Analytical investigation of singularities in two-particle irreducible vertex functions of the Hubbard atom

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Local two-particle irreducible vertex functions represent a crucial ingredient for diagrammatic extensions of dynamical mean field theory (DMFT) as well as for the calculation of dynamical response functions in the framework of DMFT. Unexpected divergences in these correlation functions have recently been identified in correlated systems. Remarkably, such singularities appear already for one of the simplest correlated systems: the atomic limit of the half-filled Hubbard model. In this paper, we calculate the exact expressions for all two-particle irreducible vertex functions of the Hubbard atom in all scattering channels and discuss their divergences. Specifically, we will classify the divergences by explicit analytical calculations of the eigenvalues and eigenvectors of the corresponding generalized susceptibilities. In order to establish a connection to the recently found multivaluedness of the exact self-energy functional $\Sigma[\omega_n]$, we show that already an approximation akin to iterated perturbation theory is sufficient to capture, qualitatively, the divergent structure of the vertex functions. Finally, we observe that the localized divergences in the density channel coincide with the appearance of an inflection point in the single-particle Matsubara Green’s function.

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I. INTRODUCTION

One of the most successful tools for the theoretical description of strongly correlated electron systems are one- and many-particle Green’s functions. They give access to a large number of experimentally measurable observables, such as the spectral function, the magnetic susceptibility and the optical conductivity, which provide essential insights into the physics of realistic as well as model many-electron systems. However, the one- and more-particle Green’s functions are often very challenging to calculate in the presence of strong correlations between the particles. A breakthrough in this respect came with the advent of DMFT which maps the problem of correlated electrons on a lattice onto a single Anderson impurity model, i.e., a site which is self-consistently embedded in a dynamic bath. The Green’s functions calculated within this approach include all purely local correlations in the system while nonlocal correlation effects are captured only on a mean-field level. DMFT has been successfully exploited for describing many fascinating phenomena in correlated materials, such as the celebrated Mott metal-to-insulator transition, the volume collapse in Ce, magnetism in transition metal, and electronic entanglement in transition metal oxides.

Apart from the single-particle self-energy $\Sigma(\nu)$, other highly relevant objects which can be calculated in DMFT are the so-called local two-particle irreducible vertex functions $\Gamma^{\nu\nu}_{\nu\nu}$. They serve as input for the Bethe-Salpeter (BS) equations to include local vertex corrections for all kind of two-particle response functions (spin-, charge-, pairing susceptibilities, optical conductivity, Hall coefficient, etc.) in the framework of DMFT. They are also the basic ingredients of diagrammatic extensions of DMFT such as the diagrammatic vertex approximation (DVA) which include nonlocal correlation effects on top of the local ones of DMFT by means of a diagrammatic perturbation theory adopting $\Gamma^{\nu\nu\nu}_{\nu\nu\nu}$ of DMFT as an effective interaction.

Recently, a lot of attention has been directed toward the properties of the irreducible vertices themselves as they, unexpectedly, show singularities in the intermediately-to-strongly correlated regime. These divergences are typically accompanied by crossings of branches of the derivative of the Luttinger-Ward functional $\Phi[G]$, i.e., the self-energy functional $\Sigma[G] = \delta \Phi[G] / \delta G$. It has been shown that such crossings lead to divergences in $\Gamma^{\nu\nu\nu}_{\nu\nu\nu}$. In this respect, apart from being an indicator for the onset of (strong) correlations in a many-electron system, these divergences also limit the applicability of so-called bold diagrammatic Monte Carlo methods which sample the functional $\Sigma[G]$ by means of a Metropolis algorithm.

Unfortunately, the irreducible vertex is highly challenging to calculate, even in the framework of DMFT where it is purely local. In this case, $\Gamma^{\nu\nu\nu}_{\nu\nu\nu}$ is obtained from the corresponding Anderson impurity model by means of an impurity solver such as exact diagonalization or quantum Monte Carlo. Although recently methods have been suggested to improve the treatment of the high-frequency asymptotic
regime of the vertex functions, many multi-orbital applications are still limited by the high numerical cost to calculate the irreducible vertex functions. Moreover, regarding the analysis of the divergences of these correlations functions, it is often difficult to draw definite conclusions from purely numerical simulations in which singularities are notoriously difficult to tackle. Hence, analytical expressions for $\Gamma_{\nu\nu'}^{\omega}$ would be highly desirable.

While for non-interacting disordered systems, such as the binary mixture (BM) or the Falicov-Kimball model (FKM), analytical results are indeed available, no exact expressions are known for interacting systems. In this paper, we will fill this gap by presenting analytical results for $\Gamma_{\nu\nu'}^{\omega}$ in a prototypical correlated system: the Hubbard model at half-filling in its atomic limit (referred to as Hubbard atom or simply AL in the following). Despite the very simple structure of this correlated model it exhibits complex two-particle correlations that even capture the above mentioned singularities in the irreducible vertices.

A subsequent analysis of the derived analytic formulas for $\Gamma_{\nu\nu'}^{\omega}$ provides therefore a deeper understanding of these divergences and the relation to the multivaluedness of the functional $\Sigma[G]$. Finally, the results of this paper can serve as starting point for approximations to more complex strongly correlated systems.

The paper is organized as follows: In Sec. II we recall the basic formalism of two-particle correlation functions for the Hubbard atom. In Sec. III we present our analytical results for the two-particle irreducible vertices in all channels while in Sec. IV we analyze their divergences in terms of their eigenvalues and eigenvectors. In Sec. V we obtain a direct relation between the singularities of the irreducible vertex and the multivaluedness of the Luttinger-Ward functional by adopting an approximate expression for the (otherwise unknown) functional $\Sigma[G]$. In Sec. VI we allow ourselves to briefly speculate on the connection between the divergences of $\Gamma_{\nu\nu'}^{\omega}$ and specific features of the single-particle Green’s function. Finally, Sec. VII is devoted to the conclusions and an outlook.

II. TWO-PARTICLE CORRELATION FUNCTIONS FOR THE AL

In the following we will introduce the one- and two-particle Green’s functions and the related generalized susceptibilities, as well as the two-particle irreducible vertex functions of a many electron system. While in Sec. II A the general definitions of these quantities are given, Sec. II B reviews the explicit expressions of the generalized susceptibilities of the half-filled Hubbard atom. As these subjects have been already discussed extensively in the literature we will here just recapitulate the main points which are relevant for the present work. For a more comprehensive discussion of the general two-particle formalism we refer the reader to the literature, in particular to Refs. 10–12

A. General definitions and formalism

The half-filled Hubbard atom corresponds to an isolated $s$-orbital with an effective Coulomb interaction $U$ between the electrons. The chemical potential is set to $U/2$ to enforce particle-hole symmetry, and in the absence of a magnetic field the system is also SU(2) symmetric with respect to the spin. Its Hamiltonian reads

$$\hat{H} = U\hat{n}_\uparrow\hat{n}_\downarrow - \frac{U}{2}(\hat{n}_\uparrow + \hat{n}_\downarrow),$$

where $\hat{n}_\sigma = \hat{c}_\sigma \hat{c}_\sigma^\dagger$ and $\hat{c}_\sigma^\dagger$ (creates) annihilates an electron with spin $\sigma = \uparrow, \downarrow$. The one-particle Green’s function of this model is given by

$$G(\nu) = \frac{1}{\nu - \frac{U}{2} + \frac{i\pi}{2}},$$

where $\nu = \frac{\pi}{\beta}(2n+1)$, $n \in \mathbb{Z}$ is a fermionic Matsubara frequency, and $\beta = 1/T$ denotes the inverse temperature. Below, we will also use bosonic Matsubara frequencies which we denote as $\omega = \frac{\pi}{\beta}2m$, $m \in \mathbb{Z}$.

The generalized susceptibility which is required for the calculation of the two-particle irreducible vertex functions is defined as

$$\chi_{\nu\nu'}^{\omega,\sigma\sigma'} = \int_0^{\beta} d\tau_1 d\tau_2 d\tau_3 e^{-i\nu\tau_1} e^{i(\nu+\omega)\tau_2} e^{-i(\nu'+\omega)\tau_3} \times \left[ \langle T_\tau \hat{c}_\sigma^\dagger(\tau_1)\hat{c}_\sigma(\tau_2)\hat{c}_{\sigma'}^\dagger(\tau_3)\hat{c}_{\sigma'}(0) \rangle - \langle T_\tau \hat{c}_{\sigma'}^\dagger(\tau_1)\hat{c}_{\sigma'}(\tau_2)\hat{c}_\sigma(\tau_3)\hat{c}_\sigma(0) \rangle \right].$$

Here $T_\tau$ is the time-ordering operator and $\langle \ldots \rangle = \frac{1}{Z} \text{Tr}(e^{-\beta \hat{H}} \ldots)$ denotes a thermal expectation value with $Z = \text{Tr}(e^{-\beta \hat{H}})$. The assignment of the frequencies $\nu$, $\nu + \omega$ and $\nu' + \omega$ to the imaginary times $\tau_1$, $\tau_2$ and $\tau_3$, respectively, corresponds to the so-called particle-hole ($ph$) notation. Analogously, one can express the generalized susceptibility in the particle-particle ($pp$) representation which is obtained from the $ph$ one by a frequency shift, here defined as

$$\chi_{\nu\nu'}^{\omega,\sigma\sigma'} \equiv \chi_{\nu\nu'}^{\omega,\sigma\sigma'}(\omega - \nu - \nu').$$

The different physical interpretations of these two notations as particle-hole and particle-particle scattering amplitudes are discussed in detail in Ref. 11. Note that with respect to the latter, here we have defined (for convenience) the $pp$ notation with an additional minus sign for the bosonic frequency $\omega$.

