Interplay between local response and vertex divergences in many-fermion systems with on-site attraction

D. Springer, P. Chalupa, S. Ciuchi, G. Sangiovanni, and A. Toschi

1 Institut f"ur Theoretische Physik und Astrophysik and W"urzburg-Dresden Cluster of Excellence ct.qmat, Universit"at W"urzburg, Germany

We investigate the problem of divergences appearing in the two-particle irreducible vertex functions of many-fermion systems with attractive on-site interactions. By means of dynamical mean-field theory calculations we determine the location of singularity lines in the phase diagram of the attractive Hubbard model at half-filling, where the local Bethe-Salpeter equations are non-invertible. We find that divergences appear both in the magnetic and in the density scattering channels. This corresponds to the propagation of one extraneous electron (or hole) added to the interacting system or -more physically- to the description of (direct/inverse) electron (or hole) added to the interacting system or level. This constitutes the propagation of one extraneous electron (or hole) added to the interacting system or -more physically- to the description of (direct/inverse) photoemission experiments. The widespread application of the QFT to one-particle processes is reflected in a fully structured textbook description and a clear physical interpretation of the different quantities appearing in the formalism, such as the electronic self-energy which can be accessed experimentally by ARPES experiments.

However, a complete understanding of the physical response in correlated systems often requires to work at the next level of complexity, namely at the “two-particle level”. This represents also a fundamental prerequisite for several cutting-edge many-body schemes which explains the increasing effort extending our knowledge in this direction. Ideally, one would like to handle the QFT description of two-particle processes at the same level of confidence we have for the one-particle ones, including a comparable understanding of their mathematical and physical properties.

In this paper, we take a step in this direction by analyzing one surprising property which characterizes the two-particle analog of the self-energy, i.e. the irreducible vertex function. In particular, we refer here to the occurrence of multiple divergences displayed by this two-particle quantity, in the Matsubara frequency domain. In this respect, we recall that the self-energy expressed as function of Matsubara diverges only in the “extreme” case of a Mott-insulating phase, reflecting the complete suppression of the one-particle Green’s function. On the contrary, an ubiquitous presence of divergences in the irreducible vertex functions has been recently demonstrated in all fundamental models of many-electron physics: from the Hubbard atom to the Falicov-Kimball model, the Anderson Impurity model, and the Hubbard model.

These divergences are a manifestation of the breakdown of self-consistent perturbation expansions in QFT and, as it was recently demonstrated, are also directly related to the intrinsic multivaluedness of the Luttinger-Ward functional for interacting many-electron systems. Mathematically, they correspond to a non-invertibility of the Bethe-Salpeter equation, through which the irreducible vertex functions are defined.

The physical processes controlling these divergences are, instead, not fully clarified yet. In fact, they do not appear to be associated to any phase-transition in the systems considered: At low $T$, they take place well inside of the metallic, Fermi-liquid phases in the AIM and the dynamical mean-field theory solution of the Hubbard model. Heuristically, their occurrence has at first been related to the appearance of kinks in the spectral functions and in the specific heat or to underlying non-equilibrium properties. A recent, more convincing interpretation, however, associates the vertex divergences (occurring in a given channel) to the suppression of the corresponding physical susceptibility caused by the electronic interaction. This interpretation works quite satisfactorily in all the cases studied hitherto and it can be regarded, to a good extent, as a two-particle
generalization of the suppression of the Green’s function.

In this paper, we study how the divergences of the irreducible vertex functions of the half-filled Hubbard model are transformed by changing the sign of the interaction from \( U \) to \(-U\). We will interpret our numerical calculations of two-particle susceptibilities and vertex functions, performed by means of the dynamical mean-field theory (DMFT)\(^{35}\), extending the existing mapping to treat also generalized two-particle quantities. This will allow us to relate our results to the underlying physical symmetries of the model considered, and to investigate the multifaceted aspects of “coupling” of two-particle vertex properties and their possible divergences to the behavior of the physical local response of the system.

These considerations do not only improve our understanding of the physics responsible for the breakdown of the (bold) perturbation expansion\(^{27}\) but allows us to make predictions about which kind of vertex divergences can be expected -on general grounds- in different physical situations. Beyond the conceptual progress of an improved mathematical and physical understanding of the two-particle QFT formalism, our results will be also of particular interest for the future development and applications of several cutting-edge many-electron algorithms (e.g., as all those based on the parquet formalism\(^{10,12}\), the diagrammatic Monte Carlo\(^{32}\), the nested cluster scheme\(^{35}\) beyond the weak-coupling, perturbative regime.

The paper is organized as follows: In Sec. II, we introduce the basic two-particle formalism needed for this study; in Sec. III, we present our numerical results for the two-particle vertex functions and their divergences in the attractive Hubbard model, as well as an interpretation of our observations, based on the mapping of the repulsive case and on the high-\( T \) behavior; in Sec. IV we exploit a properly chosen graphical representation to improve the immediate physical readability of the generalized two-particle susceptibilities while in Sec. V we discuss possible physical and algorithmic implications of our findings. Our conclusions are concisely summarized in Sec. VI.

II. MODEL AND FORMALISM

In this work we will compute, by means of the dynamical mean-field-theory (DMFT)\(^{35}\), the local two-particle susceptibilities and (irreducible) vertex functions of both, the attractive and the repulsive Hubbard model,

\[
\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} c_i^{\dagger} c_j \sigma + U \sum_i n_{i, \uparrow} n_{i, \downarrow} + \Sigma(\nu)
\]

where \( c(c^\dagger) \) are the annihilation (creation) fermionic operators at lattice position \( i \) and spin \( \sigma \), \( t \) is the hopping between next-neighboring sites on a Bethe lattice (with semielliptic DOS of half-bandwidth \( D = 2t = 1 \)), and the local Hubbard interaction \( U \) can take both positive (repulsive interaction) and negative (attractive interaction) values. The chemical potential is kept fixed to \( \frac{U}{2} \) to preserve the particle-hole symmetry of the model.

In order to extract irreducible quantities, one has to invert the Dyson equation at the one- and the Bethe-Salpeter equation (BSE) as well as the parquet equation at the two-particle level. At the one-particle level the self-energy \( \Sigma(\nu) \) may be computed from the inversion

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

of the non-interacting Green’s function \( G_0 \) and the interacting impurity Green’s function

\[
G(\nu) = -\int_{0}^{\beta} d\tau e^{i\nu\tau} \langle T_{\tau} c(\tau) c^\dagger(0) \rangle
\]

of the auxiliary AIM associated to the DMFT solution (here \( \nu = \pi T(2n + 1) \) is a fermionic Matsubara frequency). Eq. \( 2 \) illustrates that a divergence of \( \Sigma(\nu) \) is associated to a complete suppression of \( G(\nu) \), which only occurs in the Mott-insulating regime for \( T, \nu \to 0 \).

Though more complex, the formalism is extendable to the two-particle level\(^{10,12}\). The analog of \( \Sigma \) at the two-particle level is the irreducible vertex function \( \Gamma_r \), given in a specific scattering channel \( r \) (e.g., density, magnetic, see below). \( \Gamma_r \) is obtained by inverting the corresponding BSE

\[
\Gamma_r^{\nu,\nu'}(\Omega) = \beta^2 \langle \chi_r^{\nu,\nu'}(\Omega) \rangle^{-1} \chi_0^{\nu,\nu'}(\Omega)
\]

where the explicit expression of the generalized susceptibility of the impurity-site reads in particle-hole notation\(^{10,12}\)

\[
\chi^{\nu,\nu'}_{\sigma,\sigma'}(\Omega) = \int_{0}^{\beta} d\tau_1 d\tau_2 e^{-i\nu\tau_1} e^{i(\nu+\Omega)\tau_2} e^{-i(\nu'+\Omega)\tau_3}
\]

\[
\times \left[ \langle T_{\tau_1} c^\dagger_{\tau_2}(\tau_1) c_{\sigma,\tau_2}(\tau_3) \rangle c_{\sigma',\tau_3}(0) \right]
\]

(4)

