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FUNCTIONAL RENORMALIZATION-GROUP APPROACHES, ONE-PARTICLE (IR)REDUCIBLE WITH RESPECT TO LOCAL GREEN's FUNCTIONS, WITH DYNAMICAL MEAN-FIELD THEORY AS A STARTING POINT

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We consider formulations of the functional renormalization-group (fRG) flow for correlated electronic systems with the dynamical mean-field theory as a starting point. We classify the corresponding renormalization-group schemes into those neglecting one-particle irreducible six-point vertices (with respect to the local Green's functions) and neglecting one-particle reducible six-point vertices. The former class is represented by the recently introduced DMF^{2}RG approach [31], but also by the scale-dependent generalization of the one-particle irreducible representation (with respect to local Green's functions, 1PI–LGF) of the generating functional [20]. The second class is represented by the fRG flow within the dual fermion approach [16, 32]. We compare formulations of the fRG approach in each of these cases and suggest their further application to study 2D systems within the Hubbard model.

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1. INTRODUCTION

Strongly correlated electron systems demonstrate a variety of interesting phenomena, such as magnetism, (unconventional) superconductivity, "colossal" magnetoresistance, and quantum critical behavior. The dynamical mean-field theory (DMFT) [1, 2], which becomes exact in the limit of high spatial dimensions ($d \to \infty$), has allowed achieving substantial progress in describing strong electronic correlations. In particular, it allowed describing the Mott–Hubbard metal–insulator transition [3] accurately, with an important local part of electronic correlations taken into account.

In real physical systems, which are one-, two-, or three-dimensional, the nonlocal correlations neglected in DMFT are important, however. Cluster extensions of DMFT [4–8] can treat only short-range correlations due to numerical limitations of the cluster size [9]. In spite of this, diagrammatic extensions of DMFT have been developed. These are the dynamical vertex approximation (DΓA) [10–15], the dual fermion (DF) approach [16–19], and the one-particle irreducible approach with respect to the local Green's functions (1PI–LGF) [20]. The DΓA approximation starts from local two-particle irreducible vertices and sums ladder or parquet diagrams for the vertices, considering the effect of the nonlocality of the Green's functions. The DF approach on the other hand splits the degrees of freedom into local ones, treated within DMFT, and the non-local (dual), considered perturbatively, with a possibility of summation of infinite series of diagrams for dual fermions [19, 21]. The 1PI version of the dual fermion approach (the 1PI–LGF approach) performs the same splitting of the local and nonlocal degrees of freedom for 1PI (Legendre-transformed) generating functionals. This approach therefore accounts for the effect of one-particle reducible six-point and higher-order reducible vertices, which was argued to be potentially important in Ref. [22].

The above approaches typically treat nonlocal fluctuations within the ladder approximation. A more

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powerful method, the parquet approach, can bring substantial improvement over the ladder approximation [21, 23], but is often not feasible numerically for correlated electronic systems. At the same time, the recently developed functional renormalization group (fRG) approaches [24–29] allow performing approximate summation of the parquet set of the diagrams at a lower computational cost if the six-point (i. e., three-particle) interaction vertices remain sufficiently small during the flow. In particular, for the standard fRG applied to the Hubbard model, the initial one-particle irreducible six-point vertices are zero, which favors the use of the one-particle irreducible approach, where the corresponding six-point vertex can be expected to remain small during the flow. Using DMFT as the initial theory for the flow accounts exactly for the local subset of diagrams, but (in principle) yields nonzero n-point vertices of arbitrarily high orders n, so that the formulation and justification of the fRG approach requires more effort. In general, in this case, one has to choose between neglecting the six-point one-particle irreducible or reducible vertices, depending on the model under consideration. In particular, in the half-filled spinless Falikov–Kimaball model, the one-particle-reducible six-point local vertex vanishes in the infinite-dimensional limit [30], while for the Hubbard model, at least in the weak-to-intermediate coupling limit, neglecting six-point one-particle irreducible local vertices seems more preferable.

In this paper, we concentrate on the renormalization-group approaches that use DMFT as a starting point and neglect either one-particle irreducible or one-particle reducible three-particle vertices (with respect to the local Green's function). Recently, an approach of the former type, considering the functional renormalization-group flow from infinite to finite dimensions (the DMF^{2}RG approach) was introduced [31]. This flow starts from an infinite-dimensional model, which is solved by DMFT, and considers the flow to a finite number of dimensions, e. g., in the approximation of neglecting the local six-point vertices. Because of the use of the 1PI approach, the latter approximation implies the neglect of six-point vertices that are one-particle irreducible with respect to the local Green's functions. For a more general view on the possible variety of different renormalization-group approaches starting from DMFT, it is useful to formulate the fRG approach for the other two mentioned schemes, the 1PI–LGF and DF theories, and compare them with the DMF^{2}RG approach. This study is performed in the present paper (see also Ref. [32]).

