigma}\widetilde{G}^{-1}_{0k}\eta_{k,\sigma} - \eta^+_{k,\sigma}\widetilde{G}^{-1}_{0k}\widetilde{c}_{k,\sigma}\right] - \widetilde{\mathcal{V}}_{\text{DMFT}}[\widetilde{c},\widetilde{c}^+]},$$

where

$$\widetilde{G}'_k = \widetilde{G}_{0k}\frac{1 - \zeta(i\nu_n)\Sigma_{\text{loc}}(i\nu_n)}{1 - G_{0k}\Sigma_{\text{loc}}(i\nu_n)} = [1 - \zeta(i\nu_n)\Sigma_{\text{loc}}(i\nu_n)]^2 \widetilde{G}_k, \tag{15}$$

and $\widetilde{G}_k = G_k - G_{\text{loc}}(i\omega_n)$. Rescaling the fields of integration to exclude extra factor $(1 - \zeta\Sigma_{\text{loc}})^2$ and introducing the 'dual' source field

$$\widehat{\eta}_{k\sigma} = \eta_{k\sigma}/\left[1 - \Sigma_{\text{loc}}(i\nu_n)G_{0k}\right], \tag{16}$$

we obtain the effective interaction of the lattice theory in the form

$$\mathcal{V}[\eta, \eta^+] = \widehat{\mathcal{V}}[\widehat{\eta}, \widehat{\eta}^+] - \sum_{k,\sigma}\eta^+_{k,\sigma}\left\{\widetilde{G}^{-1}_{0k} - \frac{1}{[1 - \Sigma_{\text{loc}}(i\nu_n)G_{0k}]^2}\widetilde{G}^{-1}_k\right\}\eta_{k,\sigma} \tag{17}$$

$$= \widehat{\mathcal{V}}[\widehat{\eta}, \widehat{\eta}^+] + \sum_{k,\sigma}\eta^+_{k,\sigma}\frac{\Sigma_{\text{loc}}(i\nu_n)}{1 - \Sigma_{\text{loc}}(i\nu_n)G_{0k}}\eta_{k,\sigma}, \tag{18}$$

where

$$\widehat{\mathcal{V}}[\widehat{\eta}, \widehat{\eta}^+] = -\ln\int D[\widetilde{c}, \widetilde{c}^+]e^{\sum_{k,\sigma}\widetilde{G}^{-1}_k(\widetilde{c}^+_{k,\sigma} - \widehat{\eta}^+_{k,\sigma})(\widetilde{c}_{k,\sigma} - \widehat{\eta}_{k,\sigma}) - \widehat{\mathcal{V}}_{\text{DMFT}}[\widetilde{c}^+,\widetilde{c}]} \tag{19}$$

is the effective interaction of dual fermions. According to the Eq. (12), the expansion of $\widehat{\mathcal{V}}_{\text{DMFT}}[\widetilde{c}^+, \widetilde{c}]$ in fields reads

$$\widehat{\mathcal{V}}_{\text{DMFT}}[\widetilde{c}^+, \widetilde{c}] = \frac{1}{2}\Gamma_{\text{loc}} \circ (\widetilde{c}^+_{k_1,\sigma}\widetilde{c}_{k_3,\sigma})(\widetilde{c}^+_{k_2,\sigma'}\widetilde{c}_{k_4,\sigma'}) \tag{20}$$

$$+ \frac{1}{6}\Gamma^{(6)}_{\text{loc}} \circ (\widetilde{c}^+_{k_{1\sigma}}\widetilde{c}_{k_{2\sigma}})(\widetilde{c}^+_{k_{3\sigma'}}\widetilde{c}_{k_{4\sigma'}})(\widetilde{c}^+_{k_{5\sigma''}}\widetilde{c}_{k_{6\sigma''}}) + ...$$