Here, \( \sigma, \sigma' \) denote the spin directions of the impurity electrons, and \( \nu, \nu' \) and \( \Omega \) represent two fermionic and one bosonic Matsubara frequency, respectively. \( \chi_0^{\nu,\nu'} \) corresponds to the bare bubble given by \(-\beta G(\nu) G(\nu+\Omega) \delta_{\nu,\nu'} \). In the case of SU(2) symmetry, the BSE can be diagonalized in the spin sector defining the density \( (r = d) \) and magnetic \( (r = m) \) channel: \( \chi^{\nu,\nu'}_{d|m}(\Omega) = \chi^{\nu,\nu'}_{d|m}(\Omega) \) and \( \chi^{\nu,\nu'}_{d|m}(\Omega) \). Similar considerations apply to the particle-particle \( (pp) \)-sector: the expression of the generalized susceptibilities in the corresponding \( (pp) \) notation can be obtained\(^{12,49}\) via a frequency shift of the particle-hole expressions \( \chi^{\nu,\nu'}_{pp}(\Omega) = \chi^{\nu,\nu'}_{d|m}(\Omega - \nu - \nu') \). At the two-particle level the inversion of \( \chi^{\nu,\nu'}_{r} \) in Eq. \( 3 \) written in terms of its eigenvalue decomposition takes the form

\[
[\chi^{\nu,\nu'}_r]^{-1} = \sum_{\ell} V^{\nu}_{\ell}(\nu) [\chi^{\nu,\nu'}_{\ell}]^{-1} V^\dagger(\nu')
\]

(5)
Similar to the one-particle level, where $\Sigma(\nu) \to \infty$ directly corresponds to a zero of $G(\nu)$, a divergence of the “two-particle” self-energy, the irreducible vertex $\Gamma^{\nu\nu'}_r$, is related to a vanishing eigenvalue $\lambda^r_\nu$ in Eq. (5). Note, that this is merely an analogy, since a single vanishing eigenvalue $\lambda^r_\nu$ does not imply a vanishing of the whole $\chi^{\nu\nu'}_r$ matrix. Hence, a divergence of $\Gamma^r_\nu$ does not cause the corresponding static ($\Omega = 0$) physical susceptibility

$$\chi^r = \frac{1}{\beta^2} \sum_{\nu, \nu'} \chi^{\nu\nu'}_r(\Omega = 0)$$

(6)

to vanish as well. However, after crossing a divergence line the corresponding eigenvalue $\lambda^r_\nu$ becomes negative, resulting in a negative contribution in the eigenvalue decomposition of the physical susceptibility

$$\chi^r = \sum_{r} \lambda^r_\nu \sum_{\nu} V^r_\nu(\nu)^2 .$$

(7)

eventually causing a progressive suppression of the physical fluctuations in the respective channel. Therefore, a divergence of $\Gamma^{\nu\nu'}_r$ followed by the presence of a negative eigenvalue in $\chi^{\nu\nu'}_r$ can be interpreted as the analog of the suppression of the single-particle Green’s function by the single-particle self-energy.

Indeed, in all previous studies of models with repulsive interactions, negative eigenvalues have exclusively occurred in physical channels that are suppressed upon increasing the interaction strength $U$, namely in the charge and in the particle-particle sectors.

According to this observation, one may expect that vertex divergences in models with attractive interaction will occur in the magnetic channel only. This would heuristically be consistent with the known “mapping” of the physical degrees of freedom (D.o.F.) of the half-filled Hubbard model. Due to the intrinsic $O(4) = SU(2) \times SU(2)$ symmetry, the partial-particle-hole, or Shiba, transformation, acts as a mapping of all physical observables between $U > 0$ and $U < 0$. In particular, the two SU(2) spin ($\vec{S}$) and pseudospin ($\vec{S}_p$) sectors, which are related to the respective suppressed channels on the attractive and repulsive side, are transformed into each other

$$c_{i\uparrow} \rightarrow c_{i\uparrow} \quad \text{and} \quad c_{i\downarrow} \rightarrow (-1)^i c_{i\downarrow}$$

(8)

acts as a mapping of all physical observables between $U > 0$ and $U < 0$. In particular, the two SU(2) spin ($\vec{S}$) and pseudospin ($\vec{S}_p$) sectors, which are related to the respective suppressed channels on the attractive and repulsive side, are transformed into each other

$$S_x = \frac{1}{2} [c_{i\downarrow} c_{i\uparrow} + c_{i\uparrow} c_{i\downarrow}] \leftrightarrow -\frac{1}{2} [c_{i\downarrow} c_{i\uparrow} + c_{i\uparrow} c_{i\downarrow}] = S_{p,x}$$

$$S_y = \frac{i}{2} [c_{i\downarrow} c_{i\uparrow} - c_{i\uparrow} c_{i\downarrow}] \leftrightarrow \frac{i}{2} [c_{i\downarrow} c_{i\uparrow} - c_{i\uparrow} c_{i\downarrow}] = S_{p,y}$$

(9)

$$S_z = \frac{1}{2} [c_{i\uparrow} c_{i\downarrow} - c_{i\downarrow} c_{i\uparrow}] \leftrightarrow \frac{1}{2} [c_{i\uparrow} c_{i\downarrow} + c_{i\downarrow} c_{i\uparrow} - 1] = S_{p,z} .$$

This mapping of physical D.o.F. suggests that a similar “transformation” may as well apply to the vertex-divergences. However, as already noted in, the mapping of generalized two-particle quantities, and especially of dynamical irreducible vertices, is more complex than Eq. (9) would imply. We will see in the next section, how this is reflected in the appearance and the nature of the vertex divergences in attractive Hubbard model.

### III. VERTEX DIVERGENCES OF THE ATTRACTIVE HUBBARD MODEL

#### A. DMFT results

We start our analysis of the vertex functions and their divergences in the attractive Hubbard model by presenting our DMFT calculations at the two-particle level performed with a continuous time quantum Monte Carlo (CTQMC) impurity solver in the hybridization expansion precisely, the w2dynamics-package. The main outcome of our DMFT calculations are summarized in Fig. 1, where we report the location of the vertex divergences found for different values of the local attraction $U < 0$ and the temperature $T$ (left side), compared against the corresponding results for the repulsive case $U > 0$ (right side). In the large $|U|$ regime our numerical results are consistent with analytical calculation in the atomic limit. Furthermore, in the whole repulsive sector, we also reproduce the outcome of previous DMFT studies finding multiple lines in the $U$-$T$ plane, where the irreducible vertex diverges. As already observed, the first divergences are located at moderate repulsion values, well before the Mott-Hubbard MIT. With increasing interaction the occurrence of divergence lines becomes more dense, and the lines occur in alternating order starting with a divergence in the density channel (red lines) followed by a simultaneous divergence in the density and pp channel (orange lines).

In the case of attractive interaction, our DMFT results show the following: We find vertex divergences in the density channel (red lines), which are perfectly mirrored with respect to the repulsive side. These occur in alternating order with lines of divergences in the magnetic channel (green lines), which mirror, instead, the orange divergence lines of the repulsive model. As a consequence, the overall location of the vertex divergences looks highly symmetric when comparing the repulsive and the attractive sides of the phase diagram.

At first sight this symmetry may appear rather surprising, because the physical properties of a given scattering channel in the repulsive and the attractive model are very different, as dictated by the mapping of the physical degrees of freedom (cf. Eq. (9) and Fig. 1). At a closer look, we can distinguish the situation of the three-times degenerate divergences found at the orange and green lines, respectively, from that of the single degenerate divergences found at the red lines, occurring in the density sector only. Specifically, the mapping of the combined divergences in the pp and density sector (orange lines) into divergences of the magnetic sector (green...
FIG. 1. Left: Location of the divergences of the irreducible vertex in the different channels along the whole phase-diagram of the attractive and the repulsive half-filled Hubbard model, computed in DMFT. The comparison of the negative and positive $U$ sectors yields perfectly mirrored divergences in the density channel (red). The simultaneous divergences in the density and particle-particle channel (orange) in the repulsive model are mapped into divergences of the magnetic channel (green) on the attractive side. Stars refers to the position in the phase diagram of the data shown in Fig. 4. Right: Schematic sketch comparing the mapping of the singular eigenvalues $\lambda^S[\lambda^A]$ associated to symmetric [antisymmetric] eigenvectors to the mapping of different physical degrees of freedoms (D.o.F.)

(lines) is fully matching our physical expectations that (i) divergences play a role in the suppression of a scattering channel and that (ii) they are mapped consistently with the physical D.o.F., i.e. according Eq. (9). At the same time, the perfect mirroring of the density divergence lines (red) under the $U \leftrightarrow -U$ transformation looks puzzling, because (i) for $U < 0$, these divergences affect a scattering channel associated to a physical susceptibility, which is not suppressed but enhanced by the attractive interaction, and (ii) the physical degrees of freedom associated to the density channel is mapped onto one of the three spin-components.

A first understanding of this apparent discrepancy is provided by the analysis of the symmetry of the eigenvectors associated to a vanishing eigenvalue ($\chi^\ell_o = 0$ for $\ell = \alpha$ in Eq. (5)). In Figure 2 we compare the shape of eigenvectors following the first and second divergence lines at different temperatures for $U \leq 0$. Evidently, the perfect mirroring of divergence lines is also reflected in identical shapes of the eigenvectors associated to a vanishing eigenvalue for $U \leq 0$. The singular eigenvectors associated to all divergences in the density sector only (red lines), display a completely antisymmetric frequency structure $[V_\ell(-\nu) = -V_\ell(\nu)]$. In contrast, all other divergence lines (green and orange lines) are associated to frequency symmetric singular eigenvectors $[V_\ell(-\nu) = V_\ell(\nu)]$.