2. THE MODEL AND DYNAMICAL MEAN-FIELD THEORY

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

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k},\sigma} \widehat{c}^{\dagger}_{\mathbf{k},\sigma} \widehat{c}_{\mathbf{k},\sigma} + \sum_{i,\sigma} H_{int}[\widehat{c}_{i\sigma}, \widehat{c}^{\dagger}_{i\sigma}], \qquad (1)$$

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

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

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

where $c_{i\sigma}$, $c^{\dagger}_{i\sigma}$, $\eta_{i\sigma}$, $\eta^{\dagger}_{i\sigma}$ are the Grassman fields, the fields $\eta_{i\sigma}$ and $\eta^{\dagger}_{i\sigma}$ correspond to source terms, and $\tau \in$ $\in [0, \beta = 1/T]$ is the imaginary time.

The DMFT [1, 2] for model (1) can be introduced via the effecive interaction

$$\mathcal{V}_{DMFT}[\eta, \eta^{\dagger}] = -\ln \int d[c, c^{\dagger}] \times$$
$$\times \exp\left\{ -\sum_{i,\sigma} \int d\tau H_{int}[c_{i\sigma}, c^{\dagger}_{i\sigma}] + \right.$$
$$\left. + \sum_{k,\sigma} \zeta^{-1}(i\nu_n) \left(c^{\dagger}_{k,\sigma} + \eta^{\dagger}_{k,\sigma} \right)(c_{k,\sigma} + \eta_{k,\sigma}) \right\}, \quad (4)$$

assuming locality of the "Weiss field" function $\zeta(\tau)$ and its Fourier transform $\zeta(i\nu_n)$, which have to be determined self-consistently from the condition

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

where

$$\mathcal{G}(\mathbf{k}, i\nu_n) \equiv \mathcal{G}_k = \left[G^{-1}_{0k} - \Sigma_{loc}(i\nu_n) \right]^{-1}, \qquad (6)$$

$G^{-1}_{0k} = i\nu_n - \varepsilon_{\mathbf{k}}$ is the lattice noninteracting Green's function (we use the 4-vector notation $k = (\mathbf{k}, i\nu_n)$), and $\Sigma_{loc}(i\nu_n)$ is the self-energy of impurity problem (4), 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 on the corresponding vertex functions [10, 33]. This is reflected in the following expansion of the effective interaction:

$$\mathcal{V}_{DMFT}[\eta,\eta^\dagger] = \widehat{\mathcal{V}}_{DMFT}[\widehat{\eta}_{k\sigma},\widehat{\eta}^\dagger_{k\sigma}] + \\ + \sum_{k,\sigma}\eta^\dagger_{k,\sigma}\frac{\Sigma_{loc}(i\nu_n)}{1-\zeta(i\nu_n)\Sigma_{loc}(i\nu_n)}\eta_{k,\sigma}, \quad (7)$$

where

$$\widehat{\eta}_{k,\sigma} = \frac{\eta_{k\sigma}}{1-\Sigma_{loc}(i\nu_n)G_{0k}}.$$

The functional $\widehat{\mathcal{V}}_{DMFT}[\eta,\eta^\dagger]$ generates connected vertices (which are in general one-particle reducible), amputated by the local Green's function $G_{loc}(i\nu_n)$, such that its expansion in the fields has the form

$$\widehat{\mathcal{V}}_{DMFT}[\eta^\dagger,\eta] = \frac{1}{2}\Gamma_{loc}\circ(\eta^\dagger_{k_1,\sigma}\eta_{k_3,\sigma})(\eta^\dagger_{k_2,\sigma'}\eta_{k_4,\sigma'}) + \\ + \frac{1}{6}\Gamma^{(6)}_{loc}\circ(\eta^\dagger_{k_1\sigma}\eta_{k_2\sigma})(\eta^\dagger_{k_3\sigma'}\eta_{k_4\sigma'})\times \\ \times(\eta^\dagger_{k_5\sigma''}\eta_{k_6\sigma''}) + \dots, \quad (8)$$

where Γ_{loc} and $\Gamma^{(6)}_{loc}$ are the connected four- and six-point vertices amputated with the local Green's functions G_{loc}, e. g.,

$$\Gamma^{\sigma\sigma'}_{loc}(i\nu_1\dots i\nu_3) = (1+\delta_{\sigma\sigma'})^{-1}\prod_{i=1}^{4}G^{-1}_{loc}(i\nu_i)\times \\ \times\Big[G^{(4)}_{loc,\sigma\sigma'}(i\nu_1\dots i\nu_3) - \\ - G_{loc}(i\nu_1)G_{loc}(i\nu_2)(\delta_{\nu_1\nu_3}-\delta_{\sigma\sigma'}\delta_{\nu_2\nu_3})\Big], \quad (9)$$

and $\circ$ stands for summation over momentum, frequency, and spin indices satisfying the conservation laws, and $G^{(4)}_{loc}$ is the two-particle local Green's function, which can be obtained by solving the impurity problem. For the four-point vertex Γ_{loc}, the requirement of connectivity and amputation with the full local Green's functions implies the one-particle irreducibility. However, the higher-order vertices, e. g., $\Gamma^{(6)}_{loc}$ remain one-particle reducible with respect to the local Green's functions. To obtain one-particle irreducible vertices, the Legendre transformation of Eq. (4) has to be performed.

