

Origin of Misleading Convergence in Self-Consistent Many-Electron Theories: Fundamental Aspects and Practical Implications

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Self-consistent approaches in many-electron problems typically converge to an unphysical solution in strongly correlated regimes. By deriving the mathematical condition for the stability of the physical solution, we unveil the *precise relation* between two *distinct* issues previously considered equivalent: the misleading convergence in self-consistent schemes and the multivaluedness of the Luttinger-Ward functional. Although these problems are fundamentally linked through the divergences of the irreducible vertex function, we show that misleading convergence can occur even in the absence of such divergences. Eventually, a systematic procedure for stabilizing the physical solution is proposed.

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Introduction—Many fascinating phenomena in condensed matter physics, such as unusual spectral features (pseudogap [1,2], waterfalls [3,4], kinks [5], etc.), unconventional superconductivity [6–9], quantum criticality [10–13], and Mott and Hund’s metal-insulator transition [14–17] are driven by electronic correlations. This sets, for their theoretical description, the high bar of solving a full quantum many-body problem of interacting fermions. While a Feynman diagrammatic formalism could be employed, this lacks, unlike in QED, a small expansion parameter. Thus, for describing the interesting physics mentioned above, Feynman diagrammatic calculations often need to be performed in the *nonperturbative* regime.

This problem affects the important class of conserving Baym-Kadanoff approximations, constructed through self-consistent resummations of Feynman diagrams, which guarantee the thermodynamic “consistency” of the results [18–23]. Formally, self-consistent diagrammatic methods compute the electron Green’s function G as a functional f of G itself, with the implicit equation $G = f[G]$ being solved by iterations. With the exception of extremely simple models the exact map f is unknown, but can be constructed approximately, e.g., as truncated diagrammatic series in terms of G , summed to high order by the diagrammatic Monte Carlo technique [24,25], the GW scheme [26,27], or, nonperturbatively, using dynamical

mean-field theory [28] and its extensions [29,30], nested-cluster [31] or parquet-based [32] approaches.

In the last decade, an increasing number of studies have reported that an iterative solution of $G = f[G]$ can converge to a wrong answer [31,33–38], typically in the most interesting correlated regimes. These studies have ascribed the occurrence of misleading convergence in the iterative solution for G to the intrinsic multivaluedness of the Luttinger-Ward functional (LWF) of the many-electron problem [23,34,39,40]. Any crossing of two branches of the LWF (with only one being physical) [41] implies the simultaneous divergence of the two-particle irreducible (2PI) vertex function [31,36,42–49]. Physically, this divergence is intrinsically linked [44,50–52] to one of the most relevant feats of electronic correlation: the local magnetic moment formation and the associated freezing of charge fluctuations, as this huge differentiation of on site magnetic and charge responses requires extremely large vertex functions. Notably, vertex divergences also yield the necessary condition [53–57] for the onset of phase separations in the proximity of Mott-Hubbard metal-insulator transitions [14,58–60].

More formally, vertex divergences represent a key hallmark [50–53,61–63] of the breakdown of self-consistent perturbation theory (SCPT). Specifically, the skeleton diagrammatic series in terms of G was found [34,64,65] to always converge to an unphysical answer for interaction values larger than those at which the first branching point of the LWF and, hence, the first vertex divergence, occurs. However, so far, the evidence for the connection between the misleading convergence of the iterative solution of $G = f[G]$ and the crossings between the LWF branches has remained *empirical*. This is likely the reason why the misleading convergence issues affecting GW [35], parquet-based [37], and nested-cluster schemes [31], often in the proximity of vertex divergences, have been hitherto

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attributed to the branching of the LWF, even if these iterative approaches, differently from SCPT, are *not* based on perturbative series of LWF diagrams. At the same time, misleading convergences have also been reported in regions of parameter space without such crossings, i.e., vertex divergencies [31,34,65]. Evidently, a complete understanding of this problem and its implications is still lacking.

In this Letter, we aim to clarify the origin of the misleading convergence observed in iterative many-body schemes, formally *disentangling* this issue from the branching of the LWF. To this end, we first devise a rigorous, model-independent procedure to determine whether the fixed points of the map f are stable or unstable. This allows us to prove that, for the same parameters at which branch crossings of the LWF (and the associated vertex divergences) occur, the physical fixed point of the iterative procedure also becomes unstable. However, as we will also demonstrate, in the absence of vertex divergences, both the misleading convergence and the breakdown of the skeleton series can still occur but *no longer simultaneously*. Through our analytical derivation, we will be able to eventually unveil the *precise relation* between these two important issues of the self-consistent theories for the many-electron problem. Finally, we derive a systematic approach for changing the map f (to a *modified* map $\tilde{f}$) that stabilizes the physical fixed point (see the illustration in Fig. 1), thereby ensuring convergence to the correct physical solution over the entire parameter range.

Models—Our analytic theory will be illustrated by its application to the zero point (ZP) model, for which the functional f simplifies to a function, and to the Hubbard atom (HA). These are defined by the action

$$S = -\sum_{\nu,\sigma} \bar{c}_{\nu,\sigma} G_{0,\nu}^{-1} c_{\nu,\sigma} + S_{\text{int}}, \quad (1)$$

where ν is a fermionic Matsubara frequency, $\bar{c}(c)$ are Grassmann variables that represent the creation (annihilation) of an electron (see Appendix A), and $G_{0,\nu}^{-1} = i\nu + \delta\mu$ with $\delta\mu$ being the chemical potential [$\delta\mu = 0$ corresponds to particle hole (ph) symmetry]. The interacting part of the action reads as $S_{\text{int,ZP}} = (U/\beta) \sum_{\nu} \bar{c}_{\nu,\uparrow} c_{\nu,\uparrow} \bar{c}_{\nu,\downarrow} c_{\nu,\downarrow}$ for the ZP model and $S_{\text{int,HA}} = U \int_0^\beta d\tau (\bar{c}_{\tau,\uparrow} c_{\tau,\uparrow} - 1/2)(\bar{c}_{\tau,\downarrow} c_{\tau,\downarrow} - 1/2)$ for the HA, with U being the on site interaction, β the inverse temperature, and τ the imaginary time.