The symmetry of eigenvectors is clearly essential in the calculation of the physical susceptibility, as can be seen quickly in Eq. (7). Due to the summation over Matsubara frequencies, the actual value of $\chi^\ell_r$ is independent from any antisymmetric eigenvector, irrespective of whether associated to a positive or a negative eigenvalue.

Hence, the appearance of negative eigenvalues in a channel is not necessarily associated to a suppression of the respective physical susceptibility. While in the repulsive model the occurrence of divergences and the suppression of the respective channel, maybe incidentally, coincide, our calculations of the attractive model provide a clear-cut counter-example: the crossing of several divergence lines in the density sector is accompanied by an enhanced susceptibility.

To rationalize the results of our two-particle DMFT calculations on more general grounds, we investigate the effect of the attractive-repulsive mapping on generalized two-particle quantities and its relation the physical symmetries of the system under consideration.

B. The role of the underlying symmetries

As mentioned at the end of Sec. III, the mapping of the generalized two-particle quantities is less obvious than the mapping of the physical D.o.F.

When considering purely local quantities, the single-particle Green’s function $G(\tau_1, \tau_2)$ is identical for the repulsive ($U > 0$) and attractive ($U < 0$) half-filled model, while the two-particle Green’s function $G_{\uparrow\uparrow}(\tau_1, \tau_3, \tau_4), G_{\downarrow\downarrow}(\tau_1, \tau_2, \tau_3, \tau_4)$, i.e. the first time-ordered product appearing on the right hand side of Eq. (4), with anti-parallel spin orientation transforms according to

$$G_{\uparrow\uparrow}^{(U)}(\tau_1, \tau_2, \tau_3, \tau_4) = -G_{\downarrow\downarrow}^{(-U)}(\tau_1, \tau_2, \tau_4, \tau_3),$$

which, after Fourier transformation of all fermionic variables, reads

$$G_{\uparrow\uparrow}^{(U)}(\nu_1, \nu_2, \nu_3) = -G_{\downarrow\downarrow}^{(-U)}(\nu_1, \nu_2, -\nu_4)$$

$$\lambda^S = 0 \quad \lambda^A = 0 \quad U < 0 \quad U > 0 \quad \nu \quad \nu \quad \nu \quad \nu$$

$$\begin{array}{ccc}
\lambda^S = 0 & m & d, pp \\
\# D.o.F. & 3 & 1 + 2 \\
\lambda^A = 0 & d & d \\
\# D.o.F. & 1 & 1 \\
\end{array}$$
with \( \nu_4 = \nu_1 - \nu_2 + \nu_3 \). After changing to the ph-notation, as defined in Eq. \( (4) \), \( (\nu_1 = \nu, \nu_2 = \nu + \Omega, \nu_3 = \nu' + \Omega, \nu_4 = \nu') \) one can easily see how the transformation maps the generalized static (\( \Omega = 0 \)) susceptibility, \( \chi_{\nu^{\prime} \nu} = G_{\uparrow \downarrow}(\nu, \nu, \nu') \) of the \( \uparrow \downarrow \) sector according to

\[
\chi_{\nu^{\prime} \nu} = -\chi_{\nu \nu}^{\prime\prime} \quad \text{and} \quad \chi_{\nu \nu}^{\prime\prime} = -\chi_{\nu^{\prime} \nu} \quad \text{(12)},
\]

while \( \chi_{\uparrow \uparrow} \) is obviously invariant under a partial particle-hole transformation.

Hence, in general, the Shiba transformation on the two-particle level will mix the different (particle-hole) channels of generalized susceptibilities and the associated irreducible vertices. In particular, one sees that only the mapping of the generalized susceptibility expressed in the \( pp \) notation

\[
\chi_{\nu^{\prime} \nu} = \chi_{pp, \nu^{\prime} \nu} \quad \text{and} \quad \chi_{\nu \nu}^{\prime\prime} = \chi_{pp, \nu \nu} \quad \text{(13)},
\]

reflects the transformation of the physical (spin/pseudospin) degrees of freedoms, discussed in Eq. \( (9) \), in a direct fashion.

As the location of divergence lines is directly encoded in the generalized susceptibilities, it will be also subject to the mixing of channels, explaining the differences w.r.t. the mapping of the physical degrees of freedom, discussed in Sec. \( IIIA \). To fully rationalize the results observed in Sec. \( IIIA \), we will focus on the symmetry properties of the generalized susceptibilities. In this respect we note, that Eq. \( (13) \) shows already why the mirrored divergences of the particle-particle \( \uparrow \downarrow \) channel for \( U > 0 \) are observed in the magnetic channel for \( U < 0 \). Hence, the main question concerns the behavior of the particle-hole channels.

We start by considering the (spin resolved) generalized susceptibility \( \chi_{\nu^{\prime} \nu}^{\nu \nu} \), as defined in Eq. \( (4) \). Due to the particle-hole (PH) symmetry of the system considered here, \( \chi_{\nu^{\prime} \nu}^{\nu \nu} \) has all real entries. Exploiting the time-reversal (TR)- and the SU(2)-symmetry of the problem

\[
(\chi_{\nu^{\prime} \nu}^{\nu \nu})^* = \chi_{\nu^{\prime} \nu}^{\nu \nu} \quad \text{and} \quad \chi_{\nu^{\prime} \nu}^{\nu \nu} = \chi_{\nu^{\prime} \nu}^{\nu \nu} \quad \text{(14)}
\]

it is evident that \( \chi_{\nu^{\prime} \nu}^{\nu \nu} \) is a symmetric matrix of \( \nu \) and \( \nu' \). Relation \( (14) \) ensures that all matrix entries and all eigenvalues remain real for any \( \Omega \).

Another symmetry relation can be obtained by exploiting the complex conjugation (CC) of \( \chi_{\nu^{\prime} \nu}^{\nu \nu} \). For \( \Omega = 0 \) it can be shown that the generalized susceptibility is invariant under the rotation of the matrix along both of its cardinal axes \( (\nu \rightarrow \nu, \nu' \rightarrow -\nu') \)

\[
\chi_{\nu^{\prime} \nu}^{\nu \nu} = \chi_{\nu \nu}^{\nu \nu} \quad \text{and} \quad \chi_{\nu^{\prime} \nu}^{\nu \nu} = \chi_{\nu \nu}^{\nu \nu} \quad \text{CC transformation} \quad \text{(15)}
\]

A matrix obeying the conditions

\[
\chi_{\nu^{\prime} \nu}^{\nu \nu} = \chi_{\nu \nu}^{\nu \nu} \quad \text{and} \quad \chi_{\nu^{\prime} \nu}^{\nu \nu} = \chi_{\nu \nu}^{\nu \nu} \quad \text{(16)}
\]

is a so-called bisymmetric matrix, where the matrix elements are symmetric with respect to both the main diagonal \( (\nu = \nu') \) as well as the secondary diagonal \( (\nu = -\nu') \). Essentially, this particular symmetry is at the core to understand the mapping of divergence lines.

A bisymmetric matrix can always be diagonalized in blocks (here associated to positive/negative Matsubara frequencies), by applying an orthogonal matrix \( Q \), defined in terms of the counteridentity \( (J_{\nu^{\prime} \nu}^{\nu \nu} = \delta_{\nu^{\prime} \nu}^{\nu \nu} \delta_{\nu^{\prime} \nu}^{\nu \nu}) \) and identity submatrix \( I \) (see Appendix \( A \) for more details)

\[
Q = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -J \\ 1 & J \end{pmatrix} \quad \text{and} \quad Q_{\chi^{\nu \nu}} Q^T = \begin{pmatrix} A & 0 \\ 0 & S \end{pmatrix} \quad \text{(17)}
\]

The block-diagonalization of \( \chi_{\nu \nu} \) is associated with precise symmetry properties: the subspace denoted by \( A \) represents a submatrix with exclusively antisymmetric eigenvectors, while \( S \) is the subspace of purely symmetric eigenvectors. As a consequence, one can attribute, unambiguously, the occurrence of a red divergence line in \( \chi_{\nu \nu} \) to the purely antisymmetric subspace \( A \), while all other divergence lines will be accounted for by the symmetric subspace \( S \).