3. THE ONE-PARTICLE IRREDUCIBLE APPROACHES WITH RESPECT TO LOCAL GREEN's FUNCTIONS

3.1. The flow from infinite to finite dimension within the DMF^{2}RG approach

Recently, the flow from the infinite to a finite number of dimensions was introduced in Ref. [31]. This flow involves evolution of the generating functional with the action

$$\mathcal{S}_\Lambda = \sum_{k\sigma}c^\dagger_{k\sigma}G^{-1}_{0k,\Lambda}c_{k\sigma} + \sum_{i,\sigma}\int d\tau H_{int}[c_{i\sigma},c^\dagger_{i\sigma}] \quad (10)$$

with the cutoff dependence of the bare Green's function

$$G_{0k,\Lambda} = [f(k,\Lambda)G^{-1}_{0,k} + (1-f(k,\Lambda))\zeta^{-1}(i\nu_n)]^{-1} \quad (11)$$

containing some function $f(k,\Lambda)$ such that $f(k,1)=0$ and $f(k,0)=1$, allowing to interpolate between the DMFT action for $\Lambda=0$ and lattice action (3) for $\Lambda=1$; specific choices of this function are discussed in Sec. 4 ($f(k,\Lambda)=1-\Lambda$ was used in Ref. [31]). The 1PI approach applied to model (10) yields the equations for the self-energy Σ_Λ and interaction vertex V_Λ:

$$\frac{d\Sigma_\Lambda}{d\Lambda} = V_\Lambda\circ S_\Lambda, \quad (12)$$

$$\frac{dV_\Lambda}{d\Lambda} = V_\Lambda\circ(G_\Lambda\circ S_\Lambda + S_\Lambda\circ G_\Lambda)\circ V_\Lambda, \quad (13)$$

where

$$G_{k,\Lambda} = \frac{G_{0k,\Lambda}}{1-\Sigma_{k,\Lambda}G_{0k,\Lambda}}, \quad (14)$$

$$S_{k,\Lambda} = \left.\frac{dG_{k,\Lambda}}{d\Lambda}\right|_{\Sigma=\text{const}} = -(\mathcal{G}^{-1}_k - G^{-1}_{loc})\frac{\partial f}{\partial\Lambda}G^2_{k,\Lambda}. \quad (15)$$

This approach uses initial one-particle-irreducible vertices and self-energy as the initial condition for the flow: $V_{\Lambda=1}=\Gamma^{\uparrow\downarrow}_{loc}$, $\Sigma_{\Lambda=1}=\Sigma_{loc}$, which are in practice obtained from the solution of the impurity problem (4). At the same time, Eqs. (12) and (13) neglect the local 1PI six-point vertex at the initial stage of the flow.

3.2. General formulation of the 1PI–LGF approach

Another way of the treatment of nonlocal correlations, based on DMPT as a starting point, is the splitting of local and nonlocal correlations in the generating functional for the lattice theory. For the one-particle-irreducible version, this was done within the 1PI–LGF approach considered in Ref. [20]. This approach represents the partition function as a functional of the local Green's function G_{loc} and the corresponding nonlocal part $\widetilde{\mathcal{G}}_k = \mathcal{G}_k - G_{loc}$. Contrary to the dual fermion approach, considered in the next section, this representation contains two fermionic fields, one of which describes propagation of nonlocal degrees of freedom

(similarly to the DF approach) and the other provides the one-particle irreducibility of the resulting functional.

To formulate the renormalization-group treatment within this approach, we trivially generalize the representation for the partition function obtained in Ref. [20], to introduce a Λ-dependence of the lattice Green's function $\mathcal{G}_k$ by the replacement $\mathcal{G}_k \to \mathcal{G}_{k,\Lambda}$, where $\mathcal{G}_{k,\Lambda}$ is defined by

$$\mathcal{G}_{k,\Lambda} = \left[f(k,\Lambda)\mathcal{G}_k^{-1} + (1-f(k,\Lambda))G_{loc}^{-1}(i\nu_n)\right]^{-1}, \quad (16)$$

which is similar to Eq. (11). The other choice, which we consider below, is to combine the two Green's functions (and not their inverse) into a sum,

$$\mathcal{G}_{k,\Lambda} = f(k,\Lambda)\mathcal{G}_k + [1-f(k,\Lambda)]G_{loc}(i\nu_n) \quad (17)$$

such that

$$\widetilde{\mathcal{G}}_k \to \widetilde{\mathcal{G}}_{k,\Lambda} := \mathcal{G}_{k,\Lambda} - G_{loc}(i\nu_n) = \\ = f(k,\Lambda)[\mathcal{G}_k - G_{loc}(i\nu_n)]. \quad (18)$$

The resulting Λ-dependent partition function in both cases is given by [20]