These basic models are selected for illustrative purposes and for a rigorous benchmark with respect to their exact solutions. Yet, they still entail, in a crude fashion, pivotal feats of the electron-correlation physics. The HA, which describes totally localized electrons, yields a somewhat “extreme representation” of Mott insulating regimes. As for the ZP, at half filling, it essentially corresponds to a binary-mixture disorder model, precisely its coherent potential approximation solution in the limit of high-lattice coordination [36] (see the Supplemental Material [66]).

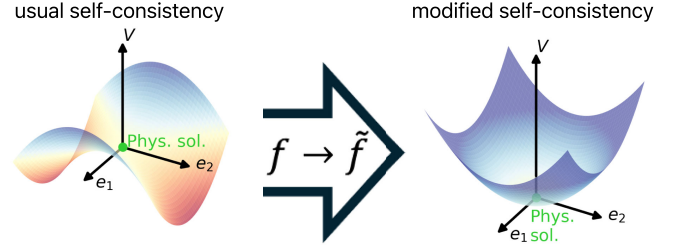


FIG. 1. Heuristic sketch of the “stability landscape” of a self-consistent scheme. Left: usual self-consistent scheme (f) in a parameter regime, where the physical fixed point is unstable in one direction (e_2). Right: modified self-consistent scheme ($\tilde{f}$), where the physical fixed point has been stabilized.

This features a metal-to-insulator transition driven by increasing disorder strength (which corresponds to U in the ZP), often used pedagogically to provide an intuition for the more complex Mott transition. Thus, not so surprisingly, both HA and ZP are plagued by qualitatively similar misleading convergence issues [34–36,39,43,49,61] as more realistic Hubbard-like models [31,36,42,44,48,50,56,61].

Self-consistent schemes—In previous literature two different iterative schemes have been exploited to investigate possible misleading convergence issues. Both use a damped iteration scheme together with the Dyson equation, which links the noninteracting Green’s function (G_0) to the interacting one (G) via the self-energy Σ , i.e., $G^{-1} = G_0^{-1} - \Sigma$. The two schemes differ, however, for the quantity that is calculated by the iterative procedure, i.e., either (I) G_0 [34] or (II) G [19,71,72]. While the two approaches have provided essentially equivalent indicators for studying misleading convergence problems, for the purposes of our investigation, it is important to precisely work out their intrinsic differences. Specifically, in scheme (I) G is fixed to the physical Green’s function G_{phys} and G_0 is found iteratively using the (unique) self-energy functional $\Sigma[G_0]$:

$$\begin{aligned} [G_{0,\nu}^{(n+1)}]^{-1} &= f_{G_0,\nu} \left[[G_0^{(n)}]^{-1} \right] \quad \text{with} \\ f_{G_0,\nu} [G_0^{-1}] &= p(G_{\text{phys},\nu}^{-1} + \Sigma_\nu[G_0]) + (1-p)G_{0,\nu}^{-1}, \end{aligned} \quad (2)$$

where n is the iteration index and the iteration damping $p \in (0, 1]$. For simplicity, we omit the momentum, spin, and orbital dependence, but the generalization is straightforward (see Appendix B). In scheme (II), which corresponds to the conventional SCPT at weak coupling, G_0 is fixed to the physical noninteracting Green’s function $G_{0,\text{phys}}$, and G is iterated using the self-energy functional $\Sigma[G]$ of the LWF formalism:

$$\begin{aligned} [G_\nu^{(n+1)}]^{-1} &= f_{G,\nu} \left[[G^{(n)}]^{-1} \right] \quad \text{with} \\ f_{G,\nu} [G^{-1}] &= p(G_{0,\text{phys},\nu}^{-1} - \Sigma_\nu[G]) + (1-p)G_\nu^{-1}. \end{aligned} \quad (3)$$

The solution of Eqs. (2) and (3) corresponds to a stable fixed point of the respective iterative map, f_{G_0} or f_G . Both schemes are affected by the intrinsic multivaluedness of the LWF [31,34,40], albeit in different ways. In scheme (I) one finds *several* G_0 functions that fulfill the condition $G[G_0] = (G_0^{-1} - \Sigma[G_0])^{-1} = G_{\text{phys}}$ [34,61]. Therefore, Eq. (2) has multiple fixed points, of which only one corresponds to $G_{0,\text{phys}}$.

For scheme (II), instead, the multivaluedness is directly reflected onto the nonuniqueness of the functional $\Sigma[G]$, i.e., unlike $\Sigma[G_0]$, several functionals $\Sigma[G]$ exist, while only one of them (depending on the parameter regime) describes the physical self-energy [34,36,39,64]. Hence, G_{phys} is only a fixed point of Eq. (3) if the correct branch of $\Sigma[G]$ is chosen.