A crucial ingredient for connecting the bisymmetry of the generalized susceptibilities to the mapping of divergence lines lies in the equivalence of the Shiba transformation for \( \chi_{\nu^{\prime} \nu}^{\nu \nu} \) to a matrix multiplication with the negative counteridentity matrix \( (\nu) \)

\[
\chi_{\nu^{\prime} \nu}^{\nu \nu} = -\chi_{\nu^{\prime} \nu}^{\nu \nu} \quad \text{and} \quad \chi_{\nu^{\prime} \nu}^{\nu \nu} = \chi_{\nu^{\prime} \nu}^{\nu \nu} \quad \text{(18)}
\]

Combining Eq. \( (17) \), \( (18) \), and the fact that \( J^2 = 1 \) one can prove (see Appendix \( B \) the remarkable result, that the antisymmetric sector \( A \) remains invariant under
$U \leftrightarrow -U$ for all $\chi_r$. This explains why the red divergence lines ($\chi_d$) and their associated antisymmetric eigenvectors are perfectly mirrored on both sides of the phase-diagram in Fig.1 and Fig.2. At the same time one finds that the symmetric parts (S) of $\chi_d$ and $\chi_m$ are mapped into one-another for $U \leftrightarrow -U$, therefore connecting the symmetric divergences, and the corresponding eigenvectors, appearing in $\chi_d^{U>0}$ (orange) and in $\chi_m^{U<0}$ (green).

Let us stress at this point that the proof made in Appendix B applies not only to singular eigenvalues, which are connected to divergence lines, but to all eigenvalues and eigenvectors of $\chi_r^{\nu \nu'}$. In this way, we have extended the mapping relation known for $\chi_{pp,\uparrow\downarrow}$ to the whole particle-hole sector, clarifying the relation with the mapping of the physical D.o.F.: the antisymmetric subspace $A$, not contributing to the sum for the physical susceptibility in Eq. (7), is invariant under the Shiba transformation, while the symmetric subspace is found to transform in accordance with Eq. (6).

As we have illustrated, the particle-hole symmetry plays a central role in determining the mirroring properties of the generalized susceptibilities. If one relaxes this constraint, the relations in Eq. (16) no longer hold in the particle-hole sector and, therefore, the bisymmetry is lost and eigenvalues are not necessarily real. This implies, in turn, that the eigenvectors of the corresponding $\chi_r$ are not necessarily symmetric or antisymmetric any longer. At the same time, it is important to stress, that even in the absence of PH-symmetry (e.g. out of half-filling) $\chi_{pp,\uparrow\downarrow}^{\nu \nu'}$ continues to fulfill both relations in Eq. (16), ensuring the validity of all associated properties (i.e. real eigenvalues as well as bisymmetry and associated properties).

C. High-Temperature Limit

To exemplify the concepts discussed in the previous section, we performed DMFT calculations in the high-temperature regime ($\beta = 5$), where the frequency structure of the two-particle generalized susceptibilities strongly simplifies. Due to the large stepsize on the Matsubara frequency grid, most information of the system is encoded in the central $2 \times 2$ matrix. The analysis of the divergences can be then restricted to the innermost $2 \times 2$ matrix defined by the smallest Matsubara frequencies ($\nu, \nu' = -\pi, \pi$).

For a $2 \times 2$ case, the bisymmetry condition (see III B) poses significant constraints on the matrix elements and a singularity can be realized only in two ways:

$$\chi_r^{A=0} = \begin{pmatrix}
a & a \\
a & a
\end{pmatrix}$$

(19)

which corresponds to the (anti-symmetric) singular eigenvector $V_A(\nu) \propto \delta_{\nu, \pi} - \delta_{\nu, -\pi}$, and

$$\chi_r^{S=0} = \begin{pmatrix}
\mp b & \pm b \\
\pm b & \mp b
\end{pmatrix}$$

(20)

with $a, b > 0$, corresponding to a (symmetric) singular eigenvector $V_S(\nu) \propto \delta_{\nu, \pi} + \delta_{\nu, -\pi}$.

On the basis of these considerations, we analyze the $U$-dependence of the diagonal ($\chi_r^D$) and off-diagonal ($\chi_r^O$) elements of the $2 \times 2$ lowest frequency-submatrix of the generalized susceptibility, extending the study of Ref. 25 to the attractive case. The corresponding data are reported in Fig.3 for the density (left) and the magnetic/pp sectors (right).

A general trend can be readily identified: Upon increasing $|U|$ all diagonal matrix elements ($\chi_r^D$) eventually...
decrease, while the off-diagonal elements ($\chi^O_d$) mostly increase in absolute values, for the considered interaction regime. The decrease of $\chi^D_r$ upon increasing $|U|$ is dominated by the bubble term ($\propto -\beta G(\nu)G(\nu')\delta_{\nu\nu'}$), reflecting the suppression of the single particle Green’s function $G(\nu)$ at low-frequencies. Vertex corrections are responsible for the asymmetry of the damping effects on $\chi^D_r$ with respect to $\pm U$ as well as for differentiating its size between the different sectors.

In particular, we find the following behavior for the diagonal entries: (i) the decrease-rate with $|U|$ of $\chi^D_r$ is stronger in those channels that correspond to a suppressed susceptibility, (ii) $\chi^D_d$ decreases faster compared to the other two channels and even turns negative for large $U > 0$, where density fluctuations are suppressed.

The off-diagonal matrix elements are obviously zero in the non-interacting case ($U = 0$) and for small values of $U$ yield positive/negative corrections to the enhanced/suppressed susceptibilities. For large $U$ values this behavior is preserved in the $m$ and $pp$ channel. An exception is the suppressed density channel where $\chi^D_d$ displays a strong increase, becoming positive again.

From these observations, we conclude that the suppression/enhancement of a static physical susceptibility is controlled by the interplay of suppressed diagonal entries and the enhanced magnitude of the (positive/negative) off-diagonal terms.

Due to the considerably milder damping of the diagonal entries in the magnetic and the $pp$ sector, one always finds that $\chi^D_r > \chi^O_r$, with $r = m, pp$. Therefore only singularities of the second kind ($\chi^D_r = -\chi^O_r$, s. Eq. (20)) can occur in these channels. This implies that singularities of the second kind can occur exclusively in sectors of suppressed susceptibilities.

On the contrary, the much stronger damping of $\chi^D_d$ plays a crucial role in suppressing the density fluctuations for $U > 0$. For $U < 0$ this decrease of $\chi^D_d$ is outperformed by an even stronger increase of $\chi^O_d$ in order to describe the corresponding enhancement of $\chi_d$. As one can easily see in Fig. 3 these conditions allow divergences of the first kind with $\chi^O_d = \chi^O_d$ (compare Eq. (19)), to occur specularly on both sides of the phase-diagram. In fact, frequency-antisymmetric divergences are the only one to be expected in sectors of enhanced physical susceptibilities, because in this regime, both diagonal and off-diagonal components of $\chi^{\nu\nu'}_r$ have the same (positive) sign.

IV. SPECTRAL REPRESENTATIONS OF PHYSICAL SUSCEPTIBILITIES

The relation between generalized and physical susceptibilities emerging from our numerical and analytical analysis can be illustrated in a physically more insightful way. As all eigenvalues in Eq. (7) are real, we introduce a susceptibility density ($\rho(\chi)$) defined as

$$\rho_r(\chi) = \sum_\ell \left| \sum_\nu V^\ell_\nu(\nu) \right|^2 \delta(\chi - \lambda^\ell_{\nu}) \geq 0 \tag{21}$$

from which the local physical susceptibility is readily obtained as an average over $\rho_r(\chi)$:

$$\langle \chi_r \rangle = \int \chi \rho_r(\chi) d\chi. \tag{22}$$

This representation has several advantages: Equations (21) and (22) enable to distinguish immediately between positive ($\chi > 0, \rho(\chi) > 0$), negative ($\chi < 0, \rho(\chi) > 0$) and vanishing ($\chi = 0$) contributions to the static response $\chi_r$. Further, its graphical conciseness will allow to comprehend, at a single glance, how the mapping of the generalized susceptibilities works for the different cases, highlighting the most relevant physical implications.

The introduced representation is applied here to analyze our susceptibility data after crossing four divergence lines at two mirrored positions in the phase diagram (light-blue stars in Fig. 1).

The corresponding results are shown in the three plots of Fig. 4 representing the three scattering channels. Here, the positions of all eigenvalues $\lambda^\ell_{\nu}$ are shown as bars in the light-blue shaded innermost panels of the three plots: Gray bars indicate eigenvalues associated to antisymmetric eigenvectors and thus to a vanishing $\rho_r$ which does not contribute to $\chi_r$. Colored bars account for eigenvalues associated to finite $\rho_r(\lambda^\ell_{\nu})$ values, corresponding to symmetric eigenvectors whose weighted sum builds up the full $\chi_r$. The actual value of the susceptibility-density $\rho_r$ for a given eigenvalue is indicated by the circle-symbols in the outermost panels of the plots in Fig. 4.

The color-shaded regions slightly above $\chi \sim 0$ represent an increasingly denser distribution of small positive eigenvalues, arising from the high-frequency behavior of $\chi^{\nu\nu} \propto 1/\nu^2$ for $\chi > 0$ (See Appendix C).

