Efficient evaluation of the polarization function in the dynamical mean-field theory

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The dynamical susceptibility of strongly correlated electronic systems can be calculated within the framework of the dynamical mean-field theory (DMFT). The required measurement of the four-point vertex of the auxiliary impurity model is however costly and restricted to a finite grid of Matsubara frequencies, leading to a cutoff error. It is shown that the propagation of this error to the lattice response function can be minimized by virtue of an exact decomposition of the DMFT polarization function into local and nonlocal parts. The former is measured directly by the impurity solver, while the latter is given in terms of a ladder equation for the Hedin vertex that features an unprecedentedly fast decay of frequency summations compared to previous calculation schemes, such as the one of the dual boson approach. Neglecting nonlocal corrections furthermore yields an improved polarization diagram for the TRILEX method. In finite dimensions the DMFT susceptibility exhibits spurious mean-field criticality, therefore, a two-particle self-consistent and frequency-dependent correction term is introduced, similar to the Moriya-λ correction of the dynamical vertex approximation. Applications to the two- and three-dimensional Hubbard models on the square and cubic lattices show that the expected critical behavior near an antiferromagnetic instability is recovered.

I. INTRODUCTION

The dynamical mean-field theory (DMFT) is a powerful non-perturbative approach to strong local correlations in the Hubbard model [1]. Although in widespread use, many aspects of the DMFT are still under investigation, which is fueled to large extent by persistent algorithmic advances in the solution of its auxiliary Anderson impurity model [2]. These improvements allow insights into the two-particle level of the DMFT approximation [3], which is also the elemental precursor for its diagrammatic extensions [4].

A basic application for DMFT at the two-particle level is the calculation of the dynamical susceptibility, which grants access, for example, to the electron energy loss spectrum [5]. Calculation of the dynamical susceptibility however requires knowledge of the impurity vertex function, which is often evaluated by means of improved estimators for continuous-time quantum Monte-Carlo (CTQMC) solvers [6, 7]. The further development of improved estimators is highly desirable, as they allow to efficiently calculate the DMFT susceptibility in multi-orbital settings, see for example Ref. [8]. Recently, progress has been reported also in the measurement of the vertex function within the exact diagonalization method [9].

The role of the improved estimators in CTQMC methods is to minimize the statistical noise of the Monte Carlo measurement, which for fixed run-time greatly increases with the number of dynamic degrees of freedom (Matsubara frequencies) of the measured quantity. A further numerical error is introduced because the measurement of the impurity vertex function \( f(\nu, \nu', \omega) \) is restricted to a finite grid of the three Matsubara frequencies \( \nu, \nu', \omega \). In order to obtain a gauge invariant lattice response function in DMFT it is necessary to account for an infinite number, that is, a ladder of vertex corrections [10]. For each vertex correction the value of \( f \) (or of the related irreducible vertex) at all frequencies enters the calculation, and therefore due to the finite Matsubara grid a cutoff error arises. Consequently, the numerical error of the DMFT response function may not only be minimized by an improved Monte Carlo measurement but also by reduction of the cutoff error. A straightforward way to do this is to account for the asymptotics of the vertex function [11–14].

A further option for improvement, the subject of this work, is to use the numerically exact impurity solver to sum local diagrams exactly. For concreteness, within the dual boson approach and in a calculation scheme by Pruschke et al. the DMFT response function \( X \) is written as the sum of local and nonlocal parts [10, 15, 16],

\[
X_q(\omega) = \chi(\omega) + \tilde{X}_q(\omega), \tag{1}
\]

where \( q \) is the lattice momentum and \( \omega \) the (bosonic) Matsubara frequency. The local part, the impurity susceptibility \( \chi \), depends only on one frequency and is calculated directly by the impurity solver, which in effect sums all local two-particle diagrams that taken together yield \( \chi \). On the other hand, the large error attached to the impurity vertex function \( f \) only enters the nonlocal corrections \( \tilde{X} \). Even when the asymptotic behavior of \( f \) is neglected this reduces the numerical error enough to allow an analytical continuation of the response function \( X \) to the real axis [5, 10]. It is however desirable to preserve numerical resources, and hence further improvements are welcome.

In this work it will be shown that the concept of breaking down the DMFT susceptibility into simpler diagrammatic pieces can be taken to a further level by separating exactly the diagrams from the vertex function \( f \) that are irreducible with respect to the bare Hubbard interaction \( U \). The main result is a decomposition of the polarization function \( \Pi \), which is \( U \)-irreducible, into local and nonlocal parts, \( \Pi_q(\omega) = \pi(\omega) + \Pi_q(\omega) \), analogous to Eq. (1). The nonlocal part \( \Pi \) is obtained via an efficient ladder equation for the Hedin three-leg vertex [17]. The lattice
polarization $\Pi_\alpha(\omega)$ in turn encapsulates all non-trivial information about the two-particle spectrum.

The Hedin vertex also plays a central role in the TRILEX approach [18]. In this method nonlocal vertex corrections to the Hedin vertex are neglected, and therefore the calculation of the four-point vertex function of the impurity model is not necessary. A byproduct of this work is an improved formula for the polarization in the TRILEX approach, which takes a large number of additional vertex corrections beyond the original formula into account while the numerical effort is the same.

Lastly, a further aspect is considered in the application of the efficient formula for the polarization: In finite dimensions the DMFT susceptibility violates the Pauli principle and suffers from a spurious mean-field instability in two dimensions. It has been shown previously that the Mermin-Wagner theorem is satisfied in the renormalized ladder dual fermion approach [19] or after introduction of the Moriya-$\lambda$ correction to the DMFT susceptibility [20]. Similar to the latter option, in this work the mean-field artifacts and the violation of the Pauli principle are removed by virtue of a frequency-dependent correction term that is fixed by a two-particle self-consistency condition.

The paper is organized as follows: The Hubbard Hamiltonian, the DMFT approximation, and the Anderson impurity model are briefly recollected in Sec. II. The reducible and irreducible vertices of the impurity model are defined in Sec. III. The efficient formula for the DMFT polarization is introduced in Sec. IV and compared to the dual boson and TRILEX formulas. A two-particle self-consistent modification of the DMFT susceptibility is presented in Sec. V and applied in Sec. VI. The conclusions follow in Sec. VII. A self-contained derivation of the ladder equation for the Hedin vertex is provided in the Appendices A-D.

II. HUBBARD HAMILTONIAN AND DMFT APPROXIMATION

The Hamiltonian of the paramagnetic two- or three-dimensional Hubbard model is given as,

$$H = -\sum_{\langle ij \rangle \sigma} t_{ij} c_{i \sigma}^\dagger c_{j \sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow},$$  

where $t_{ij}$ is the nearest neighbor hopping between lattice sites $i,j$, its absolute value $t=1$ is the unit of energy, $c,c^\dagger$ are the construction operators, $\sigma = \uparrow, \downarrow$ the spin index. $U$ is the Hubbard repulsion between the densities $n_\sigma = c_{\sigma}^\dagger c_{\sigma}$.

In the DMFT approximation the self-energy $\Sigma$ of Green’s function is local,

$$G_k = [\nu - \varepsilon_k + \mu - \Sigma_\nu]^{-1},$$  

where $k = (\mathbf{k}, \nu)$ comprises lattice momentum and fermionic Matsubara frequency, $\varepsilon_k$ is the dispersion, $\mu$ is the chemical potential. $\Sigma_\nu$ is the self-energy of an auxiliary Anderson impurity model (AIM) that is solved numerically exactly. The action of the AIM reads,

$$S_{\text{AIM}} = -\sum_{\nu \sigma} c_{\nu \sigma}^\dagger (\nu + \mu - \Delta_\nu) c_{\nu \sigma} + U \sum_\omega n_{\uparrow \omega} n_{\downarrow \omega}.$$  

Here $\Delta_\nu$ denotes the hybridization function, $\omega$ is a bosonic Matsubara frequency, summations $\sum_\nu', \sum_\omega$ imply multiplication with the temperature $T$. $c^\dagger,c$ are Grassmann numbers. In DMFT the hybridization function is fixed self-consistently according to the constraint,

$$\sum_\mathbf{k} G_k = g_\nu,$$  

where $g$ is the numerically exact local Green’s function of the AIM. Note that summation over $\mathbf{k}$ implies division by the number of lattice sites $N$.

