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 six-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 six-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 four-point vertices as the diagrams usually considered in the approach. These observations highlight an importance of six-point and higher order vertices in the dual fermion approach, and call for the development of new schemes of treatment of non-local fluctuations, which are based on one-particle irreducible quantities.

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(Some figures may appear in colour only in the online journal)

1. Introduction

Strongly correlated electron systems have become one of the touchstones 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] accurately describes the Mott–Hubbard metal–insulator transition [3].
DMFT becomes exact in the limit of high spatial dimensions \((d \to \infty)\) and accounts for an important local part of electronic correlations. Real physical systems are however one-, two- or three-dimensional. Therefore, non-local correlations, which are neglected in DMFT, may be important. Recently, progress to go beyond DMFT through cluster extensions [4–8] was achieved. These correlations are however necessarily short-range in nature due to numerical limitations of the cluster size [9].

This limitation motivated the development of the diagrammatic extensions of the DMFT. The dynamical vertex approximation (D\(\Gamma\)A) was introduced in [10–15]. Starting from the local particle–hole irreducible vertex, this approximation sums ladder diagrams for the vertex in the particle–hole channel, considering the effect of the non-locality of the Green functions. An alternative dual fermion (DF) approach was proposed in [16–19], 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 above-mentioned approaches use a four-point local vertex as an effective interaction between fermionic degrees of freedom (lattice fermions in the case of D\(\Gamma\)A and dual fermions in the DF approach), they in fact make very different assumptions on the neglect of higher order local vertices. Indeed, D\(\Gamma\)A operates with one-particle irreducible (1PI) vertices, and in the practical implementations neglects six-point and higher order 1PI local vertices. At the same time, the DF representation does not use the assumption of the one-particle irreducibility; in particular, its formulation in [16–19] neglects one-particle reducible six-point and higher vertices.

This difference appears to be important for analysing the diagrammatic consistency of the above-discussed 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 this paper, we show that the inclusion 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 \(H_{\text{int}}[\hat{c}_{i \sigma}, \hat{c}^+_{i \sigma}]\)

\[
H = \sum_{k, \sigma} \epsilon_{k, \sigma} \hat{c}_{k, \sigma}^\dagger \hat{c}_{k, \sigma} + \sum_{i, \sigma} H_{\text{int}}[\hat{c}_{i \sigma}, \hat{c}^+_{i \sigma}],
\]

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

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

\[
S[c, c^+] = \int d\tau \left\{ \sum_{\sigma} c^\dagger_{\sigma} (\tau) \frac{\partial}{\partial \tau} c_{\sigma} (\tau) + H_{\text{int}}[c^+, c^+] \right\},
\]

where \(c_{\sigma}, c^\dagger_{\sigma}, \eta_{\sigma}, \eta^+_{\sigma}\) are the Grassman fields, the fields \(\eta_{\sigma}, \eta^+_{\sigma}\) correspond to source terms. The DMFT corresponds to considering the effective single-site problem with the action

\[
S_{\text{DMFT}}[c, c^+] = \sum_{i, \sigma} \int d\tau \left\{ -\xi^{-1}(\tau) c^\dagger_{\sigma} (\tau) c_{\sigma} (\tau) + H_{\text{int}}[c_{\sigma}, c^+_{\sigma}] \right\}.
\]
where the ‘Weiss field’ function \( \zeta(\tau) \) and its Fourier transform \( \zeta(iv_n) \) has to be determined self-consistently from the condition

\[
G_{\text{loc}}(iv_n) := \frac{1}{\zeta^{-1}(iv_n) - \Sigma_{\text{loc}}(iv_n)} = \sum_k G(k, iv_n),
\]

where

\[
G(k, iv_n) := G_k = \left[ G_{0k}^{-1} - \Sigma_{\text{loc}}(iv_n) \right]^{-1},
\]

\( G_{0k}^{-1} = iv_n - \epsilon_k \) is the lattice noninteracting Green function (we use the 4-vector notation \( k = (k, iv_n) \)) and \( \Sigma_{\text{loc}}(iv_n) \) 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 [16–19] can be conveniently formulated in terms of an effective interaction of the lattice theory (see, e.g. [21]):

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

\[
= -\ln Z \left[ G_{0k}^{-1} \eta_{k,\sigma}, G_{0k}^{-1} \eta_{k,\sigma}^+ \right] - \eta_{k,\sigma} G_{0k}^{-1} \eta_{k,\sigma}.
\]

(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 \( \Sigma_k \) of the lattice problem (i.e. the 1PI two-point vertex function) can be extracted from the two-point connected vertex function \( V^{(2)} \) via the relation \( V^{(2)}_k = \Sigma_k/(1 - G_{0k} \Sigma_k) \).