The three plots of Fig. 4 graphically combine all aspects of the attractive-repulsive mapping of the generalized susceptibilities and allow a comprehensive understanding at a single glance.

The location of the colored bars together with the corresponding values of $\rho_r(\chi)$ are transformed fully consistently with the mapping of the physical D.O.F.. In accordance with our results in Sec. IIIb, not only the physical susceptibility, but the entire distribution $\rho_r(\chi)$ of the identical density and $pp$ (pseudospin) sectors are mapped onto the magnetic (spin) sector and vice versa.

On the contrary, the positions of the gray bars of each channel are unchanged in the $+U$ and $-U$ cases, reflecting the perfect invariance of the antisymmetric subspaces of all generalized $\chi_r$ under the mapping. We note that
Obviously, by replacing $U$ with $-U$ in Eq. (23), a similar property holds for all enhanced susceptibility densities

$$\rho_{\text{enh}}(U) = \rho_{\text{sup}}(-U) = \rho_m^{U<0} = \rho_d^{U>0} = \rho_{pp}^{U>0}.$$ (24)

The comparison of the attractive and repulsive panels of each channel in Fig. 4 indicates as an overall trend, that the suppression of a susceptibility is associated to a systematic shift of the colored bars towards smaller values, as well as with a change of the weight distribution, where the highest values of $\rho_{\text{sup}}$ are associated with the lowest eigenvalues. This supports the physical picture that an interaction-driven suppression of a static local susceptibility is connected to an increasing number of negative eigenvalues and therefore with the crossing of multiple vertex divergences. This corresponds to a loose generalization of the self-energy behavior at the 2P level, as discussed in Sec. II.

At the same time, this demonstrates why the “reverse” implication of the above physical picture is not correct. The perfect invariance of the gray bars under the mapping, whose physical content is totally decoupled from the static susceptibility, implies the perfect mirroring of all red-lines where only the density channel is singular (Fig. 1). Hence, the occurrence of red divergence lines is independent of the behavior of the corresponding susceptibility as well as of the SU(2)×SU(2) symmetry properties of the model considered.

Finally, important quantitative information can be also gained from Fig. 4. By analyzing the behavior of the enhanced susceptibilities, it is evident that $\rho_{\text{enh}}$ is dominated by the contribution of a single term: the one associated to largest eigenvalue $\lambda_{\text{max}}$. This property is illustrated in Fig. 5, where we compare the actual values of $\chi_d$ and $\chi_m$ obtained from Eq. (22) with the case where the summation in Eq. (21) is reduced to the largest eigenvalue only. The contribution from the largest eigenvalue $\lambda_{\text{max}}$ very well reproduces the trend across the entire repulsive and attractive regime and even well approximates the actual value of the static susceptibilities $\chi_d$ and $\chi_m$ in their respective enhanced regions. Since the relation $V_{\text{enh}}^{\text{max}} = V_m^{\text{max}} = V_d^{\text{max}} = V_{pp}^{\text{max}}$ follows from the proof in Appendix B and Eq. 13, the value of all physical susceptibilities in their respective enhanced regions can be well approximated by

$$\langle \chi_r \rangle \sim \lambda_{\text{max}} \sum_{\nu} V_{\text{enh}}^{\text{max}}(\nu)$$ (25)

According to this relation, the Curie-Weiss behavior
FIG. 5. Comparison of the static density $\chi_d(\Omega = 0)$ (red) and magnetic $\chi_m(\Omega = 0)$ (green) susceptibility with the contribution of the largest eigenvalue only, as a function of the attractive/repulsive Hubbard interaction $U$ at $T = 0.2$. In the bottom of the plot, the lowest eigenvalue of $\lambda_{\min}^{d\nu}$ is shown. The evolution of the lowest eigenvalues ($\lambda_{\min}^{d\nu}$, in dark gray) is completely decoupled from the behaviour of the static susceptibility.

of any static local susceptibility in the strong-coupling regime can be ascribed to the evolution of the corresponding $\lambda_{\max}^{d\nu}$ and the associated eigenvector.

V. PHYSICAL AND ALGORITHMIC CONSEQUENCES

The numerical and analytical results of the previous sections allow us to draw some relevant conclusions on algorithmic and physics implications of vertex divergences. As we have seen, only divergences associated to symmetric singular eigenvectors reflect an interaction-driven suppression of the corresponding static susceptibility. Our DMFT study of the attractive Hubbard model provides, indeed, a clear example where vertex divergences associated with antisymmetric singular eigenvectors do affect also the dominant scattering channel. This observation has direct implications for the usage of parquet-based schemes in the non-perturbative regime, such as, e.g., DFT$^{25}$ and QUADRILEX$^{22}$.

In fact, if the occurrence of vertex divergences could be completely confined to the secondary scattering channels, with suppressed scattering and fluctuations, their appearance could be exploited as an useful “indicator” that this channel can be safely neglected. This would considerably simplify the parquet treatment of the problem under investigation (e.g. reducing the parquet treatment to some effective BSE-based algorithm). Evidently, the occurrence of divergences in the dominant channels prevents a straightforward implementation of this idea. Hence, other ways to address this problem should be followed, such as the combination of FRG and DMFT, (DMF$^2$RG$^{21}$ or the single-boson exchange (SBE) approach$^{20}$.

At the same time, the antisymmetric nature of the divergences occurring in the dominant channels will not hinder the applicability of post-processing schemes of non-perturbative results based on the parquet equations (e.g. the parquet-decomposition of the self-energy$^{26}$), since the potentially dangerous effects of such divergences will be cancelled out by the internal summation over fermionic variables. This might suggest alternative strategies to circumvent the divergences occurring in the major channels, even at the level of parquet solves$^{21,16,29,51}$, by exploiting the odd symmetry properties of their frequencies (and/or momentum$^{23}$) structures.

We should also note that the divergences associated to antisymmetric eigenvectors are the first to be encountered upon increasing the interaction, independent of the interaction sign. As they affect the density channel, diagrammatic Monte Carlo algorithms based on bold resumptions are likely going to encounter difficulties of formal convergence towards unphysical solutions for repulsive$^{27}$ as well as attractive interactions.

It is important to stress that our results (and in particular that of Sec. III B and Sec. IV) do not only apply to the singular eigenvalues and eigenvectors. Instead, they fully define the effects of the Shiba mapping on all generalized two-particle quantities: The symmetric subspaces of $\chi_\nu$ are transformed exactly in the same way as the physical D.o.F., while the antisymmetric subspaces remain invariant.

On the basis of these considerations, and consistently with the total decoupling of the antisymmetric eigenvectors from the static susceptibilities (see Secs. III B and IV), one would be tempted to associate the whole physically relevant information with the symmetric subspace of the generalized susceptibilities. However, this is not true in general. In fact, while the antisymmetric subspace of $\chi_\nu$ does not contribute at all to the corresponding static susceptibility, it can affect the behavior of other physical quantities.

A pertinent example are energy-energy correlationfunctions, i.e. response functions which explicitly contain first-order time-derivatives (i.e., $i\hbar \frac{d}{dt} = -\hbar \frac{d}{dt} = \hat{H}$) such as the thermal conductivity$^{28}$. By Fourier transforming the (imaginary) time-derivative, one gets an additional linear dependence of the generalized response on the two fermionic Matsubara frequencies $\nu, \nu'$. This additional frequency dependence essentially inverts the symmetry effects in the final fermionic frequency summations, hence allowing for contributions arising from the antisymmetric subspace.

Finally, we note that if symmetries of the problem are lifted (e.g. by doping the system, considering further hopping terms or applying a magnetic field, etc.), correspondent changes must be expected. The high-symmetry
case we considered in this work will represent then a good "compass" to interpret the observed deviation. For instance, doping the model with electron/holes will break the SU(2) symmetry of the pseudospin D.o.F., and one will observe a corresponding splitting of the degeneracy of the "orange" (pseudospin) divergences lines, with a different location of the singularities in the density and in the \(pp\) channel. For the \(pp\) channel however, the internal symmetry subdivision into fully symmetric and antisymmetric subspaces will continue to hold. Similarly, the three-fold degenerate divergences in the magnetic channel will be split, if the SU(2) symmetry is lifted by applying a magnetic field.

VI. CONCLUSION

In the present work we conducted a comparative DMFT analysis to understand the location and physical role of vertex divergences occurring in the two-particle vertex correlation functions of the repulsive and attractive Hubbard model. Our calculations show that the location of divergences of two-particle irreducible vertices is perfectly symmetric in the attractive and repulsive Hubbard model. This result partly contradicts the expectation from the one-particle picture, where a divergence of the self-energy is accompanied by the suppression of the one-particle Green’s function. In particular the symmetric occurrence of singular eigenvalues in \(\chi_{\sigma \nu}^\nu\) for \(U \leq 0\) shows, that divergences of the two-particle self-energy \(\Gamma\) do not necessarily occur in physically suppressed channels.