Iteration in G_0 —We start by explicitly considering the map f_{G_0} in Eq. (2). In the spirit of Ref. [73], we note that the information about the stability of the fixed points of f_{G_0} is encoded in its Jacobian J_{G_0} [74]. Specifically, a fixed point is stable if the Jacobian evaluated on the given fixed point has only eigenvalues with magnitudes smaller than 1 (see, e.g., Refs. [76–78]). In our case, the Jacobian J_{G_0} , which is a functional of G_0^{-1} , can be directly expressed through the generalized (static, i.e., zero transfer frequency) charge susceptibility $\chi_c^{\nu\nu'}$ of the system considered and its bubble term counterpart, $\chi_{0,\nu\nu'} = -\beta G_{\nu}^2 \delta_{\nu\nu'}$ (see Appendixes A and C), as

$$J_{G_0}^{\nu\nu'} = \frac{\delta f_{G_0,\nu}}{\delta G_{0,\nu}^{-1}} = \delta_{\nu\nu'} - p[\chi_0^{-1}]_{\nu\nu'} \chi_c^{\nu\nu'}, \quad (4)$$

where summations are performed on repeated indices. The eigenvalues of the Jacobian in Eq. (4) are, thus, $1 - p\lambda_\alpha$, λ_α being the eigenvalues of the matrix $\chi_0^{-1}\chi_c$.

Let us first consider the case where the eigenvalue, which is responsible for the instability, i.e., $|1 - p\lambda_\alpha| > 1$, is real. In this situation, a fixed point is unstable if an eigenvalue λ_α of $\chi_0^{-1}\chi_c$ satisfies one of two conditions: (i) $\lambda_\alpha < 0$ or (ii) $\lambda_\alpha > 2/p$. These two situations are fundamentally different: the onset of condition (i), which does *not* depend on p , corresponds to a sign change of λ_α , and, hence, to a degenerate matrix χ_c , triggering a *divergence* [42] of the corresponding 2PI vertex: $\Gamma_c \sim \chi_c^{-1}\chi_0$. Hence, (i) represents an intrinsic nonperturbative property of the considered system [44,50–53,61]. On the contrary, the occurrence of the instability condition (ii) can be systematically overcome by damping the iteration scheme, i.e., choosing a smaller p . Hence, (ii) should be regarded as a mere algorithmic aspect of the self-consistency. For ph-symmetric systems, where all eigenvalues of $\chi_0^{-1}\chi_c$ are real [47,49,73,79], only these two types of instabilities can occur. However, out of ph symmetry, where the eigenvalues of $\chi_0^{-1}\chi_c$ can become complex conjugate pairs, another type of instability appears. This instability, which we classify as of type (iii), is of

particular importance: it is triggered by two complex conjugated eigenvalues of the Jacobian generically expected in the absence of ph symmetry [49,53] and appears near the change of sign of the real part of λ_α . In particular, for a complex λ_α , the real part contributes linearly in p to $|1 - p\lambda_\alpha|^2$ of J_{G_0} , while its imaginary part contributes only quadratically. Hence, for $p \rightarrow 0^+$, it is the sign switch of $\text{Re}(\lambda_\alpha)$ from positive to negative which triggers the instability. For a loose analogy with (i), the condition $\text{Re}(\lambda_\alpha) = 0$ with $\text{Im}(\lambda_\alpha) \neq 0$ has been referred to in the literature [31,49,54] as *pseudodivergence* [80].

To illustrate the applicability of our scheme we consider the ZP model and the HA. The obtained results are reported in Fig. 2, where the top row presents the data for the ZP and the bottom row for the HA model. The left panels show the location of vertex divergences and pseudodivergences in the U - $\delta\mu$ space (we chose $\beta = 1$ for our units). Further, the lines beyond which the physical solution becomes unstable for a given p [J_{G_0} has eigenvalue(s) of magnitude 1] are plotted. Note that the ZP displays vertex divergences only at ph symmetry, while in the HA they can appear also in a finite $\delta\mu$ range. Above the vertex divergence and pseudodivergence lines the physical solution is unstable at any p : according to Eq. (4), by increasing U , we will get a p -independent [type (i)] instability of the physical fixed point exactly at the vertex divergence line. For $|\delta\mu| > 0$ in the ZP model and for $|\delta\mu| > 0.6$ in the HA model, an instability of type (iii) occurs, whose location progressively approaches the pseudodivergence line for $p \rightarrow 0^+$. Note that instabilities of type (ii), i.e., $\lambda_\alpha > 2/p$, do not appear in the studied parameter regime. They would, however, appear in the case of an attractive interaction ($U < 0$). The numerical iterative solution [81] of Eq. (2), shown in the middle and right panels of Fig. 2 fully confirms these predictions. Specifically, in the middle panels the imaginary part of the physical $G_{0,\text{phys}}$ at the first Matsubara frequency $\bar{\nu} = (\pi/\beta)$ is shown together with the self-consistent solution $\bar{G}_0$ of Eq. (2) at ph symmetry for different U values: as expected, $\bar{G}_0 = G_{0,\text{phys}}$ (see the Supplemental Material [66] for the real parts) for small U up to the vertex divergence line (independent of p). Afterward, for larger U values, Eq. (2) can still be converged, but to an *unphysical* solution ($\bar{G}_0 \neq G_{0,\text{phys}}$) [34]. In the right panels of Fig. 2 the same calculations have been repeated out of ph symmetry at $\delta\mu = 2.5$, where a pseudodivergence of $\chi_0^{-1}\chi_c$ instead of a divergence occurs. Consistent with our predictions, the convergence of $\bar{G}_0$ to $G_{0,\text{phys}}$ now becomes p dependent, with its hard boundary determined by the pseudodivergence line [86].

