Using the (extended) dynamical mean field theory as a starting point for the two-particle irreducible functional renormalization-group approach for strongly-correlated systems

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Abstract

We suggest a new approach for treatment of local and non-local interactions in correlated electronic systems, which is based on the combination of the (extended) dynamical mean-field theory ((E)DMFT) and the two-particle irreducible functional renormalization-group (2PI-fRG) method. The considering approach uses self-energy and the two-particle irreducible vertices, obtained from (E)DMFT, as an input of 2PI-fRG approach. Using 2PI vertices may improve the applicability of various truncations and fulfilling conservation laws in comparison with one-particle irreducible approaches. In case of purely local interaction in a certain "ladder" truncation of the DMFT+2PI-fRG equations, the obtained equation for the self-energy has a similar, although not identical, structure to that in the ladder dynamic vertex approximation (DΓA). For the non-local interactions, in a simplest truncation we reproduce the results for the two-particle vertices/susceptibilities in the ladder approximation of the dual boson approach, but obtain different equation for the self-energy with a correct treatment of the one-particle reducible vertices of higher orders. The proposed scheme is rather general and can be applied to study various phenomena in strongly-correlated electronic systems, e.g. as a tool describing ab initio screening of the Coulomb interaction in strongly correlated systems.
I. INTRODUCTION

Strongly-correlated electronic systems attract a lot of attention, since they show a broad variety of interesting physical phenomena, such as spin- and charge-density wave instabilities, as well as superconductivity, originating from interelectron Coulomb interaction, see, e.g., Refs. [1–3]. The screened part of this interaction can be effectively described by the on-site or nearest-neighbour repulsion, which may yield charge- or spin-density wave instabilities. Even the local interactions, dressed by the particle-hole bubbles, yield non-local attractive interaction in the superconducting channel [4, 5]. Apart from that, description of the dynamic screening in solids from first principles represents an interesting problem, see, e.g., Refs. [6–8].

Developing suitable approximations for treatment of local and non-local interactions in strongly-correlated electronic systems represents an important problem. While the local correlations in strongly-correlated systems are well described by the (extended) dynamical mean-field theory ((E)DMFT), see Refs. [7, 9–11], this theory is not sufficient to describe the non-local correlations. Recent progress in diagrammatic extensions of (E)DMFT, namely dynamic vertex approximation (DΓA) [12–17], dual fermion approach [18–22], and the dual boson approach [23–26] allowed to treat non-local correlations on a non-perturbative basis. Yet, the conservation laws are fulfilled only in some special versions of these approaches (see, e.g., the discussion in Ref. [25]).

The concept of Φ-derivability, proposed long time ago [27], allows to search for new approaches, which treat non-local correlations in strongly-correlated systems. The fluctuation exchange approach (FLEX) [28] was proposed as a Φ-derivable approximation, which can yield self-energy and two-particle vertices, derived from the same functional, and therefore fulfilling the conservation laws. However, the corresponding self-energy, taken separately, contains only the result of the summation of ladder diagrams with respect to the bare interaction, and is not guaranteed to yield better results, than in the other diagrammatic approaches, see, e.g. the discussion in Refs. [29, 30]. The recently proposed TRILEX approach [31] extends the concept of Φ-derivability to merge dynamical mean-field theory with perturbation techniques; so far this approach was however applied to treat only local interactions.

Recently, the two-particle irreducible functional renormalization-group (2PI-fRG) ap-
proach was proposed \[32, 33\] and its application to quantum anharmonic oscillator \[34\] and single-impurity Anderson model \[35\] was discussed; the suitable truncation schemes were developed. In the strong coupling limit, however, the functional $\Phi[G]$, which yields the 2PI-fRG equations, may not be uniquely defined \[36\], and the diagrammatic series may converge to an unphysical self-energy. Although the 2PI-fRG is non-perturbative in principle, the standard truncations usually spoil this property. Therefore, search for non-perturbative starting points of $\Phi$ is important. In this respect, the (E)DMFT provides the natural starting point for the search of new functionals.

In the present paper we propose the scheme to merge of (E)DMFT and the 2PI-fRG approach. The suggested scheme follows earlier considered DMF$^2$RG approach \[37, 38\], which merges DMFT with one-particle irreducible (1PI) functional renormalization group \[39\] by using information from the DMFT (the self-energy and the one-particle irreducible vertices) as a starting point for the flow. In the strong-coupling regime, however, the one-particle irreducible vertices grow fast with the interaction, which may limit applicability of such an approach. The approach, considered in the present paper, uses instead two-particle irreducible vertices, which are (at least in the local theory) generally smaller, than 1PI vertices, which may improve the applicability of various truncations. Although it was shown recently that in the strong-coupling regime the charge and superconducting 2PI vertices may have negative eigenvalues \[40\] (which is likely related to the abovementioned problem of $\Phi[G]$ being not uniquely defined), this problem can be circumvented by an appropriate treatment of these channels (which will not be addressed in the present paper). We formulate the (E)DMFT+2PI-fRG method and relate it to known approaches to strongly-correlated systems. The plan of the paper is the following. In Sect. II we introduce the model and formulate the (E)DMFT approach in the notations, suitable for the following discussion. In Sect. III we describe the (E)DMFT+2PI-fRG approach, derive the respective equations, and analyse their results in simplest truncations. In Sect. IV we present conclusions and discuss perspectives of the presented approach.
II. THE MODEL AND EXTENDED DYNAMICAL MEAN-FIELD THEORY