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

\[
\sum_{k,\sigma} C_k^{-1} c_{k,\sigma} c_{k,\sigma} = \ln \int d[\tilde{c}, \tilde{c}^+] \exp \left\{ \sum_{k,\sigma} \tilde{c}_{k,\sigma}^+ B_k^{-1} \tilde{c}_{k,\sigma} + \sum_{k,\sigma} A_k^{-1} \left( \tilde{c}_{k,\sigma}^+ c_{k,\sigma} + c_{k,\sigma}^+ \tilde{c}_{k,\sigma} \right) \right\},
\]

(8)

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

\[
\mathcal{V}(\eta, \eta^+) = -\ln \int d[\tilde{c}, \tilde{c}^+] \exp \left\{ \sum_{k,\sigma} \tilde{c}_{k,\sigma}^+ \tilde{G}_{0k}^{-1} \tilde{c}_{k,\sigma} - V_{\text{DMFT}}[\eta^+ + \tilde{c}^+, \eta + \tilde{c}] \right\},
\]

(9)

where \( V_{\text{DMFT}}[\eta, \eta^+] \) is an effective interaction of the DMFT, defined by

\[
e^{-V_{\text{DMFT}}[\eta, \eta^+]} = \int d[c, \bar{c}^+] \exp \left\{ -\sum_{\sigma} H_{\text{int}}[c_{\sigma}, c_{\sigma}^+] + \sum_{k,\sigma} \zeta^{-1}(iv_n) \left( c_{k,\sigma}^+ + \eta_{k,\sigma}^+(c_{k,\sigma} + \eta_{k,\sigma}) \right) \right\},
\]

(10)

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

To simplify equation (9), we perform a shift \( \tilde{c}_{k,\sigma} \rightarrow \tilde{c}_{k,\sigma} - \eta_{k,\sigma} \), such that

\[
\mathcal{V}(\eta, \eta^+) = -\ln \int d[\tilde{c}, \tilde{c}^+] \exp \left\{ \sum_{\sigma} \tilde{c}_{k,\sigma}^+ \tilde{G}_{0k}^{-1} \tilde{c}_{k,\sigma} - V_{\text{DMFT}}[\tilde{c}, \tilde{c}^+] \right\}.
\]

(11)
To arrive at the standard dual fermion approach [16–19], we consider an expansion of $\tilde{\mathcal{V}}_{\text{DMFT}}[\tilde{\varphi}, \tilde{\varphi}^+]$ in fields

$$\tilde{\mathcal{V}}_{\text{DMFT}}[\tilde{\varphi}, \tilde{\varphi}^+] = \sum_{k,\sigma} \tilde{c}_{k,\sigma}^\dagger \frac{\Sigma_\text{loc}(iv_n)}{1 - \xi(iv_n)\Sigma_\text{loc}(iv_n)} \tilde{c}_{k,\sigma} + \tilde{\mathcal{V}}_{\text{DMFT}}^\text{loc}[\tilde{\varphi}, \tilde{\varphi}^+]$$

$$\tilde{\mathcal{V}}_{\text{DMFT}}^\text{loc}[\tilde{\varphi}, \tilde{\varphi}^+] = \frac{i}{\hbar} \Gamma^\text{loc} \circ (\tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma}^\dagger) (\tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma}^\dagger) + \frac{i}{\hbar} \Gamma^\text{loc}(6) \circ (\tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma}^\dagger) (\tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma}^\dagger) (\tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma}^\dagger) + \cdots$$

(12)

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

$$\tilde{\Gamma}_\text{loc}^{\sigma\sigma'}(iv_1..iv_4) = (1 + \delta_{\sigma\sigma'})^{-1} \prod_{n=1}^4 \xi^{-1}(iv_n)$$

$$\times [G^{(4)}_{\text{loc},\sigma\sigma'}(iv_1..iv_4) - G_{\text{loc}}(iv_1)G_{\text{loc}}(iv_2)(\delta_{\nu_1\nu_2} - \delta_{\nu_1\nu_3} - \delta_{\nu_2\nu_3})],$$

(13)