III. IMPURITY VERTICES

The calculation of the dynamical susceptibility requires knowledge of higher correlation functions of the impurity. Directly measured by the solver are the susceptibilities, $\chi_\nu = -\langle \rho_{-\omega} \rho_\nu^\dagger \rangle + \langle n \rangle \delta_{\omega,\delta_{\alpha,\text{ch}}}$, the four-point,

$$g^{(4),\alpha}_{\nu\nu'\omega} = -\frac{1}{2} \sum_{\sigma_i} s_\sigma^\alpha_{\sigma_i} s_{\sigma_i}^\dagger \langle c_{\nu \sigma_1}^\dagger c_{\nu' +\omega,\sigma_1}^\dagger c_{\nu' +\omega,\sigma_2} c_{\nu,\sigma_2}^\dagger \rangle,$$

and the three-point function,

$$g^{(3),\alpha}_{\nu\omega} = \frac{1}{2} \sum_{\sigma,\sigma'} s_\sigma^\alpha s_{\sigma'}^\dagger \langle c_{\nu \sigma_1}^\dagger c_{\nu' +\omega,\sigma_1} c_{\nu' +\omega,\sigma_2} \rangle = \sum_{\nu'} g^{(4),\alpha}_{\nu\nu'\omega},$$

where $s_\sigma^\alpha$ are the Pauli matrices ($\alpha = \text{ch,sp}$), $\rho^\dagger = n_\uparrow + n_\downarrow$ and $\rho^\dagger = n_\uparrow - n_\downarrow$ are the charge and spin densities.

A. Reducible vertices

One defines the four- and three-point vertices $f$ and $\bar{\lambda}$,

$$f^{\alpha}_{\nu\nu'\omega} = \frac{g^{(4),\alpha}_{\nu\nu'\omega} - \beta g_{\nu\nu'\omega} \delta_{\nu' +\omega} + 2\beta g_{\nu\nu'\omega} \delta_{\omega,\delta_{\alpha,\text{ch}}}}{g_{\nu\nu'\omega} g_{\nu' +\omega} g_{\nu' +\omega},}$$

$$\bar{\lambda}^{\alpha}_{\nu\omega} = \frac{g^{(3),\alpha}_{\nu\omega} + \beta g_{\nu} \langle n \rangle \delta_{\omega,\delta_{\alpha,\text{ch}}}}{g_{\nu} g_{\nu +\omega}}.$$  

Although numerically unfavorable $\bar{\lambda}$ can in principle also be obtained by attaching legs to $f$ from the right and adding $1$, $\bar{\lambda}^{\alpha}_{\nu\omega} = 1 + \sum_{\nu'} f^{\alpha}_{\nu\nu'\omega} g_{\nu' +\omega}$, therefore $\bar{\lambda}$ is a right-sided three-leg vertex [21], the left-sided one $\lambda$ is obtained by attaching the legs from the left or via the symmetry relation, $\lambda^{\alpha}_{\nu\omega} = \bar{\lambda}^{\alpha}_{\nu +\omega,-\omega}$. 
FIG. 1. Lowest order contributions to the $U^\alpha$-reducible three-leg [a]) and four-leg [b)] vertices $\lambda$ and $f$ of the impurity. Dashed lines indicate the bare interaction $\pm U$, arrows the impurity Green’s function $g$. Red crosses mark RPA-like contributions that are not included in the $U^\alpha$-irreducible $\lambda^i$ and $f^i$. The second line of diagram b) shows the relation between $f, f^i$, and $\lambda^i$, the wiggly line denotes the screened interaction $w$ of the impurity [cf. Eq. (9) and Appendix A], which is represented in diagram c) as a geometric series.

B. $U^\alpha$-irreducible vertices

In order to make the later calculation of the DMFT lattice correlation functions efficient the impurity vertices are decomposed following Hertz and Edwards [22].

The diagram a) in Fig. 1 shows that when the three-leg vertex $\lambda^\alpha$ is expanded diagrammatically one may encounter, in going from left to right, an insertion of the bare interaction $U^\alpha$, where $U^{\text{ch}} = +U$ or $U^{\text{mp}} = -U$. The Hubbard interaction is just a constant, and the incoming impurity Green’s function lines on the left of $U^\alpha$ can thus be contracted, the same is case for the out-going lines.

On the left of $U^\alpha$ there hence arises a contribution to the $U^\alpha$-irreducible polarization $\pi^\alpha$ of the impurity [related to the susceptibility via $\chi^\alpha = 2\pi^\alpha/(1 - U^\alpha \pi^\alpha)$], whereas on the right of $U^\alpha$ begins once again an expansion of the three-leg vertex. As shown algebraically in Appendix A, one thus separates diagrams from $\lambda$ that are once or manifold $U^\alpha$-reducible,

$$\lambda^\alpha_{\nu\omega} = \frac{\lambda^{i\alpha}_{\nu\omega}}{1 - U^\alpha \pi^\alpha},$$  

where $\lambda^i$ is the $U^\alpha$-irreducible three-leg vertex – the Hedin vertex – of the impurity.

Let us perform this procedure also for the four-point vertex $f$, as depicted in Fig. 1 b). $f$ obviously contains one part $f^i$ that is irreducible, whereas in the remaining terms one finds at least one insertion $U^\alpha$. At this point the incoming lines may be closed and a right-sided Hedin vertex $\lambda^i$ arises on the left of $U^\alpha$. In fact, also on the right of $U^\alpha$ the lines may be closed, which means that a true four-point contribution does not arise in the $U^\alpha$-reducible diagrams. For this reason the whole of the reducible diagrams may be split into the three- and two-point objects $\lambda^i, \lambda^\pi$ and $\pi$, respectively,

$$f^\alpha_{\nu\omega} = f^{i\alpha}_{\nu\omega} + \lambda^{i\alpha}_{\nu\omega} w^\alpha_{\nu\omega} \lambda^{i\alpha}_{\nu\omega},$$

where $w^\alpha_{\nu\omega} = U^\alpha/(1 - U^\alpha \pi^\alpha)$ is the screened interaction of the impurity [cf. Fig. 1 c)].

The equations (8) and (9) are valuable because they separate RPA-like diagrams from the vertices $\lambda$ and $f$, which are absorbed into the geometric series in Fig. 1 c), the screened interaction $w$. Similar relations are also valid for the Hubbard model (2), see Ref. [23] and Appendix A. The characteristic triangle-wiggle-triangle diagram in Fig. 1 b) is typically large when the corresponding susceptibility $\chi^\alpha$ is large, since then $U^\alpha \pi^\alpha \approx 1$.

One should note that in the reducible contribution $\lambda^{i\omega}_{\nu\omega} w^\omega_{\nu\omega}$ in Eq. (9) the dependence on $\nu$ and $\nu'$ is separated. Therefore, this term is necessarily comprised in the lowest order of a singular value decomposition of $f$ [24].

IV. LATTICE QUANTITIES

The goal is to calculate the dynamical susceptibility in the DMFT approximation,

$$\chi^\alpha_q = \frac{2\Pi^\alpha_q}{1 - U^\alpha \Pi^\alpha_q},$$  

where $q = (q, \omega)$ and $\Pi^\alpha_q$ is the lattice polarization. It is shown in Appendix C that in DMFT the latter may be decomposed into local and nonlocal parts,

$$\Pi^\alpha_q = \sum_{\nu} \Lambda^{\nu\alpha}_{\nu\omega} \chi^\nu_{\nu\omega}(q) \bar{\lambda}^{i\alpha}_{\nu\omega} = \pi^\alpha_q + \tilde{\Pi}^\alpha_q.$$

The nonlocal corrections are denoted as $\tilde{\Pi}$, analogous to the dual boson formula for the susceptibility (1) and $\bar{\lambda}^{i\alpha}_{\nu\omega}(q)$ is a nonlocal bubble,

$$\bar{\lambda}^{i\alpha}_q(q) = \sum_k G_{k+q} G_k.$$

Here, $G_k = G_k - g_k$ is the nonlocal DMFT Green’s function, which decays with the frequency as $1/\nu^2$, and $\Lambda^{\nu\alpha}$ is the left-sided lattice Hedin vertex. Equation (11) is depicted diagrammatically in Fig. 2 b).

