Breakdown of traditional many-body theories for correlated electrons

O. Gunnarsson,1 G. Rohringer,2 T. Schäfer,3 G. Sangiovanni,4 and A. Toschi4

1 Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany
2 Russian Quantum Center, Novaya street, 100, Skolkovo, Moscow region 143025, Russia
3 Institute of solid state physics, Vienna University of Technology, 1040 Vienna, Austria
4 Institute of Physics and Astrophysics, University of Würzburg, Würzburg, Germany

(Dated: November 7, 2018)

Starting from the (Hubbard) model of an atom, we demonstrate that the uniqueness of the mapping from the interacting to the noninteracting Green’s function, $G \rightarrow G_0$, is strongly violated, by providing numerous explicit examples of different $G_0$ leading to the same physical $G$. We argue that there are indeed infinitely many such $G_0$, with numerous crossings with the physical solution. We show that this rich functional structure is directly related to the divergence of certain classes of (irreducible vertex) diagrams, with important consequences for traditional many-body physics based on diagrammatic expansions. Physically, we ascribe the onset of these highly non-perturbative manifestations to the progressive suppression of the charge susceptibility induced by the formation of local magnetic moments and/or RVB states in strongly correlated electron systems.

PACS numbers: 71.10.-w; 71.27.+a; 71.10.Fd

Introduction. For more than fifty years non-relativistic quantum many-body theory (QMBT) has been successfully applied to describe the physics of many-electron systems in the field of condensed matter. Despite the intrinsic difficulty of identifying a small expansion parameter (analogously to the the fine-structure constant of quantum-electrodynamics), the formalism of QMBT — in its complementary representations in terms of Feynman diagrams and of the universal Luttinger-Ward (LW) functional — is the cornerstone of the microscopic derivation of Landau’s Fermi-liquid theory and of uncountable approximation schemes.

Yet, the actual conditions of applicability of the QMBT in the non-perturbative regime have been scarcely investigated. This is surprising, because QMBT is extensively applied to strongly correlated electron materials, where band-theory and Fermi-liquid predictions fail, and some of the most exotic physics of condensed matter systems is observed. Recently, however, the quest for such investigations became particularly strong. This is because several cutting-edge QMBT-approaches, explicitly designed for describing the crucial, but elusive, regime of intermediate-to-strong interactions, have been developed, e.g., the diagrammatic Quantum Monte Carlo (DQMC) schemes and numerous diagrammatic extensions of dynamical mean field theory (DMFT).

Pioneering analyses of the perturbation theory breakdown have been reported in the last four years. (i) We argue that there are indeed infinitely many singularities in the Bethe-Salpeter equations and (ii) the intrinsic multivaluedness of the LW functionals. The first problem appears as an infinite series of unexpected divergences in irreducible vertex functions, while the second is reflected in the convergence of the perturbative series to an unphysical solution. The intrinsic origin of these non-perturbative manifestations, their impact on the many-electron physics, as well as on the method development in the field, represent a challenge for the current theoretical understanding.

In this Letter, we report a fundamental progress in the comprehension of the perturbation theory breakdown and of its significance. In particular, going beyond the pioneering work of, (i) we show that there are many (probably an infinite number of) unphysical self-energies that become equal to the physical one at specific values of the interaction. This puts us into the position to (ii) demonstrate the actual correspondence between the vertex divergences of the Feynman diagrams and the occurrence of bifurcations of the LW functional. Finally, (iii) we generalize these results from the Hubbard atom to generic systems with strong correlations. Regarding the nature of the singularities, we show that vertex divergences of different kinds are reflected in different natures of solution crossings at the bifurcation.

The emerging scenario, which mathematically depicts an unexpectedly complex structure of the many-body formalism, will be physically related to the progressive suppression of charge fluctuations, a generic property of strongly-correlated systems with a local interaction. The improved understanding of the QMBT beyond the perturbative regime serves as a crucial guidance for future method development for non-relativistic many-electron systems.