We consider a general one-band model of interacting fermions

\[ H = \sum_{\mathbf{k}, \sigma} \varepsilon_{\mathbf{k}, \sigma} \hat{c}_{\mathbf{k}, \sigma}^+ \hat{c}_{\mathbf{k}, \sigma} + H_{\text{int}}[\hat{c}, \hat{c}^+], \]  
(1)

where \( \hat{c}_{\mathbf{i}, \sigma}, \hat{c}_{\mathbf{i}, \sigma}^+ \) are the fermionic operators, and \( \hat{c}_{\mathbf{k}, \sigma}, \hat{c}_{\mathbf{k}, \sigma}^+ \) are their Fourier transforms, \( \sigma = \uparrow, \downarrow \) corresponds to a spin index. The interaction \( H_{\text{int}} \) contains in general both, local \( U \) and non-local \( V_{ij}^{c,s} \) contributions, the latter act on charge and spin degrees of freedom,

\[ H_{\text{int}}[\hat{c}, \hat{c}^+] = \sum_{i} U n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{ij} \left( V_{ij}^{c} n_{i} n_{j} + V_{ij}^{s} \mathbf{S}_{i} \mathbf{S}_{j} \right), \]  
(2)

where \( n_{i\sigma} = \hat{c}_{i\sigma}^+ \hat{c}_{i\sigma} \) and \( \mathbf{S}_{i} = \hat{c}_{i\sigma}^{\uparrow} \sigma_{\sigma\sigma'} \hat{c}_{i\sigma'}^\downarrow, \sigma_{\sigma\sigma'} \) are the Pauli matrices.

The model is characterized by generating functional

\[ \mathcal{Z}[\eta, \eta^+] = \int \mathcal{D}[c, c^+] \exp \left\{ -\mathcal{S}[c, c^+] + \eta^+ c + c^+ \eta \right\}, \]  
(3)

\[ \mathcal{S}[c, c^+] = \int d\tau \left\{ \sum_{i, \sigma} c_{i\sigma}^+ (\tau) \frac{\partial}{\partial \tau} c_{i\sigma} (\tau) + H[c, c^+] \right\}, \]  
(4)

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 (extended) dynamical mean-field theory \([7, 11]\) for the model (1) can be introduced via the corresponding local action

\[ \mathcal{S}_{\text{E}DMFT}[c, c^+] = \int d\tau \int d\tau' \sum_{i, \sigma} c_{i\sigma}^+ (\tau) \zeta^{-1}(\tau - \tau') \xi_{i\sigma} (\tau) + H_{\text{int}}^{\text{loc}} [c_{i\sigma}, c_{i\sigma}^+] \]  
(5)

where

\[ H_{\text{int}}^{\text{loc}} [c_{i\sigma}, c_{i\sigma}^+] = \sum_{i} U n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{q} \left[ v^{c} (i\omega_{n}) n_{q} n_{-q} + v^{s} (i\omega_{n}) \mathbf{S}_{q} \mathbf{S}_{-q} \right], \]  
(6)

the ”Weiss field” functions \( \zeta (i\nu_{n}) \) and \( v (i\omega_{n}) \) have to be determined self-consistently from the conditions

\[ G_{\text{loc}} (i\nu_{n}) \equiv \frac{1}{\zeta^{-1} (i\nu_{n}) - \Sigma_{\text{loc}} (i\nu_{n})} = \sum_{\mathbf{k}} \mathcal{G} (\mathbf{k}, i\nu_{n}), \]  
(7a)

\[ \chi_{\text{loc}}^{c,s} (i\nu_{n}) \equiv \frac{1}{v^{c,s} (i\omega_{n}) + \Pi_{\text{loc}}^{c,s} (i\nu_{n})} = \sum_{\mathbf{q}} \chi_{\mathbf{q}}^{c,s} (\mathbf{q}, i\nu_{n}), \]  
(7b)

where

\[ \mathcal{G} (\mathbf{k}, i\nu_{n}) \equiv \mathcal{G}_{\mathbf{k}} = \left[ G_{\text{lok}}^{-1} - \Sigma_{\text{loc}} (i\nu_{n}) \right]^{-1}, \]  
(8)

\[ \chi_{\mathbf{q}}^{c,s} (\mathbf{q}, i\nu_{n}) \equiv \chi_{\mathbf{q}}^{c,s} = \left[ V^{c,s}_{\mathbf{q}} + \Pi_{\text{loc}}^{c,s} (i\omega_{n}) \right]^{-1} = \left[ \left( \chi_{\mathbf{q}}^{c,s} (i\omega_{n}) \right)^{-1} - v^{c,s} (i\omega_{n}) + V^{c,s}_{\mathbf{q}} \right]^{-1}, \]  
(9)
\( G_{0k}^{-1} = i\nu_n - \varepsilon_k \) is the lattice noninteracting Green function (we use the 4-vector notation \( k = (k, i\nu_n) \)) and \( \Sigma_{\text{loc}}(i\nu_n) \) and \( \Pi_{\text{loc}}^{c,s}(i\omega_n) \) is the bosonic and fermionic self-energy of the impurity problem \([5]\), which is in practice obtained within one of the impurity solvers: exact diagonalization, quantum Monte-Carlo, etc. These solvers provide information not only on the electronic self-energy, but also the corresponding vertex functions\([12, 41]\). \( F_{\text{loc}}^{\sigma\sigma'}(i\nu_1..i\nu_3) = (1 + \delta_{\sigma\sigma'})^{-1} \prod_{i=1}^{4} G_{\text{loc}}^{-1}(i\nu_i) \) \( G_{\text{loc}}^{(4)} \) is the two-particle local Green function, which can be obtained via the solution of the impurity problem. Solving Bethe-Salpeter equations in the spin- and charge channel then provides an information about the respective two-particle irreducible vertices in spin and charge channels, \( \Phi_{\text{loc}}^{(2),c}(i\nu_1..i\nu_3) \), see Refs. \([12, 41]\).

### III. THE TWO-PARTICLE IRREDUCIBLE FUNCTIONAL RENORMALIZATION-GROUP APPROACH

The considering approach is similar to the DMF\(^2\)RG approach for the flow from infinite to finite number of dimensions for the standard Hubbard model\([37]\). In particular, we consider the evolution of generating functional with the action

\[
S_{\Lambda} = S_{(\text{E})\text{DMFT}}[c, c^+] + H_{\text{non-loc}}^\Lambda[c_\sigma, c_\sigma^+],
\]

where

\[
H_{\text{non-loc}}^\Lambda[c_\sigma, c_\sigma^+] = \Lambda \sum_k c_\sigma^+ G_{0,k}^{-1} - \zeta^{-1}(i\nu_n) c_{k\sigma} + \frac{\Lambda}{2} \sum_q \left( \tilde{V}_q^c n_q n_{-q} + \tilde{V}_q^s S_q S_{-q} \right),
\]

such that \( \tilde{V}_q^c = V_q^c - v^c(s(i\omega_n)) \); for \( \Lambda = 0 \) the (E)DMFT theory is reproduced, while for \( \Lambda = 1 \) we obtain the lattice problem \([3]\).