By considering the specific symmetries that apply in the presently considered system, we show that the antisymmetric part of the generalized susceptibilities is invariant under the Shiba transformation. Therefore, we confirm that the interaction-driven suppression of a static local susceptibility is generally accompanied by an increasing number of negative eigenvalues, if they are associated to symmetric eigenvectors, which actively contribute to the suppression of the channel. However, the reversed implication, that the occurrence of negative eigenvalues is in general indicative of the suppression of a channel, is not valid, because of the antisymmetric divergence lines being invariant under \(U \leftrightarrow -U\).

Therefore, this suggests the physically relevant information in terms of a susceptibility density distribution which naturally distinguish the symmetric from the vanishing antisymmetric eigenvector subspace. This representation allows to summarize the \(U \leftrightarrow -U\) mapping behavior of the generalized susceptibilities and its relation to the mapping of the physical (spin and pseudospin) degrees of freedom at a single glance. Moreover, since the associated spectral distribution is identical for all suppressed as well as all enhanced channels, the introduced representation provides a universal description of all physical susceptibilities relevant for this problem.

Further studies are required to clarify the role of the antisymmetric subspace for other physical quantities such as the thermal conductivity, the effect of a progressive reduction of the symmetry conditions and, on a broader perspective, the relation with the non-equilibrium properties of the system under investigation.

Acknowledgments: We are indebted for insightful discussions with Sabine Andergassen, Massimo Capone, Lorenzo Del Re, James Freericks, Anna Kauch, Olle Gunnarsson, Andreas Hausoel, Cornelia Hille, Friedrich Krien, Erik van Loon, Matthias Reitner, Georg Rohringer, Thomas Schäfer, Agnese Tagliavini, Patrik Thunström, and Angelo Valli. We acknowledge financial support from the Austrian Science Fund (FWF) through the projects: SFB ViCoM F41 (DS) and I 2794-N35 (PC, AT). Calculations have been performed on Vienna Scientific Cluster (VSC).

Appendix A: Bisymmetric Matrices

The following part is a short summary of mathematical literature on bisymmetric and centrosymmetric matrices. It is reported here to present the reader the possibility to follow more easily the proof in part \(\text{[1]}\).

Note that at this point we focus on the matrix properties related to Eq. (16), without taking into account that the matrix is also symmetric. In this case one speaks of centrosymmetric matrices.

In the following we consider a centrosymmetric matrix \(H\), a \(2n \times 2n\) matrix, where \(n\) is the number of positive/negative fermionic Matsubara frequencies. As \(H\) is a centrosymmetric matrix it fulfills the following condition:

\[
JHJ = H \tag{A1}
\]

where \(J\) is the counteridentity matrix \((J^2 = 1)\), given in Eq. (A2).

\[
J = \begin{pmatrix}
0 & \ldots & 0 & 1 \\
\vdots & \ddots & \vdots & \vdots \\
0 & 1 & \ddots & \vdots \\
1 & 0 & \ldots & 0
\end{pmatrix}
= \begin{pmatrix}
0 & J \\
J & 0
\end{pmatrix} \tag{A2}
\]

If \(J\) is multiplied from the right it inverts the columns of a matrix, if it is multiplied from left the rows are inverted. As one can easily see, for \(\chi_{\sigma \nu}^\nu\) this means...
where \( J_{\lambda \sigma \sigma'} = J_{\lambda' \sigma' \sigma} = \lambda_{\sigma \sigma'} \), which is true for our case, see Eq. [16] in the main text.

If \( H \) is a centrosymmetric matrix, the following condition holds, where the submatrices \( A, B, C, D \) are \( n \times n \) matrices.

\[
H = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \quad \text{and} \quad JHJ
\]

\[
\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix}
\]

\[
= \begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix} \begin{pmatrix} B & AJ \\ DJ & AJ \end{pmatrix}
\]

\[
= (JDJ) \begin{pmatrix} JCJ & AJ \\ C \end{pmatrix}
\]

\[
\Rightarrow D = JAJ \quad \& \quad B = JCJ
\]

This means that the centrosymmetric matrix \( H \) can be written in the following form:

\[
H = \begin{pmatrix} A & JCJ \\ JCJ & JAJ \end{pmatrix}
\]

### Eigenvalues and Eigenvectors

Centrosymmetric matrices have a very useful property. Their eigenvalues can be obtained from the diagonalization of specific combinations of the submatrices \( A \) and \( C \), corresponding to either symmetric or antisymmetric eigenvectors. This can be seen as follows:

Consider \( \mathbf{v} \), an eigenvector of \( H \)

\[
H\mathbf{v} = \lambda\mathbf{v} \quad | \cdot J \rightarrow \quad (A10)
\]

\[
JH\mathbf{v} = \lambda J\mathbf{v} \quad (A11)
\]

\[
HJ\mathbf{v} = \lambda J\mathbf{v} \quad (A12)
\]

where we used Eq. [A1] and \( J^2 = 1 \). From this it follows that \( J\mathbf{v} \) is also an eigenvector of \( H \) corresponding to the eigenvalue \( \lambda \), i.e.

\[
J\mathbf{v} = a\mathbf{v} \quad , \quad (A13)
\]

with \( a \neq 0 \), being the eigenvalue of \( J \) and since \( J \) is an orthogonal matrix, \( a = \pm 1 \). This leads to antisymmetric or symmetric eigenvectors \( \mathbf{v} \). In our terms this means that:

\[
\mathbf{v} = \begin{pmatrix} \mathbf{v} \\ J\mathbf{v} \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} \mathbf{v} \\ -J\mathbf{v} \end{pmatrix} \quad \text{with} \quad \begin{pmatrix} \text{neg. Matsubara} \\ \text{frequencies} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \text{pos. Matsubara} \\ \text{frequencies} \end{pmatrix}
\]

\[
(\text{A14})
\]

where \( \mathbf{v} \) is a \( 2n \times 1 \) vector and \( \mathbf{v} \) is a \( n \times 1 \) subpart of it.

Next, we consider \( \lambda_S \), an eigenvalue corresponding to a symmetric eigenvector \( H\mathbf{v}_S = \lambda_S\mathbf{v}_S \):

\[
\begin{pmatrix} A & JCJ \\ C & JAJ \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ J\mathbf{v} \end{pmatrix} = \lambda_S \begin{pmatrix} \mathbf{v} \\ J\mathbf{v} \end{pmatrix} \quad (A15)
\]

\[
\downarrow
\]

\[
\begin{pmatrix} A + JC \end{pmatrix}\mathbf{v} = \lambda_S\mathbf{v} \quad (A16)
\]

In a similar fashion for \( \lambda_A \), corresponding to an antisymmetric eigenvector:

\[
\begin{pmatrix} A & JCJ \\ C & JAJ \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ -J\mathbf{v} \end{pmatrix} = \lambda_A \begin{pmatrix} \mathbf{v} \\ -J\mathbf{v} \end{pmatrix} \quad (A17)
\]

\[
\downarrow
\]

\[
\begin{pmatrix} A - JC \end{pmatrix}\mathbf{v} = \lambda_A\mathbf{v} \quad (A18)
\]

This shows that the centrosymmetric matrix \( H \) has eigenvalues \( \lambda_S \) obtained from diagonalizing \( A + JC \), which also gives the non-trivial parts \( \mathbf{v} \) of the symmetric eigenvectors \( \mathbf{v}_S \). In our case they correspond to the orange and green divergence lines, for \( \lambda_S = 0 \). On the other hand we observe that \( \lambda_A \) corresponds to antisymmetric eigenvectors obtained from the diagonalization of the submatrices \( A - JC \) - the red divergence lines.

In the following a very elegant way to see this block structure of \( H \) is presented, which will be used later in the proof.