Multivaluedness of the Luttinger-Ward functional. The Luttinger-Ward (LW) functional $\Phi[G]$ plays a crucial role in traditional many-body physics. It is a universal functional of the full single-particle Green’s function $G$, which only depends on the electron-electron interaction but not on the external potential. From $\Phi[G]$ the free energy can be determined. One can also obtain the electron self-energy $\Sigma[G] \sim \delta \Phi[G]/\delta G$, entering the Dyson...
equation
\[ G_0^{-1} - G^{-1} = \Sigma, \] (1)
where \( G_0 \) is the noninteracting Green's function determined by the external potential. From \( \Sigma[G] \) one can compute all irreducible vertices \( \Gamma \) entering the Bethe-Salpeter equations [8] for response functions. For instance, the charge susceptibility is determined by the vertex [8][9][19][20]

\[ \Gamma_c = \frac{\delta \Sigma[G]}{\delta G}. \] (2)

Approximations built within this approach are guaranteed to be conserving [3], therefore it is exploited for numerous formal derivations [11][29][31]. Moreover, the full two-particle nature of the vertices \( \Gamma \) represents an ideal building block for approximations designed to preserve the Pauli principle properties, and related sum rules. In this respect, it is believed that the parquet equations [8] are one of the most fundamental ways of performing diagrammatic summations.

In order for QMBT methods to be meaningful, an important property of the functional \( G[G_0] \) needs to be fulfilled: The introduction of \( \Sigma \) in QMBT implicitly assumes that there is a unique mapping between \( G \) and \( G_0 \), \( G \to G_0 \). Otherwise, several branches of \( \Sigma \) would exist, corresponding to different \( G_0 \), posing the general problem of an intrinsic multivaluedness of any QMBT-based scheme. This is not just a formal issue. If two such branches cross, \( \Gamma \) in Eq. (2) might become ill-defined and diverge. This would challenge important aspects of the traditional many-body theory, such as, e.g., the definition of physically meaningful parquet summations [32].

Fig. 1 schematically illustrates such a scenario. The general functional relation between \( G \) and \( G_0 \) is depicted by several red curves for different values of the electronic interaction \( U \) [33]. \( G \) and \( G_0 \) are here treated as numbers rather than functions (of frequency/momentum/spin, etc.). For \( U = 0 \), \( G[G_0] = G_0 \), and for any physical \( G \) (horizontal blue line) the corresponding \( G_0 \) is univalently determined. When \( U > 0 \), however, \( G[G_0] \) becomes 

\[ \text{"wavier"}, \] displaying several maxima/minima in the functional space. This way, the intersection with \( G_{\text{phys}} \) would correspond to several \( G_0 \) (blue dots), of which only one describes the physical system (\( G_{0 \text{phys}} \)). Even if unphysical \( G_0 \)’s exist, many standard numerical algorithms are able to converge to the solution that is adiabatically connected with the \( U = 0 \) one. This can however turn into an actual problem, if for some values of \( U \) the intersection with \( G_{\text{phys}} \) occurs at one extreme of \( G[G_0] \). This would correspond to the intersection of two different solutions of \( G_0 \) (and thus of \( \Sigma \), see green dashed lines in Fig. 1). At this point we would expect \( \delta G/\delta G_0 = 0 \). Combining this with the Dyson equation and the definition [Eq. (2)] of \( \Gamma_c \), one would conclude that \( \Gamma_c \) diverges.

To go beyond the sketch of Fig. 1 we present calculations for the Hubbard atom [34] and show that different \( G_0 \) indeed do cross for certain values of \( U \). In Sec. IA of the Supplemental Material [28] we then show that such a crossing indeed does lead to divergences of \( \Gamma_c \).

Method. We have developed a method for finding different \( G_0 \)’s which lead to the physical \( G \) for the Hubbard atom. We use the Hirsch-Fye algorithm [35] to obtain \( G \) from a guess for \( G_0 \). This method involves a summation over auxiliary spins, which is usually done stochastically. Here we perform a complete summation using the Gray code [36], thereby avoiding stochastic errors. We guess a \( G_0 \), and then use a Metropolis method to search for improved guesses for \( G_0 \). When a promising guess has been found, the Hirsch-Fye equations are repeatedly linearized and solved, until a \( G_0 \) has been found which accurately reproduces the physical \( G \) (see Sec. II of [28]). It is crucial that there are no stochastic errors in this approach. The method makes it possible to determine if two \( G_0 \) really become equal for some \( U \) and to determine how they approach each other as \( U \) is varied.