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

$$\mathcal{V}[\eta, \eta^+] = -\sum_{k,\sigma} \eta_{k,\sigma}^+ \tilde{c}_{k,\sigma}^\dagger \eta_{k,\sigma} - \int D[\tilde{\varphi}, \tilde{\varphi}^+] e^{\xi \sum_{i} \frac{1}{\Sigma_\text{loc}(iv_n)} \Sigma_\text{loc}(iv_n) \tilde{\Gamma}_\text{loc} - \eta_{\text{loc}} [1 - \Sigma_\text{loc}(iv_n)G_{\text{loc}}] \tilde{\Gamma}_\text{loc}^\dagger} \eta_{\text{loc}},$$

(14)

where

$$\tilde{G}_k = \frac{\tilde{\eta}_\text{loc}}{1 - \xi(iv_n)\Sigma_\text{loc}(iv_n)} = [1 - \xi(iv_n)\Sigma_\text{loc}(iv_n)]^2 \tilde{G}_k,$$

(15)

and $\tilde{\Gamma}_\text{loc} = \tilde{G}_k - G_{\text{loc}}(io_0)$. Rescaling the fields of integration to exclude extra factor $(1 - \xi \Sigma_\text{loc})^2$ and introducing the ‘dual’ source field

$$\tilde{\eta}_{\text{loc}} = \eta_{\text{loc}}/[1 - \Sigma_\text{loc}(iv_n)G_{\text{loc}}],$$

(16)

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

$$\mathcal{V}[\eta, \eta^+] = \tilde{\mathcal{V}}[\tilde{\eta}, \tilde{\eta}^+] = \sum_{k,\sigma} \tilde{\eta}_{k,\sigma}^+ \left\{ \tilde{G}_{k}^\dagger - \frac{1}{1 - \Sigma_\text{loc}(iv_n)G_{\text{loc}}} \tilde{\Gamma}_{k}^\dagger \right\} \eta_{k,\sigma}$$

(17)

$$\tilde{\mathcal{V}}[\tilde{\eta}, \tilde{\eta}^+] = \sum_{k,\sigma} \tilde{\eta}_{k,\sigma}^+ \frac{\Sigma_\text{loc}(iv_n)}{1 - \Sigma_\text{loc}(iv_n)G_{\text{loc}}} \eta_{k,\sigma},$$

(18)

where

$$\tilde{\mathcal{V}}[\tilde{\eta}, \tilde{\eta}^+] = -\int D[\tilde{\varphi}, \tilde{\varphi}^+] e^{\xi \sum_{i} \frac{1}{\Sigma_\text{loc}(iv_n)} \Sigma_\text{loc}(iv_n) \tilde{\Gamma}_\text{loc} - \tilde{\eta}_{\text{loc}} [1 - \Sigma_\text{loc}(iv_n)G_{\text{loc}}] \tilde{\Gamma}_\text{loc}^\dagger} \tilde{\mathcal{V}}_{\text{DMFT}}[\tilde{\varphi}, \tilde{\varphi}^+]$$

(19)

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

$$\tilde{\mathcal{V}}_{\text{DMFT}}[\tilde{\varphi}, \tilde{\varphi}^+] = \frac{i}{\hbar} \Gamma_\text{loc} \circ (\tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma}^\dagger) (\tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma}^\dagger) + \frac{i}{\hbar} \Gamma_\text{loc}(6) \circ (\tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma}^\dagger) (\tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma}^\dagger) (\tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma}^\dagger) + \cdots$$

(20)

where $\Gamma_\text{loc} = \Gamma_\text{loc}^{\text{loc}} \prod_{n=1}^4 (1 - \xi \Sigma_\text{loc})_{iv}$ and $\Gamma_\text{loc}^{(6)} = \Gamma_\text{loc}^{(6)} \prod_{n=1}^6 (1 - \xi \Sigma_\text{loc})_{iv}$ are the connected four- and six-point vertices, amputated with the local Green functions $G_{\text{loc}}$. For the four-point vertex $\Gamma_{\text{4-point}}$, the requirement of connectivity and amputation with the full local Green functions implies one-particle irreducibility. However, the higher order vertices, e.g. $\Gamma_{\text{6-point}}$, remain one-particle reducible.
In the described approach, the relation between the self-energies $\Sigma_d(k)$ of the dual fermions $\tilde{c}_k$ and $\Sigma_k$ of the lattice fermions $c_k$ is easily obtained by equating the corresponding two-point vertices in equation (17):