We now come to the main result, which a nonlocal ladder equation for the Hedin vertex in the DMFT approximation. It is shown in Appendix D that,

$$\Lambda^{\nu\alpha}_{\nu\omega} = \bar{\lambda}^{i\alpha}_{\nu\omega} + \sum_{\nu'} \Lambda^{i\alpha}_{\nu'\omega} \bar{\lambda}^{i\alpha}_{\nu'\omega}(q) f^{i\alpha}_{\nu'\omega},$$  

which is depicted in Fig. 2 a). Note that $f^i$ is the $U^\alpha$-irreducible four-leg vertex of the impurity model, it is the only true four-point object needed in the calculation.
A. Comparison to dual boson formula

It will now be shown that the formula (11) for the polarization is numerically more efficient than the dual boson formula (1). To this end, let us recall that in the latter case the nonlocal corrections are given as [see Appendix C, Refs. [5, 10], and Fig. 2 c)],

$$
\tilde{X}_q^\alpha = 2 \sum_\nu \Lambda^\alpha_{\nu q} \tilde{X}_0^0(q) \tilde{\lambda}^\alpha_{\nu \omega},
$$

(14)

similar to \( \tilde{\Pi} \) in Eq. (11), except that the \emph{U-reducible} three-leg vertices \( \Lambda, \lambda \) are in place of the Hedin vertices \( \Lambda^i, \lambda^i \) (and the factor 2). Furthermore, the vertex \( \lambda \) of the lattice is given by the same ladder equation (13) [see also Fig. 2 a)], albeit the label \( i \) needs to be omitted, and there is hence a complete formal analogy in the calculation of \( \tilde{\Pi} \) and \( X \).

Let us compare the first four-point vertex contribution to the nonlocal correction terms \( \tilde{X} \) and \( \tilde{\Pi} \), by expanding the ladder equations for the three-leg vertices \( \Lambda, \lambda \), respectively, see also Eq. (13),

$$
\tilde{X}_q/2 (or \tilde{\Pi}_q) = \sum_\nu \Lambda^\alpha_{\nu q} \tilde{X}_0^0(q) \tilde{\lambda}^\alpha_{\nu \omega},
$$

(15)

where the flavor label \( \alpha \) was omitted for readability.

Typically the calculation of the impurity three-leg vertices \( \tilde{\lambda}^{\alpha i} \) is more efficient than that of the four-leg vertices \( f^{(i)} \), in the latter case one likes to minimize the domain of measurement for \( \nu, \nu', \omega \). The question is therefore how the cutoff error in the four-point corrections that arise in the second line of Eq. (15) affects the calculation. It is useful to analyze the convergence of the term that is written out in the second line of Eq. (15), let us consider first the limit \( |\nu| \to \infty \) while \( \nu' \) and \( \omega \) are kept constant:

According to Eq. (8) the decay of the vertices \( \lambda_{\nu\omega} \) and \( \lambda^i_{\nu\omega} \), with the frequency \( \nu \) is the same except for a prefactor \( [1 - U^{\alpha} \pi_{\nu\omega}^{\alpha}]^{-1} \), therefore, the difference in the three-leg vertices does not lead to a different convergence of the \( \nu \)-summations in \( X \) and \( \tilde{\Pi} \). Also in both cases the nonlocal bubble \( \tilde{X}_0^0(q) \) defined in Eq. (12) decays as \( 1/\nu^4 \). However, the vertices \( f \) and \( f^i \) behave differently, which follows from an observation in Ref. [25]: In the limit \( |\nu| \to \infty \) all diagrams contributing to \( f \) that depend on \( \nu \) have decayed, and hence asymptotically this vertex is given by the diagrams that do not depend on \( \nu \) at all. According to the argument in the reference these diagrams are all \( U \)-reducible, one can write for fixed \( \nu' \),

$$
f_{\nu\nu'\omega}^0 + U^\alpha \sum uv \sum_{\nu'} g_{\nu \nu'} g_{\nu' \omega} f_{\nu\nu'\omega}^0 + O \left( \frac{1}{\nu} \right).
$$

(16)

Factoring out \( U^\alpha \) one identifies the reducible three-leg vertex \( \tilde{\lambda} \) [see below Eq. (7)], therefore,

$$
\lim_{|\nu| \to \infty} f_{\nu\nu'\omega}^0 = U^\alpha \lambda_{\nu\omega}^\alpha = w_{\omega}^\alpha \lambda_{\nu\omega}^{i,\alpha}.
$$

(17)

In the last step Eq. (7) and \( w_{\omega}^\alpha = U^\alpha \pi_{\nu\omega}^{\alpha} \) were used. Let us now compare to the exact relation between the vertices \( f \) and \( f^i \) in Eq. (9). The asymptotic limit of \( f \) in Eq. (17) is given exactly by the asymptotic limit of the \( U \)-reducible diagrams \( \tilde{\lambda}_{\nu\omega}^i \lambda_{\nu\omega}^\alpha \) (note that \( \lambda^i_{\nu\omega} \to 1 \) for \( |\nu| \to \infty \)). This is not surprising in view of the observation of Ref. [25] that only \( U \)-reducible diagrams can be independent of \( \nu \). As a result, the irreducible vertex \( f_{\nu\nu'\omega}^i \) decays to zero for \( |\nu| \to \infty \) and fixed \( \nu' \),

$$
f_{\nu\nu'\omega}^i = U^\alpha \lambda_{\nu\omega}^\alpha = w_{\omega}^\alpha \lambda_{\nu\omega}^{i,\alpha}.
$$

(18)

For this reason the four-point corrections in Eq. (15) decay at least one order of magnitude more quickly for \( \tilde{\Pi} \) than for \( \tilde{X} \), which is the central observation of this work. As a result, compared to the dual boson formula (1), for a fixed cutoff error the domain of the frequencies \( \nu \) and \( \nu' \) can be chosen significantly smaller in the new calculation scheme.

A comprehensive discussion of the asymptotics of \( f \) can be found in Ref. [12], where it is also shown that in the double limit \( |\nu|, |\nu'| \to \infty \) one needs to consider separately the two cases \( \nu - \nu' = \text{const} \) and \( \omega - \nu - \nu' = \text{const} \), that is, the elements of \( f \) near the main and secondary diagonal. However, as regards the scope of this work these cases can be ignored, because then the nonlocal bubbles in Eq. (15) decay as \( 1/\nu^4 \) and \( 1/(\nu')^4 \), respectively, leading to a still faster decay than when only one frequency is large. In summary, in the dual boson formula each four-point correction comes with a factor \( \tilde{X}_0^0(q) f_{\nu\nu'\omega} \), which decays like the nonlocal bubble as \( 1/\nu^4 \) due to the constant background of \( f \), whereas in the new calculation scheme the corrections enter as \( \tilde{X}_0^0(q) f_{\nu\nu'\omega}^i \), which decays at least as \( 1/\nu^4 \) by virtue of the combined decay of nonlocal bubble and vertex \( f^i \).
B. TRILEX-like approximation

Despite all optimizations it may be unfeasible to take four-point corrections due to \( f \) or \( f' \) into account, for example, in multi-orbital settings. In this case one may consider to neglect vertex corrections to the Hedin vertex in Eq. (13), \( \Lambda' \approx \lambda' \), which is also the philosophy of the TRILEX approach. However, Fig. 2 b) shows that in the present case one is left with two bare triangles \( \lambda' \) and \( \lambda' \), respectively, whereas in the original TRILEX approach there is only one triangle [18]. In fact, a similar result arises when the vertex corrections to \( \Lambda' \) are neglected in the relation \( \Pi_{q}^{\alpha} = \sum_{\nu} \Lambda_{q}^{\alpha} G_{k} G_{k+q} \), which in DMFT is equivalent to Eq. (11). It seems however favorable to neglect the vertex corrections not before that equation (11) has been derived [see also Appendix C]. The approximation \( \Lambda' \approx \lambda' \) is further discussed in the applications VI.