How to stabilize the physical solution—To stabilize the physical solution in the entire range of parameters, we introduce the modified iterative map $\tilde{f}$:

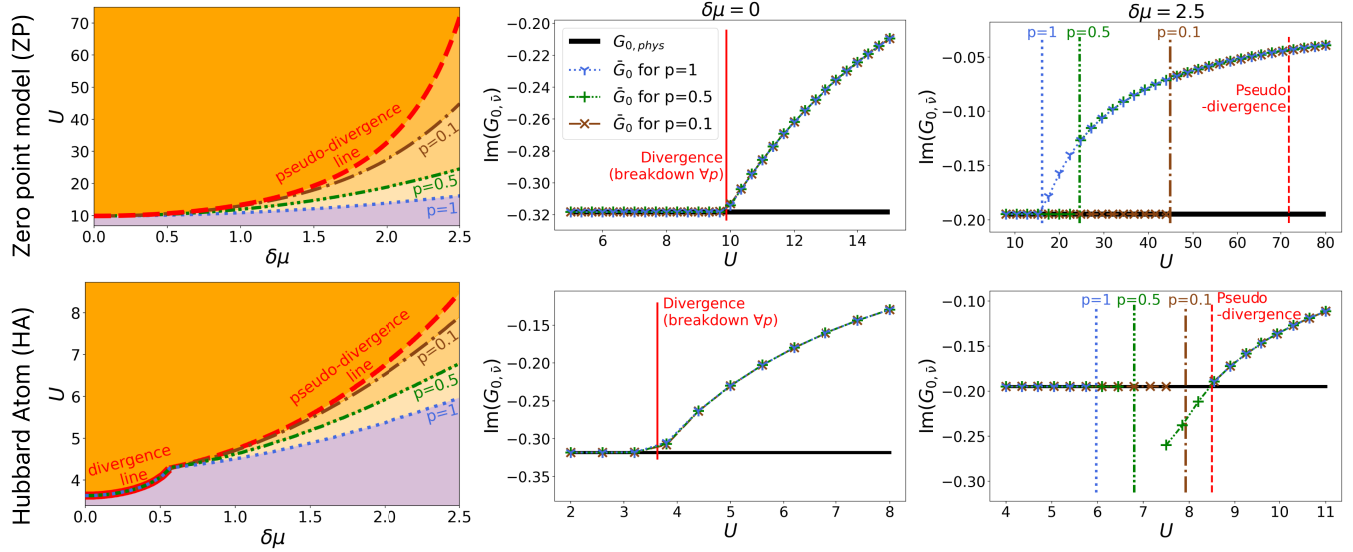


FIG. 2. Misleading convergence for the scheme of Eq. (2) in the ZP model (upper panels) and HA (lower panels). Left panels: phase space of both models, where the lines corresponding to the instability condition of the iterative scheme are shown for different dampings together with the (pseudo)divergence lines (red solid or dashed lines). The imaginary part of $\tilde{G}_{0,\bar{\nu}=\pi/\beta}$ obtained via iteration of Eq. (2) is compared to the physical solution $G_{0,\text{phys},\bar{\nu}}$ at or out of ph symmetry (middle or right panels).

$$\begin{aligned} [G_{0,\nu}^{(n+1)}]^{-1} &= \tilde{f}_{G_{0,\nu}} [[G_0^{(n)}]^{-1}] \\ \text{with } \tilde{f}_{G_{0,\nu}}[G_0^{-1}] &= \mathcal{P}^{\nu\nu_1} (G_{\text{phys},\nu_1}^{-1} + \Sigma_{\nu_1}[G_0]) \\ &\quad + (\delta_{\nu\nu_1} - \mathcal{P}^{\nu\nu_1}) G_{0,\nu_1}^{-1}, \end{aligned} \quad (5)$$

where $\mathcal{P}$ is defined as $\mathcal{P}^{\nu\nu'} = \mathcal{U}^{\nu\alpha_1} \mathcal{D}^{\alpha_1\alpha_2} [\mathcal{U}^{-1}]^{\alpha_2\nu'}$, with $\mathcal{U}$ being the similarity transformation that diagonalizes J_{G_0} , Eq. (4), (and therefore also $\chi_0^{-1}\chi_c$), and

$$\mathcal{D}^{\alpha\alpha'} = \begin{cases} p\delta_{\alpha\alpha'}, & \text{if } \text{Re}(\lambda_\alpha) > 0 \\ -p\delta_{\alpha\alpha'}, & \text{if } \text{Re}(\lambda_\alpha) \leq 0. \end{cases} \quad (6)$$

Hence, $\mathcal{P}$ can be readily computed through *eigenvalues* and *eigenvectors* of $\chi_0^{-1}\chi_c$ [87]. The Jacobian of the modified iterative scheme, Eq. (5), then reads as

$$\tilde{J}_{G_0} = \frac{\delta \tilde{f}_{G_{0,\nu}}}{\delta G_{0,\nu}^{-1}} = \delta_{\nu\nu'} - \mathcal{P}^{\nu\nu_1} [\chi_0^{-1}]_{\nu_1\nu_2} \chi_c^{\nu_2\nu'}. \quad (7)$$

Its eigenvalues are $1 - \mathcal{D}^{\alpha\alpha}\lambda_\alpha$, hence (for a small enough p) the Jacobian of $\tilde{f}$ has no eigenvalue of magnitude greater than 1, even after the (pseudo)divergence lines. Note that this procedure can be directly applied, *mutatis mutandis*, to other (exact or approximated) self-consistent schemes exhibiting unstable physical fixed points.