For the SU(2) symmetric case considered here, it is convenient to use the spin-diagonalized versions of the generalized susceptibilities in the particle-hole as well as in the particle-particle notation. This corresponds to defining the $r = d(\text{ensity}), m(\text{agnetic}), s(\text{inglet}), t(\text{ripplet})$
The irreducible vertex functions $\Gamma$ and susceptibilities by means of the BS equations are defined as

$$\chi^\nu_{\nu'\omega} = \chi^\nu_{\nu'\omega}^{\text{B}} + \chi^\nu_{\nu'\omega}^{\text{ph}},$$

(5a)

$$\chi^\nu_{m} = \chi^\nu_{m}^{\text{B}} - \chi^\nu_{m}^{\text{ph}},$$

(5b)

$$\chi^\nu_{\nu'\omega} = (-\chi^\nu_{\nu'\omega}^{\text{B}} + 2\chi^\nu_{\nu'\omega}^{\text{ph}} - 2\chi^\nu_{\nu'\omega}^{\text{pp}})/4,$$

(5c)

$$\chi^\nu_{\nu'\omega} = (\chi^\nu_{\nu'\omega}^{\text{B}} + 2\chi^\nu_{\nu'\omega}^{\text{pp}})/4,$$

(5d)

where the bare particle-hole and particle-particle susceptibilities are defined as

$$\chi^\nu_{\nu'\omega}^{\text{ph}} = \chi^\nu_{\nu'\omega}^{\text{pp}},$$

(6a)

$$\chi^\nu_{\nu'\omega}^{\text{pp}} = \frac{1}{\beta} \sum_{\nu'\nu'\omega} \Gamma_{\nu'\nu'\omega}^{\text{pp}} \chi^\nu_{\nu'\omega},$$

(7)

The irreducible vertex functions $\Gamma_{r}^{\nu'\omega}$ in all four channels $(d, m, s, t)$ can be obtained from the generalized and bare susceptibilities by means of the BS equations

$$\pm \chi^\nu_{r} = \chi^\nu_{d} - \frac{1}{\beta^2} \sum_{\nu'\nu'\omega} \chi^\nu_{0,\nu'\omega} \Gamma_{r}^{\nu'\nu'\omega} \chi^\nu_{r}.$$  

B. Explicit expressions for the atomic limit

As shown in Appendix A, the particle-hole and spin SU(2) symmetry of the Hubbard atom entail the relation

$$\chi_{\sigma\sigma'}^{\nu'\omega} = \chi_{\sigma\sigma'}^{\nu'\omega},$$

(9)

in both the particle-hole and particle-particle notation. Its generalized susceptibilities can therefore be decomposed into a symmetric ($\chi_{\sigma\sigma'}^{\nu'\omega}$) and an anti-symmetric ($\chi_{\sigma\sigma'}^{\nu'\omega}$) part with respect to the transformation $\nu \rightarrow -\nu - \omega$. In the following, it is also convenient to explicitly keep track of the diagonal terms proportional to $\delta_{\nu\nu'}$ and $\delta_{\nu(-\nu'-\omega)}$. A particular feature of the atomic limit at half-filling is that its non-diagonal contributions can be factorized with respect to $\nu$ and $\nu'$. Hence, the general expression for the generalized susceptibility can be written in a unified form for all four channels as (see Refs. 11, 27 and 40)

$$\chi^\nu_{r} = \chi_{r}^{\nu'\omega} = \sum_{\nu'\nu'\omega} \chi_{r}^{\nu'\omega} = \chi_{r}^{\nu'\omega} = \sum_{l=1}^{2} b_{\nu'\nu'\omega}^{l} b_{\nu'\nu'\omega}^{l},$$

(10a)

The functions $b_{0,\nu'\nu'\omega}^{0}, b_{0,\nu'\nu'\omega}^{1}, b_{1,\nu'\nu'\omega}^{1},$ and $b_{2,\nu'\nu'\omega}^{2}$ are defined as

$$a_{0,\nu'\nu'\omega}^{0} = \frac{\beta}{2} \frac{1}{\nu^{2} + \frac{U_{2}}{4}}(\nu^{2} + \frac{U^{2}}{4})^{2},$$

(11a)
\[ b_{1,r}^{\nu\omega} = B_1 \frac{\sqrt{U(1-C_\omega^\nu)} \nu(\nu+\omega) - D_r^\nu}{(\nu^2 + \frac{U^2}{4})(\nu + \omega)^2 + \frac{U^2}{4}}, \]  
(11c)

\[ b_{2,r}^{\nu\omega} = B_2 \frac{\sqrt{\frac{U^3}{4} - \frac{U^2}{2} C_\omega^\nu + \omega^2}}{(\nu^2 + \frac{U^2}{4})(\nu + \omega)^2 + \frac{U^2}{4}}, \]  
(11d)

where \( D_r^\nu \) is given by

\[ D_r^\nu = \frac{U^2}{4} 1 + C_r^\nu \frac{\nu(\nu+\omega) - D_r^\nu}{4 - 1 - C_r^\nu}. \]  
(12)

The channel dependent prefactors \( A_r^0, B_r^0, B_r^1 \) and \( B_r^2 \) as well as the channel dependent constants \( A_r, B_r \) and \( C_r^\nu \) (which depends on \( \omega \) only via \( \delta_0 \)) are given in Tab. I. Here we note that the factor \( \sqrt{3} \) in \( A_d \) arises from the addition of the anti-symmetric parts of \( \chi_\nu^{\nu\nu'} \) and \( \chi_\nu^{\nu'\nu} \) in Eq. (5a) and, hence, reflects the spin-1/2 nature of the particles (see also Sec. V).

### III. Analytical Calculation of \( \Gamma_r \)

Due to the special structure (10) of \( \chi_\nu^{\nu\nu'} \), the matrix inversion in Eq. (8) can be performed analytically via the Woodbury matrix identity. In the following we will go through the explicit inversion procedure as the actual calculation highlights how the divergences of different types (localized vs. global) develop in \( \chi_\nu^{\nu\nu'} \).

The defining equation of the inverse susceptibility, which we will denote by \( \chi_r^{\nu\nu'} \equiv (\chi_\nu^{\nu\nu'})^{-1} \) in the following, is given by

\[ \sum_{\nu'} \chi_r^{\nu\nu'} \chi_r^{\nu'\nu} = \delta_{\nu\nu'}. \]  
(13)

Inserting the explicit expression for \( \chi_r^{\nu\nu'} \) in Eq. (10) into Eq. (13) and the corresponding relation for \( \chi_r^{(-\nu'-\nu)\nu} \), yielding the following two equations for \( \chi_r^{\nu\nu'} \) and \( \chi_r^{(-\nu'-\nu)\nu} \):

\[ \delta_{\nu\nu'} = (a_{0,r}^{\nu\omega} + b_{0,r}^{\nu\omega}) \chi_r^{\nu\nu'} + (-a_{0,r}^{\nu\omega} + b_{0,r}^{\nu\omega}) \chi_r^{(-\nu'-\nu)\nu'} + \sum_{l=1}^2 b_{l,r}^{\nu\omega} Q_{l,r}^{\nu\nu'}, \]  
(14a)

\[ \delta_{(-\nu'-\nu)\nu'} = (a_{0,r}^{\nu\omega} + b_{0,r}^{\nu\omega}) \chi_r^{(-\nu'-\nu)\nu'} + (-a_{0,r}^{\nu\omega} + b_{0,r}^{\nu\omega}) \chi_r^{\nu\nu'} + \sum_{l=1}^2 b_{l,r}^{\nu\omega} Q_{l,r}^{\nu\nu'}. \]  
(14b)

where we have defined

\[ Q_{l,r}^{\nu\nu'} = \sum_{\nu_1} b_{l,r}^{\nu\omega} \chi_{l,\nu_1}^{\nu\nu'}, \]  
(15)

and used the symmetries of the quantities \( a_{0,r}^{\nu\omega}, b_{0,r}^{\nu\omega} \) and \( b_{l,r}^{\nu\omega} \) under the (fermionic) frequency transformation \( \nu \leftrightarrow -\nu - \omega \). The two Eqs. (14) can be combined to yield

\[ \chi_r^{\nu\nu'} = \frac{1}{4a_{0,r}^{\nu\omega}} [\delta_{\nu\nu'} - \delta_{\nu(-\nu'-\omega)}] + \frac{1}{4b_{0,r}^{\nu\omega}} [\delta_{\nu\nu'} + \delta_{\nu(-\nu'-\omega)}] - \frac{1}{2b_{0,r}^{\nu\omega}} \sum_{l=1}^2 b_{l,r}^{\nu\omega} Q_{l,r}^{\nu\nu'}. \]  
(16)

The remaining task is now to determine \( Q_{l,r}^{\nu\nu'} \). To this end we substitute Eq. (16) into Eq. (15) to obtain a system of two linear equations for the two unknowns \( Q_{1,r}^{\nu\nu'} \) and \( Q_{2,r}^{\nu\nu'} \):

\[ \sum_{l=1}^2 M_{kl}^{\nu\nu'} Q_{l,r}^{\nu\nu'} = b_{k,r}^{\nu\omega}, \]  
(17a)

\[ M^{\nu\nu'} = \delta_{kl} + \frac{b_{k,r}^{\nu\omega} b_{l,r}^{\nu\omega}}{2b_{0,r}^{\nu\omega}}. \]  
(17b)

Equation (17a) is solved straightforwardly by inverting the matrix \( M_{kl}^{\nu\nu'} \) (see Appendix C). The final expression for the inverse of the generalized susceptibility then reads

\[ \chi_r^{\nu\nu'} = \frac{1}{4a_{0,r}^{\nu\omega}} [\delta_{\nu\nu'} - \delta_{\nu(-\nu'-\omega)}] + \frac{1}{4b_{0,r}^{\nu\omega}} [\delta_{\nu\nu'} + \delta_{\nu(-\nu'-\omega)}] - \frac{1}{4b_{0,r}^{\nu\omega}} b_{0,r}^{\nu\omega} \sum_{k,l=1}^2 b_{l,r}^{\nu\omega} M_{kl}^{\nu\nu'} b_{k,r}^{\nu\omega}, \]  
(18)

where \( M^{\nu\nu'} = (M^{\nu\nu'})^{-1} \) is the inverse of \( M^{\nu\nu'} \). The matrix \( M_{kl}^{\nu\nu'} \) in Eq. (17b) can be obtained using the explicit definitions of \( b_{0,r}^{\nu\omega}, b_{1,r}^{\nu\omega} \) and \( b_{2,r}^{\nu\omega} \) [see Eqs. (11)]. The actual calculations involve lengthy, but analytically evaluable, sums over fermionic Matsubara frequencies which have been performed using Mathematica. The corresponding explicit calculations and results are reported in Appendix B as well as the supplemental material (SM) where the Mathematica notebooks, which have been employed for this task, are given.