V. TWO-PARTICLE SELF-CONSISTENCY

The DMFT susceptibility \( X^{\text{imp}} \) in Eq. (10) may diverge in two dimensions, in violation of the Mermin-Wagner theorem, and it shows the mean-field critical behavior near an antiferromagnetic instability in three dimensions [26, 27]. As discussed in the context of the two-particle self-consistent (TPSC) approach, these drawbacks are due to the violation of local sum rules [28]. In order to alleviate the mean-field artifacts a frequency-dependent correction is introduced,

\[
X_{q}^{\alpha} \rightarrow \chi_{q}^{\alpha} = \frac{2\Pi_{q}^{\alpha}}{1 - (U^{\alpha} + U_{q}^{\alpha})\Pi_{q}^{\alpha}}, \tag{19}
\]

where \( \Pi \) is the DMFT polarization (11). The correction term \( U_{q}^{\alpha} \) is fixed by the self-consistency condition,

\[
\sum_{q} \chi_{q}^{\alpha} = \chi_{\alpha}, \tag{20}
\]

thereby \( \chi \) yields the same kinetic and potential energy as the impurity model of DMFT [29]. The decomposition of the impurity vertex function in Eq. (11) and hence \( \chi_{\alpha} \) is similar to \( \omega \) in the static limit for \( T > 0 \), because then the integral \( \sum_{\alpha} \) over the divergent integrand remains finite [28]. In the limit \( d \rightarrow \infty \) the constraint (20) is satisfied by the DMFT susceptibility (10) and hence \( \chi \) is zero in this limit, as expected. Finally, \( \chi \) preserves the feature \( \omega \chi_{q}^{\alpha} = 0 \) that is satisfied by the conserving DMFT polarization \( \Pi \) in the nominator of Eq. (19). The two-particle spectrum described by \( \chi \) is therefore ungapped, as required by the global conservation law [29] [31].

For all these reasons the correction \( U_{q} \) in Eq. (19) and the constraint (20) appear as suitable in order to remove the mean-field artifacts from the DMFT susceptibility (10). Note that the self-consistency (20) does not lead to a feedback on the impurity model of DMFT, which would in general invalidate the conserving features of the polarization [29]. The correction \( U_{q} \) is similar to the constant Moriya-\( \lambda \) correction [20], it can however not be interpreted straightforwardly as a renormalization of the correlation length, nor is it a retarded interaction. Instead, one may interpret \( U_{q} \) as an effective vertex correction to the susceptibility, which takes diagrams beyond DMFT into account that are needed to satisfy the constraint (20). This interpretation is consistent with the TPSC approach [28], whose non-perturbative features follow due to effective vertex corrections to the RPA susceptibility. Due to the similarities equation (19) and the constraint (20) are referred to in this work as a two-particle self-consistent dynamical mean-field (TPSC-DMF) approach to the susceptibility.

VI. NUMERICAL RESULTS

The decomposition of the impurity vertex function in Sec. III, the efficient evaluation of the polarization in Sec. IV, and the TPSC-DMF approach in Sec. V are applied to the two- and three-dimensional Hubbard models (2) at half-filling. In the calculations firstly the DMFT cycle of Sec. II was completed, then the two- and three-point correlation functions (6) and (7) of the AIM were evaluated, where a CTQMC solver based on the ALPS libraries [32] with improved estimators [6] was used. The polarization was then evaluated according to Sec. IV, then the TPSC-DMF susceptibility was obtained according to Sec. V. The implementation is based on the dual boson code by E.G.C.P van Loon and H. Hafermann.

A. Impurity vertex function

Figure 6 further below shows a phase diagram of the three-dimensional Hubbard model. Stars mark two points at \( T/t = 6 \) and \( T/t = 14 \) for \( T/t \approx 0.4 \), in DMFT these regimes correspond to a bad metal and to an insulator with local moments, respectively [27].

For the metallic regime \( (U/t = 6) \) the left panels of Fig. 3 show the impurity spin vertex function \( f_{\nu\nu}^{\text{imp}} \) in the static limit \( \omega_{0} = 0 \) and for \( \omega_{3} = 6\pi T \). In most directions
f^{sp} decays with increasing ν, ν′ to a constant, however, it also shows two persistent structures with shapes + and ×, see also Ref. [3]. For finite ω_3 these patterns are shifted along the diagonal.

Important in this work is the exact decomposition \( f = f^i + \lambda^i w^\alpha \lambda^i \) discussed in Sec. III. The part that is given by the impurity Hedin vertex \( \lambda^i \) and by the screened interaction \( w \) is shown for \( \alpha = \text{sp} \) in the center panels of Fig. 3. This object merely shows a + pattern, while the right panels show the \( U^{\text{sp}} \)-irreducible vertex \( f^{i,\text{sp}} \), which features the × shape. This correspondence is also there in the charge channel and in different parameter regimes (not shown).

As shown above, a feature of the irreducible vertex \( f^i \) is that it has no constant background, and the one of the reducible vertex \( f \) originates from the term \( \lambda^i w^\alpha \lambda^i \). The large frequency behavior of the four-point vertices is compared qualitatively in Fig. 4, which shows cuts of \( f \) and \( f^i \) in absolute values on a logarithmic scale. The constant background of the reducible vertex \( f^\alpha \) is determined by the quantity \( [1 - U^{\alpha} \pi^{\alpha}]^{-1} \), cf. Eq. (17), which can be very large near a quantum critical point \( U^{\alpha} \pi^{\alpha}=0 \approx 1 \), where the impurity susceptibility \( \chi^{\alpha} \) is large. On the other hand, the irreducible vertex \( f^{i,\alpha} \) quickly decays to values that are indistinguishable from noise of the CTQMC measurement. The difference between \( f \) and \( f^i \) at large frequencies therefore depends on the physical regime. For example, the left panels of Fig. 4 show the metallic regime \( U/t = 6 \), where the charge and spin susceptibilities \( \chi^{\text{ch}} \) and \( \chi^{\text{sp}} \) are of comparable and non-negligible magnitude, and hence \( f \) is very large compared to \( f^i \) at high frequencies. On the other hand, \( \chi^{\text{ch}} \) is very small in the insulating regime \( U/t = 14 \), and there is no big difference between \( f^{\text{ch}} \) and \( f^{i,\text{ch}} \). Instead, in this regime the static spin susceptibility \( \chi^{\text{sp}}(\omega_0) \) dominates, as can be seen in the top right panel of Fig. 4, where \( f^{\text{sp}} \) is almost three orders of magnitude larger than \( f^{i,\text{sp}} \) for most frequencies.

### B. Two-particle self-consistent susceptibility

The TPSC-DMF susceptibility \( \chi \) is calculated according to Sec. V. Firstly, it is verified for the Hubbard model on the square lattice that \( \chi^{\text{sp}}(Q, \omega_0) \) obeys the exponential scaling with temperature required by the Mermin-Wagner theorem, where \( Q = (\pi, \pi) \). This is shown in the top panel of Fig. 5 for \( U/t = 8 \), at low temperature this corresponds in the DMFT approximation to a strongly correlated Fermi liquid (when paramagnetism is enforced). With increasing \( \beta = \frac{1}{T} \) the DMFT susceptibility \( \chi^{\text{sp}} \) quickly diverges, whereas the self-consistent correction term \( \mathcal{U} \) prevents that the same happens to \( \chi^{\text{sp}} = [\chi^{\text{sp}}(Q, \omega_0) - U/2] \). For large \( \beta \) the correlation length \( \xi \) eventually exceeds any fixed system size. Finite-size effects are noticeable when \( \xi \) is of order of the half linear system size, then the self-consistent calculation of \( \mathcal{U} \) becomes inaccurate (arrows).