In Fig. 3 the modified iterative scheme of Eq. (5) is applied to the ZP model (top) and the HA (bottom) at ph symmetry (whereas it can be successfully exploited also out of ph symmetry; see the Supplemental Material [66]). Note that, in practice, the knowledge of the physical fixed point is *not* needed for the application of our scheme (see

Appendix D and the Supplemental Material [66]) and, further, that the Jacobian is *not* computed during the self-consistency, but only for the last iteration. Our results make it evident that the modified iterative scheme $\tilde{f}$ does actually converge to the physical solution also after the crossing of (multiple in the case of the HA [36,46,49]) vertex divergence lines. This result is highlighted by the flow diagrams (see Appendix E) in the middle panel of Fig. 3 showing the evolution of the iteration procedure toward the solution for the ZP model at $U = 15$, i.e., after the vertex divergence line, both for the usual f (left) and the modified $\tilde{f}$ scheme (right).

Iteration in G —We turn to stabilizing the physical solution in its practical calculations via Eq. (3), i.e., when G_{phys} is the unknown. Assuming that the correct branch for $\Sigma[G]$ is chosen [i.e., G_{phys} is indeed a fixed point of Eq. (3)], we can now calculate the Jacobian of Eq. (3), which reads as

$$J_G^{\nu\nu'} = \frac{\delta f_{G,\nu}}{\delta G_{\nu'}^{-1}} = \delta_{\nu,\nu'} - p[\chi_c^{-1}]^{\nu\nu_1} \chi_{0,\nu_1\nu'}. \quad (8)$$

As the eigenvalues of J_G are $1 - p/\lambda_\alpha$, it is clear that the instability of the physical solution (for $p \rightarrow 0^+$) will occur at vertex divergences and pseudodivergences of $\chi_0\chi_c^{-1}$. As this quantity is the inverse of the term $\chi_0^{-1}\chi_c$, relevant for the scheme of Eq. (2), all pseudodivergence lines have the same location in both schemes, while the vertex divergence lines now correspond to odd poles instead of zero crossing for the eigenvalues of $\chi_0\chi_c^{-1}$.

In order to stabilize the physical fixed point after the corresponding (pseudo)divergence lines, we can adopt a similar approach as before, introducing a modified iterative

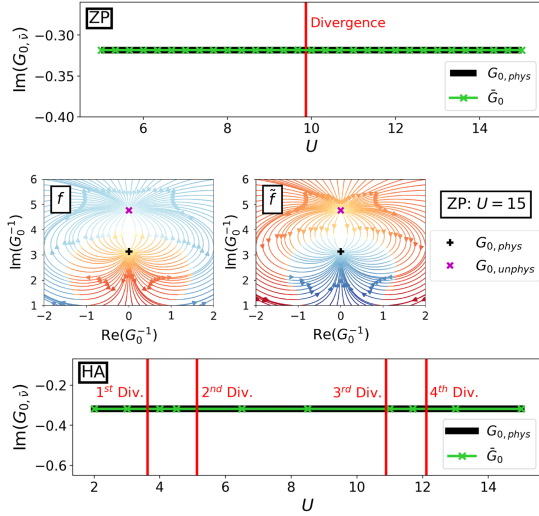


FIG. 3. $\text{Im}(G_{0,\nu})$ obtained via the modified iterative scheme $\tilde{f}$, Eq. (5), at ph symmetry ($\delta\mu = 0$, $p = 0.1$) for both the ZP model (top) and the HA (bottom), compared with the corresponding physical solution. Middle panel: flow diagram in the complex plane of G_0^{-1} for the ZP model in the nonperturbative regime ($U = 15$) for the conventional, Eq. (2) (left), and the modified scheme, Eq. (5) (right), where the stability region of a fixed point is indicated by the blue color.

scheme $\tilde{f}_G$, Eq. (9), which is defined as

$$G_{\nu}^{(n+1)} = \tilde{f}_{G,\nu}[G^{(n)}]$$

$$\text{with } \tilde{f}_{G,\nu}[G] = \mathcal{P}^{\nu\nu_1}(G_{0,\text{phys},\nu_1}^{-1} - \Sigma_{\nu_1}[G]) + (\delta_{\nu\nu_1} - \mathcal{P}^{\nu\nu_1})G_{\nu_1}^{-1}, \quad (9)$$

with $\mathcal{P}$ as in Eqs. (5) and (6). The corresponding Jacobian is

$$\tilde{J}_{G'}^{\nu\nu'} = \frac{\delta \tilde{f}_{G,\nu}}{\delta G_{\nu'}^{-1}} = \delta_{\nu,\nu'} - \mathcal{P}^{\nu\nu_1}[\chi_c^{-1}]^{\nu_1\nu_2}\chi_{0,\nu_2\nu'}, \quad (10)$$

whose eigenvalues are $1 - \mathcal{D}^{\alpha\alpha}/\lambda_{\alpha}$. Hence, as in Eq. (5), the Jacobian of the modified scheme will not have eigenvalues of magnitude larger than 1 for $p \rightarrow 0^+$.