where $\Gamma_{\text{loc}} = \widetilde{\Gamma}_{\text{loc}}\prod_{i=1}^{4}(1 - \zeta\Sigma_{\text{loc}})_{i\nu_i}$ and $\Gamma^{(6)}_{\text{loc}} = \widetilde{\Gamma}^{(6)}_{\text{loc}}\prod_{i=1}^{6}(1 - \zeta\Sigma_{\text{loc}})_{i\nu_i}$ are the connected 4- and 6-point vertices, amputated with the local Green functions G_{loc}. For the four-point vertex Γ_{loc} the requirement of connectivity and amputation with the full local
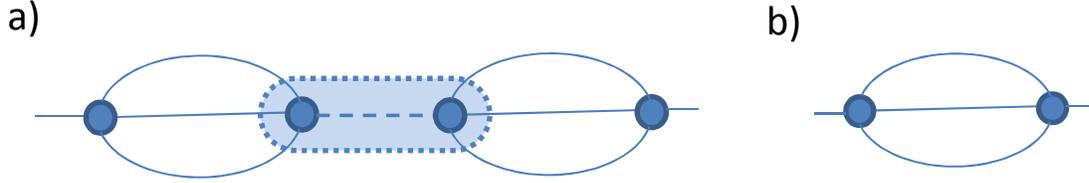
Figure 1. (Color online) (a) The one-particle reducible contributions to the lattice two-point Green function, coming from one-particle reducible six-point local vertex (shaded). The circles correspond to the four-point local vertices, solid line - the propagator $\widetilde{G}_k$, dashed line corresponds to the local propagator G_{loc}. (b) The corresponding contribution to the non-local self-energy, which is of the second order in the local 4-point vertices.

Green functions implies one-particle irreducibility. However, the higher-order vertices, e.g. $\Gamma_{\text{loc}}^{(6)}$ remain one-particle reducible.

In the described approach the relation between the self-energies $\Sigma_{\text{d}}(k)$ of the dual fermions $\widetilde{c}_k$ and Σ_k of the lattice fermions c_k is easily obtained by equating the corresponding two-point vertices in Eq. (17):

$$
\frac{\Sigma_k}{1 - \Sigma_k G_{0k}} = \frac{\Sigma_{\text{loc}}(i\nu_n)}{1 - \Sigma_{\text{loc}}(i\nu_n)G_{0k}} \\
+ \frac{\Sigma_{\text{d}}(k)}{1 - \Sigma_{\text{d}}(k)\left[G_k - G_{\text{loc}}(i\nu_n)\right]} \frac{1}{\left[1 - \Sigma_{\text{loc}}(i\nu_n)G_{0k}\right]^2}, \tag{21}
$$

which implies

$$
\Sigma_k = \frac{\Sigma_{\text{d}}(k)}{1 + G_{\text{loc}}(i\nu_n)\Sigma_{\text{d}}(k)} + \Sigma_{\text{loc}}(i\nu_n). \tag{22}
$$

The result (22) was derived in Ref. [16].

3. The effect of the six-point vertex

3.1. Relation between the dual and lattice self-energy

The relation (22) does not change its form in the approximation, when one neglects six-point (and higher order) local vertices in Eq. (12). This however does not necessarily mean, that it remains correct in this case. Instead, as becomes clear from the following discussion, the relation (22) implicitly assumes that the one-particle reducible diagrams for six- and higher order vertices are taken into account.

Let us consider the diagrams for the self-energy, which include six-point one particle reducible vertex, such as the diagram shown in Fig. 1a. These diagrams, being 1PI in terms of the vertices $V_{\text{loc}}^{(6)}$, produce nevertheless one-particle reducible contributions to the self-energy, which should be excluded. The denominator in the relation (22) aims to remove the corresponding one-particle reducible diagrams for self-energy. Formulated differently, the quantity Σ' in Eq. (22) must contain one-particle reducible diagrams, which are cancelled by the denominator in the first term in Eq. (22).