The center panel of Fig. 5 shows \( \chi^{\text{sp}} \) in the Brillouin zone for the largest lattice size \( 256 \times 256 \) and the lowest considered temperature \( T = 1/7 \). The figure demonstrates simultaneously features of the Mermin-Wagner theorem and of the conservation law: On the one hand the static susceptibility \( \chi^{\text{sp}}(Q \approx Q, \omega_0) \) shows the re-
required Lorentzian (Ornstein-Zernike) form [25], while on the other hand \( \chi^{sp}(q,\omega) \) [dashed red] shows a \( |q|^2 \)-scaling near \( \Gamma \). Fits are shown as black lines, vertical dashed lines indicate the fitting interval. Bottom: Self-consistent correction term \( U^{sp}(\omega) \) to the spin susceptibility for different temperatures.

C. Criticality in three dimensions

A further benchmark for the TPSC-DMF susceptibility is to consider criticality when a spontaneous phase transition is indeed allowed, as is the case in the half-filled three-dimensional Hubbard model. Figure 6 shows the Néel temperature predicted by the ladder dual fermion approach (LDFA) and by the Moriya-\( \lambda \)-corrected DMFT susceptibility [4]. The figure also shows the phase boundary predicted by the TPSC-DMF susceptibility, where \( \chi^{sp,-1}(Q,\omega_0) \) was fitted with the function \( a(T - T_c)^{-\gamma} \) in order to obtain the critical temperature \( T_c \) and the critical exponent \( \gamma \). The fit interval needs to be bounded from above by the high-\( T \) mean-field regime and from below by finite size effects. The upper bound was determined as in Ref. [26], the lower bound is the temperature where the correlation length \( \xi \) exceeds 1/6 of the linear system size of the \( 16 \times 16 \times 16 \) lattice, as in Ref. [27]. The boundary obtained by fitting \( a, T_c, \) and \( \gamma \) is in excellent agreement with the Moriya-\( \lambda \) correction.

The maximum of \( T_c \) at \( U/t = 10 \) marks the crossover from the bad metal to the insulating regime [27]. It was found that already at this point the three-dimensional Hubbard model exhibits the Heisenberg universality class [26], where \( \gamma \approx 1.4 \). Consistent with this the fit of \( \chi' \) for \( U/t \geq 10 \) yields an exponent of roughly 1.35, which compares to the mean-field exponent 1 of DMFT. In this regime \( T_c \) was also estimated with \( \gamma \) assumed to be known from the Heisenberg model, see red crosses in Fig. 6, which leads to an even better agreement with the Moriya-\( \lambda \) correction.
tions to the Hedin vertex are neglected, $\Lambda^i \approx \lambda^i$, as in TRILEX. Note that once again the constraint $x_{\text{loc}} = \chi$ is satisfied by self-consistent adjustment of $U$ in Eq. (19). In fact, also this approximation clearly deviates from the mean-field criticality near the transition and for $U/t \geq 10$ is well-described by the Heisenberg critical exponent, as shown in the right panel of Fig. 6. Without vertex corrections $T_c$ lies reasonably close to the result with the vertex corrections (left panel, yellows and red lines) but the deviation depends on the physical regime: For large coupling the vertex corrections have negligible influence on $T_c$, but play an important role in the region where DMFT predicts a bad metal. The good result at strong coupling may seem counter-intuitive, since the top right panel of Fig. 4 shows that $f^{\text{sp}}$ is not small in the insulator. However, one should recall that all vertex corrections to $\Lambda^i$ come with a bubble of nonlocal Green’s functions $GG$, see also Fig. 2, which represent the propagation of charge carriers that is strongly suppressed in the insulator.

### VII. CONCLUSIONS

A novel method to evaluate the DMFT susceptibility was presented by making use of the Hedin three-leg vertex. Vertex corrections to the latter arise in the form of a four-point vertex $f^i$ of the Anderson impurity model that is irreducible with respect to the bare interaction $\pm U$. This vertex has no constant background, in contrast to the full impurity vertex $f$. Furthermore, the ladder equation for the Hedin vertex is formulated in terms of nonlocal Green’s functions, as in the dual fermion approach [34]. The combination of the fast decay of the nonlocal Green’s functions with the decay of the irreducible vertex $f^i$ leads to a convergence of frequency summations in the vertex corrections that is at least one order of magnitude faster than in the dual fermion and dual boson approaches [16]. As a result, the measurement of the four-point vertex can be restricted to a smaller frequency window. An obvious objective for the future is a generalization to the multi-orbital case.

The new calculation scheme implicitly takes vertex asymptotics into account, which were discussed, for example, in Refs. [11–14]. In the implementation it is nevertheless not necessary to consider the large frequency limits explicitly, because the contributions to the DMFT susceptibility that originate from the constant background of the reducible vertex $f$ are handled in an exact way. The main difference to the previously presented approaches to reduce the cutoff error by taking vertex asymptotics into account is that a diagrammatic decomposition of $f$ is employed that is exact for all frequencies, leading to a particularly simple calculation scheme. The formulation in terms of nonlocal Green’s functions further accelerates the convergence of frequency summations substantially. There may nevertheless be more options to minimize cutoff errors by taking the asymptotic behavior of the irreducible vertex $f^i$ into account.

The mean-field instability of the DMFT susceptibility was removed by introduction of a frequency-dependent correction $U(\omega)$ that is fixed by adjusting the local susceptibility to the impurity, $x_{\text{loc}}(\omega) = \chi(\omega)$. This approach ensures an unzipped two-particle spectrum and the expected critical behavior in two dimensions in agreement with the Mermin-Wagner theorem, reminiscent of the two-particle self-consistent (TPSC) approach that is based on the Hartree/RPA approximation [28]. In the half-filled three-dimensional Hubbard model with one band the criticality of the thus corrected DMFT susceptibility is consistent with the similar Moriya-λ correction used in the dynamical vertex approximation [20], which leads to a renormalized correlation length.

The interpretation of $U(\omega)$ is however different as a somewhat intransparent vertex correction beyond DMFT, it is therefore necessary to consider the domain of validity of the approach: To do this for the weak-coupling limit, one may recall that the TPSC approach requires that the Hartree approximation provides a reasonable description of the Fermi surface nesting [28]. However, in the half-filled two-dimensional Hubbard model on the square lattice a pseudogap opens at low temperature due to antiferromagnetic fluctuations [35–37]. In this case neither the Harttree approximation nor DMFT provide a good starting point, because they predict a homogeneous Fermi surface with strong nesting. On the other hand, even when the feedback of the pseudogap on the two-particle spectrum is taken into account it leads to similar results as the Moriya-λ-corrected DMFT susceptibility [4, 9]. In the large coupling limit an artifact may arise due to the self-consistency $x_{\text{loc}} = \chi$, because the impurity spin susceptibility diverges at zero temperature, although in some settings the local moment may be screened due to short-ranged correlations. In general, the effect of arbitrary two-particle self-consistency conditions must be considered carefully [29].

In the future it may be investigated whether the $U(\omega)$ correction yields a similar feedback on the single-particle spectrum as the Moriya-λ correction [25], where an intriguing perspective is to consider the effect of the frequency-dependence of $U(\omega)$. It may also be possible to make use of the efficient evaluation of the ladder approximation within the dual fermion and dual boson formalisms [16, 34]. Finally, it was shown that for large coupling vertex corrections to the Hedin vertex play a minor role for the Néel temperature of the half-filled three-dimensional Hubbard model. This strengthens the case for the TRILEX approximation in this regime [18], in fact, a byproduct of this work is an improved polarization diagram for this method that takes additional local vertex corrections into account.

During the completion of this work a manuscript was preprinted [24] where it is shown that near a local moment phase of the Anderson impurity model a singular value decomposition of the generalized spin susceptibility may be truncated after the lowest order, which leads to
a significant simplification of the DMFT spin susceptibility. A possible outlook for the future is to establish a relationship between the results of Ref. [24] and the diagrammatic decomposition of the vertex function used in this work, which leads to a separation of variables reminiscent of the singular value decomposition.