From Eq. (18) we can now easily derive the explicit analytical expressions for the irreducible vertex functions \( \Gamma_r^{\nu\nu'} \) by subtracting the inverse of \( \chi_r^{\nu\nu'} \) according to Eq. (8). This finally yields:
where the plus sign in the denominator of the first term of the second line corresponds to \( r = d, s \) while the minus sign has to be taken for \( r = m \). The choice of sign does not affect the triplet vertex \( \Gamma_{r}^{\nu' \nu} \omega \) since \( B_{3}^{2} = 0 \) (see Tab. I). The terms in the first line of Eq. (19) represent the di- 

gonal contributions to the vertex irreducible in channel \( r \) while the lower line corresponds to the contributions which factorize with respect to the fermionic Matsubara frequencies \( \nu \) and \( \nu' \).

Let us mention that the analytical expression for \( \Gamma_{r}^{\nu' \nu} \omega \) and \( \Gamma_{r}^{\nu' \nu} \omega \) can be inserted into the parquet equations (10, 11, 43, 44) to yield an analytic expression also for the fully irreducible vertex \( \Lambda_{r}^{\nu' \nu} \omega \) in the atomic limit (not shown). However, although \( \Lambda_{r}^{\nu' \nu} \omega \) represents just a subset of the scattering processes found in \( \Gamma_{r}^{\nu' \nu} \omega \), no drastic simplification of the analytical expressions occur.

In particular, the diverging terms described in the next section do not cancel out but remain in \( \Lambda_{r}^{\nu' \nu} \omega \).

### A. Divergences of \( \Gamma_{r} \)

The explicit expression for the irreducible vertex \( \Gamma_{r}^{\nu' \nu} \omega \) in Eq. (19) allows us now to identify and classify all divergences of this correlation function in all channels. Obviously, a singularity in \( \Gamma_{r}^{\nu' \nu} \omega \) has to be expected when one of the denominators in Eq. (19) vanishes. If this happens for a single frequency \( \nu \) (and its crossing symmetric counterpart \( -\nu - \omega \)) we are dealing with a localized divergence while the vanishing of a \( \nu \)-independent denominator gives rise to a global divergence. A closer inspection of Eq. (19) indicates three possible types of divergences:

(i) The denominator of the first summand in the first line of Eq. (19) vanishes if

\[
\nu(\nu + \omega) = A_{r}^{2},
\]

which corresponds to \( a_{r}^{\omega} = 0 \) in Eq. (18). This condition gives clearly rise to a localized divergence in the \( \nu, \nu' \) frequency space since, for a given value of \( A_{r} \) and \( \beta \), it can be fulfilled by only one Matsubara frequency \( \nu' \) and its symmetric conjugate \(-\nu' - \omega\). For the density, magnetic, and triplet channels \( (r = d, m, t) \) Eq. (20) can be fulfilled for specific values of \( U \) if \( \omega \neq 0 \). For the singlet channel this is never possible at finite temperature since \( A_{s} = 0 \) (see Tab. I). For the special case of \( \omega = 0 \), on the other hand, a solution to Eq. (20) can be found only for the density channel since \( A_{r} \) is imaginary (and, hence, \( A_{r}^{2} \) is negative) for the magnetic and triplet channels. This leads to localized divergences in \( \Gamma_{d}^{\nu' \nu}(\omega = 0) \) at frequencies \( \nu' = \pm \frac{\pi}{\beta} \sqrt{3} \) which have already been reported in Refs. 13, 18 and 40.

(ii) From the second and the third summand of \( \Gamma_{r}^{\nu' \nu} \omega \) in Eq. (19) we would expect the emergence of localized divergences if

\[
\nu(\nu + \omega) = B_{r}^{2}.
\]

However, the rule of l’Hôpital yields that the divergences in the two terms cancel. The analysis of the eigenvalues of \( \chi_{r}^{\nu' \nu} \omega \) in the next section shows that the cancellation of these divergences is not accidental, but is directly linked to the shape of the eigenvectors.

(iii) Finally, \( \Gamma_{r}^{\nu' \nu} \omega \) will diverge when the \( \nu \)-independent denominator in the second line of Eq. (19) vanishes, i.e.,

\[
f_{r}(\beta U/2, \omega) \equiv \frac{U \tan[\frac{\pi}{2} \sqrt{4 B_{r}^{2} + \omega^{2} + \omega}]}{\sqrt{4 B_{r}^{2} + \omega^{2}}} \pm 1 = 0.
\]

where the upper (plus) sign has to be taken for the density and singlet \((r = d, s)\) and the lower (minus) one for the magnetic \((r = m)\) channel, respectively. For the triplet channel there is obviously no global divergence since the corresponding \( \chi_{r} \) consists of diagonal terms only. Eq. (22) corresponds to a singularity of the matrix \( \mathcal{M}_{r}^{\nu' \nu} \) in Eq. (18), i.e., to the vanishing of the determinant of this matrix [see Eq. (C2) in Appendix C]. Condition (22) obviously gives rise to a global divergence of \( \Gamma_{r}^{\nu' \nu} \omega \) since it is associated with a divergence of the prefactor in the second line of Eq. (19) which does not depend on the fermionic Matsubara frequencies \( \nu \) and \( \nu' \).

Eq. (22) represent a transcendental equation for the quantity \( f_{r}(\beta U/2, \omega) \) (cf. the definitions of \( B_{r} \) in Tab. I), which can be solved numerically. \( f_{r}(\beta U/2, \omega) \) is plotted in Fig. 1 in the density and singlet (upper panel) as well as for the magnetic channel (lower panel). A divergence occurs whenever a curve crosses 0. The three different colors in the respective plots refer to the three lowest values of the bosonic Matsubara frequencies.
at \( \beta U \) Eq. (22) in the limit the magnetic channel leads to condition \( \tanh(\beta U/4) = 1 \) which cannot be satisfied for any finite values of \( \beta \) and \( U \), confirming the absence of global divergences for \( \Gamma_m^{\nu\nu} \) in the half-filled (repulsive) AL.

\[ \sum_{\nu'} \chi^{\nu\nu}_{r,A} V^{\nu\nu}_{r,A} = \lambda^\omega_{r,A} V^{\nu\nu}_{r,A}, \tag{23} \]

where \( \lambda^\omega_{r} \) denotes the eigenvalue and \( V^{\nu\nu}_{r,A} \) is the corresponding eigenvector.

In order to solve the eigenvalue Eq. (23), let us first recall that the generalized susceptibility \( \chi^{\nu\nu}_{r,A} \) can be decomposed into an anti-symmetric (\( \chi^{\nu\nu}_{r,A} \)) and a symmetric (\( \chi^{\nu\nu}_{r,S} \)) part [see Eq. (10)] with respect to the transformation \( \nu \to -\nu \). This observation implies that the eigenvector \( V^{\nu\nu}_{r,A} \) is either antisymmetric (\( V^{\nu\nu}_{r,A} \)) or symmetric (\( V^{\nu\nu}_{r,S} \)), where \( V^{\nu\nu}=(V_{r,A}/V_{r,S}) \). Consequently, the eigenvalue problem splits into

\[ \sum_{\nu'} \chi^{\nu\nu}_{r,A} V^{\nu\nu}_{r,A} = \lambda^\omega_{r,A} V^{\nu\nu}_{r,A}, \tag{24a} \]

\[ \sum_{\nu'} \chi^{\nu\nu}_{r,S} V^{\nu\nu}_{r,S} = \lambda^\omega_{r,S} V^{\nu\nu}_{r,S}. \tag{24b} \]

We will analyze these two eigenvalue problems separately in the following two subsections.

A. Antisymmetric eigenvectors of \( \chi^{\nu\nu}_{r,A} \)

The eigenvalue equation [Eq. (24a)] for the antisymmetric eigenvector explicitly reads [see Eq. (10)]:

\[ \sum_{\nu'} a^{\nu\nu}_{0,r} [\delta_{\nu\nu'} - \delta_{\nu(-\nu'-\omega)}] V^{\nu\nu}_{r,A} = \lambda^\omega_{r,A} V^{\nu\nu}_{r,A}. \tag{25} \]

Using the symmetry properties of \( a^{\nu\nu}_{0,r} \) and \( V^{\nu\nu}_{r,A} \) under the transformation \( \nu \to -\nu - \omega \) one obtains the relation

\[ 2 a^{\nu\nu}_{0,r} V^{\nu\nu}_{r,A} = \lambda^\omega_{r} V^{\nu\nu}_{r,A}. \tag{26} \]
which corresponds to an eigenvalue equation of an already diagonal matrix. The normalized eigenvectors read

$$V_{r,A}^{\nu\omega} = \frac{1}{\sqrt{2}} \left[ \delta_{\nu\nu^*} - \delta_{\nu(-\nu^-\omega)} \right].$$

and the corresponding eigenvalues for the fixed frequency $\nu^*$ are given by [see Eq. (11a)]

$$\lambda_{r,A}^{\nu,\omega} \equiv \lambda_{r,A}^{\nu\omega} = 2\delta_{0,r}^{\nu\omega} = \frac{A_0^{\nu,\omega}(\nu^* + \omega) - A_1^{\nu,\omega}}{((\nu^*)^2 + \frac{\nu^2}{4})((\nu^* + \omega)^2 + \frac{\omega^2}{4})}.$$

The eigenvalue $\lambda_{r,A}^{\nu,\omega}$ clearly vanishes if $\nu^*(\nu^* + \omega) = A_1^{\nu,\omega}$, and the outer product of the eigenvector $V_{r,A}^{\nu\omega}$ is indeed identical to the shape of the corresponding localized divergences in $\Gamma_{r}^{\nu\omega}$ discussed in Sec. IIIA.