$$\frac{\Sigma_k}{1 - \Sigma_k G_{0k}} = \frac{\Sigma_{\text{loc}}(iv_n)G_{0k}}{1 - \Sigma_{\text{loc}}(iv_n)G_{0k}} + \frac{\Sigma_d(k)}{1 - \Sigma_d(k)[G_k - G_{\text{loc}}(iv_n)]} \frac{1}{1 - \Sigma_{\text{loc}}(iv_n)G_{0k}}[1 - \Sigma_{\text{loc}}(iv_n)G_{0k}]^2, \ (21)$$

which implies

$$\Sigma_k = \frac{\Sigma_d(k)}{1 + G_{\text{loc}}(iv_n)\Sigma_d(k)} + \Sigma_{\text{loc}}(iv_n). \ (22)$$

Result (22) was derived in [16].

3. The effect of the six-point vertex

3.1. Relation between the dual and lattice self-energy

Relation (22) does not change its form in the approximation, when one neglects six-point (and higher order) local vertices in equation (19). This however does not necessarily mean that it remains correct in this case. Instead, as becomes clear from the following discussion, relation (22) implicitly assumes that at least one-particle reducible contributions to six- and higher order vertices are taken into account.

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

To prove this statement for the diagrams, similar to that of figure 1(a), containing repeating lowest (second-order) diagram of figure 1(b), it is sufficient to consider the tree diagram contribution to the six-point vertex of the form $\Gamma^{(6)}_{\text{loc}} = \sum G_{\text{loc}} G_{\text{loc}}$, the sum is taken over different combinations of 4-momenta, assigned to four-point vertices. Decoupling the resulting six-particle interaction in equation (19) with the fermionic Hubbard–Stratonovich transformation by introducing auxiliary fermionic field $\phi_k$, we obtain

$$e^{-\hat{\mathcal{V}}[\pi,\pi^+ \phi^+] = \int d[\tilde{c}, \tilde{\phi}^+] \exp \left\{ \sum_{k,\sigma} \left[ \hat{G}_k^{-1}(\hat{e}_{k,\sigma} - \tilde{\eta}_{k,\sigma}) (\hat{e}_{k,\sigma} - \tilde{\eta}_{k,\sigma}) \right] + \hat{G}_{\text{loc}}^{-1}(iv_n)(\phi_{k,\sigma}^+ - \tilde{\zeta}_{k,\sigma}^+)(\phi_{k,\sigma} - \tilde{\zeta}_{k,\sigma}) \right\} - \hat{\mathcal{V}}_{\text{DMFT}}[\tilde{c}^+, \tilde{\phi}^+, \phi] \} \ (23)$$

$$\hat{\mathcal{V}}_{\text{DMFT}}[\tilde{c}^+, \tilde{\phi}^+, \phi] = \frac{1}{2} \Gamma_{\text{loc}} \circ (\hat{c}_{k,\sigma}^+ \tilde{c}_{k,\sigma}^+)(\hat{c}_{k,\sigma} \tilde{c}_{k,\sigma}^+) + \Gamma_{\text{loc}} \circ (\tilde{c}_{k,\sigma}^+ \tilde{c}_{k,\sigma}^+)(\hat{c}_{k,\sigma}^+ \hat{c}_{k,\sigma}^+) + \Gamma_{\text{loc}} \circ (\hat{c}_{k,\sigma} \tilde{c}_{k,\sigma}^+)(\hat{c}_{k,\sigma}^+ \tilde{c}_{k,\sigma}^+), \ (24)$$

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

$$e^{-\hat{\mathcal{V}}[\pi,\pi^+] = \int d[\Phi, \Phi^+] \exp \left\{ \sum_{k,\sigma} (\Phi_{k,\sigma} - \Pi_{k,\sigma})(\Phi_{k,\sigma}^+ - \Pi_{k,\sigma}^+) - \hat{\mathcal{V}}_{\text{DMFT}}[\Phi^+, \Phi] \right\}, \ (25)$$

where the corresponding matrix bare Green function reads

$$\hat{G}_k = \begin{pmatrix} \hat{G}_k & 0 \\ 0 & G_{\text{loc}}(iv_n) \end{pmatrix}. \ (26)$$
Figure 1. (a) The one-particle reducible contributions to the lattice two-point Green function, coming from the one-particle reducible six-point local vertex (shaded). The circles correspond to the four-point local vertices, solid line—the propagator $\tilde{G}_k$, 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 four-point vertices.