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Appendix A: \( U^\alpha \)-irreducible vertices

It is shown how diagrams that are reducible with respect to the bare interaction \( U^\alpha \) can be separated from the three-leg vertex \( \Lambda \) and from the vertex function \( F \), following an approach of Hertz and Edwards [22]. The relations in this section of the appendix are formally exact for the paramagnetic Hubbard model (2), for the Anderson impurity model (4) capital letters may be replaced by small letters \( (\Lambda \rightarrow \lambda, F \rightarrow f, \text{and so on}) \) and four-momenta are replaced by frequencies \( [k = (k, \nu) \rightarrow \nu, q = (q, \omega) \rightarrow \omega] \).

1. Correlation functions

The four-point function is defined as,
\[
G^{(4),\alpha}_{kk'q} = \frac{1}{2} s^\alpha_{\sigma_1\sigma_3} s^\alpha_{\sigma_2\sigma_4} \langle T_{\sigma_1} c_{k\sigma_1} c^\dagger_{k+q,\sigma_2} c_{k'\sigma_3} c^\dagger_{k'+q,\sigma_4} \rangle ,
\]
where definitions are as in the main text. It is convenient to define the generalized susceptibility,
\[
X^{\alpha}_{kk'q} = G^{(4),\alpha}_{kk'q} + 2\beta G_k G_{k'} \delta_{\alpha,\chi} ,
\]
(A1)

the latter can be represented in terms of a ladder equation \( X = X^0 + X^0 \Gamma X \), where \( \Gamma \) is the two-particle self-energy and all quantities denote matrices in the labels \( k, k' \) and \( X^0_{kk'} = \beta G_k G_{k+q} \delta_{kk'} \) is the bubble. Matrix multiplication implies a factor \( (N\beta)^{-1} \), the labels \( q, \alpha \) are suppressed.

2. \( U^\alpha \)-irreducible generalized susceptibility

The goal is to separate the diagrams from \( \hat{X} \) that are reducible with respect to \( U^{\text{ch}} = +U \) and \( U^{\text{sp}} = -U \), respectively. To this end, one defines \( \hat{\Gamma}^i = \hat{\Gamma} - \hat{\Gamma}^0 \), where \( \Gamma^{\alpha}_{kk'} = U^\alpha \) is the bare two-particle self-energy. The ladder equation for \( \hat{X} \) can therefore be written as,
\[
\hat{X} = \hat{X}^0 + \hat{X}^0 (\hat{\Gamma}^i + \hat{\Gamma}^0) \hat{X} ,
\]
\[
\Leftrightarrow \hat{X}^{0,-1} = \hat{X}^{-1} + \hat{\Gamma}^i + \hat{\Gamma}^0 ,
\]
(A2)

which implies super-matrix inversion with respect to \( k, k' \). Let us now define the \( \Gamma^0\)-irreducible generalized susceptibility \( \hat{\Pi} \),
\[
\hat{\Pi} = \hat{X}^0 + \hat{X}^0 \hat{\Gamma} \hat{\Pi} ,
\]
\[
\Leftrightarrow \hat{X}^{0,-1} = \hat{\Pi}^{-1} + \hat{\Gamma}^i .
\]
(A3)

There are no diagrams in \( \Pi \) that can be separated into two parts by removing a single vertex \( \Gamma^0 \) [in the sense of Fig. 7]. Subtracting Eq. (A3) from (A2) eliminates \( \Gamma^i \) and \( X^0 \),
\[
0 = \hat{X}^{-1} + \hat{\Gamma}^0 - \hat{\Pi}^{-1} ,
\]
\[
\Leftrightarrow \hat{X} = \hat{\Pi} + \hat{\Pi} \Gamma^0 \hat{\Pi} .
\]
(A4)

In explicit notation this relation simplifies (the label \( \alpha \) remains dropped),
\[
X_{kk'q} = \Pi_{kk'q} + \sum_{k_1 k_2} \Pi_{k_1 k_2 q} X_{k_2 k' q}^0
\]
\[
= \Pi_{kk'q} + \left( \sum_{k_1} \Pi_{k_1 k q} \right) \Gamma^0 \left( \sum_{k_2} X_{k_2 k' q} \right) ,
\]
(A5)

where \( \Gamma^0 = \pm U \), summations imply \( (N\beta)^{-1} \).

3. Three-leg vertices and polarization

\( X \) and \( \Pi \) will now be related to the left- and right-sided three-leg vertices \( \Lambda^{(l)} \) and \( \Lambda^{(i)} \), using the definitions,
\[
\sum_k X_{kk'q} = \Lambda_{k'q} X_{k'q}^0 , \quad \sum_{k'} X_{kk'q} = X_{kq}^0 \Lambda_{kq} ,
\]
(A6)

\[
\sum_k \Pi_{kk'q} = \Lambda_{k'q} X_{k'q}^0 , \quad \sum_{k'} \Pi_{kk'q} = X_{kq}^0 \Lambda_{kq} ,
\]
(A7)

where in the second line the \( \Gamma^0\)-irreducible (Hedin) three-leg vertex \( \Lambda^i \) was introduced and \( X_{kq}^0 = G_{k+q} G_k \) is the
bubble. The reducible and irreducible three-leg vertices are related via Eq. (A5), which is seen by summation over \( k' \),
\[
\sum_{k'} X_{kk'q} = \sum_{k'} \Pi_{kk'q} + \sum_{k_i} \Pi_{kk_{i}k_{i}q} \Gamma^{0} \sum_{kk_{i}q} X_{kk_{i}k_{i}q}, ~ (A8)
\]
\[
\Leftrightarrow X_{kk'q} \tilde{\Lambda}_{kq} = X_{kk'q} \tilde{\Lambda}_{kq} + X_{0}^{q} \tilde{\Lambda}_{kq} \Gamma^{0} \sum_{kk_{i}q} X_{kk_{i}k_{i}q}. ~ (A9)
\]

Finally, dividing by \( X_{0}^{q} \) and identifying the susceptibility, \( X_{q} = 2 \sum_{kk'} X_{kk'q} \), one arrives at the simple relation,
\[
\tilde{\Lambda}_{kq} = \tilde{\Lambda}_{kq}^{\alpha} \left( 1 + \frac{1}{2} U^{\alpha} X_{0}^{q} \right), ~ (A10)
\]
\[
= \tilde{\Lambda}_{kq}^{\alpha} / (1 - U^{\alpha} \Pi_{kq}^{\alpha}). ~ (A11)
\]
where the label \( \alpha \) was reintroduced. In the second line the polarization was defined,
\[
\Pi_{kq}^{\alpha} = \frac{1}{2} X_{kk'q} / \left( 1 + \frac{1}{2} U^{\alpha} X_{0}^{q} \right). ~ (A12)
\]
By summing Eq. (A8) over \( k \) one sees that,
\[
\Pi_{q} = \sum_{kk'} \Pi_{kk'q} = \sum_{k} X_{kk'q} \tilde{\Lambda}_{kq}. ~ (A13)
\]

Note that in contrast to the susceptibility \( X_{q} \) a factor 2 does not occur [see above Eq. (A10)]. Similar to Eq. (A11) one derives in an analogous way the relation for the left-sided three-leg vertex,
\[
\Lambda_{kq}^{\alpha} = \tilde{\Lambda}_{kq}^{\alpha} / (1 - U^{\alpha} \Pi_{kq}^{\alpha}). ~ (A14)
\]