The 2PI approach\([33, 34]\), applied to the model \( \Pi(\text{II}) \), considers the evolution of the partition function

\[
Z_{\Lambda}[J] = \int D[c, c^+] e^{-S_{\Lambda} + \sum_{km} J_{k,q,m} M_{k,q,m}},
\]

where \( J_m \) are the source fields, \( M_{k,q,c} = \sum_{\sigma} c_{k\sigma}^+ c_{k+q,\sigma} \), \( M_{k,q,s} = \sum_{\sigma\sigma'} c_{k,\sigma}^+ \sigma_{\sigma\sigma'} c_{k+q,\sigma'} \), \( M_{k,q,ssc} = \sum_{\sigma\sigma'} ic_{k,\sigma}^+ \sigma_{\sigma\sigma'} c_{-k+q,\sigma'} \), \( M_{k,q,tsc} = \sum_{\sigma\sigma'} ic_{k,\sigma}^+ (\sigma\sigma')_{\sigma\sigma'} c_{-k+q,\sigma'} \) are the respective
combinations of Grassman variables. Performing Legendre transform, we obtain the 2PI effective action

$$\Gamma_{\Lambda}[G] = -\ln Z_{\Lambda}[J] - \sum_m \text{sp} [J_m \cdot G_m] - \frac{1}{2} \sum_{mm'} \text{sp} [G_m R_{\Lambda}^{mm'} G_{m'}], \quad (14)$$

where \(\text{sp}\) is taken with respect to momentum/frequency indices, which we omit for brevity, and we have introduced the counterterm \(R_{\Lambda}^{mm'}\), which will be determined later. Following the standard strategy, we introduce the Luttinger-Ward functional [27],

$$\Gamma_{\Lambda}[G] = -\frac{1}{2} \text{Sp} \ln (-\hat{G}) - \frac{1}{2} \text{Sp} \left[ I - \hat{G}_{0,\Lambda}^{-1} \right] + \Phi_{\Lambda}[G], \quad (15)$$

where \(\hat{G}_{k,k'} = \sum_m G_{k,k'-m} \hat{M}_{k,k'-m} \hat{G}_{0,\Lambda}^{-1} = \left[ (1/2) \sum_\sigma c_\sigma^+ G_{0,\Lambda,k} c_\sigma \delta_{kk'} \right] \) and \(\hat{M}_{kqm} = [M_{kqm}]\) are considered as matrices in space of fermionic variables \(c, c^+\), \(\text{Sp}\) is taken with respect to fermionic, momenta, and frequency indices, and

$$G_{0,\Lambda,k}^{-1} = (1 - \Lambda) \zeta^{-1}(i\nu_n) + \Lambda G_{0,\Lambda,k}^{-1}, \quad (16)$$

the (non-stationary) Green function \(G_{k,q,m}\) depends on the two momenta indices, corresponding to incoming and outgoing momenta \(k\) and \(k + q\), respectively. This yields the following derivatives:

$$\Gamma_{\Lambda,k,q}^{(1),m} = \frac{\delta \Gamma}{\delta G_{k,q,m}} = -\frac{1}{2} \text{Sp} \left[ \hat{G}_{k+q,k}^{-1} \hat{M}_{k,q,m} \right] + G_{0,\Lambda,k}^{-1} \delta_{m,c} + \frac{\delta \Phi_{\Lambda,k,q}}{\delta G_{k,q,m}} = -J_{k,q,m} - \sum_{k',m'} R_{q,mm'}^{\Lambda} G_{k',q,m'}, \quad (17a)$$

$$\Gamma_{\Lambda,k,k'q}^{(2),mm'} = \frac{\delta^2 \Gamma}{\delta G_{k,q,m} \delta G_{k',q,m'}} = \Pi_{k,k'q,mm'}^{1} + \Phi_{\Lambda,k,k'q}^{(2),mm'} = \left[ W_{\Lambda,k,k'q}^{(2),mm'} \right]^{-1} - R_{q,mm'}^{\Lambda}, \quad (17b)$$

where \(\Pi_{k,k'q,mm'}^{1} = (1/2) \text{Sp} \left[ \hat{G}_{k+q,k}^{-1} \hat{M}_{k',q,m} \hat{G}_{k',q,k}^{-1} \hat{M}_{k,q,m} \right]\) is the inverse polarization bubble (cf. Refs. [33, 34]), and \(W_{\Lambda,k,k'q}^{(2),mm'} = \left[ \Gamma_{\Lambda,k,k'q}^{(2),mm'} + R_{q,mm'}^{\Lambda} \right]^{-1} = \left[ \Pi^{-1} + \Phi_{\Lambda,k,k'q}^{(2),mm'} + R_{q,mm'}^{\Lambda} \right]^{-1}\) is the corresponding susceptibility, the inversion is performed with respect to momentum \(k, k'\) and channel \(m, m'\) indices. The stationary one- and two-particle quantities (which we denote by bar) are determined by the condition \(\Gamma^{(1)} = 0\), such that

$$\overline{G}_{\Lambda,k}^{-1} = 2\overline{G}_{\Lambda,k,c}^{-1} = G_{0,\Lambda,k}^{-1} - \Sigma_{\Lambda,k},$$

$$\Sigma_{\Lambda,k} = -\overline{\Phi}_{\Lambda,k}^{(1),c}.$$

(18)
At $\Lambda = 0$ we have

$$\Phi_{\Lambda=0}[G] = \Phi_{\text{loc}}[G] - \frac{1}{2} \sum_{mm'} \text{sp} \left[ G_m R^{\Lambda=0}_{mm'} G_{m'} \right],$$