To prove this statement for the diagrams, similar to that of Fig. 1a, containing repeating lowest (second-order) diagram of Fig. 1b, it is sufficient to consider the tree diagram contribution to the six-point vertex of the form $V_{\mathrm{loc}}^{(6)} = \sum \Gamma_{\mathrm{loc}} G_{\mathrm{loc}} \Gamma_{\mathrm{loc}}$, the sum is taken over different combinations of 4-momenta, assigned to 4-point vertices. Decoupling the resulting six-particle interaction with the fermionic Hubbard-Stratonovich transformation by introducing auxiliary fermionic field ϕ_k, we obtain

$$
\begin{aligned}
e^{-\widehat{\mathcal{V}}[\widehat{\eta},\widehat{\eta}^+,\widehat{\zeta},\widehat{\zeta}^+]} &= \int d[\widetilde{c},\widetilde{c}^+]\exp\Bigg\{\sum_{k,\sigma}\Big[\widetilde{G}_k^{-1}\left(\widetilde{c}_{k,\sigma}^+ - \widehat{\eta}_{k,\sigma}^+\right)\left(\widetilde{c}_{k,\sigma} - \widehat{\eta}_{k,\sigma}\right) \\
&\quad + G_{\mathrm{loc}}^{-1}(i\nu_n)(\phi_{k,\sigma}^+ - \widehat{\zeta}_{k,\sigma}^+)(\phi_{k,\sigma} - \widehat{\zeta}_{k,\sigma})\Big] \\
&\quad - \widehat{\mathcal{V}}'_{DMFT}[\widetilde{c}^+,\widetilde{c},\phi^+,\phi]\Bigg\}
\end{aligned}
\tag{23}
$$

$$
\begin{aligned}
\widehat{\mathcal{V}}'_{DMFT}[\widetilde{c}^+,\widetilde{c},\phi^+,\phi] &= \frac{1}{2}\Gamma_{\mathrm{loc}}\circ(\widetilde{c}_{k_1,\sigma}^+\widetilde{c}_{k_3,\sigma})(\widetilde{c}_{k_2,\sigma'}^+\widetilde{c}_{k_4,\sigma'}) \\
&\quad + \Gamma_{\mathrm{loc}}\circ(\widetilde{c}_{k_1,\sigma}^+\widetilde{c}_{k_3,\sigma})(\widetilde{c}_{k_2,\sigma'}^+\phi_{k_4,\sigma'}) \\
&\quad + \Gamma_{\mathrm{loc}}\circ(\widetilde{c}_{k_1,\sigma}^+\widetilde{c}_{k_3,\sigma})(\phi_{k_2,\sigma'}^+\widetilde{c}_{k_4,\sigma'})
\end{aligned}
\tag{24}
$$

where we have introduced source fields $\widehat{\zeta}$ for fermions ϕ. The effective interaction (23) can be put in more compact form by introducing spinors $\Phi_{k,\sigma} = (\widetilde{c}_{k,\sigma},\phi_{k,\sigma})$ and $\Pi_{k\sigma} = (\widehat{\eta}_{k,\sigma},\widehat{\zeta}_{k,\sigma})$, such that

$$
e^{-\widehat{\mathcal{V}}[\Pi,\Pi^+]} = \int d[\Phi,\Phi^+]e^{\sum_{k,\sigma}\left(\Phi_{k\sigma}^+ - \Pi_{k\sigma}^+\right)\widehat{G}_k^{-1}(\Phi_{k\sigma} - \Pi_{k\sigma}) - \widehat{\mathcal{V}}'_{DMFT}[\Phi^+,\Phi]}
\tag{25}
$$

where the corresponding matrix bare Green function reads

$$
\widehat{G}_k = \begin{pmatrix} \widetilde{G}_k & 0 \\ 0 & G_{\mathrm{loc}}(i\nu_n) \end{pmatrix}
\tag{26}
$$

It is of crucial importance that the matrix Green function, Eq. (26), contains both, the non-local $\widetilde{G}_k$ and the local $G_{\mathrm{loc}}(i\omega_n)$ components, which are mixed through the non-local dual self-energy, as considered below.