4. Four-leg vertices and screened interaction

Next, also the vertex function \( F \) will be expressed in terms of a \( \Gamma^{0} \)-irreducible counterpart \( F^{0} \). To do this, the following relation between the generalized susceptibility \( X \) and \( F \) will be used,
\[
X_{kk'q} = X_{0}^{q} \delta(kk') F_{kk'q} + X_{0}^{q} F_{kk'q} X_{kk'q}, ~ (A15)
\]
\[
\Pi_{kk'q} = X_{0}^{q} \delta(kk') \tilde{\Lambda}_{kq} + X_{0}^{q} F_{kk'q} X_{kk'q}. ~ (A16)
\]
Inserting these relations into Eq. (A5), and using once again Eqs. (A6) and (A7) leads to,
\[
X_{kk'q} F_{kk'q} X_{kk'q} = X_{0}^{q} F_{kk'q} X_{kk'q} + (X_{0}^{q} \tilde{\Lambda}_{kq} \Gamma^{0} \Lambda_{kq} X_{kk'q}).
\]
Finally, dividing by \( X_{0}^{q} X_{kk'q} \) and using Eq. (A14), the reducible vertex \( F \) can be expressed in terms of the irreducible vertices \( F^{0} \) and \( \Lambda^{i} \),
\[
F_{kk'q}^{\alpha} = F^{i}_{kk'q} + \tilde{\Lambda}_{kk'q} \gamma_{kk'}^{\alpha} \Lambda_{kk'}^{i}, ~ (A17)
\]
where the label \( \alpha \) was reintroduced and the screened interaction \( W \) is defined as,
\[
W_{qq}^{\alpha} = U^{\alpha} / (1 - U^{\alpha} \Pi_{q}^{\alpha}). ~ (A18)
\]
For the impurity model one makes in Eqs. (A14), (A17), and (A18) the replacements \( F \rightarrow f \), \( \Lambda \rightarrow \lambda \), \( W \rightarrow w \), and \( \Pi \rightarrow \pi \), leading to Eqs. (8) and (9) in the main text.

Appendix B: Ladder equation for the reducible three-leg vertex

Ladder equations for the reducible and irreducible three-leg vertices \( \Lambda \) and \( \Lambda^{i} \) are derived in the DMFT approximation, where the two-particle self-energy is approximated with the one of the impurity model \( (4) \), \( \Gamma_{kk'q}^{\alpha} = \gamma_{kk'}^{\alpha} \). In this case the Bethe-Salpeter equation for the lattice vertex function \( F \) reads,
\[
F_{kk'q}^{\alpha} = \gamma_{kk'q}^{\alpha} + \sum_{k''} \gamma_{kk''q}^{\alpha} F_{kk''q}^{\alpha} F_{kk'q}^{\alpha}, ~ (B1)
\]
where it was used that for a local two-particle self-energy \( \Gamma \) the vertex function does not depend on the momenta \( k, k' \). \( X_{0}^{q}(q) = \sum_{k} G_{k} G_{k+q} \) denotes the bubble of DMFT Green’s functions \( (3) \).

By \( \nu, \nu' \)-matrix inversion one obtains from Eq. (B1) in a short notation, \( \tilde{\gamma}_{kk'}^{\nu, \nu'} = \tilde{F}_{q}^{\nu, \nu'} + \tilde{X}_{0}^{q}(q) \delta_{\nu, \nu'} \). Similarly, there exists an impurity Bethe-Salpeter equation, \( \tilde{\gamma}_{kk'}^{\nu, \nu'} = \tilde{f}_{q}^{\nu, \nu'} + \tilde{\chi}^{\nu}(\omega) \), where \( f \) denotes the impurity vertex function and \( \lambda_{kk'}^{\nu, \nu'} = \tilde{g}_{\nu, \nu'+\omega} \delta_{\nu, \nu'} \). Thereby, \( \gamma \) is eliminated in favor of \( f \), leading to the exact reformulation of Eq. (B1),
\[
F_{kk'q}^{\alpha} = f_{kk'q}^{\alpha} + \sum_{\nu, \nu'} f_{kk'q}^{\nu, \nu'} \tilde{X}_{0}^{q}(q) F_{kk'q}^{\nu, \nu'}(q), ~ (B2)
\]
where \( \tilde{X}_{0}^{q}(q) = \sum_{k} (G_{k} G_{k+q} - g_{\nu} g_{\nu'+\omega}) \) is the nonlocal bubble, see also Ref. [10].

In order to arrive at an analogous ladder equation for the three-leg vertex \( \Lambda \), Eq. (B2) is multiplied by \( G_{k'} G_{k'+q} \), summed over \( k' \), and I is added on both sides,
\[
1 + \sum_{k'} F_{kk'q}^{\alpha}(q) G_{k} G_{k'+q} = 1 + \sum_{k'} f_{kk'q}^{\alpha}(q) G_{k} G_{k'+q} + \sum_{\nu, \nu'} f_{kk'q}^{\nu, \nu'}(q) \tilde{X}_{0}^{q}(q).
\]
On the left-hand-side (LHS) arises the right-sided three-leg vertex, \( \tilde{\Lambda}_{kk'q} = 1 + \sum_{k'} f_{kk'q}^{\nu, \nu'}(q) G_{k} G_{k'+q} \), on the right-hand-side (RHS) \( \sum_{k} G_{k} G_{k+q} = \tilde{X}_{0}^{q}(q) + g_{\nu} g_{\nu'+\omega} \) is inserted,
\[
\tilde{\Lambda}_{kk'q}^{\nu, \nu'} = 1 + \sum_{\nu, \nu'} f_{kk'q}^{\nu, \nu'}(q) G_{k} G_{k'+q} + \sum_{\nu, \nu'} f_{kk'q}^{\nu, \nu'}(q) \tilde{X}_{0}^{q}(q), ~ (B3)
\]
On the RHS one identifies the right-sided impurity three-leg vertex \( \tilde{\Lambda}_{kk'q} = 1 + \sum_{\nu, \nu'} f_{kk'q}^{\nu, \nu'}(q) G_{k} G_{k'+q} \), and \( \nu, \nu' \) \( f_{kk'q}^{\nu, \nu'}(q) \tilde{X}_{0}^{q}(q) \) is factored out,
\[
\tilde{\Lambda}_{kk'q}^{\nu, \nu'} = \tilde{\Lambda}_{kk'q}^{\nu, \nu'} + \sum_{\nu, \nu'} f_{kk'q}^{\nu, \nu'}(q) \tilde{X}_{0}^{q}(q) \left( 1 + \sum_{k'} F_{kk'q}^{\nu, \nu'}(q) G_{k'} G_{k'+q} \right), ~ (B4)
\]
The term in brackets is again \( \tilde{\Lambda} \), leading to the ladder equation for the right-sided three-leg vertex,

\[
\tilde{\Lambda}^\alpha_{\nu q} = \tilde{\chi}^\alpha_{\nu \omega} + \sum_{\nu'} f^{\nu \alpha}_{\nu' \omega} \tilde{X}^0_{\nu'}(q) \Lambda^\alpha_{\nu' q}.
\]  

(B6)

The analoguous ladder equation for the left-sided three-leg vertex \( \Lambda \) follows from the symmetry of the impurity vertex, \( f_{\nu \nu' \omega} = f_{\nu' \nu \omega} \).

\[
\Lambda^\alpha_{\nu q} = \chi^\alpha_{\nu \omega} + \sum_{\nu'} \Lambda^\alpha_{\nu' q} \tilde{X}^0_{\nu'}(q) f^{\nu' \alpha}_{\nu \omega}.
\]  

(B7)

**Appendix C: Efficient formulae for susceptibility and polarization**

Efficient formulae for the susceptibility and polarization are derived. The susceptibility may be calculated from the reducible three-leg vertex \( \Lambda \) as,

\[
X^\alpha_q = - \langle \rho^\alpha_q \rho^0_q \rangle + \beta \langle \rho^\alpha_q \langle \rho^\alpha_q \rangle \delta_q \delta_{\alpha, ch}
= 2 \sum_k \Lambda^\alpha_q G_k G_{k+q}.
\]  

(C1)

In the DMFT approximation \( \Lambda \) does not depend on \( k \), hence, \( X^\alpha_q = 2 \sum_k \Lambda^\alpha_q X^0(q) \), where \( X^0(q) = \sum_k G_k G_{k+q} \). This relation will be rewritten as the sum of impurity susceptibility \( \chi \) and nonlocal corrections \( \tilde{X} \).

To do this, the bubble \( X^0 \) is expressed in terms of the nonlocal bubble \( \tilde{X}^0 \) and the impurity bubble \( g \tilde{g}_{\nu \nu' \omega} \).

\[ X^0_{\nu q} = \tilde{X}^0_{\nu q} + g_{\nu q} \tilde{g}_{\nu q} \].