$$Z_\Lambda[\eta^\dagger,\eta] = \int D[\phi^\dagger,\phi]D[\psi^\dagger,\psi] \times \\ \times \exp\left\{\sum_{k,\sigma}\eta_{k\sigma}^\dagger\left(\psi_{k\sigma}+\phi_{k\sigma}\right) + \left(\psi_{k\sigma}^\dagger + \phi_{k\sigma}^\dagger\right)\eta_{k\sigma} + \right. \\ + \frac{1}{\beta}\sum_{k,\sigma}\mathcal{G}_{k,\Lambda}^{-1}\left(\phi_{k\sigma}^\dagger\phi_{k\sigma} + \psi_{k\sigma}^\dagger\phi_{k\sigma} + \phi_{k\sigma}^\dagger\psi_{k\sigma}\right) + \\ + \left(\mathcal{G}_{k,\Lambda}^{-1} - G_{loc,\nu}^{-1}\right)\psi_{k\sigma}^\dagger\psi_{k\sigma} - \frac{1}{\beta^3}\times \\ \times \sum_{kk'q}\sum_{\sigma\sigma'}\widetilde{\Gamma}_{loc,\sigma\sigma'}^{\nu\nu'\omega}\left[\left(\psi_{k\sigma}^\dagger\phi_{k+q,\sigma}\right)\left(\phi_{k'+q,\sigma'}^\dagger\phi_{k'\sigma'}\right) + \right. \\ + \left(\phi_{k\sigma}^\dagger\phi_{k+q,\sigma}\right)\left(\phi_{k'+q,\sigma'}^\dagger\psi_{k'\sigma'}\right) + \\ \left.\left. + \frac{1}{2}\left(\phi_{k\sigma}^\dagger\phi_{k+q,\sigma}\right)\left(\phi_{k'+q,\sigma'}^\dagger\phi_{k'\sigma'}\right)\right]\right\} J[\phi^\dagger,\phi], \quad (19)$$

where $J[\phi^\dagger,\phi]$ is the Jacobian, defined in terms of local degrees of freedom in Ref. [20], and

$$\widetilde{\Gamma}_{loc,\sigma\sigma'}^{\nu\nu'\omega} = \left(1 - \frac{\delta_{\sigma\sigma'}}{2}\right)\Gamma_{loc,\sigma\sigma'}^{\nu\nu'\omega}.$$

Equation (19) contains integration over two fermionic fields ϕ and ψ; the latter appears after the fermionic Hubbard–Stratanovich transformation of the Legendre transform of the action and provides the one-particle irreducibility of the resulting approach with respect to the local Green's functions. The diagrammatic meaning of Eq. (19), as well as the summation of the ladder diagrams for the vertex and their effect on the self-energy, was discussed in detail in Ref. [20]; here, we consider the renormalization-group approach to this representation.

The bare propagator of representation (19), which fully includes the effect of the local self-energy, can be conveniently written in the spinor representation [20]

$$\Phi_{k\sigma} = \begin{pmatrix} \phi_{k\sigma} \\ \psi_{k\sigma} \end{pmatrix} \quad (20)$$

and is given by

$$\mathbf{G}_{k,\Lambda} = -\frac{1}{\beta}\langle\langle\Phi_k|\Phi_k^\dagger\rangle\rangle_0 = \\ = \begin{pmatrix} \mathcal{G}_{k,\Lambda}^{-1} & \mathcal{G}_{k,\Lambda}^{-1} \\ \mathcal{G}_{k,\Lambda}^{-1} & \mathcal{G}_{k,\Lambda}^{-1} - G_{loc,\nu}^{-1} \end{pmatrix}^{-1} = \\ = \begin{pmatrix} \widetilde{\mathcal{G}}_{k,\Lambda} & G_{loc,\nu} \\ G_{loc,\nu} & -G_{loc,\nu} \end{pmatrix}. \quad (21)$$

The corresponding equations for the vertex $\mathbb{V}_\Lambda^{\alpha\beta\gamma\delta}(k_1, k_2; k_3, k_4)$ (where k_1, k_2 and k_3, k_4 are the momenta and frequencies of the incoming and outgoing electrons, $k_i = (\mathbf{k}_i, i\nu_n^{(i)})$, and $\alpha,\beta,\gamma,\delta = 1,2$ respectively correspond to ϕ and ψ fields) and the nonlocal part of the self-energy $\widetilde{\Sigma}_\Lambda^{\alpha\beta}(\mathbf{k}, i\nu_n)$ are

$$\frac{d\widetilde{\Sigma}_\Lambda}{d\Lambda} = \mathbb{V}_\Lambda \circ \mathbb{S}_\Lambda, \quad (22)$$

$$\frac{d\mathbb{V}_\Lambda}{d\Lambda} = \mathbb{V}_\Lambda \circ (\mathbb{G}_\Lambda \circ \mathbb{S}_\Lambda + \mathbb{S}_\Lambda \circ \mathbb{G}_\Lambda) \circ \mathbb{V}_\Lambda, \quad (23)$$

where

$$\mathbb{G}_{k,\Lambda} = [\mathbf{G}_{k,\Lambda}^{-1} - \widetilde{\mathbf{\Sigma}}_{k,\Lambda}]^{-1} \quad (24)$$

is the dressed spinor Green's function. For the choice of the propagators in (16), we obtain

$$\mathbb{S}_{k,\Lambda} = -(\mathcal{G}_k^{-1} - G_{loc}^{-1})\frac{\partial f(k,\Lambda)}{\partial\Lambda}[\mathbf{G}_{k,\Lambda}^{-1} - \widetilde{\mathbf{\Sigma}}_{k,\Lambda}]^{-1} \times \\ \times \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}[\mathbf{G}_{k,\Lambda}^{-1} - \widetilde{\mathbf{\Sigma}}_{k,\Lambda}]^{-1}, \quad (25)$$

while for propagator (17), we find

$$\mathbb{S}_{k,\Lambda} = -(\mathcal{G}_k - G_{loc})\mathcal{G}_{k,\Lambda}^{-2}\frac{\partial f(k,\Lambda)}{\partial\Lambda}[\mathbf{G}_{k,\Lambda}^{-1} - \widetilde{\mathbf{\Sigma}}_{k,\Lambda}]^{-1} \times \\ \times \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}[\mathbf{G}_{k,\Lambda}^{-1} - \widetilde{\mathbf{\Sigma}}_{k,\Lambda}]^{-1}. \quad (26)$$