Results for the Hubbard atom. We start to present our results by showing in Fig. 2 (left panel) \( \text{Tr} \Sigma G_{\text{phys}}/(\beta U) \) as a function of \( U \) corresponding to the different \( G_0 \) and, hence \( \Sigma \), via Eq. (1). For \( G_0 = G_{0 \text{phys}} \), this quantity yields the double occupancy. The black curve displays the values obtained with \( G_0 = G_{0 \text{phys}} \), while the colored (red, orange) curves are the results for the other (unphysical) \( G_0 \), collapsing to \( G_{0 \text{phys}} \) in the several crossing points shown in the Figure. The latter ones do coincide -within our numerical accuracy- with the locations (marked by vertical arrows) of the first six divergences of \( \Gamma_c \) in the Hubbard atom [19]. The red \( G_0 \)'s are associ-
variations at localized arrows mark the divergences of $\Gamma$ to the vanishing of one values. While the divergences of $\Gamma$ with $V$ et al. found by Kozik [20], although, there, it could not be converged around the crossing with $G_{0}^{\text{phys}}$.

There are important connections between the frequency dependence of the divergences of $\Gamma_{c}$, coded by red/orange colors [19], and the detailed behavior of $G_{0}$ at a crossing. The divergences of $\Gamma_{c}$ can be divided into two classes [18, 19]. To this end, we consider the generalized charge susceptibility $\chi_{c}^{\nu\nu'}(\omega=0)$ [37], which depends on two fermionic Matsubara frequencies, $\nu$ and $\nu'$, and a bosonic frequency $\omega = 0$. $\Gamma_{c}$ is then given by

$$\Gamma_{c} = \beta^{2}[\chi_{c}^{-1} - \chi_{0}^{-1}],$$

where $\chi_{0}$ is the noninteracting generalized susceptibility $\chi_{c}$, and $\chi_{c}$ and $\chi_{c,0}$ are treated as matrices of $\nu$ and $\nu'$. These matrices can be diagonalized

$$\chi_{c}^{\nu\nu'}(\omega=0) = \sum_{l} V_{l}(\nu)^{*} \varepsilon_{l} V_{l}(\nu'),$$

with $V_{l}(\nu)$ and $\varepsilon_{l}$ being the corresponding eigenvectors/values. While the divergences of $\Gamma_{c}$ always correspond to the vanishing of one $\varepsilon_{l}$, they differ in the frequency-structure of $V_{l}(\nu)$: For the divergences marked by the red arrows, $V_{l}(\nu)$ has only two non-zero elements (at $\nu = \pm \nu_{n} = \pm (2n - 1)\pi/\beta$, with $n = 1, 2, 3, ...$) reflecting a localized divergence at $\nu = \pm \nu_{n}$, while for the orange arrows, $V_{l}(\nu) \neq 0 \forall \nu$, reflecting a global divergence of $\Gamma_{c}$ [19].