### Block-diagonalization

Using the following orthogonal matrix \( Q \) (\( QQ^T = 1 \)) one can block-diagonalize a centrosymmetric matrix \( H \):

\[
Q = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -J \\ 1 & J \end{pmatrix} \quad (A19)
\]

\[
QHQ^T = \frac{1}{2} \begin{pmatrix} 1 & -J \\ 1 & J \end{pmatrix} \begin{pmatrix} A & JCJ \\ C & JAJ \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -J & J \end{pmatrix} \quad (A20)
\]

\[
= \frac{1}{2} \begin{pmatrix} 1 & -J \\ 1 & J \end{pmatrix} \begin{pmatrix} A - JC & A + JC \\ C - JA & C + JA \end{pmatrix} \quad (A21)
\]

\[
= \frac{1}{2} \begin{pmatrix} 2(A - JC) & 0 \\ 0 & 2(A + JC) \end{pmatrix} \quad (A22)
\]

\[
\begin{pmatrix} A - JC & 0 \\ 0 & A + JC \end{pmatrix} \quad (A23)
\]

Where immediately the block-structure described before is found.
Bisymmetric Matrices

As stated in the main text, due to the SU(2)- and the time-reversal-symmetry the centrosymmetric matrix $H$ considered is in fact bisymmetric. This has important consequences for the submatrices $A$ and $C$ introduced earlier:

$$H = H^T \quad (A_{24})$$

as $J = J^T$ one finds $A = A^T$ immediately. For $C$ the following equation holds:

$$C^T = JCJ \rightarrow C^T J^T = JC \rightarrow (JC)^T = JC \quad (A_{26})$$

This means that the combination of submatrices yielding the eigenvalues and the corresponding symmetric or antisymmetric eigenvectors is symmetric, ensuring together with the particle-hole symmetry that the obtained eigenvalues are real.

$$(A \pm JC)^T = A^T \pm (JC)^T \quad (A_{27})$$

Appendix B: The mapping of divergence lines

Because of the specific mapping from $U > 0$ to $U < 0$ of $\chi^{\uparrow \uparrow}$ and $\chi^{\uparrow \downarrow}$, it is possible to show, that the red divergence lines for $U < 0$ have to be the mirrored ones of $U > 0$. As it turns out it also follows that the symmetric density divergences $(U > 0)$ are mapped to symmetric divergences in the magnetic channel for $U < 0$.

The starting point is to consider the bisymmetric $\chi^{\uparrow \uparrow}$ and $\chi^{\uparrow \downarrow}$ matrices, where the fermionic Matsubara frequency indices will be omitted in the following. $\chi^{\uparrow \uparrow}$ and $\chi^{\uparrow \downarrow}$ fulfill the following relations, discussed in the main text in Sec. III B, when mapped from positive to negative $U$.

$$\chi^{U>0}_{\uparrow \uparrow} = \chi^{U<0}_{\uparrow \downarrow} = A \begin{pmatrix} J & B \\ D & J \end{pmatrix} \quad (B_1)$$

$$\chi^{U>0}_{\uparrow \downarrow} = \chi^{U<0}_{\uparrow \downarrow} = \begin{pmatrix} C & JDJ \\ D & JCJ \end{pmatrix} \quad (B_2)$$

$$\chi^{U<0}_{\uparrow \downarrow} = \chi^{U>0}_{\downarrow \uparrow} = \begin{pmatrix} C & JDJ \\ D & JCJ \end{pmatrix} \begin{pmatrix} 0 & -J \\ -J & 0 \end{pmatrix}$$

$$= \begin{pmatrix} -JD & -CJ \\ -JC & -JD \end{pmatrix} \quad (B_3)$$

Now, block-diagonalization of $\chi^{\uparrow \uparrow}$ and $\chi^{\uparrow \downarrow}$ for both cases leads to:

$$Q\chi^{U<0}_{\uparrow \downarrow} = \begin{pmatrix} A - JB & 0 \\ 0 & A + JB \end{pmatrix} \quad (B_4)$$

$$Q\chi^{U>0}_{\uparrow \downarrow} = \begin{pmatrix} C - JD & 0 \\ 0 & C + JD \end{pmatrix} \quad (B_5)$$

$$Q\chi^{U<0}_{\uparrow \downarrow} = \begin{pmatrix} -JD - J(-JC) & 0 \\ 0 & JD + J(-JC) \end{pmatrix}$$

$$= \begin{pmatrix} C - JD & 0 \\ 0 & -[C + JD] \end{pmatrix} \quad (B_6)$$

This shows immediately that the antisymmetric block of $\chi^{\downarrow \uparrow}$, $(C - JD)$, is unchanged, whereas the symmetric one changes sign for $U > 0 \leftrightarrow U < 0$. Considering $\chi_d$ and $\chi_m$ for $U < 0$ and $U > 0$ the following conclusions can be drawn, where we use the trivial relation:

$$Q\chi^{d+,-}_m Q^T = Q\chi^{\downarrow \uparrow} Q^T = Q\chi^{\uparrow \downarrow} Q^T \quad (B_7)$$

$$Q\chi^{U>0}_d Q^T = \begin{pmatrix} \pm |A - JB| + |C - JD| & 0 \\ 0 & |A + JB| \pm |C + JD| \end{pmatrix} \quad (B_8)$$

$$Q\chi^{U<0}_m Q^T = \begin{pmatrix} |A - JB| - |C - JD| & 0 \\ 0 & |A + JB| \pm |C + JD| \end{pmatrix} \quad (B_9)$$

where in the density case the + sign corresponds to $U > 0$ and the − to $U < 0$, for the magnetic case it is the other way around.

From Eqs. [B_4], [B_5], [B_6] three things can be learned:

(i) The antisymmetric block of $Q\chi^{U>0}_m Q^T$ is independent of the sign of $U$. The diagonalization of $[A - JB] + [C - JD]$ will yield the eigenvalues and the corresponding antisymmetric eigenvectors of $\chi_d$. Their singularity corresponds to a red divergence line - independent of the sign of $U$. This is the mathematical reason for the perfect mapping of the red divergence lines reported in Fig. 1 and the equality of the singular eigenvectors seen in Fig. 2 of the main text. Note that this statement is crucially dependent on the perfect particle-hole symmetry of the problem analyzed - otherwise the bisymmetry property is lost.

(ii) The antisymmetric block of $Q\chi^{U>0}_m Q^T$ is also independent of the sign of $U$. This means that, irrespective of the sign of $U$, the eigenvalues corresponding to antisymmetric eigenvectors of $\chi_m$ can be calculated by diagonalizing $[A - JB] - [C - JD]$. However, so far none of these eigenvalues were found to be singular.

(iii) The symmetric parts of $\chi_d$ and $\chi_m$ are mapped in the following way: $[A + JB] + [C + JD]$ is the symmetric blockmatrix of $\chi^{U>0}_d$ and $\chi^{U<0}_m$. This explains why the symmetric density channel divergences for $U > 0$ are
mapped to divergences with symmetric eigenvectors in the magnetic channel for $U < 0$.

Analogously, $[A + JB] - [C + JD]$ is the symmetric blockmatrix of $\chi_d^{U<0}$ and $\chi_m^{U>0}$, exactly the parameter regime where these channels exhibit the dominant, non-suppressed physics. Here the bisymmetry explains the mapping of the eigenvalues, as discussed in Sec. IV.

Finally we note that also the matrix causing the divergences in the particle-particle up-down channel $\chi_{pp,\uparrow\downarrow}^{\nu,-\nu'} - \chi_{0,pp}^{\nu,-\nu'}$, is bisymmetric, having hence the same properties as mentioned above. Combining this insight with Eq. 13 we have now fully clarified how the mapping of the generalized susceptibilities works and its exact relation with the physical degrees of freedom. The antisymmetric sectors are not mapped along the lines of Eq. 9, but they cancel in the sum in Eq. 7. The symmetric subparts on the other hand follow the mapping of the physical D.o.F.

Appendix C: Susceptibility density in the binary mixture disordered model

We calculate analytically the $\rho_d(\chi)$ in the Binary Mixture (BM) disordered case defined by the Hamiltonian

$$ H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + \sum_i \epsilon_i c_i^\dagger c_i. \quad (C1) $$

Here spin indices can be omitted and we can safely consider spinless electrons moving in a random background with equal probability for $\epsilon_i = \pm W/2$.

The Green’s function at half-filling can be easily calculated within DMFT

$$ G(\nu) = \frac{1}{2} \left( \frac{1}{G_{0}^{-1}(\nu) - \frac{W}{2}} + \frac{1}{G_{0}^{-1}(\nu) + \frac{W}{2}} \right), \quad (C2) $$

where $G_{0}^{-1}(\nu) = \nu - D^2 G(\nu)/4$ in the Bethe lattice case. This result is in perfect analogy with the Hubbard III

![FIG. 6. Eigenvalues from Eq. (C3) evaluated a $T = 0.0$. (CPA) approximation for the Hubbard model, where $W$ must be understood as $U$. The BM shows divergences in the irreducible vertex function as well as negative eigenvalues in the generalized susceptibility for the density channel. They appear at sufficiently large $W$ beyond the Mott-like transition in which the DOS at vanishes at the Fermi level.](image)

The BM shows divergences in the irreducible vertex function as well as negative eigenvalues in the generalized susceptibility for the density channel. They appear at sufficiently large $W$ beyond the Mott-like transition in which the DOS at vanishes at the Fermi level. The susceptibility $\chi_d^{\nu,\nu'}$ can be easily calculated as

$$ \chi_d^{\nu,\nu'} = \frac{2}{W^2} \sqrt{1 + W^2 G^2(\nu)} \left[ \sqrt{1 + W^2 G^2(\nu)} \pm 1 \right] \delta_{\nu,\nu'}, \quad (C3) $$

where the ± sign is a consequence of the multivaluedness of the electronic self-energy and must hence be taken into account properly, in order to access the physical solution.