It is of crucial importance that the matrix Green function, equation (26), contains both, the non-local $\tilde{G}_k$ and the local $G_{loc}(i\nu_n)$ 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 $(\tilde{\eta}, \tilde{\zeta})$. The relation between the lattice and dual two-point vertices then has the form, similar to the equation (17),

$$V^{(2)}_k = \left( \begin{array}{cc} \Sigma_{loc}(i\nu_n) & 0 \\ 0 & \Sigma^{1PI}_d(k) \end{array} \right) + \tilde{V}^{(2)}_k,$$

$$\tilde{V}^{(2)}_k = \tilde{\Sigma}_d(k)[1 - \tilde{G}_k \tilde{\Sigma}_d(k)]^{-1}, \quad (27)$$

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

$$\tilde{\Sigma}_d(k) = \Sigma^{1PI}_d(k) \left( \begin{array}{cc} 1 & 1 \\ 1 & 1 \end{array} \right), \quad (28)$$

where $\Sigma^{1PI}_d(k)$ is the 1PI dual fermion self-energy, given by the diagram of figure 1(b). From this we obtain the relation between the local and lattice self-energies:

$$V^{(2)^{\nu,\tau}}_k = \frac{\Sigma_{loc}(i\nu_n)}{1 - \Sigma_{loc}(i\nu_n)G_{0k}} + \frac{\Sigma^{1PI}_d(k)}{1 - G_k \Sigma^{1PI}_d(k)[1 - \Sigma_{loc}(i\nu_n)G_{0k}]} = \frac{\Sigma_k}{1 - \Sigma_kG_{0k}}, \quad (29)$$

which yields

$$\Sigma_k = \Sigma_{loc}(i\nu_n) + \Sigma^{1PI}_d(k). \quad (30)$$

Result (30) is essentially different from equation (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 equation (22). Equations (22) and (30) also imply the analogue of the Dyson equation for the dual fermion self-energy:

$$\Sigma_d(k) = \Sigma^{1PI}_d(k) \frac{1}{1 - G_{loc}(i\nu_n)\Sigma^{1PI}_d(k)}. \quad (31)$$

Having the 1PI self-energy $\Sigma^{1PI}_d(k)$, result (30) should be used to obtain the lattice self-energy instead of the equation (22), suggested by [16–19].

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 $\tilde{c}$ and $\phi$, as it happens for the diagram in figure 1(b). The above-mentioned 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 relations (30) and (31) fulfilled in more general situations [23].
Figure 2. 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 figure 1.

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 figure 2(a). These diagrams, being formally of the same order in the local four-point vertices, as considered by the dual fermion approach (figure 2(b)), 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 figure 2(a), can produce an even larger contribution to the self-energy than the diagrams of the dual fermion approach, neglecting six-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 the functional renormalization-group approach (see, e.g., [24, 21]), except that the latter splits 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], 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 also be shown to be important for the evaluation of multi-loop contributions to the self-energy. In the following 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:

\[
\tilde{G}_k = \tilde{G}_k/[1 - \tilde{G}_k \Sigma_1^{1PI}(k)].
\] (32)

However, the function \(\tilde{G}_k\), 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

\[
\tilde{G}_k = G_k/[1 - G_k (\Sigma_k - \Sigma_{loc})]
= G_k/[1 - G_k \Sigma_1^{1PI}(k)],
\] (33)

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

Again, we argue, that the six- and higher order local vertices are crucially important to obtain (33). To see this, let us insert $G_k = \tilde{G}_k + G_{\text{loc}}$ into equation (33), use equations (31) and (32) to represent the result in terms of $\tilde{G}_k$ and $\Sigma_d^{\text{1PI}}(k)$, and expand the result in a series of $\Sigma_d^{\text{1PI}}(k)$:

$$G_k = \sum_{n=1}^{\infty} [G_{\text{loc}}(iv_n) + n\tilde{G}_k][G_{\text{loc}}(iv_n)\Sigma_d^{\text{1PI}}(k)]^{n-1}. \quad (34)$$

The term with $n = 1$ represents the combination $G_{\text{loc}} + \tilde{G}_k$, discussed above, while the terms with $n \geq 2$ in this series expansion can be ascribed to the respective diagrams (see figure 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, therefore neglects a difference between $\tilde{G}_k$ and $\tilde{G}_k + G_{\text{loc}}$.

4. Conclusion

In this paper, we have considered the 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 us to obtain the correct relation between the dual and lattice self-energies, as well as correctly treat 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 are to be performed (see, e.g., [23]). This also calls for the development of 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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