(19)

$$\tilde{\Phi}^{(1),c}_{\Lambda=0,k} = -\Sigma_{\Lambda=0,k} = -\Sigma_{\text{loc}}(i\nu_n) - 2R^{\Lambda=0}_{q=0,cc} \int d\nu / G_{\text{loc}}(i\nu'),$$

$$\tilde{\Phi}^{(2),mm'}_{\Lambda=0} = \Phi_{\text{loc}} \delta_{mm'} - R^{\Lambda=0}_{mm'},$$

and $G_{k,\Lambda=0} = (\zeta^{-1}(i\nu_n) - \Sigma_{\text{loc}}(i\nu_n))^{-1} = G_{\text{loc}}(i\nu_n)$. From this setup we obtain the following 2PI-fRG equation (see Appendix A, cf. Refs. [33, 34]):

$$\Phi_{\Lambda}[G] = \frac{1}{2} \sum_{kk'q,m} \tilde{v}_m \left[ \Pi^{-1} + \Phi^{(2)}_{\Lambda} + R^{\Lambda}_{kk',mm} \right]^{-1} G_{k,q,m} G_{k',-q,m},$$

$$- \frac{1}{2} \sum_{kk'q,mm'} R^{\Lambda}_{q,mm'} G_{k,q,m} G_{k',-q,m'}.$$

(20)

Taking functional derivatives, choosing $R^{\Lambda}_{q,mm} = -\tilde{v}_m \delta_{mm'}$, and considering stationary quantities, we find the equations of the (E)DMFT+2PI-fRG approach (see Appendix A)

$$\frac{d\Sigma_{\Lambda,k}}{d\Lambda} = 2 \sum_{q,m=c,s} a^{(c)}_m \partial_{H^{m}_{\Lambda,k,k,q}} G_{\Lambda,k+q} - 2 \sum_{k'} \tilde{\Phi}^{(2),c}_{k',k} \partial_{\Lambda} G_{k',k'},$$

(21a)

$$\frac{d\Phi^{(2),c,s}_{\Lambda,k,k,q}}{d\Lambda} = - \sum_{m=c,s} a^{(c,s)}_m \partial_{H^{m}_{\Lambda,k,k+q,k'-k}} G_{\Lambda,k+q} \circ \partial_{\Lambda} G_{k',k'},$$

$$+ \sum_{m,n=c,s,ssc,tsc} b^{(c,s)}_{mn} \Phi^{(2),m}_{\Lambda,k,k+q,m} \circ \partial_{\Lambda} G_{k',k'} \circ \Phi^{(2),n}_{\Lambda,k,k+q}.$$  

(21b)

where the coefficients in the charge- and spin channels are given by $a^{(c)}_c = a^{(s)}_c = -a^{(s)}_s = b^{(c)}_{cc} = b^{(s)}_{cs} = b^{(s)}_{sc} = 1/2$, $a^{(s)}_s = b^{(c)}_{ss} = 3/2$, $b^{(s)}_{ss} = 1$, $b^{(c)}_{cc} = b^{(s)}_{cs} = b^{(c)}_{sc} = 0$

$$\tilde{\partial}_{\Lambda} H^{m}_{\Lambda,k,k'} = \left[ \Pi^{-1}_{\Lambda} W^{(2)}_{\Lambda} \tilde{v}_m W^{(2)}_{\Lambda} \Pi^{-1}_{\Lambda} \right]_{kk',mm'},$$

(22a)

$$\tilde{W}^{(2)}_{\Lambda,k,k',mm'} = \left[ \Pi^{-1}_{\Lambda} + \tilde{\Phi}^{(2)}_{\Lambda} + R^{\Lambda}_{kk',mm'} \right]^{-1},$$

(22b)

$$\Pi^{\Lambda}_{\Lambda,k,k',mm'} = \Pi^{\Lambda}_{k,q} \delta_{kk'} \delta_{mm'}; \quad \Pi^{\Lambda}_{k,q} = 2G_{\Lambda,k} G_{\Lambda,k+q}$$

(22c)

(we omit momenta/frequency indices in the matrix products with respect to $k, k'$), the circle $\circ$ corresponds to the summation over momenta, frequencies, and internal indices according to the diagrammatic rules (see below). With the choice $R^{\Lambda}_{q,mm} = -\tilde{v}_m \delta_{mm'}$, removing the tadpole (Hartree) contributions from Eqs. (21), $\tilde{\partial}_{\Lambda} H^{c,s}_{\Lambda,k,k'}$ can be represented as a certain scale derivative, $\tilde{\partial}_{\Lambda} = (\partial R^{\Lambda}_{c,s}/\partial \Lambda) \partial_{R^{\Lambda}_{c,s}}$ of the sum of ladder diagrams

$$H^{c(s)}_{\Lambda,k,k'} = \left[ \left( \Phi^{(2),c(s)}_{\Lambda} + R^{\Lambda}_{c(s),c(s)} \right) - 1 + \Pi^{\Lambda}_{k,q} \delta_{kk'} \right]^{-1}. $$

(23)
FIG. 1: (Color online) The diagrammatic form of Eqs. 21 for the self-energy $\Sigma_\Lambda$ (a) and the two-particle irreducible vertex $\Phi^{(2),c,s}_\Lambda$ (b). The wavy lines with triangular vertices correspond to the two-particle interaction $H^m_\Lambda$, or, equivalently, $\gamma^m W^m_\Lambda \gamma^m$ (see below), the solid lines correspond to the stationary Green functions $G_\Lambda$, and the square box - to the two-particle irreducible vertex $\Phi^{(2),c,s}_\Lambda$. The dash on the wavy lines corresponds to the partial derivative $\tilde{\partial}_\Lambda$, on the solid lines - to the derivative $\partial_\Lambda$.

Note that in contrast to Refs. 33–35, the above mentioned choice of $R$ cancels only part of second-order diagrams in $\Phi$, the remaining second-order diagrams are present in $H^m_\Lambda$. The diagrammatic form of Eqs. 21 is shown in Fig. 1. The terms in the right-hand side describe contributions from the non-local interaction (first term) and local interaction, as well as mixed contributions (last term).