The numerical results of the calculation of G in the ZP model are shown in Fig. 4, comparing the conventional iteration Eq. (3) (top) and the modified scheme Eq. (9) (bottom). Note that in both cases, the correct branch of the $\Sigma[G]$ functional has been taken [i.e., the weak-coupling branch Σ_w for $U < U_{\text{branch}}$ (gray line in Fig. 4) and the strong-coupling one Σ_s for $U > U_{\text{branch}}$, which are exactly known for the ZP model [39,64]]. However, even if the correct functional branch has been used, the conventional scheme f_G converges to physical solution only up to the (p -dependent) predicted instability border (cf. Fig. 4, top panel), approaching the pseudodivergence line for $p \rightarrow 0^+$. The data of the bottom panel demonstrate, instead, how the problem gets solved by using the modified scheme $\tilde{f}$: we

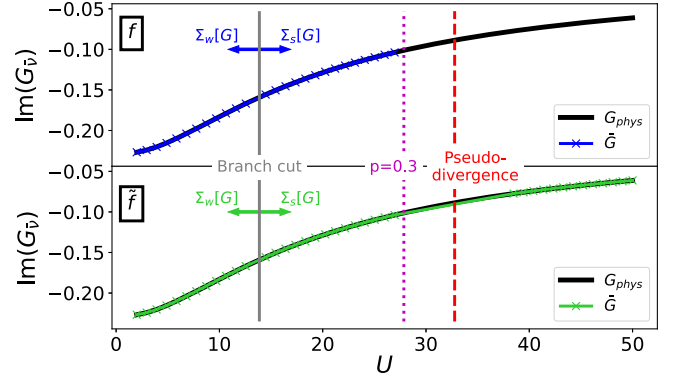


FIG. 4. Self-consistently calculated G for the ZP model out of ph symmetry ($\delta\mu = 2$, $p = 0.3$) with the conventional Eq. (3) (top) and the modified scheme Eq. (9) (bottom); see text.

find a convergence to the physical solution *both* before and after the pseudodivergence line [88].

Conclusion—By means of our analysis, we were able to separate two issues, which affect self-consistent approaches for the many-electron problem, previously considered somewhat intertwined [31,33–36,39,61,64,89]: the convergence of the iterative procedure and the multiple branches of the LWF. Specifically, we introduced a *model-independent* method to rigorously determine the stability of the physical solution in self-consistent approaches based on the electron Green's function, and illustrate the modification needed to avoid the associated misleading convergence problems.

The separate problem of multivaluedness of the LWF reveals itself in the fact that the skeleton series for $\Sigma[G]$ always converges to the weak coupling branch of the LWF [34], despite this branch being incorrect in the strong coupling regime [48,90]. The origin of such unphysical convergence is *not* the instability of the physical fixed point, since this also happens if $\Sigma[G]$ is evaluated at the exact Green's function G_{phys} [34]. Despite recent progress in rectifying the SCPT instabilities caused by divergences in the series for $\Sigma[G]$ [65], capturing the strong-coupling branch(es) of the LWF through diagrammatic expansion remains an unsolved problem. On the other hand, as the instability of the physical fixed point revealed here can occur *even if* the correct branch of the LWF is used for $\Sigma[G]$ (Fig. 4, top panel), understanding how and at which parameters the iterative procedure should be adjusted will allow future studies to focus exclusively on the remaining problem of constructing the correct functional $\Sigma[G]$ in the nonperturbative regime. Meanwhile, the misleading convergence issues reported for approaches such as GW, parquet, or nested-cluster-based schemes [31,35,37]—which do not rely on an explicit resummation of the skeleton expansion (and are thus free from the problem of selecting the correct branch of the LWF)—could be directly amendable using the prescription presented here.

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Data availability—A dataset containing all numerical data and scripts for calculating and plotting these data is publicly available in the TU Wien Research Data repository [91].

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End Matter

Appendix A: Definition of one- and two-particle quantities—The one-particle Green's function in the local, SU(2)-symmetric, single-orbital case is defined as

$$G_\nu = \frac{1}{Z} \int \mathcal{D}[\bar{c}, c] \frac{1}{2} \sum_\sigma \bar{c}_{\nu,\sigma} c_{\nu,\sigma} e^{-S}, \quad (\text{A1})$$

where $Z = \int \mathcal{D}[\bar{c}, c] e^{-S}$ and S is the action that depends on the considered model [see Eq. (1)]. $\bar{c}$ and c are Grassmann variables whose Fourier transformation we define as $\bar{c}_{\nu,\sigma} = (1/\sqrt{\beta}) \int_0^\beta d\tau \bar{c}_{\tau,\sigma} e^{-i\nu\tau}$ and $c_{\nu,\sigma} = (1/\sqrt{\beta}) \int_0^\beta d\tau c_{\tau,\sigma} e^{i\nu\tau}$ where $\nu = (2n+1)\pi/\beta$, $n \in \mathbb{Z}$ are fermionic Matsubara frequencies. Further, the static (bosonic transfer frequency $\omega = 0$) generalized susceptibility in the charge channel is defined as

$$\begin{aligned} \chi_c^{\nu\nu'}[G_0^{-1}] &= \beta \frac{\delta G_\nu[G_0^{-1}]}{\delta G_{0,\nu'}^{-1}} \\ &= \frac{\beta}{Z} \int \mathcal{D}[\bar{c}, c] \frac{1}{2} \sum_\sigma \bar{c}_{\nu,\sigma} c_{\nu,\sigma} \sum_{\sigma'} \bar{c}_{\nu',\sigma'} c_{\nu',\sigma'} e^{-S} \\ &\quad - 2\beta G_\nu G_{\nu'}. \end{aligned} \quad (\text{A2})$$