### B. Symmetric eigenvectors of $\chi_{r}^{\nu\nu^*\omega}$

The calculation of the symmetric eigenvectors $V_{r,S}^{\nu\omega}$ and the corresponding eigenvalues $\lambda_{r,S}^{\nu,\omega}$ is more difficult than in the antisymmetric case since the symmetric part of the susceptibility $\chi_{r}^{\nu\nu^*\omega}$ exhibits non-diagonal terms. However, since its non-diagonal contribution corresponds to a matrix of only rank 2 we can follow a similar strategy as for the inversion of $\chi_{r}^{\nu\nu^*\omega}$. The explicit eigenvalue equation [Eq. (24b)] is given by

$$\sum_{\nu'} \left[ b_{0,r}^{\nu\omega} \delta_{\nu\nu'} + \delta_{\nu(-\nu^-\omega)} \right] + \sum_{l=1}^2 b_{l,r}^{\nu\omega} V_{r,S}^{\nu\omega} = \lambda_{r,S}^{\nu,\omega} V_{r,S}^{\nu\omega}.$$  \hspace{1cm} (29)

Using the symmetry of both $b_{0,r}^{\nu\omega}$ and $V_{r:S}^{\nu\omega}$ under the transformation $\nu \rightarrow -\nu - \omega$ one obtains the equivalent relation

$$\sum_{l=1}^2 b_{l,r}^{\nu\omega} P_{r,l} = (-2b_{0,r}^{\nu\omega} + \lambda_{r,S}^{\nu,\omega}) V_{r,S}^{\nu\omega},$$  \hspace{1cm} (30a)

$$P_{r,l} = \sum_{\nu'} b_{l,r}^{\nu\omega} V_{r,S}^{\nu\omega}. $$  \hspace{1cm} (30b)

Assuming that we know $P_{r,l}^{\nu\omega}$ and $\lambda_{r,S}^{\nu,\omega}$, the eigenvector $V_{r,S}^{\nu\omega}$ is in general given as

$$V_{r,S}^{\nu\omega} = \frac{1}{N} \left[ \sum_{l=1}^2 \lambda_{r,S}^{\nu,\omega} P_{r,l} + \delta(\lambda_{r,S}^{\nu,\omega} - 2b_{0,r}^{\nu\omega}) \right] V_{r,S}^{\nu\omega},$$

where $\mathbf{P}$ takes the principal value, i.e. excludes any point for which $\lambda_{r,S}^{\nu,\omega} = 2b_{0,r}^{\nu\omega}$, and $c_{\nu\omega}$ is a constant to be determined.

Let us first consider the triplet channel $r = t$. In this case $b_{1,r}^{\nu\omega} = b_{2,r}^{\nu\omega} \equiv 0$, which implies that $P_{r,t} = 0$. The symmetric eigenvectors of $\chi_{t}^{\nu\nu^*\omega}$ are, hence, given by

$$V_{t,S}^{\nu\omega} = \frac{1}{\sqrt{2}} \left[ \delta_{\nu\nu^*} - \delta_{\nu(-\nu^-\omega)} \right].$$

and the corresponding eigenvalue $\lambda_{t,S}^{\nu,\omega}$ reads

$$\lambda_{t,S}^{\nu,\omega} \equiv \lambda_{t,S}^{\nu\omega} = 2\delta_{0,t}^{\nu\omega} = \frac{-\beta\nu^*(\nu^* + \omega) - \lambda_t^{\nu,\omega}}{2((\nu^*)^2 + \frac{\nu^2}{4})((\nu^* + \omega)^2 + \frac{\omega^2}{4})},$$

which is always different from zero.

Now we consider Eq. (30) for the remaining cases $r = d, m, s$ where $b_{1,r}^{\nu\omega}, b_{2,r}^{\nu\omega} \neq 0$. Let us first analyse the case when $\lambda_{r,S}^{\nu,\omega} \neq 2b_{0,r}^{\nu\omega}$. This condition simplifies the eigenvector to the form

$$V_{r,S}^{\nu\omega} = \sum_{l=1}^2 \lambda_{r,S}^{\nu,\omega} b_{l,r}^{\nu\omega} P_{r,l}^{\nu\omega}.$$  \hspace{1cm} (34)

In order to determine the values of the quantities $P_{r,l}^{\nu\omega}$ we substitute this expression into Eq. (30b), which yields the following homogenous linear equation for $P_{r,t}^{\nu\omega}$:

$$\sum_{l=1}^2 L_{r,t}^{\nu\omega} (\lambda_{r,S}^{\nu,\omega}) P_{r,l}^{\nu\omega} = 0,$$  \hspace{1cm} (35a)

$$L_{r,t}^{\nu\omega} (\lambda_{r,S}^{\nu,\omega}) = \delta_{kl} + \sum_{\nu'} \frac{b_{l,r}^{\nu\omega} b_{k,r}^{\nu\omega}}{2b_{0,r}^{\nu\omega} - \lambda_{r,S}^{\nu,\omega}}.$$  \hspace{1cm} (35b)

Clearly, Eq. (35a) has only a non-trivial solution if $L_{r,t}^{\nu\omega} (\lambda_{r,S}^{\nu,\omega})$ becomes singular. Formally, this corresponds to the condition Det$[L_{r,t}^{\nu\omega} (\lambda_{r,S}^{\nu,\omega})] = 0$ which represents a transcendental equation for $\lambda_{r,S}^{\nu,\omega}$. After the value of $\lambda_{r,S}^{\nu,\omega}$ has been determined by means of this equation, Eq. (35b) can be solved for $P_{r,t}^{\nu\omega}$ (or, more precisely, for the ratio $P_{r,t}^{\nu\omega}/P_{r,t}^{\nu\omega}$) which yields the final expression for $V_{r,S}^{\nu\omega}$ in Eq. (34).

The matrix $L_{r,t}^{\nu\omega} (\lambda_{r,S}^{\nu,\omega})$ is similar to $M_{r,t}^{\nu\omega}$ in Eq. (18) and can be in principle calculated analytically. However, for $\lambda_{r,S}^{\nu,\omega} \neq 0$ the structure of the poles of the summand in the Matsubara frequency sum in Eq. (35) is considerably more complicated compared to the corresponding expression for $M_{r,t}^{\nu\omega}$ and we, hence, refer the reader to App. D for the final (rather lengthy) results.

The most interesting case is, however, when $\lambda_{r,S}^{\nu,\omega} = 0$ which signals a global divergence of the corresponding vertex $\Gamma_{r}^{\nu\nu^*\omega}$. In this situation, the matrix $L_{r,t}^{\nu\omega} (\lambda_{r,S}^{\nu,\omega} = 0)$ becomes equivalent to $M_{k,t}^{\nu\omega}$ whose determinant vanishes when the condition in Eq. (22) is fulfilled. In fact, all matrix elements $L_{r,t}^{\nu\omega} (\lambda_{r,S}^{\nu,\omega} = 0) = M_{k,t}^{\nu\omega}$ become 0 except for $L_{r,t}^{\nu\omega} (\lambda_{r,S}^{\nu,\omega} = 0)$ and, hence, $P_{r,t}^{\nu\omega} = 0$. This is indeed consistent with the requirement that $V_{r,S}^{\nu\omega}$ should be normalizable which would not be the case for the term $b_{1,r}^{\nu\omega} b_{2,r}^{\nu\omega}$ which appears for $\lambda_{r,S}^{\nu,\omega} = 0$ in Eq. (34). The eigenvector to a vanishing eigenvalue is therefore $\propto b_{2,r}^{\nu\omega} b_{2,r}^{\nu\omega}$ and explicitly reads

$$V_{r,S}^{\nu\omega} |_{\lambda_{r,S}^{\nu,\omega} = 0} = \frac{N}{\nu(\nu^* + \omega) - B_r^2},$$

where $N$ can be easily obtained from the normalization.
condition \( \sum_i (v^{\sigma \nu}_i)^2 = 1 \). The outer product of this eigenvector indeed reproduces the globally divergent component in \( \Gamma^{0 \nu}_e \omega \) in the second line of Eq. (19).

Let us finally consider the case when \( \lambda^{\nu}_r, S = 2 b'_{0, r} \omega \), for some fixed frequency \( \nu^* \). This condition reduces Eq. (30a), evaluated at \( \nu^* \), to the constraint

\[
P^{\nu}_r = - \frac{b'_{0, r} \omega}{b''_{0, r} \omega} P^{\nu}_r.
\]

Substituting Eqs. (31) and (37) into Eq. (30b) gives now two (non-trivial) linear equations \( l = 1, 2 \) but only one free parameter \( \epsilon'_{r} \omega / P^{\nu}_r \). This implies that there are in general no solutions fulfilling \( \lambda^{\nu}_r, S = 2 b'_{0, r} \omega \) for a fixed frequency \( \nu^* \) and interaction strength \( U \). Instead, any valid solution of this type can be reached by intersecting the condition in Eq. (37) with the closure of the solutions with \( \lambda^{\nu}_r, S \neq 2 b'_{0, r} \omega \). In particular, for \( \lambda^{\nu}_r, S = 0 \) there are no solutions for the condition \( (2) \) in the neighborhood of \( b''_0 \omega = 0 \), for any finite frequency \( \nu^* \). This implies that \( \nu^* \omega / \lambda^{\nu}_r, S \) has no zero at the points \( b''_0 \omega = 0 \) and, hence, any divergence in \( \Gamma^{0 \nu}_e \omega \) at these points must cancel (c.f. Sec. IIIA).