For the local bare interaction we put $V = \tilde{V} = R = 0$. The equation (21b) then provides analogue of the parquet equations with the bare local interactions. The solution of the Eq. (21b) then corresponds to dressing the bare vertices $\Phi^{(2),c,s}_\text{loc}$ by particle-hole and particle-particle bubbles in the "transverse" direction with respect to that, in which $\Phi^{(2),c,s}_\Lambda$ is defined. Since the contribution of the charge and spin channel are mixed ($b_{ss}^{(c)} \neq 0$), this yields finite contribution in the charge channel even for the vanishing (or neglected) bare one. Keeping only the particle-hole contributions in Eq. (21b) yields the result

$$[\Phi^{(2),\tilde{c},\tilde{s}}_\Lambda]^{-1} = [\Phi^{(2),\tilde{c},\tilde{s}}_\text{loc}]^{-1} + G_\Lambda \circ G_\Lambda - G_{\text{loc}} \circ G_{\text{loc}},$$

which is identical with the ladder version of DΓA 12, 13. Note that the indices $\tilde{c}, \tilde{s}$ refer
here to the 'transverse' direction. The corresponding vertices are related to those in the "longitudinal" direction $c, s$ by the relations

\[
\Phi^{(2),c}_{\Lambda,k,k'q} = -\frac{1}{2} \Phi^{(2),c}_{\Lambda,k,k+q,k'-k} - \frac{3}{2} \Phi^{(2),c}_{\Lambda,k,k+q,k'-k},
\]

\[
\Phi^{(2),s}_{\Lambda,k,k'q} = -\frac{1}{2} \Phi^{(2),s}_{\Lambda,k,k+q,k'-k} + \frac{1}{2} \Phi^{(2),s}_{\Lambda,k,k+q,k'-k}.
\]

Approximating the particle-particle contributions, which are generated by Eq. (21b) and contribute to the right-hand side of (24), by a constant $\lambda$ yields $\lambda$-corrected DΓA type of approach [14] (for fulfillment the sum rules and Mermin-Wagner theorem see discussion of the self-consistency procedure below), while keeping all contributions from the last term in Eq. (21b), we arrive at the scheme, which is similar to parquet DΓA [12].

The equation for the self-energy (21a) for purely local bare interaction reads

\[
\Sigma_{\Lambda,k} = -2 \sum_{k'} H^{c}_{\Lambda,k,k'0} \Pi^{c}_{k',0} G_{\Lambda,k'}^{-1},
\]

and with account of (24) it has the form, similar to that in dynamic vertex approximation. As follows from Eq. (27), the equation (28) can be rewritten in a form, which is similar to 1PI fRG approach [39] (cf. Ref. 34)

\[
\dot{\Sigma}_{\Lambda,k} = 2 \sum_{k'} H^{c}_{\Lambda,k,k'0} \Pi^{c}_{k',0} G_{\Lambda,k'}^{-1} = -2 \sum_{k'} H^{c}_{\Lambda,k,k'0} S_{\Lambda,k'},
\]

where we have defined the "single-scale" propagator $S_{\Lambda,k} = -\Pi^{c}_{k,0} G_{0,\Lambda,k}^{-1}$.

In the presence of the non-local interactions, we choose $R^{A}_{q,mm'} = (1 - \Lambda) \tilde{V}^{m}_{q} \delta_{mm'}$ to fulfill the abovementioned condition $\dot{R}^{A}_{q,mm'} = -\tilde{V}^{m}_{q} \delta_{mm'}$. Then we obtain the initial two-particle irreducible vertices and self-energy $\Phi^{(2),c,s}_{\Lambda=0,k,k'q} = \Phi^{(2),c,s}_{\Lambda=0,k,k'q} - V^{c,s}_{q} + v^{c,s}(i\omega_{n})$, $\Sigma_{\Lambda=0}(i\nu) = \Sigma_{\text{loc}}(i\nu) + 2(V^{c}_{q=0} - v^{c}(0)) \int d\nu' G_{\text{loc}}(i\nu')$; the local quantities are in practice obtained from the solution of the Anderson impurity model, and the last term in the initial self-energy, substracting the corresponding local Hartree contribution and replacing it with the one, containig non-local interaction, can be absorbed in the redefinition of the chemical potential.

We note that due to special choice of $R$, only "longitudinal" component of the initial vertices is momentum dependent, while the vertex remain local with respect to "transverse" momenta $k, k'$. In the simplest truncation, one can neglect for simplicity the flow of $\Phi^{(2)}_{\Lambda}$ to obtain

\[
H^{c,s}_{\Lambda,k,k'q} = \left\{ \Phi^{(2),c,s}_{\text{loc},\nu\nu'\omega} - \Lambda(V^{c,s}_{q} - v^{c,s}(i\omega_{n})) \right\}^{-1} + \Pi^{c,s}_{k,q} \delta_{kk'q},
\]
where $\Pi_{k,q}^\Lambda$ is calculated with the initial local self-energy. The corresponding susceptibilities are

$$\chi_{c,s}^{\Lambda,\mathbf{q},\omega} = - \sum_{k,k'} \Pi_{k,q}^\Lambda \left( \delta_{kk'} + H_{kk'q}^c \Pi_{k',q}^\Lambda \right)$$

$$= \int d\nu d\nu' \left[ (\lambda_{c,s}^0)^{-1} \delta_{\nu\nu'} - \Phi_{\lambda_{c,s}^0,\nu\nu'}^{(2)} + \Lambda (V_{\mathbf{q}} - v_{c,s}(i\omega_n)) \right]^{-1}_{\nu\nu'},$$  \hspace{1cm} (30)

where

$$\chi_{c,s}^0_{\mathbf{q},\omega} = -2 \sum_k \overline{G}_{\mathbf{k},0} \overline{G}_{\mathbf{k},\mathbf{q},\nu\nu'} \omega.$$