Furthermore, the three-leg vertex \( \Lambda \) is expanded to first order using Eq. (B7), hence,

\[
X^\alpha_q = 2 \sum_k \Lambda^\alpha_q G_k G_{k+q}.
\]  

(C2)

Four terms arise, the impurity susceptibility can be identified, \( \chi^\alpha_{\nu \omega} = 2 \sum_{\nu'} \Lambda^\alpha_{\nu' \omega} g_{\nu q} \tilde{g}_{\nu q} \).

Furthermore,

\[
2 \sum_{\nu'} \Lambda^\alpha_{\nu' \omega} \tilde{X}^0_{\nu'}(q) f^{\nu' \alpha}_{\nu \omega} = 2 \sum_{\nu'} \Lambda^\alpha_{\nu' \omega} \tilde{X}^0_{\nu'}(q) \Lambda^\alpha_{\nu' q} - 2 \sum_{\nu'} \Lambda^\alpha_{\nu' \omega} \tilde{X}^0_{\nu'}(q),
\]  

(C3)

where the right-sided impurity three-leg vertex was identified, \( \tilde{\lambda}^\alpha_{\nu \omega} = 1 + \sum_{\nu'} f^{\nu \alpha}_{\nu' \omega} g_{\nu q} \tilde{g}_{\nu q} \) [its trivial part 1 is canceled by the second term on the RHS of Eq. (C3)].

Using these relations in Eq. (C2) leads to,

\[
X^\alpha_q = \chi^\alpha_{\nu \omega} + 2 \sum_{\nu'} \Lambda^\alpha_{\nu' \omega} \tilde{X}^0_{\nu'}(q) \Lambda^\alpha_{\nu' q}
- 2 \sum_{\nu'} \Lambda^\alpha_{\nu' \omega} \tilde{X}^0_{\nu'}(q)
+ 2 \sum_{\nu' \nu''} \Lambda^\alpha_{\nu' \omega} \tilde{X}^0_{\nu'}(q) + 2 \sum_{\nu' \nu''} \Lambda^\alpha_{\nu' \omega} \tilde{X}^0_{\nu'}(q) f^{\nu' \alpha}_{\nu \omega} \tilde{X}^0_{\nu''}(q).
\]

Using the ladder equation (B7) for \( \Lambda \) it is seen that the second line cancels the third, hence,

\[
X^\alpha_q = \chi^\alpha_{\nu \omega} + 2 \sum_{\nu'} \Lambda^\alpha_{\nu' \omega} \tilde{X}^0_{\nu'}(q) \tilde{\lambda}_{\nu' \omega} = \chi^\alpha_{\nu \omega} + X^\alpha_{\nu q},
\]  

(C5)

which is the dual boson formula (1) [10, 16].

A similar relation will be derived for the polarization \( \Pi \). To do this, let us invoke the local analogue of Eq. (A11),

\[
\tilde{\chi}^\alpha_{\nu \omega} = \tilde{\lambda}^\alpha_{\nu \omega} (1 - U^\alpha \pi^\omega_{\nu q}).
\]  

(C6)

where \( \tilde{\lambda}, \tilde{\chi} \), and \( \pi \) are the three-leg vertices and the polarization of the impurity. The latter is related to \( \chi \) analogous to Eq. (A12),

\[
\pi^\omega_{\nu q} = \frac{1}{2} \chi^\omega_{\nu \omega} + \left( 1 + \frac{1}{2} U^\alpha \chi^\omega_{\nu \omega} \right)
\]  

(C7)

Using Eqs. (C6), (C7) for the impurity quantities, and Eqs. (A14), (A12) for the lattice quantities in Eq. (C5) leads to,

\[
\Pi^\alpha_q = \pi^\alpha_{\nu q} + \sum_{\nu'} \Lambda^\alpha_{\nu' q} \tilde{X}^0_{\nu'}(q) \tilde{\lambda}_{\nu' \omega}.
\]  

(C9)

Again, compared to Eq. (C5) a factor 2 does not occur.

**Appendix D: Ladder equation for the Hedin vertex**

Equation (B7) is now reformulated for the irreducible three-leg vertex \( \Lambda \). To do this, Eq. (A14) and its local analogue \( \lambda_{\nu \omega} = \lambda_{\nu \omega}^1 / (1 - U^\alpha \pi^\omega_{\nu q}) \) are inserted into the ladder equation (B7) for \( \Lambda \),

\[
\Lambda^\alpha_{\nu q} = \frac{1 - U^\alpha \Pi^\omega_{\nu q}}{1 - U^\alpha \pi^\omega_{\nu q}} \lambda^\alpha_{\nu \omega} + \sum_{\nu'} \Lambda^\alpha_{\nu' q} \tilde{X}^0_{\nu'}(q) f^{\nu' \alpha}_{\nu \omega}.
\]  

(D1)

both sides were multiplied by a factor \( 1 - U^\alpha \Pi^\omega_{\nu q} \). On the RHS appears the reducible impurity vertex function \( f \), which will be eliminated in favor of its irreducible counterpart \( f^1 \) using the local analogue of Eq. (A17),

\[
f^{\nu \alpha}_{\nu' \omega} = f^{1 \alpha}_{\nu' \omega} + \tilde{\lambda}^\alpha_{\nu \omega} \omega_{\nu' \omega} \lambda^1_{\nu' \omega}.
\]  

(D2)

where \( \omega \) is the screened interaction of the impurity,

\[
\omega^\alpha_{\nu q} = U^\alpha / (1 - U^\alpha \pi^\omega_{\nu q}).
\]  

(D3)
Inserting Eq. (D2) into Eq. (D1) leads to,

\[
\Lambda^{i,\alpha}_{\nu q} = \frac{1 - U^\alpha \Pi^{\alpha}_{\nu q}}{1 - U^\alpha \Pi^{\alpha}_{\nu q}} \lambda^{i,\alpha}_{\nu q} + \sum_{\nu'} \Lambda^{i,\alpha}_{\nu' q} \tilde{X}^0_{\nu'}(q) f^{i,\alpha}_{\nu' q} \\
+ \sum_{\nu'} \Lambda^{i,\alpha}_{\nu' q} \tilde{X}^0_{\nu'}(q) \tilde{\lambda}^{i,\alpha}_{\nu' q} w_{\nu' q} \lambda^{i,\alpha}_{\nu' q}. \tag{D4}
\]

Using Eqs. (D3) and (A18) the fraction on the RHS can be expressed as \( w_{\nu q} \). Furthermore, Eq. (C9) can be used to identify in the second line, \( \sum_{\nu'} \Lambda^{i,\alpha}_{\nu' q} \tilde{X}^0_{\nu'}(q) \tilde{\lambda}^{i,\alpha}_{\nu' q} = \Pi^\alpha_{\nu q} \).

\[
\pi^\alpha_{\nu q}. \quad \text{Eq. (D4) thus becomes,}
\]

\[
\Lambda^{i,\alpha}_{\nu q} = \frac{u_{\nu q}^\alpha}{W^\alpha_{\nu q}} \lambda^{i,\alpha}_{\nu q} + \sum_{\nu'} \Lambda^{i,\alpha}_{\nu' q} \tilde{X}^0_{\nu'}(q) f^{i,\alpha}_{\nu' q} \\
+ (\Pi^\alpha_{\nu q} - \pi^\alpha_{\nu q}) w_{\nu q} \lambda^{i,\alpha}_{\nu q}. \tag{D5}
\]

Using the relation (D3) between \( w \) and \( \pi \), and the relation (A18) between \( W \) and \( \Pi \) leads to the desired ladder equation (13) for the Hedin vertex,

\[
\Lambda^{i,\alpha}_{\nu q} = \lambda^{i,\alpha}_{\nu q} + \sum_{\nu'} \Lambda^{i,\alpha}_{\nu' q} \tilde{X}^0_{\nu'}(q) f^{i,\alpha}_{\nu' q}. \tag{D6}
\]
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