V. APPROXIMATE SELF-ENERGY FUNCTIONAL \( \Sigma[G] \)

In DMFT, the lattice problem is mapped onto an Anderson impurity model through the non-interacting one-particle bath green’s function \( G_0 \). The impurity solver can formally be seen as functional \( G [G_0] \) that for each \( G_0 \) returns the corresponding fully interacting local Green’s function \( G \). This functional is in general not injective \( (21)(22) \), i.e., there are several different non-interacting bath Green’s functions \( G_0 \) that can produce the same interacting Green’s function \( G \). This implies a multivaluedness \( (18)(21)(22)(38) \) of the inverse functional \( G_0[G] \) and —via the Dyson equation— of the self-energy functional \( \Sigma[G] \). Fortunately, there can be at most one of these \( G_0 \)’s, which we will call the physical \( G_0^{\text{phys}} \), that corresponds to a non-interacting impurity problem \( (19)(39) \).

In Refs. [21] and [24] it has been numerically shown for the AL at specific values of \( U \), \( G_0^{\text{phys}} \) and another \( G_0 \) become identical (cross) and that such a crossing implies the divergence of the irreducible density vertex \( \Gamma_d \) (see SM in Ref. [24]).

Analytically such a scenario has been first demonstrated for the simple cases of the one-point model \( (30)(31)(32) \) and disordered systems \( (33)(34) \) such as the BM or the FKM in infinite dimensions, where explicit expressions for the functional \( G[G_0] \) and the irreducible vertices \( \Gamma_r \) are available.

On the contrary, for the AL of the Hubbard model no analytical expression for the exact functional \( G[G_0] \) is known. In Ref. [24] some of the present authors used a numerically exact quantum Monte Carlo solver to obtain the different \( G_0 \)’s which yield the physical \( G \) of Eq. (2). In this paper we will follow a complementary path. Instead of adopting a numerically exact solver we will use the Dyson equation

\[
G[G_0] = (G_0^{-1} - \Sigma[G_0])^{-1},
\]

and approximate the self-energy functional \( \Sigma[G_0] \) by the Iterated Perturbation Theory \( (IPT) \) expression

\[
\Sigma[G_0](\nu) = - \frac{U}{\beta^2} \sum_{\nu_1, \nu_2} G_{0,(-\sigma)}(\nu_1) + \frac{U^2}{\beta^2} \sum_{\nu_1, \omega} G_{0,(-\sigma)}(\nu_1 + \omega) G_0(\nu + \omega).
\]

\( \Sigma[G_0](\nu) \) yields the exact self-energy of the Hubbard atom when it is evaluated with \( G_0^{\text{phys}}(\nu) = 1/i\nu \). Within DMFT, it captures strong coupling phenomena such as the Mott metal-insulator \( (3) \). The analytical form allows us to investigate which physical ingredients cause the crossings of different \( G_0 \)’s with the physical \( G_0^{\text{phys}} \) and the associated emergence of divergences in \( \Gamma_r \). In the following we will restrict ourselves, for simplicity, to the case of spin-independent \( G_{0,\sigma}(\nu) = G_0(\nu) \) without any anomalous contributions, as in the numerical calculations of Ref. [24]. This limits the following analysis to the density channel \( (51) \).

A. Unphysical \( G_0 \) solutions for the IPT functional

Substituting Eq. (39) into Eq. (38) gives \( N \) coupled fourth-order equations in \( G_0(\nu) \) where \( N \) is the number of Matsubara frequencies which we consider. Hence, one has to expect \( 4^N \) solutions for \( G_0(\nu) \) for a given \( G(\nu) \). For the numerical calculation we have fixed \( G(\nu) \) to the physical Green’s function \( [\text{Eq. (2)}] \), \( N = 8, 0 \leq U < 2.6, \beta = 2 \), and set \( G_0(\nu) \) for all frequencies \( |\nu| > 15\pi / \beta \) to its physical value \( 1/i\nu \). In order to obtain different solutions of Eq. (38) we start with an initial guess for \( G_0(\nu) \). By means of a Metropolis search we find an improved guess for \( G_0(\nu) \) that become identical to (cross) the physical \( G_0^{\text{phys}}(\nu) = 1/i\nu \) around which we repeatedly linearize Eq. (38) \( (39) \) until a divergence of \( \Gamma_r \) at \( \nu^* \) is found which reproduces the physical \( G(\nu) \) up to a given accuracy. This way it is possible to identify different unphysical \( G_0^{\text{phys}}(\nu) \) with a \( 1/i\nu \) asymptotic high-frequency behavior.

For the \( U \)-range considered in our numerical calculations we find two unphysical \( G_0^{(1)}(\nu) \) and \( G_0^{(2)}(\nu) \) which become identical to (cross) the physical \( G_0^{\text{phys}}(\nu) \) at \( U^{(1)} = \pi / \sqrt{3} \) and \( U^{(2)} = \pi / 2 \), respectively. The unphysical nature of \( G_0^{(1)}(\nu) \) and \( G_0^{(2)}(\nu) \) is reflected in an increase of double occupancy with increasing \( U \) as shown in appendix \( (\text{E}) \). The direct comparison of the physical with the two unphysical \( G_0(\nu)'s \) in Fig. 2 is similar to the corresponding results of Ref. [24] (where an exact Monte Carlo solver has been used for the functional \( G[G_0] \), ex-
cept for the value of $U_c^{(2)}$. In the upper panel we show the imaginary part of $G_0^{(1)}(\nu)$ normalized by the imaginary part of the physical $G_0^{\text{phys}}(\nu)$ for the first two Matsubara frequencies as a function of $U$. While for $\nu = \pm \pi/\beta$ the unphysical $G_0^{(1)}(\nu)$ crosses the physical one linearly in $U - U_c^{(1)}$, for the higher Matsubara frequencies the crossing occurs quadratically. Let us note that $G_0^{(1)}(\nu)$ is purely imaginary and fulfills the standard relation for complex conjugation which renders the result for the positive and negative frequencies equivalent. In the lower panel of Fig. 3 $G_0^{(2)}(\nu)$ is shown as a function of $U$ for the two lowest Matsubara frequencies. The imaginary part is again normalized by $\text{Im} G_0^{\text{phys}}(\nu)$ while the real part is plotted in absolute values. $G_0^{(2)}(\nu)$ crosses the physical $G_0^{\text{phys}}(\nu)$ at $U_c^{(2)} \approx \pi/2$. Before this crossing the relation $G_0^{(2)}(\nu) = G_0^{(2)}(-\nu)$ is violated for $G_0^{(2)}(\nu)$ and, hence, we obtain different results for positive and negative Matsubara frequencies. For $U > U_c^{(2)}$ on the other hand this relation is fulfilled but $G_0^{(2)}(\nu)$ acquires a finite real part. Our numerical results indicate that for $G_0^{(2)}(\nu)$ the crossing with $G_0^{\text{phys}}(\nu)$ is proportional to $\sqrt{U - U_c}$ for all frequencies, within the imposed numerical accuracy.

Let us stress that our findings coincide (at least qualitatively) with the numerically exact results of Ref. [24]. This demonstrates the applicability of our approximate IPT functional to analyze the physical origin of the multi-valuedness of $G_0[G]$ and its connection to the divergences of $\Gamma_r$ in the Hubbard atom.

**B. IPT susceptibilities**

The generalized susceptibility in the density channel at the bosonic Matsubara frequency $\omega = 0$ ($\chi_{\nu \nu'}^{\text{phys}}(\omega = 0)$) can be calculated from $G[G_0]$ in Eq. (38) as $\chi_{\nu \nu'}(\omega = 0) = \beta \frac{\delta G_{\sigma}(\nu)}{\delta G_{\sigma}^{\text{phys}}(\nu)} + \beta \frac{\delta G_0(\nu)}{\delta G_0^{\text{phys}}(\nu)}$. Using the Dyson equation (38) and the IPT self-energy functional in Eq. (39) these derivatives can be straightforwardly performed. Since we are interested in the divergences of the physical branch we evaluate the resulting expressions at the spin independent physical $G_0^{\text{phys}}(\nu)$ and $G(\nu)$ which yields

\[
\frac{\delta G_{\uparrow}(\nu)}{\delta G_{\downarrow}^{\text{phys}}(\nu')} = -G^2(\nu)[1 + \frac{U^2}{4} G_0^{\text{phys}}(\nu')] \delta_{\nu \nu'}, \tag{40a}
\]

\[
\frac{\delta G_{\downarrow}(\nu)}{\delta G_{\downarrow}^{\text{phys}}(\nu')} = -\frac{U^2}{4} G_0^{\text{phys}}(\nu') \delta_{\nu \nu'} - \frac{U}{\beta} G^2(\nu) G_0^{\text{phys}}(\nu'), \tag{40b}
\]

where we have used that at half filling $G_0(\nu)^2 = G_0(\nu)^2$. The non-diagonal term on the right hand side of Eq. (40b) arise directly from the (bare) Hartree term in