An analogous classification is also applicable to the different $G_{0}$ resolved in frequency space: In Fig. [2] we plot the ratio $\text{Im } G_{0}(\nu)/\text{Im } G_{0}^{\text{phys}}(\nu)$ corresponding to the first two crossings and for the three lowest $\nu$. As $G_{0}^{\text{phys}}$ is purely imaginary, the condition $G_{0}(\nu) = G_{0}^{\text{phys}}(\nu)$ is reflected in their ratio being 1 and $\text{Re } G_{0}/\text{Im } G_{0}^{\text{phys}} = 0$ (shown in Supplemental Material [28]). Fig. [2] demonstrates that the red/orange crossings observed in $\text{Tr } \Sigma G/(\beta U)$ indeed corresponds to an actual identity of $G_{0}(\nu) = G_{0}^{\text{phys}}(\nu)$, $\forall \nu$ both at $U = 1.81$ (red) and 2.58 (orange). Yet, the corresponding zooms in the insets show a qualitative difference between the two cases. For the red case, the crossing of $G_{0}$ with $G_{0}^{\text{phys}}$ is linear in $U$ only for $\nu = \pi/\beta$ (solid line), while it is $O(U^{2})$ for all other $\nu_{n}$ (dashed line). In the orange case, the crossings display the same behavior for all the frequencies (see insets of Fig. [2] and the discussion in Sec. IA of [28]). This leads to a divergence of $\Gamma_{c}$ for $\nu, \nu' = \pm \pi/\beta$ at the red crossing and for all frequencies at the orange crossing. Similar results are found for the second and third red/orange crossings, but for the former the linear crossing happens for $\nu_{2} = 3\pi/\beta$ (second) and $\nu_{4} = 5\pi/\beta$ (third). This is consistent with the result in Ref. [19] that the corresponding divergences of $\Gamma_{c}$ happens at these specific $\nu_{n}$.

The one-to-one correspondence of red/orange crossings with the local/global divergences of $\Gamma_{c}$ illustrates how the heuristic scenario of Fig. [1] is actually realized for the Hubbard atom. The result also indicates the existence of an infinite number of unphysical $G_{0}$, since infinitely many red and orange divergences were found for the Hubbard atom [19]. Furthermore, there are indications that the
positive. As \( \varepsilon \) becomes larger, one finds a very large, probably infinite divergence of \( \Pi_{\omega} \) (5).

The corresponding DMFT results are reported in Fig. 3. By increasing \( U \), the electrons gradually localize, building up local magnetic moments with longer lifetimes. These, in turn, freeze the local charge dynamics, with \( \chi_{\text{ch}} \) becoming very small especially in the proximity/after the Mott metal-insulator transition (between \( U = 2.3 \) and \( U = 2.4 \) for \( \beta = 40 \)). While the physics of this generic trend is known, the projection of \( \chi_{\text{ch}} \) in its eigenvalue-basis yields highly non-trivial information. We analyze \( \chi_{\text{ch}} \) in terms of the contributions from positive and negative \( \varepsilon_l \). For small/moderate \( U \) all \( \varepsilon_l \) are positive. As \( U \) increases, one \( \varepsilon_l \) after the other goes through zero (see inset of Fig. 3). Each time \( \Gamma_c \) diverges [see Eqs. (5)] a new \( G_0 \) becomes identical to \( G_0^{\text{phys}} \), and the negative component of \( \chi_{\text{ch}} \) becomes more important. Such a negative component of \( \chi_{\text{ch}} \) plays a crucial role in realizing the correct strong coupling physics. Its neglect would lead to a \( \chi_{\text{ch}} \) approximately saturating at some sizable value in the Mott phase, instead of being strongly suppressed. We also note, that a small value of \( \chi_{\text{ch}} \) in itself is not sufficient for this scenario to be realized (e.g., in a dilute system \( \chi_{\text{ch}} \) can be small, but all \( \varepsilon_l > 0 \)). Here, the crucial factor is the mechanism responsible for the reduction of \( \chi_{\text{ch}} \): the gradual local moment formation which manifests itself in a progressively larger contribution of the negative \( \varepsilon_l \). This is thus, the underlying physics responsible for the occurrence of the (infinitely many) unphysical \( G_0 \) crossing \( G_0^{\text{phys}} \), and the related divergences of \( \Gamma_c \). This also applies to the corresponding breakdown of perturbative expansions, such as parquet-based approximations. A certain class of diagrams can give a positive infinite contribution, which is canceled by another class of diagrams [32]. Then the diagrammatic expansion is not absolutely convergent, as was also found in Ref. [20]. This makes conventional diagrammatic expansions highly questionable for intermediate-to-strong correlations. While it is not surprising that perturbative approaches might break down at the Mott transition, it is interesting that this happens well before the Mott transition occurs, where Fermi-liquid physical properties still control the low-energy physics.