We note that the nonlocal (physical) Green's function can be directly obtained from Eq. (24) by summing all the components of the matrix Green's function $(\mathbf{G}^{-1}_{k,\Lambda}-\widetilde{\mathbf{\Sigma}}_{k,\Lambda})^{-1}$; the corresponding "physical" self-energy is then extracted in the standard way from the physical Green's function and the flowing bare Green's function $(\mathcal{G}^{-1}_{k,\Lambda}+\Sigma_{loc})^{-1}$.

For $\Lambda \geq \Lambda_0$ (where Λ_0 is the upper scale of the problem), we have $\widetilde{G}_\Lambda = 0$, and hence only the $\mathbf{G}^{12}$, $\mathbf{G}^{21}$, and $\mathbf{G}^{22}$ elements of the Green's function are nonzero, which corresponds to a purely local theory. It can be shown that the contribution of these Green's functions are exactly compensated by the "counterterms" that arise from the Jacobian of the transformation. The initial conditions for the vertex and the self-energy are

$$\begin{aligned}&\mathbb{V}^{1111}_\Lambda(k_1,k_2;k_3,k_4) = \mathbb{V}^{1211}_\Lambda(k_1,k_2;k_3,k_4) = \\ &= \mathbb{V}^{2111}_\Lambda(k_1,k_2;k_3,k_4) = \mathbb{V}^{1121}_\Lambda(k_1,k_2;k_3,k_4) = \\ &= \mathbb{V}^{1112}_\Lambda(k_1,k_2;k_3,k_4) = \\ &= \Gamma^{\uparrow\downarrow}_{loc},\end{aligned} \tag{27}$$

$$\widetilde{\mathbf{\Sigma}}^{\alpha\beta}(k) = 0. \tag{28}$$

3.3. Comparison with the DMF^{2}RG approach

To compare the fRG flow within the 1PI–LGF and DMF^{2}RG approaches, we consider the choice of propagators (16) and (25). We assume in what follows that the self-energy correction has the structure

$$\mathbf{\Sigma}_{k,\Lambda} = \Sigma^{(1)}_{k,\Lambda}\begin{pmatrix}1&1\\1&1\end{pmatrix} + \Sigma^{(2)}_{k,\Lambda}\begin{pmatrix}1&1\\1&0\end{pmatrix}, \tag{29}$$

which was obtained in the ladder approximation in Ref. [20] and is justified self-consistently below. With this assumption, the Green's function $\mathbb{G}_{k,\Lambda}$ can be represented in the form

$$\mathbb{G}_{k,\Lambda} = G_{k,\Lambda}\begin{pmatrix}1&0\\0&0\end{pmatrix} + \frac{G_{loc,\nu}}{1-G_{loc,\nu}\Sigma^{(2)}_{k,\Lambda}}\times \times\begin{pmatrix}-1&1\\1&-1\end{pmatrix}, \tag{30}$$

where $G_{k,\Lambda}$ is given by Eq. (14) with $\Sigma_{k,\Lambda} = \Sigma^{(1)}_{k,\Lambda} + \Sigma^{(2)}_{k,\Lambda}$. For the single-scale propagator, we obtain

$$\mathbb{S}_{k,\Lambda} = \begin{pmatrix}S_{k,\Lambda}&0\\0&0\end{pmatrix}, \tag{31}$$

where $S_{k,\Lambda}$ is identical to the single-scale propagator (15) considered in Ref. [31].

Considering the

$$\mathbf{\Sigma}^{11}_{k,\Lambda} = \Sigma_{k,\Lambda} \equiv \Sigma^{(1)}_{k,\Lambda} + \Sigma^{(2)}_{k,\Lambda}$$

component of the self-energy and the $\mathbb{V}^{1111}_\Lambda(k_1, k_2; k_3, k_4)$ component of the vertex, the first term in Eq. (30) yields the equations of the DMF^{2}RG approach, while the second term yields zero under the assumption that the vertex keeps its structure (27). But we have to verify that Eqs. (27), (30), and (31) are preserved by the considering approach. We first consider the self-energy. Assuming ansatz (27) for the vertices and using the result in (31) for the single-scale propagator, we find that

$$\mathbf{\Sigma}^{11}_{k,\Lambda} = \mathbf{\Sigma}^{12}_{k,\Lambda} = \mathbf{\Sigma}^{21}_{k,\Lambda}.$$

This implies Eq. (30). We next verify the fulfillment of vertex ansatz (27). Starting with (30) and (31), we find that the first term in Eq. (30) provides the fulfillment of the first three lines in (27). For the vertices $\mathbb{V}^{1211}_\Lambda$, $\mathbb{V}^{2111}_\Lambda$, $\mathbb{V}^{1121}_\Lambda$, and $\mathbb{V}^{1112}_\Lambda$, the second term involves vertices with two indices "2", like $\mathbb{V}^{1212}_\Lambda$, which turn out to cancel each other. Therefore, we find that the representations given by the first three lines of Eq. (27) and Eqs. (30) and (31) preserve their form under the flow, and the considered approach appears to be equivalent to the DMF^{2}RG approach.