![FIG. 2. First two crossings of the physical $G_0^{\text{phys}}(\nu)$ with two unphysical ones $[G_0^{(1)}(\nu) \text{ and } G_0^{(2)}(\nu)]$ as a function of $U$ at the first two Matsubara frequencies ($\nu_1 = \pm \pi/\beta$ and $\nu_2 = \pm 3\pi/\beta$). The imaginary part is normalized by $\text{Im} G_0^{\text{phys}}(\nu)$. Note that for the red solution $G_0^{(1)}(\nu)$ the relation $[G_0^{(1)}]^*(\nu) = G_0^{(1)}(-\nu) = G_0^{(1)}(\nu)$ holds and, hence, the results for positive and negative Matsubara frequencies are the same. For the orange solution $G_0^{(2)}(\nu)$ this is only true after the crossing with the physical $G_0^{\text{phys}}(\nu)$ where it, however, acquires a real part. $\text{Im} G_0^{(2)}(\nu = \pm 3\pi/\beta)$ has been rescaled by a factor of 10 for a better visibility. $\beta = 2$.](image)

$\Sigma_2[G_0] \cdot \chi_{\nu \nu'}^{\text{phys}}(\omega = 0)$ now becomes

\[
\chi_{\nu \nu'}^{\text{phys}}(\omega = 0) = -\beta \frac{G^2(\nu)}{2} \left[1 + \frac{3U^2}{4} G_0^{\text{phys}}(\nu)\right] \delta_{\nu \nu'} - \delta_{\nu \nu'} \tag{41}
\]

One can clearly see that this susceptibility has the form of Eq. (10) with the only difference that it consists of only one non-diagonal term. Furthermore we see that the generalized susceptibility produced by IPT is not symmetric with respect to $\nu \leftrightarrow \nu'$, which means it violates time reversal symmetry. We can, nevertheless, use Eq. (18) to
calculate the inverse of $\chi^{\nu\nu'}(\omega=0)$, as given in Eq. (41), which yields

$$\chi^{\nu\nu'}(\omega=0) = -\frac{1}{2\beta G^2(\nu)} + \frac{1}{1 - \frac{\nu}{4\pi} \left[ \delta_{\nu\nu'} - \delta_{\nu(-\nu')} \right]}$$

Let us now analyze the possible divergences in Eq. (42):

(i) In the first line of Eq. (42) we encounter a local divergence when $\nu = \nu^* = \frac{U}{2} \sqrt{3}$ which is equivalent to the one found by the exact calculation for the atomic limit in Eq. (20). Hence, the approximate self-energy functional of IPT indeed reproduces correctly the localized divergences in the AL at $\omega = 0$. Moreover, consistent with the proof in Ref. 24 the divergence occurs only for the frequencies for which the crossing of the physical and unphysical $G_0$'s is of lowest order, in this case linear. Just as for the exact susceptibility, the factor $\sqrt{3}$ originates from adding the two spin combinations $\uparrow \uparrow$ and $\uparrow \downarrow$ in Eqs. (40).

(ii) In line two and three of Eq. (42) we would expect a divergence at $\nu = \frac{U}{2}$. However, just as in Sec. III these divergences cancel. This is also consistent with the fact that no unphysical $G_0$ crosses the physical $G_0$ at $U = \pi$ for $\beta = 2$.

(iii) If $\tan(\frac{\beta U}{4}) = 1$ in the denominator in the last line of Eq. (42) we will get a global divergence of $\chi$. This expression is not the same as the exact result in Eq. (22), but instead consistent with the observed crossing of $G_0$'s in the lower panel of Fig. 2 obtained from IPT. The global nature of the divergence is also consistent with the fact that the corresponding crossing seems to happen for all Matsubara frequencies in the same way $(\sqrt{U-U_c})$. Following Eqs. (11) and (12), we can trace the origin of the global divergence back to the Hartree term in Eq. (19), which is typically present in a correlated system such as the AL but absent in the self-energy functional of the disordered models as the BM where, hence, no global divergence can be found.

VI. RELATION TO THE ONE-PARTICLE GREEN'S FUNCTION

In this section, we want to comment briefly on possible connections between the divergences of $\Gamma^{\nu\nu'}(\omega)$ and specific features in the single-particle Green's function $G(\nu)$. We do this by first showing a rigorous proof of such connection for disordered systems (BM). In a second step, we point out the inapplicability of this BM analysis to the fully interacting Hubbard atom for which we find quantitatively different results.

A. Binary Mixture

It has been demonstrated\(^{13}\) that in the BM a localized vertex divergence in $\Gamma^{\nu\nu'}(\omega=0)$ occurs at a frequency $\nu_{BM}^\ast = U/2$ where the corresponding single-particle Matsubara Green's function $G_{BM}(\nu)$ exhibits a minimum. To prove this connection in a more general way, we note that the self-energy functional of the BM model is local in Matsubara frequencies, i.e., $\Sigma_{BM}(\nu) = \Sigma_{BM}(G_{BM}(\nu))$. Consequently, the functional derivative $\delta \Sigma_{BM}(G_{BM}(\nu)) \partial G_{BM}(\nu)| = \Gamma^{\nu\nu'}(\omega=0)$ corresponds to a normal derivative. Considering the Dyson equation for the BM in its atomic limit

$$G_{BM}(\nu) = \frac{1}{i\nu + \mu - \Sigma_{BM}(G_{BM}(\nu))},$$

and differentiating this relation with respect to $\nu$, we obtain

$$\partial G_{BM}/\partial \nu = -G_{BM}^2(\nu) \left[ i - \Gamma^{\nu\nu'(\omega=0)}(\nu) \partial G_{BM}/\partial \nu \right].$$

Solving this equation for $\partial G_{BM}/\partial \nu$ yields

$$\partial G_{BM}/\partial \nu = -\frac{i}{G_{BM}^2(\nu) - \Gamma^{\nu\nu'(\omega=0)}(\nu)}.$$\(^{(45)}\)

Obviously, for a divergence of $\Gamma^{\nu\nu'(\omega=0)}(\nu) = \nu_{BM}^\ast$ the right hand side of this equation vanishes which implies that $\partial G_{BM}/\partial \nu |_{\nu = \nu_{BM}^\ast} = 0$. This proofs that the single-particle Green's function of the BM exhibits an extremal point, in this case a minimum, exactly at the frequency $\nu_{BM}^\ast = \nu_{BM}^\ast$ where the corresponding density vertex diverges. Let us note that this also holds in the case of a finite dispersion when the system is treated in the framework of DMFT (see App. F and Ref. 18).

B. Hubbard atom

Let us now turn our attention to the case of the fully interacting Hubbard atom. In this case, the functional $\Sigma[G_0](\nu)$ is non-local, i.e., it depends in general on $G_0(\nu')$ with $\nu' \neq \nu$. Hence, the analysis of the previous section is not applicable here.

Since the single particle Green's function $G(\nu)$ of the Hubbard atom is equivalent to that of the BM in its atomic limit, its minimum is also located at $\nu_{min} = U/2$. The first (localized) divergence of $\Gamma^{\nu\nu'(\omega=0)}$ instead occurs at a larger value of $\nu$, i.e., at $\nu^* = \sqrt{3}U/2$. Considering, on the other hand, the second derivative of $G(\nu)$ with respect to $\nu$

$$\partial^2 G/\partial \nu^2(\nu) = -i\nu \left( \nu - \frac{3\nu^2}{(\nu^2 + U^2/4)^2} \right),$$

we can see that the latter vanishes precisely at $\nu_{inf} =
\( \nu^* = \sqrt{3}U/2 \). This means, in the atomic limit of the fully interacting Hubbard model the local divergence of the density vertex coincides with an inflection point of the corresponding single-particle Green’s function. However, in contrast to the BM model it is still unclear whether this relation is ‘accidental’ or also extends also to the case of finite band width (i.e., to a corresponding AIM). This question is currently under investigation.

VII. CONCLUSIONS AND OUTLOOK

In this work, we have presented analytical expressions for the irreducible vertex functions \( \Gamma_{r\nu'\omega} \) of the half-filled Hubbard atom. In spite of its simple Hamiltonian, the corresponding vertices exhibit a complex frequency structure which captures important features originating from (strong) correlation effects. Our results can, hence, serve as an analytical approximation for vertex functions of more complex correlated systems, such as the Hubbard model, which will possibly allow for a more comprehensive understanding of strong coupling phenomena in many electron models and correlated materials. Specifically, our exact results for \( \Gamma_{r\nu'\omega} \) might be used in approximate Bethe-Salpeter equations in strongly interacting lattice systems, in order to determine physical response functions in the framework of DMFT and/or nonlocal correlation effects by means of diagrammatic extensions of DMFT. Moreover, the techniques which have been used for the calculation of \( \Gamma_{r\nu'\omega} \), as well as for the eigenvalues and eigenvectors of the corresponding generalized susceptibilities, can potentially guide the development of approximate schemes for the (semi-) analytic evaluation of the BS equations. For instance, one might use the spectral representation of the irreducible vertex, truncated at a finite (low) number of eigenvalues, to solve the BS equation for obtaining the generalized susceptibilities and corresponding response functions in a semi-analytical way, following the procedure shown in Sec. [11]

The second main outcome of this paper is the full classification of all eigenvalues and eigenvectors of the generalized susceptibilities \( \chi_{\nu'\omega} \) in all channels \( r \) and for all bosonic Matsubara frequencies \( \omega \). The low-frequency divergences of \( \Gamma_{r\nu'\omega} \) arise as these eigenvalues pass through zero, and take the form of the outer product of their corresponding eigenvectors. Specifically, we have identified localized singularities at \( \nu(\nu + \omega) = A^2_\nu \) which set an energy scale at which a perturbative treatment breaks down [13]. Interestingly, in the density channel for \( \omega = 0 \) this energy scale corresponds to an inflection point in the single-particle Green’s function. In addition, through the decomposition of the generalized susceptibility we were able to connect the factor \( \sqrt{3} \) in \( A_\nu \) of the density channel to the spin-1/2 nature of the particles. The global divergences in \( \Gamma_{r\nu'\omega} \) occur instead when a transcendental equation [Eq. (22)] is fulfilled, and takes the shape of the outer product of the eigenvector \( N/(\nu(\nu + \omega) - B^2_\nu) \).