In the end of the flow (at $\Lambda = 1$) $G_{\mathbf{k},0} = G_{\mathbf{k},0}$, which is given by the Eq. (8) with the shifted chemical potential, and we reproduce the result of the ladder approximation in the dual boson approach with purely local two-particle vertices, see, e.g., Refs. [24, 25] and Appendix B. The result (30) can be also rewritten in terms of the triangular vertices (cf. Ref. [14])

$$\gamma_{c,s}^{\Lambda,\mathbf{q},kq} = (\Pi_{k,q}^\Lambda)^{-1} \sum_{k'} \left[ (\Pi_{k',q}^\Lambda)^{-1} \delta_{kk'} + \Phi_{\lambda_{c,s}^0,\nu\nu'}^{(2)} \pm U/2 \right]^{-1}$$

in the form (see Appendix B)

$$\chi_{c,s}^{\Lambda,\mathbf{q},\omega} = \frac{\phi_{c,s}^{\Lambda,\mathbf{q}}}{1 + U_{\Lambda,q}^{c,s} \phi_{c,s}^{\Lambda,\mathbf{q}}},$$

where $U_{\Lambda,q}^{c,s} = \pm U/2 + \Lambda (V_{\mathbf{q}}^m - v^m(\omega))$ and

$$\phi_{c,s}^{\Lambda,\mathbf{q}} = \sum_{kk'} \left[ (\Pi_{k,q}^\Lambda)^{-1} \delta_{kk'} + \Phi_{\lambda_{c,s}^0,\nu\nu'}^{(2)} \pm U/2 \right]^{-1} = - \sum_k \gamma_{c,s}^{\Lambda,\mathbf{k},kq} \Pi_{k,q}^\Lambda$$

is the polarization operator (particle-hole irreducible susceptibility).

The non-local corrections to self-energy can be obtained from the Eq. (21a). Keeping the result (20) for $H_{\Lambda,\mathbf{k}k',\mathbf{q}}^{c,s}$, Eq. (21a) can be again rewritten in terms of the triangular vertices as

$$\frac{d\Sigma_{\Lambda,k}}{d\Lambda} = -2 \sum_{q,m=c,s} a_{m}^{(c)} i_{m,k,q} \frac{\partial W_{\Lambda,q}^m}{\partial \Lambda} \gamma_{k,q,-q} \overline{G}_{\Lambda,k+q}$$

$$+ 2 \sum_{k'} \left[ V_{\mathbf{q}}^{c} - v^{c}(\omega) - \Phi_{\lambda_{c,s}^0,\nu\nu'}^{(2)} \right] \partial_{\Lambda} \overline{G}_{\Lambda,k'},$$

where

$$\overline{W}_{\Lambda,q}^{c,s} = \frac{U_{\Lambda,q}^{c,s}}{1 + U_{\Lambda,q}^{c,s} \phi_{c,s}^{\Lambda,\mathbf{q}}},$$
is the effective interaction. While this interaction has also the same form, as in the dual boson approach of Refs. [24, 25], the equation for the self-energy (35) is different. The second term in the Eq. (35) can be excluded by representing
\[
\Sigma_{\Lambda,k} = \Sigma_{0,k} + 2 \sum_{k'} \left[ V^c_q - v^c(\omega) - \Phi^{(2),c}_{loc,\nu\nu'} \right] \left[ G_{\Lambda,k'} - G_{loc}(i\nu') \right] + \tilde{\Sigma}_{\Lambda,k}
\]
(37)
\[
= \Sigma_{loc}(i\nu) + 2 \left[ V^c_q = v^c(\omega) \right] \sum_{k'} G_{\Lambda,k'} - 2 \sum_{k'} \Phi^{(2),c}_{loc,\nu\nu'} \left[ G_{\Lambda,k'} - G_{loc}(i\nu') \right] + \tilde{\Sigma}_{\Lambda,k},
\]
such that the final equation for the self-energy in our approach takes the form
\[
\frac{d\tilde{\Sigma}_{\Lambda,k}}{d\Lambda} = -2 \sum_{q,m=c,s} \tilde{a}^m_{\gamma,k,q} \frac{\partial \tilde{W}^m_{\Lambda,q}}{\partial \Lambda} \tilde{\gamma}^m_{k+q,-q} G_{\Lambda,k+q+q}.
\]
(38)
Similarly to TRILEX [31] and DBγ [26] approaches, one can approximate the triangular vertices \(\gamma\) in Eqs. (34) and (38) by their local values. Although, similarly to the so called DBγ approximation [26], the equation for the self-energy contains two \(\gamma\)-vertices, the corresponding polarization operator (34) contains only first power of \(\gamma\) (which occurs naturally in a ladder summation), which differs the considering theory also from DBγ approach.

The presented approach can be applied self-consistently: the non-local self-energy, determined in the end of the flow, can produce the new local Green function, which allows to adjust the bath Green functions \(\zeta(i\nu_n)\) and \(v^{c,s}(i\omega_n)\) with the new self-consistency conditions (17); if the self-consistency condition \(\sum_{k'} G_{\Lambda=1,k'} = G_{loc}(i\nu')\) is fulfilled, we find \(\Sigma_{\Lambda=1,k} = \Sigma_{loc}(i\nu) + 2 \left[ V^c_q = 0 - v^c(\omega) \right] \sum_{\nu'} G_{loc}(i\nu') + \tilde{\Sigma}_{\Lambda=1,k}\). Note that the self-energy (37) does not contain spurious corrections, which appear due to neglect of one-particle reducible contributions to the six-point vertices in the dual fermion or boson approaches [42].

Assuming fulfillment of Eq. (7b), the Mermin-Wagner theorem in two or less dimensions in the spin channel is guaranteed to be fulfilled as well, since otherwise the integral in the right-hand side of Eq. (7b) will be divergent.

**IV. CONCLUSIONS**

In conclusion, we have presented a general EDMFT+2PI-fRG approach, which considers the 2PI functional renormalization-group flow, starting from the (extended) dynamical mean-field theory. In the simplest truncations, we have shown that for purely local interactions the considering approach yields the susceptibilities and vertices, identical to the
earlier proposed dynamic vertex approximation (DΓA) \[12, 14\], and the equation for the self-energy, which has a structure, similar to that in DΓA. For the non-local interaction, the susceptibilities coincide with those of the ladder approximation in the dual boson (DB) approach\[23–25\], but the equation for the electronic self-energy is different: it has a differential form and treats correctly the one-particle reducible parts of the vertices.