It is important to stress that the non-perturbative manifestations discussed in this Letter are affecting not only models dominated by purely local physics (such as the Hubbard atom or its DMFT version). In fact, divergences of \( \Gamma_c \) have also been found [32] studying the 2d Hubbard model, by means of the dynamical cluster approximation (DCA) [30]. In this case, the underlying physics behind the change of sign of the \( \varepsilon_l \) could be related to the formation of an RVB state [38], also responsible [39] for the opening of a spectral pseudogap [40]. Increasing the size of the DCA cluster might even push the occurrence of the first \( \varepsilon_l = 0 \) and the pseudogap towards lower \( U \), due to strong antiferromagnetic fluctuation extended on larger length scales [32, 41, 42].

**Conclusions.** We have reported important progress towards the understanding of the mathematical structures of quantum many body theories in the non-perturbative regime, and of the physics behind them. The structure of the LW functionals is even richer than the pioneering work by Kozik et al. suggested [20]. We find a very large, probably infinite, number of noninteracting \( G_0 \) leading to the same dressed \( G \). This can be regarded as a formal problem, as long as the unphysical and physical \( G_0 \) do not intersect, as it is the case in the perturbative regime. However, in the nonperturbative regime we find many crossings. These crossings reflect the analytical structure of the LW functional for physical systems. We show that they lead to divergences of irreducible vertex functions. This challenges current quan-
tum many-body algorithms in several respects, e.g., causing non-invertibility of the Bethe-Salpeter equation and breakdown of the parquet resummations. These problems, which occur when the correlation is still substantially weaker than in a Mott insulator, are, nonetheless, originated in underlying strong-coupling physical mechanisms, e.g. the formation of local moments and RVB states. This is reflected in the progressive suppression of the charge susceptibility in correlated systems. Further investigations of the theoretical foundations beyond the perturbative regime should play a central role for future method developments in condensed matter physics.

Acknowledgments. – We thank S. Ciuchi, P. Thunström, M. Capone, S. Andergassen and K. Held for insightful discussions and P. Chalupa also for carefully reading the manuscript. The authors would like to thank S. Ciuchi, P. Thunström, M. Capone, S. Andergassen and K. Held for insightful discussions and P. Chalupa also for carefully reading the manuscript. The authors would like to thank for insightful discussions and P. Chalupa also for carefully reading the manuscript. The authors would like to thank for insightful discussions and P. Chalupa also for carefully reading the manuscript. The authors would like to thank for insightful discussions and P. Chalupa also for carefully reading the manuscript.
J. Merino, G. Sangiovanni, G. Rohringer, and A. Toschi, Phys. Rev. Lett. 114, 236402 (2015).
I. RELATION BETWEEN DIVERGENCES OF IRREDUCIBLE VERTICES AND MULTIPLE $G_0$

A. Analytic analysis

In this Section we show that the crossing between the physical $G_0$ and a nonphysical $G_0$ in Figs. 2 and 3 of the main text is directly related to divergences of the irreducible charge vertex $\Gamma_c$ and zero eigenvalues of the corresponding generalized charge susceptibility $\chi_c$ observed in Ref. 1. In particular, we will demonstrate that the different ways how the $G_0$’s cross at a given interaction strength $U = U_0$ can be unambiguously related to the two types of vertex divergences (localized vs. global) found in Refs. 1 and 2 (see also Eq. (4) in the main text and the discussion below).

Let us start by considering a generating functional for the one-particle Green’s function and the susceptibility of our system

$$\mathcal{F}[G_0^{-1}; U, \nu] = \frac{1}{\mathcal{F}[G_0; U]} \int D[c^+, c] c_{\nu\sigma}^+ c_{\nu\sigma} \exp \left[ \sum_{\nu'\sigma'} G_0^{-1}(\nu') c_{\nu'\sigma'}^+ c_{\nu'\sigma'} - U \int_0^\beta d\tau_c c_{\nu\sigma}^+ c_{\nu\sigma} c_{\nu\sigma}^+ c_{\nu\sigma} \right],$$