Finally, we have also shown that the divergencies of \( \Gamma_{r\nu'\omega} \) in the Hubbard atom can be modeled qualitatively by using the self-energy functional of iterated perturbation theory. In this way, we could identify the (bare) Hartree term to be responsible for the emergence of global divergences.

Our analytical derivations have been simplified by the particle-hole symmetry of the half-filled Hubbard atom. In realistic material calculations, it is however rare that particle-hole symmetry is fulfilled, which makes a study of the Hubbard atom away from half-filling an interesting future research direction.

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Appendix A: Symmetry decomposition

| Symmetry                   | Relation |
|----------------------------|----------|
| Complex Conjugation        | \(\chi_{\nu'\omega} = (\chi_{\nu'\omega})^*\) |
| Swapping (ph)              | \(\chi_{\nu'\omega} = \chi_{\nu'\omega}\) |
| Swapping (pp)              | \(\chi_{\nu'\omega} = \chi_{\nu'\omega}\) |
| Spin-SU(2)                 | \(\chi_{\nu'\omega} = \chi_{\nu'\omega}\) |
| Time reversal              | \(\chi_{\nu'\omega} = \chi_{\nu'\omega}\) |
| Particle-hole              | \(\chi_{\nu'\omega} = (\chi_{\nu'\omega})^*\) |

Table II. Symmetry relations of the generalized susceptibilities \(\chi_{\nu'\omega}\). The particle-hole and particle-particle notation is only indicated when the results differ. Note that frequency shift needed to switch between the particle-hole and the particle-particle notation is defined as \(\omega \rightarrow -\omega - \nu - \nu'\).
notation only needs to respect spin-SU(2) (su) symmetry, in addition to the swapping symmetry (ss), in order to fulfill Eq. [9]:

\[
\chi_{\nu'\nu,\omega}^{ss} = \chi_{\nu'\nu,\omega}^{ss},
\]

\[
\chi_{\nu'\nu,\omega}^{su} = \chi_{\nu'\nu,\omega}^{su}.
\]

The generalized susceptibility in the particle-hole notation on the other hand does not require spin-SU(2) symmetry to conform with Eq. [9], but instead requires complex conjugation (cc) and particle-hole (ph) symmetry,

\[
\chi_{\nu'\nu,\omega}^{cc} = \chi_{\nu'\nu,\omega}^{cc},
\]

\[
\chi_{\nu'\nu,\omega}^{ph} = \chi_{\nu'\nu,\omega}^{ph}.
\]

\[
M_{11}^{r,\omega} = 1 + \frac{(B_1^r)^2}{B_0^r} \left(1 - C_r^\omega\right) \frac{1}{\beta} \sum_\nu \frac{\nu(\nu + \omega) - D_r^\omega}{(\nu + \omega)^2 + \frac{U^2}{4}}\,[\nu(\nu + \omega) - B_r^2],
\]

\[
M_{12}^{r,\omega} = \frac{B_0^r B_2^r U^2}{2 \sqrt{U^2 + \omega^2}} \frac{1}{\beta} \sum_\nu \frac{\nu(\nu + \omega) - D_r^\omega}{(\nu + \omega)^2 + \frac{U^2}{4}}\,[\nu(\nu + \omega) - B_r^2],
\]

\[
M_{22}^{r,\omega} = 1 + \frac{(B_2^r)^3 U^3}{B_0^r} \left(1 - C_r^\omega\right) \frac{1}{\beta} \sum_\nu \frac{\nu(\nu + \omega) - D_r^\omega}{(\nu + \omega)^2 + \frac{U^2}{4}}\,[\nu(\nu + \omega) - B_r^2],
\]

where all constants are defined in Tab. I and Eq. (12), respectively, and we have used that \(\omega^2 C_r^\omega \equiv 0\) since \(C_r^\omega \propto \delta_{s,0}\). The prefactors \((B_1^r)^2/B_0^r\), \(B_0^r B_2^r/B_0^r\) and \((B_2^r)^3/B_0^r\) evaluate to mere phase factors being \(-1\), \(1\) and \(-1\) for the density and singlet \((r = d, s)\) channels while they correspond to \(1\), \(i\) and \(-1\) for the magnetic channel \((r = m)\), respectively. Moreover, as one can infer from the corresponding definitions of \(B_r\) and \(C_r^\omega\) in Tab. I the matrix elements for the density and the singlet channel are entirely equivalent. We can, hence, restrict ourselves to the calculation of the matrix elements \(M_{ij}^{r,\omega}\) for the density and the magnetic channel in the following.

The frequency sums in Eqs. (B1) can be evaluated analytically by means of standard methods. Since either \(\omega\) or \(C_r^\omega\) is non-zero (but not both at the same time) it is convenient to consider the cases \(\omega = 0\) and \(\omega \neq 0\) separately, for both the density and the magnetic channel. In spite of these simplifications the actual explicit calculations are still rather involved and, hence, have been carried out with Mathematica scripts (See the Supplementary Material).

To conclude, in order for all the parquet channels to decompose into a symmetric and an antisymmetric part the systems needs to be paramagnetic and particle-hole symmetric.

**Appendix B: The Matrix \(M^{r,\omega}\)**

In this section we will give the explicit results for the matrix elements of the matrix \(M^{r,\omega}\) defined in Eq. (17a) for the density, magnetic and singlet channels. Inserting the explicit expressions for \(b_{0,0,r}^{\omega}, b_{1,0,r}^{\omega}\) and \(b_{2,0,r}^{\omega}\) into this definition one obtains for the matrix elements \(M_{ij}^{r,\omega}\)

\[
(M^{r,\omega})^{-1} = \frac{1}{\det M^{r,\omega}} \begin{pmatrix}
M_{11}^{r,\omega} & -M_{12}^{r,\omega} \\
-M_{12}^{r,\omega} & M_{11}^{r,\omega}
\end{pmatrix}
\]

where \(\det M^{r,\omega} = M_{11}^{r,\omega} M_{22}^{r,\omega} - (M_{12}^{r,\omega})^2\) is explicitly given by

\[
\det M^{r,\omega} = \frac{U^2 + \omega^2}{4U^2(1+e^{\pm B_r U/2})^2+\omega^2} \left(1 \pm \frac{\sqrt{4B_r^2 + \omega^2}}{\sqrt{4B_r^2 + \omega^2}} \right).
\]

Here, the plus sign has to be adopted for \(r = d, s\) and the minus sign for \(r = m\). The last contribution in Eq. (18) in the main text can now explicitly written as

\[
\chi_{\nu'\nu,\omega}^{cc} = \chi_{\nu'\nu,\omega}^{ph} = \chi_{\nu'\nu,\omega}^{cc},
\]

\[
\chi_{\nu'\nu,\omega}^{ph} = \chi_{\nu'\nu,\omega}^{cc}.
\]
where we recall that $\bar{M}^{\nu,\omega} = (M^{\nu,\omega})^{-1}$ [see Eq. (18)]. Although the actual expressions for the matrix elements $M^{\nu,\omega}$ are rather complicated some simplifications are possible for Eq. (C3). First, we note that the denominator $(\nu^{2}+\omega^{2})(\nu^{2}+\omega^{2}+\frac{U^{2}}{4})$ appears in all $b_{0,\nu,\omega}^{r}$ as well as in $b_{1,\nu,\omega}^{r}$, $i=1,2$, and, hence, cancels. This observations suggests the following definitions

$$\bar{b}_{0,\nu,\omega}^{r} = \frac{1}{B_{0}^{\nu,\omega}}[\nu(\nu + \omega) - B_{2}^{2}], \quad (C4a)$$

$$\bar{b}_{1,\nu,\omega}^{r} = \frac{1}{B_{1}^{\nu,\omega}}\sqrt{U(1 - C_{\nu}^{\omega})}[\nu(\nu + \omega) - D_{\nu}^{\omega}]$$
$$= \frac{1}{B_{1}^{\nu,\omega}}\sqrt{U(1 - C_{\nu}^{\omega})}\left[\frac{2{\nu}^{\nu,\omega}}{B_{0}^{\nu,\omega}} + (B_{2}^{2} - D_{\nu})\right], \quad (C4b)$$

$$\bar{b}_{2,\nu,\omega}^{r} = \frac{1}{B_{2}^{\nu,\omega}}\sqrt{\frac{U^{2}}{4}}\sqrt{\frac{U^{2}}{4} - C_{\nu}^{\omega} + \omega^{2}}. \quad (C4c)$$