4. THE DUAL FERMION APPROACH

The renormalization of the dual fermion approach of Refs. [16–19] was formulated and related to the renormalization of the original lattice theory (2), (3) in Ref. [32]. Here we consider the functional form of this approach, expressed in terms of the effective interactions. The DF approach can be conveniently formulated by splitting the effective interaction of the lattice theory (see, e. g., Ref. [24]),

$$\begin{aligned}\mathcal{V}[\eta,\eta^\dagger] &:= -\ln\int d[c,c^\dagger]\times \\ &\times\exp\left\{\sum_{k,\sigma} G^{-1}_{0k}\left(c^\dagger_{k\sigma}+\eta^\dagger_{k\sigma}\right)(c_{k\sigma}+\eta_{k\sigma}\right) - \\ &- \sum_{i,\sigma}\int d\tau H_{int}[c_{i\sigma},c^\dagger_{i\sigma}]\right\} = \\ &= -\ln Z[G^{-1}_{0k}\eta_{k\sigma}, G^{-1}_{0k}\eta^\dagger_{k\sigma}] - \eta^\dagger_{k\sigma}G^{-1}_{0k}\eta_{k\sigma},\end{aligned} \tag{32}$$

without performing its Legendre transformation. The expansion of $\mathcal{V}[\eta,\eta^\dagger]$ in source fields generates connected (in general, one-particle reducible) Green's func-

tions, amputated by the noninteracting Green's functions G_{0k} of the lattice theory. Applying the covariation splitting formula to Eq. (32) yields the relation between the lattice and dual effective interactions [22]

$$\mathcal{V}[\eta,\eta^\dagger] = \widehat{\mathcal{V}}[\widehat{\eta},\widehat{\eta}^\dagger] + \\ + \sum_{k,\sigma} \eta^\dagger_{k,\sigma} \frac{\Sigma_{loc}(i\nu_n)}{1-\Sigma_{loc}(i\nu_n)G_{0k}} \eta_{k,\sigma}, \quad (33)$$

where the effective interaction for the dual theory is defined by

$$\widehat{\mathcal{V}}[\widehat{\eta},\widehat{\eta}^\dagger] = -\ln \int D[\widetilde{c},\widetilde{c}^\dagger] \times \\ \times \exp\left\{ \sum_{k,\sigma} \widetilde{\mathcal{G}}_k^{-1} \left(\widetilde{c}^\dagger_{k,\sigma} - \widehat{\eta}^\dagger_{k,\sigma}\right)(\widetilde{c}_{k,\sigma} - \widehat{\eta}_{k,\sigma}) - \right. \\ \left. - \widehat{\mathcal{V}}_{DMFT}[\widetilde{c}^\dagger,\widetilde{c}] \right\}, \quad \widehat{\eta}_{k\sigma} = \frac{\eta_{k\sigma}}{1-\Sigma_{loc}(i\nu_n)G_{0k}}. \quad (34)$$

As in the preceding section, we set $\widetilde{\mathcal{G}}_k = \mathcal{G}_k - G_{loc}$.

To introduce a Λ-dependence of the effective interaction, similarly to the preceding section, we again replace $\mathcal{G}_k \to \mathcal{G}_{k,\Lambda}$ (see, e. g., Eq. (16) or Eqs. (17) and (18)). To generalize relation (33) to arbitrary Λ, we also adjust the lattice bare Green's function according to

$$G_{0k} \to G_{0k,\Lambda} := [\mathcal{G}^{-1}_{k,\Lambda} + \Sigma_{loc}(i\nu_n)]^{-1}.$$

Equation (33) then becomes

$$\mathcal{V}_\Lambda[\eta,\eta^\dagger] = \widehat{\mathcal{V}}_\Lambda[\widehat{\eta}_\Lambda,\widehat{\eta}^\dagger_\Lambda] + \\ + \sum_{k,\sigma} \widehat{\eta}^\dagger_{k,\Lambda,\sigma} \frac{\Sigma_{loc}(i\nu_n)}{1+\mathcal{G}_{k,\Lambda}\Sigma_{loc}(i\nu_n)} \widehat{\eta}^\dagger_{k,\Lambda,\sigma}, \quad (35) \\ \widehat{\eta}_{k,\Lambda,\sigma} = \eta_{k\sigma}[1+\Sigma_{loc}(i\nu_n)\mathcal{G}_{k,\Lambda}].$$

This allows us to perform a consistent renormalization of the lattice and dual theory, in particular, keeping the relation between the dual $\Sigma_d(k,\Lambda)$ and lattice $\Sigma_{k,\Lambda}$ self-energies [16, 22] unchanged (cf. Ref. [32]):

$$\Sigma_{k,\Lambda} = \frac{\Sigma_d(k,\Lambda)}{1+G_{loc}(i\nu_n)\Sigma_d(k,\Lambda)} + \Sigma_{loc}(i\nu_n). \quad (36)$$