Eq. (C3) states that $\chi_d^{\nu,\nu'}$ is diagonal in Matsubara frequency space. This is a consequence of the locality of the functional relation which relates the self-energy and the local single-particle propagator $\Sigma[G]$.

The phase-diagram of the BM model shows an accumulation point of vertex divergences at $T = 0$ located at $W_c/D = 1/\sqrt{2}$, before the Mott-like transition. As we shall see below, this implies a continuous eigenvalue distribution that exhibits a tail towards negative values above $W_c$.

Eigenvalues of $\chi_d^{\nu,\nu'}$ can be directly obtained from Eq. (C3) once the self-consistency condition has been enforced. A singular eigenvalue occurs when

$$ 1 + W^2 G^2 = 0 \quad (C4) $$

at zero frequency. The schematic behavior of eigenvalues as a function of Matsubara frequencies is shown in Fig. 6. The behavior of the distribution of eigenvalues which turns out to be continuous in the $T = 0$ limit is shown in Fig. 6. Notice the logarithmic scale in Fig. 6, which means that the weight associated to negative eigenvalues is very small. However, the zero-crossing of a small amount of eigenvalues marks the onset of the strong disorder limit at $W_c$ before the Mott-like transition where the local $\chi$ vanishes.
FIG. 7. Map of the eigenvalue distribution at $T = 0$. The green curve is the local charge susceptibility.

1. A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1975).
2. G. D. Mahan, *Many-Particle Physics* (Plenum Press, New York, 1976).
3. M. Liu, L. W. Harriger, H. Luo, M. Want, R. A. Ewings, T. Guidi, H. Park, K. Haule, G. Kotliar, S. M. Hayden, and P. Dai, *Nature Physics* 8, 376 (2012).
4. A. Toschi, R. Arita, P. Hansmann, G. Sangiovanni, and K. Held, Phys. Rev. B 86, 064411 (2012).
5. A. Gallier, C. Taranto, M. Wallerberger, M. Kaltak, G. Kresse, G. Sangiovanni, A. Toschi, and K. Held, Phys. Rev. B 92, 205132 (2015).
6. A. Haussel, M. Karolak, E. Sasoğlu, A. Lichtenstein, K. Held, A. Katanin, A. Toschi, and G. Sangiovanni, Nature Communications 8, 16062 (2017).
7. A. Kaufch, P. Pudleiner, A. Kastl, T. Ribic, and K. Held, (2019), arXiv:1902.09342 [cond-mat.str-el].
8. T. Maier, M. Jarrell, T. Pruschke, and M. H. Hettler, Rev. Mod. Phys. 77, 1027 (2005).
9. W. Metzner, M. Salmhofer, C. Honerkamp, V. Meden, and K. Schönhammer, Rev. Mod. Phys. 84, 299 (2012).
10. G. Rohringer, H. Hafermann, A. Toschi, A. A. Katanin, A. E. Antipov, M. I. Katsnelson, A. I. Lichtenstein, A. N. Rubtsov, and K. Held, Rev. Mod. Phys. 90, 025003 (2018).
11. J. Kunes, Phys. Rev. B 83, 085102 (2011).
12. G. Rohringer, A. Valli, and A. Toschi, Phys. Rev. B 86, 125114 (2012).
13. H. Hafermann, Phys. Rev. B 89, 235128 (2014).
14. O. Gunnarsson, T. Schäfer, J. P. F. LeBlanc, E. Gull, J. Merino, G. Sangiovanni, G. Rohringer, and A. Toschi, Phys. Rev. Lett. 114, 236402 (2015).
15. N. Wentzell, G. Li, A. Tagliavini, C. Taranto, G. Rohringer, K. Held, A. Toschi, and S. Andergassen, arXiv:1610.06520 (2016).
16. J. Kaufmann, P. Gunacker, and K. Held, preprint (2017), arXiv:1703.09407.
17. A. Tagliavini, S. Hummel, N. Wentzell, S. Andergassen, A. Toschi, and G. Rohringer, Phys. Rev. B 97, 235140 (2018).
18. P. Thunström, O. Gunnarsson, S. Ciuchi, and G. Rohringer, Phys. Rev. B 98, 235107 (2018).
19. R. Nourafkan, M. Côté, and A.-M. S. Tremblay, Phys. Rev. B 99, 035161 (2019).
20. F. Krien, A. Valli, and M. Capone, Phys. Rev. B 100, 155149 (2019).
21. T. Schäfer, S. Ciuchi, M. Wallerberger, T. P., O. Gunnarsson, G. Sangiovanni, G. Rohringer, and A. Toschi, Phys. Rev. B 94, 235108 (2016).
22. V. Janiš and V. Pokorný, Phys. Rev. B 90, 045143 (2014).
23. P. Chalupa, P. Gunacker, T. Schäfer, K. Held, and A. Toschi, Phys. Rev. B 97, 245136 (2018).
24. T. Schäfer, G. Rohringer, O. Gunnarsson, S. Ciuchi, G. Sangiovanni, and A. Toschi, Phys. Rev. Lett. 110, 246405 (2013).
25. O. Gunnarsson, T. Schäfer, J. P. F. LeBlanc, J. Merino, G. Sangiovanni, G. Rohringer, and A. Toschi, Phys. Rev. B 93, 245102 (2016).
26. O. Gunnarsson, G. Rohringer, T. Schäfer, G. Sangiovanni, and A. Toschi, Phys. Rev. Lett. 119, 056402 (2017).
27. E. Kozik, M. Ferrero, and A. Georges, Phys. Rev. Lett. 114, 156402 (2015).
28. A. Stan, P. Romaniello, S. Rigamonti, L. Reining, and J. A. Berger, New J. Phys. 17, 093045 (2015).
29. W. Tarantino, B. S. Mendoza, P. Romaniello, J. A. Berger, and L. Reining, Journal of Physics: Condensed Matter 30, 135602 (2018).
30. K. Byczuk, M. Kollár, K. Held, Y.-F. Yang, I. A. Nekrasov, T. Pruschke, and D. Vollhardt, Nature Physics 3, 168 (2007).
31. A. Toschi, M. Capone, C. Castellani, and K. Held, Phys. Rev. Lett. 102, 076402 (2009).
32. K. Held, R. Peters, and A. Toschi, Phys. Rev. Lett. 110, 246402 (2013).
with this definition, a BSE, formally similar to Eq. (3), can be written for the quantity
\[ \tilde{\chi}_{\nu'\nu}(\Omega) = \chi_{\nu'\nu}(\Omega) - \chi_{0,\nu'\nu}(\Omega) \]
with
\[ \chi_{0,\nu'\nu}(\Omega) = -\beta G(\nu)G(\Omega - \nu')\delta_{\nu'\nu}. \]

H. Shiba, Prog. Theor. Phys. 48, 2171 (1972).

R. Micnas, J. Ranninger, and S. Robaszkiewicz, Rev. Mod. Phys. 62, 113 (1990).

L. Del Re, M. Capone, and A. Toschi, Phys. Rev. B 99, 045137 (2019).

For previous DMFT studies of the attractive Hubbard model at the one-particle level see, e.g., [50] [55] [61].

G. Li, N. Wentzell, P. Pudleiner, P. Thunström, and K. Held, Phys. Rev. B 93, 195134 (2016).

Note that the thermal conductivity expression would also contains the spatial derivatives of the heat-current. This would preventing any kind of vertex-corrections in the single-orbital model at the DMFT level [35]. The latter are possible, however, at the level of DCA [8], where vertex-divergences with antisymmetric structure have been also reported [25]. Furthermore, the correlation functions containing time-derivatives, where the effects of the antisymmetric part of the vertex functions are important, are the most suited to establish a connection with non-equilibrium phenomena.

M. Keller, W. Metzner, and U. Schollwöck, Phys. Rev. Lett. 86, 4612 (2001).

A. Toschi, M. Capone, and C. Castellani, New J. Phys. 7, 7 (2005).

M. Keller, W. Metzner, and U. Schollwöck, Phys. Rev. Lett. 86, 4612 (2001).

A. Privitera, M. Capone, and C. Castellani, Phys. Rev. B 84, 023638 (2011).

M. Wallerberger, A. Hausoel, P. Gunacker, A. Kowalski, N. Parragh, F. Goth, K. Held, and G. Sangiovanni, Computer Physics Communications 235, 388 (2019).

The small differences arise from the different lattice (here: Bethe lattice) used in the DMFT calculations.