The resulting two-point vertices can be also considered as matrices in the space $(\widehat{\eta},\widehat{\zeta})$. The relation between the lattice and dual two-point vertices then has the form, similar to the Eq. (17),

$$
V_k^{(2)} = \begin{pmatrix} \frac{\Sigma_{\mathrm{loc}}(i\nu_n)}{1-\Sigma_{\mathrm{loc}}(i\nu_n)G_{0k}} & 0 \\ 0 & 0 \end{pmatrix} + \widehat{V}_k^{(2)}
\tag{27}
$$

$$
\widehat{V}_k^{(2)} = \widehat{\Sigma}_{\mathrm{d}}(k)[1 - \widehat{G}_k\widehat{\Sigma}_{\mathrm{d}}(k)]^{-1},
$$

where $\widehat{\Sigma}_{\mathrm{d}}(k)$ is the self-energy matrix of $\widetilde{c}_{k,\sigma}$ and $\phi_{k,\sigma}$ fields, having both, diagonal and off-diagonal contributions. For the second-order diagram of Fig. 1b the self-energy is equal for both fermion species:

$$
\widehat{\Sigma}_{\mathrm{d}}(k) = \Sigma_{\mathrm{d}}^{\mathrm{1PI}}(k)\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.
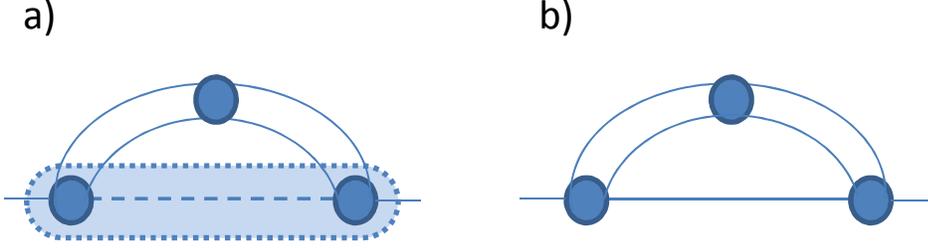\tag{28}
$$

a)

b)

Figure 2. (Color online) The non-local contributions to the lattice self-energy, which are of the third order in four-point local vertices. (a) The contribution, containing the local Green function, coming from the one-particle reducible six-point vertex. (b) Similar contribution of the dual fermion approach, neglecting six-point vertices. Notations are the same, as in Fig. 1

where $\Sigma_{\mathrm{d}}^{\mathrm{1PI}}(k)$ is the value of the 1PI diagram of Fig. 1b. From this we obtain the relation between the local and lattice self-energies

$$V_k^{(2)\widetilde{c},\widetilde{c}} = \frac{\Sigma_{\mathrm{loc}}(i\nu_n)}{1 - \Sigma_{\mathrm{loc}}(i\nu_n)G_{0k}} + \frac{\Sigma_{\mathrm{d}}^{\mathrm{1PI}}(k)}{1 - G_k\Sigma_{\mathrm{d}}^{\mathrm{1PI}}(k)}\frac{1}{[1 - \Sigma_{\mathrm{loc}}(i\nu_n)G_{0k}]^2}$$

$$= \frac{\Sigma_k}{1 - \Sigma_k G_{0k}}, \tag{29}$$

which yields

$$\Sigma_k = \Sigma_{\mathrm{loc}}(i\nu_n) + \Sigma_{\mathrm{d}}^{\mathrm{1PI}}(k). \tag{30}$$

The result (30) is essentially different from Eq. (22) and implies that the one-particle reducible contributions in the self-energy, occurring due to the one-particle reducible contributions to the six-point vertex, are indeed cancelled by the denominator in Eq. (22). Equtions (22) and (30) also imply the analogue of the Dyson equation for the dual fermion self-energy

$$\Sigma_{\mathrm{d}}(k) = \frac{\Sigma_{\mathrm{d}}^{\mathrm{1PI}}(k)}{1 - G_{\mathrm{loc}}(i\nu_n)\Sigma_{\mathrm{d}}^{\mathrm{1PI}}(k)}. \tag{31}$$

Having the 1PI self-energy $\Sigma_{\mathrm{d}}^{\mathrm{1PI}}(k)$ the result (30) should be used to obtain the lattice self-energy instead of the equation (22), suggested by Refs. [16, 17, 18, 19].