The proposed scheme is rather general, and more sophisticated truncations can be used to improve the results of the mentioned approaches. Numerical investigations of the presented equations will allow to study the concrete phenomena, such as charge- or spin-density wave instabilities in strongly-correlated systems, as well as screening of the long-range Coulomb interaction in the presence of strong electronic correlations.

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Appendix A. Derivation of 2PI fRG equations for self-energy and vertex

To derive the 2PI-fRG equations, we follow the standard strategy, outlined in Refs. \[33, 34\]. Differentiating Eqs. (13) and (14) with respect to \(\Lambda\), we find (\(W_\Lambda = \ln Z_\Lambda\)):

\[
\dot{W}_\Lambda[J] = \frac{1}{2Z} \sum_k \partial G^{-1}_{0A,k} \frac{\delta Z_\Lambda}{\delta J_{k,0,c}} - \frac{1}{2Z} \sum_{kk'q,m} \tilde{V}_q^m \frac{\delta^2 Z_\Lambda}{\delta J_{kqm} \delta J_{k',-q,m}} \\
= \frac{1}{2} \sum_{kk'q,m} \tilde{V}_q^m \left( \frac{\delta^2 W_\Lambda}{\delta J_{kqm} \delta J_{k',-q,m}} + \frac{\partial W_\Lambda}{\partial J_{kqm}} \frac{\partial W_\Lambda}{\partial J_{k',-q,m}} \right) + \frac{1}{2} \sum_k \partial G^{-1}_{0A,k} \frac{\delta W_\Lambda}{\delta J_{k,0,c}}, \quad (39)
\]

\[
\dot{\Gamma}_\Lambda[G] = \frac{1}{2} \sum_{kk'q,m} \tilde{V}_q^m \left[ \Pi^{-1} + \Phi^{(2)}_\Lambda + R^\Lambda \right]^{-1}_{kk'q,mm} G_{k,q,m} G_{k',-q,m'} + \frac{1}{2} \sum_k \partial G^{-1}_{0A,k} \frac{\delta W_\Lambda}{\delta J_{k,0,c}} \\
- \frac{1}{2} \sum_{q,k,k',mm'} \left( \tilde{V}_q^m \delta_{mm'} + \tilde{R}^\Lambda_{q,mm'} \right) G_{k,q,m} G_{k',-q,m'}, \quad (40)
\]

\[
\dot{\Phi}_\Lambda[G] = -\frac{1}{2} \sum_{kk'q,m} \tilde{V}_q^m \left[ \Pi^{-1} + \Phi^{(2)}_\Lambda + R^\Lambda \right]^{-1}_{kk'q,mm} \\
- \frac{1}{2} \sum_{kk'q,mm'} \left( \tilde{V}_q^m \delta_{mm'} + \tilde{R}^\Lambda_{q,mm'} \right) G_{k,q,m} G_{k',-q,m'}. \quad (41)
\]
Taking variational derivatives over $G$, we obtain

$$
\Phi^{(1)}_{A,k,q,m} = \frac{\delta \Phi_A}{\delta G_{k,q,m}} = -\frac{1}{2} \sum_{k'k',q',m'} \tilde{\nu}_{q'}^{m'} \left\{ \left[ \Pi^{-1} + \Phi^{(2)}_A + R^A \right]^{-1} \Pi^{-1} \frac{\delta \Pi}{\delta G_{kqm}} \Pi^{-1} \right. \\
\times \left[ \Pi^{-1} + \Phi^{(2)}_A + R^A \right]^{-1} \right\}_{k'k',q',m'} - \sum_{k',m'} \left( \tilde{\nu}_{q'}^{m'} \delta_{mm'} + R^A_{q,m} \right) G_{k',q,m}(42)
$$

$$
\Phi^{(2)}_{A,k,k'q,mm'} = \frac{\delta \Phi_A}{\delta G_{k,q,m} \delta G_{k',q,m'}} = \tilde{\nu}_{q'}^{m'} \delta_{mm'} - R^A_{q,m}(42)
$$

$$
-\frac{1}{2} \sum_{k'k''q'm''} \tilde{\nu}_{q'}^{m'} \left\{ \left[ \Pi^{-1} + \Phi^{(2)}_A + R^A \right]^{-1} \Pi^{-1} \frac{\delta \Pi}{\delta G_{kqm}} \Pi^{-1} \right. \\
\times \left[ \Pi^{-1} + \Phi^{(2)}_A + R^A \right]^{-1} \right\}_{k'k''q',m'm''}
$$

$$
-\tilde{\nu}_{q'}^{m'} \left[ \Pi^{-1} + \Phi^{(2)}_A + R^A \right]^{-1} \Pi^{-1} \frac{\delta \Pi}{\delta G_{kqm}} \Pi^{-1} \delta \Pi_{G_{kqm} \delta G_{k',q,m'}}
$$

$$
\times \Pi^{-1} \left[ \Pi^{-1} + \Phi^{(2)}_A + R^A \right]^{-1} + (k \leftrightarrow k', q \leftrightarrow -q, m \leftrightarrow m')
$$

$$
-\frac{1}{2} \sum_{k'k''m''} \tilde{\nu}_{k'k''}^{m''} \left\{ \left[ \Pi^{-1} + \Phi^{(2)}_A + R^A \right]^{-1} \Pi^{-1} \frac{\delta \Pi}{\delta G_{kqm}} \Pi^{-1} \right. \\
\times \left[ \Pi^{-1} + \Phi^{(2)}_A + R^A \right]^{-1} \right\}_{k'k''k''m''m''}
$$