The renormalization of the dual fermion effective interaction $\widehat{\mathcal{V}}_\Lambda[\widehat{\eta},\widehat{\eta}^\dagger]$ can be performed in the standard way. The Polchinskii equation for $\widehat{\mathcal{V}}_\Lambda$ is

$$\partial_\Lambda \widehat{\mathcal{V}}_\Lambda[\widehat{\eta},\widehat{\eta}^\dagger] = -\Delta_{\partial_\Lambda \widetilde{G}_{k,\Lambda}} \widehat{\mathcal{V}}_\Lambda + \Delta^{12}_{\partial_\Lambda \widetilde{G}_{k,\Lambda}} \widehat{\mathcal{V}}^{(1)}_\Lambda \widehat{\mathcal{V}}^{(2)}_\Lambda.$$

We note that the Λ-derivative here does not act on the source fields $\widehat{\eta}$ and $\widehat{\eta}^\dagger$, whose Λ-dependent values are substituted in the resulting effective interaction. This Λ-dependence determines the flow of the lattice effective interaction (35) in accordance with

$$\partial_\Lambda \mathcal{V}_\Lambda[\eta,\eta^\dagger] = \partial_\Lambda \widehat{\mathcal{V}}_\Lambda[\widehat{\eta}_\Lambda,\widehat{\eta}^\dagger_\Lambda] + \left\{ \eta \frac{\delta \widehat{\mathcal{V}}_\Lambda}{\delta \widehat{\eta}_\Lambda} + \frac{\delta \widehat{\mathcal{V}}_\Lambda}{\delta \widehat{\eta}^\dagger_\Lambda} \eta^\dagger \right\} \times \\ \times (\Sigma_{loc}\partial_\Lambda G_{k,\Lambda}) + \sum_{k,\sigma} \eta^\dagger_{k,\sigma} \Sigma^2_{loc}(i\nu_n)(\partial_\Lambda \mathcal{G}_{k,\Lambda})\eta_{k,\sigma}. \quad (37)$$

Assuming

$$\mathcal{V}_\Lambda[\eta,\eta^\dagger] = \sum \overline{V}_{n,\Lambda} \eta^\dagger_1 \dots \eta^\dagger_{n/2} \eta_{n/2+1} \dots \eta_n, \\ \widehat{\mathcal{V}}_\Lambda[\widehat{\eta},\widehat{\eta}^\dagger] = \sum \overline{v}_{n,\Lambda} \widehat{\eta}^\dagger_1 \dots \widehat{\eta}^\dagger_{n/2} \widehat{\eta}_{n/2+1} \dots \widehat{\eta}_n, \quad (38)$$

we hence obtain the standard relation between the lattice and dual self-energies, Eq. (36), and the higher-order vertices

$$\overline{V}_{n,\Lambda} = \overline{v}_{n,\Lambda} \prod_{i=1}^{n} [1+\Sigma_{loc}(i\nu_i)\mathcal{G}_{k_i,\Lambda}], \quad n>2. \quad (39)$$

The last relation accounts for the effect of the missing local self-energy insertions in the effective interaction $\widehat{\mathcal{V}}_{DMFT}[\widetilde{c}^\dagger,\widetilde{c}]$, which determines $\widehat{\mathcal{V}}_\Lambda[\widehat{\eta},\widehat{\eta}^\dagger]$ according to Eq. (34).

The Legendre transformation of $\widehat{\mathcal{V}}_\Lambda$ can also be performed in the standard way. The resulting 1PI fRG equations (irreducible with respect to $\widetilde{G}_k$) for the fully amputated vertex (cf. Ref. [32])

$$v_\Lambda = \overline{v}_\Lambda \prod\nolimits_{i=1}^{4} \widetilde{\mathcal{G}}_{k_i,\Lambda} \widetilde{G}^{-1}_{k_i,\Lambda}, \quad \overline{v}_\Lambda \equiv \overline{v}_{4,\Lambda},$$

are given by

$$\frac{d\Sigma_d}{d\Lambda} = v_\Lambda \circ S_\Lambda, \quad (40)$$

$$\frac{dv_\Lambda}{d\Lambda} = v_\Lambda \circ (\widetilde{G}_\Lambda \circ S_\Lambda + S_\Lambda \circ \widetilde{G}_\Lambda) \circ v_\Lambda, \quad (41)$$

where

$$\widetilde{G}_{k,\Lambda} = \frac{\widetilde{\mathcal{G}}_{k,\Lambda}}{1-\Sigma_d(k,\Lambda)\widetilde{\mathcal{G}}_{k,\Lambda}}, \quad (42)$$

$$v_\Lambda = \overline{v}_\Lambda \prod_{i=1}^{4} (1-\Sigma_d(k_i,\Lambda)\widetilde{\mathcal{G}}_{k_i,\Lambda}), \quad (43)$$

and

$$S_{k,\Lambda} = \left.\frac{d\widetilde{G}_{k,\Lambda}}{d\Lambda}\right|_{\Sigma_d=\text{const}} = \\ = -(\mathcal{G}^{-1}_k - G^{-1}_{loc})\mathcal{G}^2_{k,\Lambda} \frac{\partial f(k,\Lambda)}{\partial \Lambda} \times \\ \times \frac{1}{[1-\Sigma_d(k,\Lambda)\widetilde{\mathcal{G}}_{k,\Lambda}]^2} \quad (44)$$