For the considered theory with only six-point one-particle reducible contributions included, the newly derived relation (30) between the dual and lattice self-energy is fulfilled if (and only if) the self-energy is equal for both fermion species $\widetilde{c}$ and ϕ, as it happens for the diagram of Fig. 1b. The abovementioned assumption does not necessarily hold in higher orders of dual perturbation theory. However, the inclusion of one-particle reducible contributions of higher order (eight and more point vertices) makes the relations (30) and (31) fulfilled in more general situations[23].

The one-particle reducible contributions to the six-point vertex can also produce 1PI self-energy diagrams, containing local Green functions, such as shown in Fig. 2a. These diagrams, being formally of the same order in the local 4-point vertices, as considered by the dual fermion approach (Fig. 2b), are not taken into account when the six-point and higher vertices are not taken into account. At the same time, the diagrams,

similar to that shown in Fig. 2a, can produce even larger contribution to the self-energy, than the diagrams of the dual fermion approach, neglecting 6-point and higher vertices, since the sum of the local Green function over momentum does not vanish. Therefore, accounting one-particle reducible parts of six- and higher-order local vertices appears to be crucially important for both, the diagrammatic consistency of the dual fermion approach and keeping all the diagrams of the same order in the four-point local vertices.

We also note that the covariation splitting method, used in the dual fermion approach (9), is similar to that applied in functional renormalization-group approach (see, e.g., Refs. [24, 21]), except that the latter considers integration of degrees of freedom in many infinitesimally small steps, while the former – only in two steps. Similarly to the discussion above, in the Polchinski formulation of the functional renormalization-group approach [24, 21] one-particle reducible contributions to six-point vertices were argued to be important for proper calculation of the four-point vertices already in one-loop approximation [25]. The same contributions can be also shown to be important for evaluation of multi-loop contributions to the self-energy. In the next subsection we address another aspect, where the six- and higher-order vertices appear to be important in the dual fermion approach.

3.2. Self-energy feedback

The dual fermion approach accounts for the self-energy feedback by dressing the Green function of the non-local degrees of freedom:

$$\widetilde{\mathbb{G}}_k = \widetilde{G}_k / [1 - \widetilde{G}_k \Sigma_{\mathrm{d}}(k)]. \tag{32}$$

However, the function $\widetilde{G}_k$, which represents a difference of two propagators, does not correspond to a physically observable quantity, and it is informative to trace, how dressing it one can finally obtain the physical propagator

$$\mathbb{G}_k = G_k / [1 - G_k(\Sigma_k - \Sigma_{\mathrm{loc}})] \tag{33}$$
$$= G_k / [1 - G_k \Sigma_{\mathrm{d}}^{\mathrm{1PI}}(k)],$$

which is constructed by dressing the Green function G_k, see Eq. (6), containing only the local self-energy, by the remaining self-energy difference $\Sigma_k - \Sigma_{\mathrm{loc}}$. We have observed in Sect. 3.1, that in the lowest orders of perturbation theory, propagators $\widetilde{\mathbb{G}}_k$, appearing in the diagram technique for Eq. (19), are added by G_{loc}, coming either from either adding local quantities to their non-local counterparts (such as in Eq. (30)), or from the contributions, containing one-particle reducible six-point and higher order vertices, such as the diagram of Fig. 2a. Adding G_{loc} to $\widetilde{\mathbb{G}}_k$ is however still not sufficient to reproduce (33) for $\Sigma_{\mathrm{d}}^{\mathrm{1PI}}(k) \neq 0$.