$$\mathcal{F}[G_0^{-1}; U] = \int D[c^+, c] \exp \left[ \sum_{\nu\sigma} G_0^{-1}(\nu) c_{\nu\sigma}^+ c_{\nu\sigma} - U \int_0^\beta d\tau_c c_{\nu\sigma}^+ c_{\nu\sigma} c_{\nu\sigma}^+ c_{\nu\sigma} \right],$$

where we have assumed SU(2) symmetry, i.e., $\mathcal{F}$ and $\mathcal{Z}$ do not depend on the spin $\sigma$. Evaluating $\mathcal{F}$ at the physical $G_0$ yields the interacting Green’s functions of the system:

$$G(\nu) \equiv \mathcal{F}[G_0^{-1}; U, \nu].$$

The functional derivative of $\mathcal{F}[G_0^{-1}; U, \nu]$ w.r.t. $G_0^{-1}(\nu')$ on the other hand gives rise to the generalized charge susceptibility $\chi_c$:

$$\chi_c^{\nu\nu'}(\omega = 0) = \frac{\delta \mathcal{F}[G_0^{-1}; U, \nu]}{\delta G_0^{-1}(\nu')}.$$

We now consider two non-interacting Green’s functions $G_0^{(1)}$ and $G_0^{(2)}$ which yield the same $G$ and cross at $U = U_0$, which implies $1/G_0^{(1)}(\nu) - 1/G_0^{(2)}(\nu) = 0$ for all Matsubara frequencies $\nu$ at $U = U_0$.

In the next step we formally express $\mathcal{F}[1/G_0^{(2)}; U, \nu]$ in terms of a (functional) Taylor expansion of $\mathcal{F}$ around $1/G_0^{(1)}(\nu)$:

$$\mathcal{F}[1/G_0^{(2)}; U, \nu] = \mathcal{F}[1/G_0^{(1)}; U, \nu] + \sum_{\nu'} \frac{\delta \mathcal{F}[G_0^{(1)}; U, \nu]}{\delta G_0^{(1)}(\nu')} \times \left[ 1/G_0^{(2)}(\nu') - 1/G_0^{(1)}(\nu') \right] + O \left( \left( 1/G_0^{(2)} - 1/G_0^{(1)} \right)^2 \right).$$

(3)

Since both $G_0^{(1)}$ and $G_0^{(2)}$ yield (by definition) the same $G$ (for all values of $U$) we have $\mathcal{F}[1/G_0^{(2)}; U, \nu] = \mathcal{F}[1/G_0^{(1)}; U, \nu] = G(\nu)$. Considering, moreover, the definition of the generalized susceptibility in Eq. (2) we can express Eq. (3) as

$$\sum_{\nu'} \chi_c^{\nu\nu'}(\omega = 0) \left[ 1/G_0^{(2)}(\nu') - 1/G_0^{(1)}(\nu') \right] = O \left( \left( 1/G_0^{(2)} - 1/G_0^{(1)} \right)^2 \right).$$

(4)

We now turn our attention to the $U$-dependence of this equation for $U$ values close to $U_0$ where $G_0^{(1)}$ and $G_0^{(2)}$ cross. Our numerical results in Fig. 2 in the main text (Fig. 1 in this Supplemental Material) show that this crossing follows a power law behavior, i.e.,

$$1/G_0^{(2)}(\nu) - 1/G_0^{(1)}(\nu) \sim (U - U_0)^{\eta_c} \text{ for } U \to U_0$$

where the (real and positive) coefficient $\eta_c$ can be different for different Matsubara frequencies $\nu$. This observation can be expressed, more formally, as

$$\lim_{U \to U_0} \frac{1}{U - U_0} \frac{1/G_0^{(2)}(\nu) - 1/G_0^{(1)}(\nu)}{\eta_c} = \text{const}(\neq 0),$$

(5)

where $\eta_c > 0$ for all Matsubara frequencies $\nu$ and the constant on the r.h.s. of the equation can be different for different $\nu$. Let us now consider the smallest among all $\eta_c$, i.e.,

$$\eta^* = \min_\nu \{\eta_c\}.$$

(6)