An explicit calculation yields

$$
\Pi_{kk'q,c(s),c} = (G_{k,k'q,c}G_{k'q,k,c} + G_{k,k'q,k,c}G_{k'q,k,c})/2,
$$

$$
\Pi_{kk'q,++} = G_{k,k'q,k}G_{k'q,k} - G_{k,k'q,k}G_{k'q,k},
$$

$$
\Pi_{kk'q,c} = (G_{k,k'q,c}G_{k'q,k} + G_{k,k'q,k}G_{k'q,k})/2,
$$

$$
\Pi_{kk'q,c,s} = (G_{k,k'q,c}G_{k'q,k} + G_{k,k'q,k}G_{k'q,k})/2,
$$

$$
\Pi_{kk'q,c(s),\pm} = (G_{k,k'q,c(s)}G_{k'q,k,\pm} + G_{k,k'q,k,\pm}G_{k'q,k,c(s)})/2,
$$

(44)
where $G_{ks}$ corresponds to $S_z = 0$ component of the Green function in the spin channel, and $G_{k\pm}$ corresponds to its $S_z = \pm 1$ components. Simplifying, we find at the stationary point

$$\Phi^{(1)}_{k,m} \equiv \Phi^{(1)}_{k,0,m} = - \sum_{q,m'} a^{(m)}_{m'} \left[ \Pi^{-1} W^{(2)}_A \tilde{V}_q^{(2)} W^{(2)}_A \Pi^{-1} \right]_{k,k,q,m',m'} G_{k+q,m}$$

(45)

$$\Phi^{(2)}_{kk',q,mm'} = - \sum_{q,m''} c_{m''m}^{(m,m')} \left[ \Pi^{-1} W^{(2)}_A \tilde{V}_q^{(2)} W^{(2)}_A \Pi^{-1} \right]_{m''m'''} G$$

(46)

$$\times \left[ \Pi^{-1} W^{(2)}_A \tilde{V}_q^{(2)} W^{(2)}_A \Pi^{-1} \right]_{k,k',-k,m'',m'''} G_{k+q,-k,m''m'''} \delta_{mm''}$$

with the coefficients $a^{(m)}_{m'}$, given after the Eqs. (21) of the main text, and some $c_{m''m}^{(m,m')}$. Choosing $\tilde{R}_q_{mm'} = \tilde{V}_q^{(2)} \delta_{mm'}$, neglecting 'Aslamazov-Larkin' contribution (first term in the r.h.s. of Eq. (46)), considering stationary quantities, and representing $\Phi^{(3)}$ as all possible combinations of $\Phi^{(2)} G_A \Phi^{(2)}$ (cf. Refs. [32, 34]), we obtain Eqs. (21) of the main text.

Appendix B. The equivalence of the susceptibility (30) to the result of the dual boson approach

The physical charge or spin susceptibility in the dual boson approach is given by

$$X_{q\omega} = \frac{1}{1/[\Pi^{(1)}_{q\omega} + V_q - v(\omega)],}$$

(47)

where

$$\Pi^{(1)}_{q\omega} = \int \nu'' \int \nu''' \chi_{q,v''v'''}^0 \left[ 1 - \Phi^{(2)}_{loc,v''v'''} \chi_{q,v''v'''}^0 \right]^{-1},$$

$$\chi_{q,v}^0 = -2 \sum_k G_k G_{k+q}$$ is the $\Lambda = 1$ limit of the Eq. (31), and we consider here only one specific channel (charge or spin). Now we introduce the quantities

$$\Phi_{q\nu\nu'} = \left[ (\chi_{q\nu}^0) -1 - \Phi^{(2)}_{loc,\nu\nu'} + U_{q\nu} \right]^{-1} = (\chi_{q\nu}^0) [1 - \Phi^{(2)}_{loc,\nu\nu'} \chi_{q\nu}^0 + U_{q\nu} \chi_{q\nu}^0]^{-1},$$

$$\phi_{q\nu} = \int \nu \nu' \Phi_{q\nu\nu'\nu},$$

(48)
with some \( U_{q,\omega} \). Then we obtain

\[
\Pi^{(1)}_{q,\omega} = \int d\nu d\nu' d\nu'' d\nu''' \chi^0_{q,\omega} \left[ 1 - \Phi^{(2)}_{\text{loc},\nu\nu',\omega} \chi^0_{q,\omega} + U_{q,\omega} \chi^0_{q,\omega} \right]^{-1} \\
\times \left[ 1 - \Phi^{(2)}_{\text{loc},\nu'\nu''\omega} \chi^0_{q,\omega} + U_{q,\omega} \chi^0_{q,\omega} \right] \left[ 1 - \Phi^{(2)}_{\text{loc},\nu''\nu'''\omega} \chi^0_{q,\omega} \right]^{-1} \\
= \int d\nu d\nu' \Phi_{q,\omega} \left\{ 1 + U_{q,\omega} \int d\nu'' d\nu''' \chi^0_{q,\omega} \left[ 1 - \Phi^{(2)}_{\text{loc},\nu''\nu'''\omega} \chi^0_{q,\omega} \right]^{-1} \right\} \\
= \phi_{q,\omega} (1 + U_{q,\omega} \Pi^{(1)}_{q,\omega}).
\]

(49)

Therefore,

\[
\Pi^{(1)}_{q,\omega} = \frac{1}{\phi^{-1}_{q,\omega} - U_{q,\omega}},
\]

(50)

and

\[
X_{q,\omega} = \frac{1}{\phi^{-1}_{q,\omega} - U_{q,\omega} + V_q - v(\omega)}.
\]

(51)

The choice \( U_{q,\omega} = V_q - v(\omega) \) yields \( X_{q,\omega} = \phi_{q,\omega} = \int d\nu d\nu' [(\chi^0_{q,\omega})^{-1} \delta_{\nu\nu'} - \Phi^{(2)}_{\text{loc},\nu\nu'\omega} + V_q - v(\omega)]^{-1} \), which is equivalent to the Eq. \((30)\) of the main text at \( \Lambda = 1 \). On the other hand, choosing \( U_{q,\omega} = -U/2 \) leads us to the \( \Lambda = 1 \) limit of the Eqs. \((34)\) and \((33)\) of the main text.
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