Appendix B: Generalization to nonlocal, SU(2)-broken, multiorbital systems—In the main text, the formalism is worked out for local, SU(2)-symmetric, single-orbital systems. Here, we want to give a sketch on how to generalize the method to nonlocal, SU(2)-broken, multiorbital systems. First, we define the iterative map for this case as

$$\begin{aligned} f_{G_0,k,\sigma}^{\alpha\beta}[G_0^{-1}] &= p([G_{k,\sigma,\text{phys}}^{-1}]^{\alpha\beta} + \Sigma_{k,\sigma}^{\alpha\beta}[G_0]) \\ &\quad + (1-p)[G_{0,k,\sigma}^{-1}]^{\alpha\beta}, \end{aligned} \quad (\text{B1})$$

with $k = (\nu, k_x, k_y, k_z)$, spin σ , and α, β being orbital indices (we still assume energy, momentum, and spin conservation). The Jacobian can be written as

$$J_{G_0}^{ij} = \frac{\delta f_{G_0,i}}{\delta G_{0,j}^{-1}} = \delta_{ij} - p[\chi_0^{-1}]_{ij} \chi^{lj}, \quad (\text{B2})$$

where we group $(k, \sigma, \alpha, \beta)$ in superindices i and j . Then J_{G_0} can be viewed as a matrix in this superindex space and G_0^{-1} and f_{G_0} are vectors in the same superindex space. The matrices for the generalized susceptibilities χ_{ij} and $[\chi_0^{-1}]_{ij}$ are defined as

$$\begin{aligned} [\chi_0^{-1}]_{ij} &= [\chi_0^{-1}]_{k\sigma\alpha\beta,k'\sigma'\alpha'\beta'} = -\frac{1}{\beta} [G_{k\sigma}^{-1}]^{\alpha\alpha'} [G_{k'\sigma'}^{-1}]^{\beta'\beta} \delta_{kk'} \delta_{\sigma\sigma'}, \\ \chi^{ij} &= \chi_{k\sigma\alpha\beta,k'\sigma'\alpha'\beta'} = \beta \frac{\delta G_{k\sigma}^{\alpha\beta}}{\delta [G_{0,k'\sigma'}^{-1}]^{\alpha'\beta'}}. \end{aligned} \quad (\text{B3})$$

Therefore, all of the following steps can be proceeded analogously to the main text by just extending the fermionic Matsubara frequency to the superindex space. In the following, we want to investigate the spin degree of freedom in more detail. For this, we start by introducing two bases, the spin-index basis [left-hand side of Eq. (B4)] and the charge-spin basis [right-hand side of Eq. (B4)], which are transformed into each other by S [32]:

$$\begin{pmatrix} \chi_{\uparrow\uparrow} & \chi_{\uparrow\downarrow} \\ \chi_{\downarrow\uparrow} & \chi_{\downarrow\downarrow} \end{pmatrix} = S \begin{pmatrix} \chi_c & \chi_{cs} \\ \chi_{sc} & \chi_s \end{pmatrix} S \quad \text{with} \quad S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad (\text{B4})$$

where $\chi_{\sigma\sigma'} = (\delta G_\sigma / \delta G_{0,\sigma'}^{-1})$, $\chi_{c/s} = [\chi_{\uparrow\uparrow} + \chi_{\downarrow\downarrow} \pm (\chi_{\uparrow\downarrow} + \chi_{\downarrow\uparrow})]/2$ and $\chi_{cs/sc} = [\chi_{\uparrow\uparrow} - \chi_{\downarrow\downarrow} \pm (-\chi_{\uparrow\downarrow} + \chi_{\downarrow\uparrow})]/2$. In order to use the charge-spin-basis in our context, we also need to transform the iterative map into this basis

$$\begin{pmatrix} f_\uparrow \\ f_\downarrow \end{pmatrix} \xrightarrow{S} \frac{1}{\sqrt{2}} \begin{pmatrix} f_\uparrow + f_\downarrow \\ f_\uparrow - f_\downarrow \end{pmatrix}. \quad (\text{B5})$$

Enforcing SU(2) symmetry, as it is done in the main text, implies $f_\uparrow = f_\downarrow =: f$. Then expanding the iterative map in the charge-spin basis around the fixed point with a small perturbation η gives

$$\begin{pmatrix} \eta^{(n+1)} \\ 0 \end{pmatrix} = \left[\mathbb{1} - p \begin{pmatrix} \chi_0^{-1} \chi_c & 0 \\ 0 & \chi_0^{-1} \chi_s \end{pmatrix} \right] \begin{pmatrix} \eta^{(n)} \\ 0 \end{pmatrix} + \mathcal{O}((\eta^{(n)})^2). \quad (\text{B6})$$

From Eq. (B6), it becomes clear why only the charge channel contributes to the Jacobian in the main text. Note, however, that if one does not suppress the spin degree of freedom, the statistical noise from, e.g., Monte Carlo can be enough to trigger the instabilities in the spin channel also for SU(2)-symmetric parameters.

Appendix C: Functional representation of the Jacobian—We want to emphasize that the Jacobians of the iterations in G_0 , [Eq. (4)], and G , [Eq. (8)], are very different regarding their functional form. To make this more visible, we explicitly write the functional dependence in the following. By using $\Sigma[G_0^{-1}] = G_{0,\nu}^{-1} - G_\nu^{-1}[G_0^{-1}]$ and Eq. (A2), we get

$$J_{G_0}^{\nu\nu'}[G_0^{-1}] = \frac{\delta f_{G_0,\nu}}{\delta G_{0,\nu'}^{-1}} = \delta_{\nu\nu'} - p \frac{\chi_c^{\nu\nu'}[G_0^{-1}]}{-\beta G_{0,\nu}^2[G_0^{-1}]}, \quad (\text{C1})$$

and with the help of $\delta \Sigma_\nu / \delta G_\nu = \beta \Gamma_c^{\nu\nu'}$ we obtain

$$J_G^{\nu\nu'}[G^{-1}] = \frac{\delta f_{G,\nu}}{\delta G_\nu^{-1}} = (1-p)\delta_{\nu\nu'} + p \Gamma_c^{\nu\nu'}[G] \beta G_\nu^2, \quad (\text{C2})$$

where the Bethe-Salpeter equation $\Gamma_c = \chi_c^{-1} - \chi_0^{-1}$ was used for Eq. (8) in the main text. Hence, even though the functional form of both Jacobians is different, both expressions can be brought to a very similar form.