We divide both sides of Eq. (4) by $(U - U_0)^\eta^*$ and take the limit $U \to U_0$. The r.h.s. of this equation then vanishes as it is of at least quadratic order in $1/G_0^{(2)} - 1/G_0^{(1)}$ and, hence, goes to zero as $(U - U_0)^\eta^*$ for $U \to U_0$. On the l.h.s. of Eq. (4) $\chi_c^{\nu\nu'}(\omega = 0)$ takes just its value at $U = U_0$ while $1/G_0^{(2)}(\nu) - 1/G_0^{(1)}(\nu)$ yields a finite value $V(\nu)$ for Matsubara frequencies $\nu$ where $\eta_\nu = \eta^*$ and $V(\nu) = 0$ when $\eta_\nu > \eta^*$. Hence, Eq. (4) transforms into the following eigenvector equation

$$\sum_{\nu'} \chi_c^{\nu\nu'}(\omega = 0) V(\nu') = 0.$$

(7)
for χ_c for the eigenvalue 0 with the eigenvector

\[ V(ν) = \lim_{U→U_0} \frac{1/G^{(2)}_0(ν) - 1/G^{(1)}_0(ν)}{(U - U_0)^{η^*}}. \] (8)

According to Refs. 1 and 2 and the discussion below Eq. (4) in the main text such vanishing eigenvalue is related to a divergence of the irreducible charge vertex Γ_c. The way how Γ_c diverges (local vs. global) is given by the structure of the corresponding eigenvector V(ν):

a divergence of Γ_c occurs at frequencies ν where \(V(ν) \neq 0\). According to the above discussion these are exactly the frequencies where \(1/G^{(2)}_0(ν) - 1/G^{(1)}_0(ν) \sim (U - U_0)^{η^*}\), i.e., where the crossing between \(G^{(1)}_0\) and \(G^{(2)}_0\) is governed by the minimal exponent \(η^*\).

For the red crossings \(η^* = 1\), i.e., we observe a linear crossing at one (positive and negative) Matsubara frequency ±\(ν^*\) while our numerical data indicate \(η_ν = 2\) for all other \(ν \neq ν^*\). This is indeed consistent with the divergence of \(Γ^{(ν')(ω=0)}_c\) at \(ν, ν' = ν^*\) observed in Ref. 4.

On the contrary, for the orange line the crossing between \(G^{(1)}_0\) and \(G^{(2)}_0\) happens, at the lowest order, in the same way for all Matsubara frequencies ν, i.e. \(η_ν = η^* (∼ 0.5\) according to our numerical data) for all ν. To see this, one should consider separately the behavior of both Re \(G_0\) and Im \(G_0\), as shown in the lower panel of Fig. 1 (left and right, respectively). In particular, one observes that on the left side of the crossing \((U < U_0)\) Re \(G_0\) displays the leading (square-root) behavior, while Im \(G_0\) shows a linear (subleading) behavior for the first Matsubara frequency. On the right side after the crossing \((U > U_0)\), Re \(G_0\) = 0, and the leading (square-root) behavior appears for Im \(G_0\) at all frequencies. Correspondingly, according to Eq. (5), \(V(ν) \neq 0\) for all frequencies which corresponds to a global divergence of Γ_c.

1 T. Schäfer, G. Rohringer, O. Gunnarsson, S. Ciuchi, G. Sangiovanni, and A. Toschi, Phys. Rev. Lett. 110, 246405 (2013).
2 T. Schäfer, S. Ciuchi, M. Wallerberger, P. Thunström, O. Gunnarsson, G. Sangiovanni, G. Rohringer, and A. Toschi, Phys. Rev. B 94, 235108 (2016).
3 M. Potthoff, Condens. Mat. Phys. 9, 557 (2006).
4 Taking into account that, at the red crossings, the numerical date for \(G^{(1)}_0\) and \(G^{(2)}_0\) show that \(G^{(2)}_0(ν^*) - G^{(1)}_0(ν^*) = -[G^{(2)}_0(-ν^*) - G^{(1)}_0(-ν^*)]\), the singularity in Γ_c originates from the fact that the two lines and two columns ν = ν* and ν' = ν*, respectively, in χ_c are becoming equal (and, hence, the matrix χ_c becomes singular).