Again, we argue, that the six- and higher order local vertices are crucially important to obtain (33). To see this, let us insert $G_k = \widetilde{G}_k + G_{\mathrm{loc}}$ into Eq.(33), use Eqs. (31) and (32) to represent the result in terms of $\widetilde{\mathbb{G}}_k$ and $\Sigma_{\mathrm{d}}^{\mathrm{1PI}}(k)$, and expand the result in a
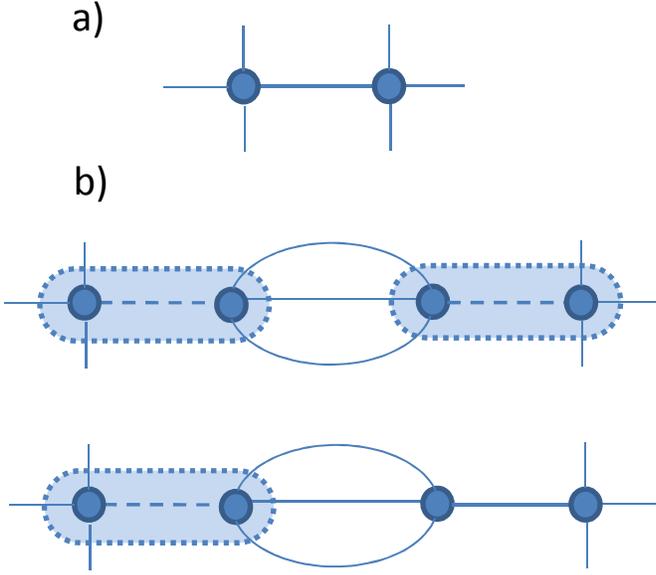
Figure 3. (Color online) Dressing of the non-local Green function $\widetilde{\mathbb{G}}_k$, shown by bold line and appearing as a part of diagram (a) by the two contributions of the lowest-order in $\Sigma_{\mathrm{d}}^{\mathrm{1PI}}(k)$ (b). Notations are the same, as in Fig. 1

series of $\Sigma_{\mathrm{d}}^{\mathrm{1PI}}(k)$:

$$\mathbb{G}_k = \sum_{n=1}^{\infty} [G_{\mathrm{loc}}(i\nu_n) + n\widetilde{\mathbb{G}}_k][G_{\mathrm{loc}}(i\nu_n)\Sigma_{\mathrm{d}}^{\mathrm{1PI}}(k)]^{n-1} \tag{34}$$

The term with $n = 1$ represents the combination $G_{\mathrm{loc}} + \widetilde{\mathbb{G}}_k$, discussed above, while the terms with $n \geq 2$ in this series expansion can be ascribed to the respective diagrams (see Fig. 3 for $n = 2$), where the one-particle irreducible local vertices are connected by local propagators, forming one-particle reducible six-point and higher vertices. The dual fermion approach, which does not account for the six-point and higher order vertices, neglects therefore a difference between $\mathbb{G}_k$ and $\widetilde{\mathbb{G}}_k + G_{\mathrm{loc}}$.

4. Conclusion

In the present paper we have considered effect of one-particle reducible six- and higher-point vertices in the dual fermion approach. We have argued that the one-particle reducible contributions to these vertices are important to make the dual fermion approach diagrammatically consistent. Neglecting the six-point and higher order vertices does not allow to obtain correct relation between the dual and lattice self-energies, as well as treat correctly the feedback of the dual self-energy on the dual Green functions. Apart from that, the one-particle reducible six-point and higher order vertices lead to the self-energy corrections, which contain both, local and non-local Green functions.

Further numerical investigations of the (un)importance of the described contributions of six-point and higher-order vertices to be performed (see, e.g., Ref.

[23]). This also calls for developing a new method of treatment of non-local degrees of freedom, which avoids the described problems of the dual fermion approach and operates with the one-particle irreducible quantities.

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