Appendix D: Practical implementation and numerical efficiency of the modified iteration—In our procedure, the Jacobian to stabilize the physical solution should be evaluated at the (in principle unknown) physical fixed point. For the data presented in this Letter (e.g., Fig. 3) the analytically known matrices for $\chi_0^{-1}\chi_c$, computed exactly at the considered parameter set, have been used to construct $\mathcal{P}$. However, we want to emphasize that, in practice, an *a priori* knowledge of the physical fixed point is *not* needed in order to apply our modified scheme to more realistic, nonanalytically solvable cases. The crucial insight is that all quantities needed for defining our modified scheme evolve smoothly by tuning U (with the obvious exception of phase transitions). Therefore, $\chi_0^{-1}\chi_c$ and/or $\mathcal{P}$ do not need to be evaluated exactly at each specific value of U at which the calculation is performed (see the Supplemental Material [66] for a detailed discussion). This can also be used to reduce the overall numerical cost considerably by evaluating $\chi_0^{-1}\chi_c$ on a coarser U grid than the one-particle quantity. We also note that a further reduction of numerical cost for our modified scheme can be obtained (i) by computing $\chi_0^{-1}\chi_c$ on a smaller Matsubara frequency grid than the one-particle quantity, and (ii) by calculating only a few eigenvalues instead of the full spectra of $\chi_0^{-1}\chi_c$, e.g., with Arnoldi iteration [92,93], provided that the unstable eigenvalues are included (see the Supplemental Material [66] for more detail). Our finding that several misleading convergence issues, previously attributed to the branching of the LWF, can be in fact be ascribed to intrinsic stability conditions of the physical fixed point of the iterative schemes were considered to pave the route to systematically explore the performances of other iterative algorithms able to converge to the physical fixed point. One concrete possibility, beyond the procedure presented here, is offered by (quasi)Newton methods, for which we provide a first preliminary comparison with respect to our scheme. Specifically, a more in-depth comparison is done

for a specific quasi-Newton method, namely the Chord method, and our modified iteration in the Supplemental Material [66].

Appendix E: Flow diagram for iterations—The Jacobian only gives information about the stability of the fixed point in its respective local neighborhood. In the worst case, this could mean that the fixed point is only stable for starting points in an infinitesimal neighborhood around the fixed point, which would be practically useless. Therefore it is also important to gain information about the nonlocal (in the space of the iterated quantity, e.g., G_0^{-1}) behavior around the fixed point. For this, we will define two quantities: first,

$$\Delta G_{0,\nu}^{-1}[G_0^{-1}] = f_{G_0,\nu}[G_0^{-1}] - G_{0,\nu}^{-1}, \quad (\text{E1})$$

which represents the change between two iterations and second the Lyapunov function V [75–78], which gives information about the stability. A Lyapunov function needs to fulfill the following conditions: (i) $V[\tilde{G}_0^{-1}] = 0$ where $\tilde{G}_0^{-1}$ is a fixed point of f_{G_0} , (ii) $V[G_0^{-1}] > 0$ for $G_0^{-1} \neq \tilde{G}_0^{-1} \in \mathcal{D}$ where $\mathcal{D}$ is an open domain around $\tilde{G}_0^{-1}$, (iii) V is continuous in $\mathcal{D}$, and (iv) $V[G_0^{-1}] \rightarrow \infty$ as $\|G_0^{-1}\| \rightarrow \infty$. $\tilde{G}_0^{-1}$ is globally (over the entire domain $\mathcal{D}$) and asymptotically stable in $\mathcal{D}$ if $\Delta V[[G_0^{(n)}]^{-1}] := V[[G_0^{(n+1)}]^{-1}] - V[[G_0^{(n)}]^{-1}] < 0$ for all $[G_0^{(n)}]^{-1} \neq \tilde{G}_0^{-1}$ in $\mathcal{D}$. Therefore $\mathcal{D}$ refers to a *stability region* that consists of initial points which converge to the fixed point $\tilde{G}_0^{-1}$ [78]. For our purpose, we define V as

$$V[G_0^{-1}] := \|f_{G_0}[G_0^{-1}] - G_0^{-1}\|^2, \quad (\text{E2})$$

where $\|\cdot\|$ denotes the usual Euclidean norm for complex vector spaces. Since the frequencies in the ZP model are decoupled, one can view all quantities essentially as complex scalars. Therefore we adapted $V_\nu[G_0^{-1}] := |f_{\nu,G_0}[G_0^{-1}] - G_{\nu,0}^{-1}|^2$ when considering the ν th frequency. A visualization of this tool is done in Fig. 3 (middle panel) in the main text for the ZP model. There $\Delta G_{0,\nu}^{-1}$ is plotted as a flow diagram in the complex plane of $G_{0,\nu}^{-1}$. The color grading of this plot is done with ΔV where red means $\Delta V[G_0^{-1}] > 0$ and blue means $\Delta V[G_0^{-1}] < 0$. We can therefore consider the blue region around a stable fixed point as the *stability region* $\mathcal{D}$ around a stable fixed point. Note that this concept is worked out explicitly for the iterative scheme in G_0 but can be also done for the iteration in G by simply changing $G_0 \rightarrow G$ and $f_{G_0} \rightarrow f_G$.