for the choice in (16) and

$$S_{k,\Lambda} = \left.\frac{d\widetilde{G}_{k,\Lambda}}{d\Lambda}\right|_{\Sigma_d=\text{const}} = -(\mathcal{G}_k - G_{loc})\frac{\partial f(k,\Lambda)}{\partial\Lambda} \times \\ \times \frac{1}{[1-\Sigma_d(k,\Lambda)\widetilde{\mathcal{G}}_{k,\Lambda}]^2}$$

for the choice in (17). The initial condition is $\Sigma_d = 0$, $V_\Lambda = \Gamma_{loc}$. As discussed above, Eqs. (40) and (41) neglect the local six-point vertex, which is one-particle reducible with respect to the local Green's function.

To compare Eqs. (40) and (41) with those of the DMF^{2}RG approach, we again consider the cutoff dependence in (16). The vertices $v_{n,\Lambda}$ with $n > 2$ can be related to the corresponding vertices $V_{n,\Lambda}$ of the DMF^{2}RG approach by amputating $\overline{V}_{n,\Lambda}$ by the respective full Green's functions and using relations (39) and (43):

$$V_{n,\Lambda} = \overline{V}_{n,\Lambda}\prod_{i=1}^{n} G_{0k_i,\Lambda}G^{-1}_{k_i,\Lambda} = \\ = v_{n,\Lambda}\prod_{i=1}^{n}\left\{[1+\Sigma_{loc}(i\nu_i)\mathcal{G}_{k_i,\Lambda}]\frac{1-\Sigma_{k_i,\Lambda}G_{0k_i,\Lambda}}{1-\Sigma_d(k_i,\Lambda)\widetilde{\mathcal{G}}_{k_i,\Lambda}}\right\}.$$

It can be verified that this factor exactly cancels the difference between the single-scale propagator and Green's functions in the dual fermion approach (Eqs. (42) and (44)) and the DMF^{2}RG approach (Eqs. (14) and (15)), see Ref. [32]. However, the corresponding equations differ because of the Λ-derivative of the corresponding factors [32].

5. CUTOFF SCHEMES AND SELF-CONSISTENCY

Here, we compare different cutoff schemes and analyze their applicability to the renormalization-group treatment discussed in the preceding Sections.

We start with the simple momentum cutoff

$$f(k,\Lambda) = \theta(|\varepsilon_{\mathbf{k}}| - \Lambda). \tag{45}$$

Combined with Eq. (17), the choice (45) has a simple physical meaning: we put the Green's function equal to the local Green's function inside the shell $|\varepsilon_{\mathbf{k}}| < \Lambda$ and equal to the nonlocal function outside this shell. This cutoff, however, does not preserve the important property of vanishing of the average of $\widetilde{G}_\Lambda$ over momentum space under the flow:

$$\sum_{\mathbf{k}}\widetilde{G}_\Lambda(\mathbf{k},i\nu_n) = \\ = \sum_{\mathbf{k}:|\varepsilon_{\mathbf{k}}|>\Lambda}[G(k,i\nu_n) - G_{loc}(i\nu_n)] \neq 0, \quad \Lambda > 0, \tag{46}$$

and, therefore, is not physical.

A possible physical choices are the "interaction flow" cutoff

$$f(k,\Lambda) = 1 - \Lambda \tag{47}$$

and the frequency cutoff used by Husemann and Salmhofer [34],

$$f(k,\Lambda) = \frac{\nu_n^2}{\nu_n^2 + \Lambda^2/(1-\Lambda)^2}, \tag{48}$$

which allow flowing from the theory not interacting nonlocally ($\Lambda = 1$) to the fully interacting theory ($\Lambda = 0$). These two cutoffs preserve the local part of the Green's function if decomposition (17) is used. The possible difficulty of using these two cutoffs is the large computational effort: because one cannot project momenta to the Fermi surface, one has to deal with many "patches" in the whole Brillouin zone.

Finally, we comment on the effect of self-consistency. In the dual fermion approach, two ingridients of a self-consistent procedure were used. The first is to obtain the self-consistent self-energy using the diagram series in the auxiliary space. This self-consistency is fully implemented in the discussed approaches by flowing the self-energy. At the same time, the second step (the so-called external self-consistency) requires adjusting the initial local problem according to the local part of the obtained self-energy. A similar procedure can be applied to the approaches considered in this paper. This type of self-consistency is expected to be important at relatively strong couplings, where it increases the resulting self-energy, making it more "insulating" (see, e. g., Ref. [20]).

6. CONCLUSION

We have considered the application of the functional renormalization-group approach to strongly correlated electronic systems within the one-particle irreducible approaches with respect to the local Green's functions and the dual fermion approach. Both these approaches allow consistent renormalization; the dual fermion approach is expected to be applicable if the one-particle-reducible vertices (with respect to the local Green's functions) of sixth and higher orders are small, while the 1PI approaches with respect to local Green's functions assume the smallness of one-particle-irreducible vertices.

Further numerical investigations of the validity of these assumptions, as well as comparison of the results of the our approaches to the flow from infinite to finite dimensions [31] remain to be performed.

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