We can now replace $\bar{b}_{0,\nu,\omega}^{r}$, $\bar{b}_{1,\nu,\omega}^{r}$ and $\bar{b}_{2,\nu,\omega}^{r}$ in Eq. (C3) by $\tilde{b}_{0,\nu,\omega}^{r}$, $\tilde{b}_{1,\nu,\omega}^{r}$ and $\tilde{b}_{2,\nu,\omega}^{r}$, respectively. Moreover, in Eq. (C4b) we have expressed $\tilde{b}_{1,\nu,\omega}^{r}$ in terms of $\tilde{b}_{0,\nu,\omega}^{r}$ plus a constant. This allows us to split the terms in Eq. (C3) into three groups: (i) The first group contains all terms where both, $\tilde{b}_{0,\nu,\omega}^{r}$ and $\tilde{b}_{0,\nu,\omega}^{r}$, are canceled. These terms do not depend on the fermionic Matsubara frequencies $\nu$ and $\nu'$ (but only on the bosonic transfer frequency $\omega$). (ii) The second group of terms includes contributions which are proportional to either $1/\tilde{b}_{0,\nu,\omega}^{r}$ or $1/\tilde{b}_{0,\nu,\omega}^{r}$, i.e., the fermionic frequency dependence of such contributions is given by $1/\nu(\nu + \omega) - B_{2}^{2}$ or $1/\nu(\nu + \omega) - B_{2}^{2}$, respectively. (iii) The third class of terms is proportional to $1/\tilde{b}_{0,\nu,\omega}^{r}$ and $\tilde{b}_{0,\nu,\omega}^{r}$, and, hence, its frequency dependence is given by $1/\nu(\nu + \omega) - B_{2}^{2}$. More explicitly, we obtain for the three different types of contributions the following expressions

$$\frac{1}{\beta^{2}} \left[\frac{(B_{1}^{\nu,\omega})^{2}}{B_{0}^{\nu,\omega}} U(1 - C_{\nu}^{\omega})\right]\quad (C5a)$$

$$\frac{1}{\beta^{2}} \left[\frac{(B_{1}^{\nu,\omega})^{2}}{B_{0}^{\nu,\omega}} U(1 - C_{\nu}^{\omega})(B_{2}^{2} - D_{\nu}^{\omega}) - M^{\nu,\omega}_{12} B_{0}^{\nu,\omega} U^{2}/2\right]/ \ det M^{\nu,\omega} \quad (C5b)$$

$$\frac{1}{\beta^{2}} \left[\frac{(B_{1}^{\nu,\omega})^{2}}{B_{0}^{\nu,\omega}} U(1 - C_{\nu}^{\omega})(B_{2}^{2} - D_{\nu}^{\omega}) - M^{\nu,\omega}_{12} B_{0}^{\nu,\omega} U^{2}/2\right]/ \ det M^{\nu,\omega} \quad (C5c)$$

The corresponding prefactors (in front of the $\nu, \nu'$ dependent contributions) have been evaluated with Mathematica (see SM). For the $\nu, \nu'$ independent term this simplifies to $U(B_{1}^{\nu,\omega})^{2}/(B_{0}^{\nu,\omega})^{2}$ which corresponds to the constant $U$ term present in the irreducible vertex functions in the density, magnetic and singlet channels (with the corresponding channel dependent numerical prefactor). The prefactor in Eq. (C5a) vanishes and, hence, there are no terms depending either on $\nu$ or $\nu'$ only. Finally, the $\nu, \nu'$ independent prefactor in Eq. (C5c) evaluates to a finite value giving rise to a term in $\Gamma_{r}$ which factorizes with respect to the fermionic Matsubara frequencies $\nu$ and $\nu'$. The explicit result is given in the final

$$L_{11}^{\nu,\omega}(\lambda_{\nu,\omega}) = 1 + \frac{(B_{1}^{\nu,\omega})^{2}}{B_{0}^{\nu,\omega}}(1 - C_{\nu}^{\omega}) \frac{1}{\beta} \sum_{\nu} \frac{[(\nu + \omega) - D_{\nu}^{\omega}]^{2}}{[\nu^{2} + \frac{U^{2}}{4} + (\nu + \omega)^{2} + \frac{U^{2}}{4}]} \frac{1}{\nu^{2} + \frac{U^{2}}{4} + (\nu + \omega)^{2} + \frac{U^{2}}{4}} \quad (D1a)$$

expression for $\Gamma_{r}^{\nu,\omega}$ in Eq. (19) in the main text.
where we have used the definition $\lambda \equiv \lambda_{c, \beta} G_0(\beta)$ for convenience. In principle, the Matsubara sums in Eqs. (D1) can be performed analytically. However, in view of their complexity it is advantageous to split up the respective second terms inside the $\nu$-sum (i.e., the ones which contain the $\lambda$) by means of a partial fraction decomposition which gives

\[
\frac{1}{[\nu(\nu + \omega) - B_0^2] - \lambda[\nu^2 + \frac{U^2}{4}][\nu + \omega + \frac{U^2}{4}]} = \frac{-1}{\lambda(G_0^{\omega} - G_0^{\omega})} \left[ \frac{1}{\nu(\nu + \omega) - G_0^{\omega}} - \nu(\nu + \omega) - G_0^{\omega} \right],
\]

where the poles $G_0^{\omega}$ of the denominators are given by

\[
G_0^{\omega} = \frac{U^2}{4} \left[ -1 + \frac{2}{\lambda U^2} \pm \frac{2}{\lambda U^2} \sqrt{1 - \lambda(U^2 + 4B_0^2) - \lambda^2 U^2 \omega^2} \right].
\]

Inserting the partial fraction composition in Eq. (D2) into Eqs. (D1) one obtains $\nu$-sums which are completely analogous to the ones for $M_{kl}^{\omega}$ in Eqs. (B1) with the only difference that $B_r$ is replaced by $G_0^{\omega}$. The actual expressions are rather lengthy transcendental functions of $\lambda$ and can be evaluated with Mathematica with slightly modified versions of the scripts given in the Supplemental Material. The condition for $\lambda$ being an eigenvalue (i.e., $\text{Det}[L_{kl}^{\omega}(\lambda)] = 0$) corresponds to Eq. (22) but with $B_r$ replaced by $G_0^{\omega}$. Also for a vanishing eigenvalue $\lambda = 0$ this relation reduces to Eq. (22) which defines the $U\beta/2$ values at which a global divergence of $\Gamma^{\nu\nu\omega}$ occurs.

### Appendix E: Unphysical behavior of the double occupancy

In this appendix, we show the unphysical behavior of the double occupancy when calculated using one of the unphysical solution $G_0^{(1)}(\nu)$ or $G_0^{(2)}(\nu)$ discussed in Sec. V.A.

The double-occupancy has been obtained by the Galitskii-Migdal formula \[ \text{Tr}(\Sigma) = \text{Tr}(\Sigma G)/(U\beta) \] where $\text{Tr}(\Sigma G) = \sum_\nu \Sigma(\nu)G(\nu)$ and $G(\nu)$ is given in Eq. (2). $\beta = 2$.

### Appendix F: Vertex divergences in the BM in DMFT

In this appendix, we will demonstrate that the relation between the (localized) divergence of the irreducible density vertex in the BM ($\Gamma^{\nu\nu\omega}_{\nu d,\beta}$) and a corresponding minimum in the single-particle Green’s function is valid, more generally, for the case of finite bandwidth, when the system is treated in the framework of DMFT. To this end we rewrite the single-particle Green’s function as

\[
G(z) = \frac{1}{z - \Sigma}. \tag{F1}
\]
where \( z = i\nu - \Delta(\nu) \) with the hybridization function \( \Delta(\nu) \) describing the DMFT bath.

Let us define the derivative:

\[
G^{(2)} = \frac{d}{dz} G(z),
\]

as well as

\[
\gamma^{(2)} = \frac{d}{dG} \Sigma(z),
\]

where we have used that for the BM the self-energy \( \Sigma \) can be recast as a function of \( G \) by appropriately choosing the physical solution of the corresponding self-energy functional of the system:\[18\]

\[
\Sigma^\pm[G] = \frac{\pm R - 1}{2G}.
\]

Here, \( R = \sqrt{1 + U^2G^2} \) and, for a given value of the disorder strength \( U \), one has to choose the respective physical branch \( \pm \) (for details see Ref.\[18\]).

The quantity \( \gamma^{(2)} \) can be then expressed using Eqs. (F4)

\[
\gamma^{(2)} = \frac{R \mp 1}{2G^2 R}.
\]

Via the above relations we, hence, get

\[
G^{(2)} = -\frac{1}{G^2 - \gamma^{(2)}},
\]

from which we can easily obtain the derivatives of the Green’s function with respect to its frequency argument \( \nu \) irrespective of the lattice structure (defined by the hybridization):

\[
\frac{d}{d\nu} G(\nu) = G^{(2)} \left( i - \frac{d}{d\nu} \Delta(\nu) \right)
\]

In the BM \( \gamma^{(2)} \) coincides with the diagonal part of the vertex function \( \Gamma^{(2)}_{\alpha\nu\beta\nu} \) which diverges when

\[
1 + U^2G^2 = 0,
\]

Considering \( \gamma^{(2)} \to \infty \) in Eqs. (F6) and (F7) then proves that a divergence of the irreducible charge vertex is always accompanied with the vanishing of the first derivative of the corresponding single-particle Green’s function with respect to its frequency argument \( \nu \) and, hence, to an extremal point (minimum) in this quantity.

Let us finally stress, that the above analysis cannot be applied to the case of the Hubbard model as in this situation the quantity \( \gamma^{(2)} \) does not represent the corresponding two-particle irreducible vertex of the system (see Sec. VII).

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Hence, the transformation between the bare particle-hole and particle-particle susceptibility requires, in addition to the frequency shift discussed above for the full generalized susceptibilities, an additional factor 2.

Note that for $\omega = 0$ this relation slightly differs from the corresponding one reported in Ref. [18] [see Eq. (49) therein] for the density channel due to a typo in the latter: In fact, the term $\beta U$ on the l.h.s. of Eq. (49) in Ref. [18] has to be replaced by $1/(\beta U)$. 

The calculation of a response function $\chi_r$ by means of the functional derivative $\delta G/\delta G_0$ [see Eqs. (40)] requires the introduction of a symmetry breaking field in channel $r$. 

\[ \text{Note that the definitions for the singlet(s) and triplet(t) susceptibilities differ slightly from the corresponding ones given in Ref. [11] (Eqs. B19 therein) in order to render the BS equations uniform in all channels.} \]

\[ \text{A factor } \frac{1}{2} \text{ is included in the bare particle-particle susceptibility in order to take into account the indistinguishability of two particles which requires exactly such prefactor in the BS equation in the } pp \text{ channel (see Appendix B in Ref. [11]).} \]