The Bethe-Salpeter equation at the critical end-point of the Mott transition

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Strong repulsive interactions between electrons can lead to a Mott metal-insulator transition. The Dynamical Mean-Field Theory (DMFT) explains the critical end-point and hysteresis region with single-particle concepts such as the spectral function and the quasiparticle weight. In this work, we reconsider the critical end point of the metal-insulator transition on the two-particle level. A divergence of the Bethe-Salpeter equation necessarily occurs at the critical point and simultaneously explains the thermodynamics of the hysteresis region and the iterative stability of the DMFT equations. In this way, the relevant eigenvalue and eigenvector of the Bethe-Salpeter equation provides a unified picture of the hysteresis region and of the critical end point of the Mott transition. This analysis paves the way for a deeper understanding of phase transitions in correlated materials.

The interplay of interactions, correlations and quantum statistics in quantum many-body physics is responsible for the appearance of complicated new phases, with the Mott transition [1] as a prominent example. The simplest theoretical realization of this correlation driven metal-insulator transition occurs in the (single-band) Hubbard model [2–5]. Quantum simulators using ultra-cold fermions in optical lattice are providing unprecedented experimental insight into this transition [6–10].

From the theory side, the Dynamical Mean-Field theory [11, 12] (DMFT) provides a rare example of an exact solution to a strongly correlated problem, namely to the Hubbard model in the limit of infinite dimensions. During the first decade after DMFT’s invention, the essence [15] of the Mott transition was ascertained [16–23]: At the zero temperature transition to the insulating phase, the quasiparticle weight vanishes and the self-energy is divergent at small frequency, in contrast to the Fermi liquid. The $U$-$T$ (interaction-temperature) DMFT phase diagram of the particle-hole symmetric model can be summarized as follows (sketched in Fig. 1, for an overview see Refs. [23–26]): at low temperature, there is a metallic phase at small $U < U_{c1}$ and an insulating phase at large $U > U_{c2}$. In between, for $U_{c1} < U < U_{c2}$, both metallic and insulating solutions can be stabilized. This hysteresis region (shaded blue area) ends at a critical temperature $T_c$, where $U_{c1} = U_{c2} = U_c$ (purple dot). No phase separation occurs in the particle-hole symmetric system [24].

Although the single-particle properties (Green’s function, self-energy, quasiparticle weight) are sufficient to understand the essentials of the metal-insulator transition, two-particle properties provide another rich layer of information about the response to external fields, spatial correlations and optical properties. The simplifications of infinite dimensions allowed early studies at the two-particle level [19, 20, 27–30], but a systematic investigation of the DMFT two-particle physics had to wait [31–36] for computational improvement, especially the invention of continuous-time Quantum Monte Carlo solvers [37–39].

There has recently been a flurry of activity on divergences on the two-particle level [40–43], from simple toy models [44, 45] and the Hubbard atom [46] to cluster approaches [47], relating these divergences to unphysical solutions [41, 43, 48] and to the suppression of fluctuations [49], but without a clear link to the Mott transition. On the other hand, previous work [50] has established that the zero temperature critical point features a divergence of a two-particle quantity, namely the charge forward scattering amplitude.

Here we show that the two-particle level provides an intriguing new view on the Mott transition across the hys-
The Hamiltonian $H = -\sum_{k,\sigma} t_{k} c_{k\sigma}^{\dagger} c_{k\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$, (1)

where $c_{k\sigma}^{\dagger}$ is the creation operator for a fermion with momentum $k$ and spin $\sigma = \uparrow, \downarrow$ and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ is the number operator of electrons with spin $\sigma$ on site $i$.

We consider the Hubbard model describing the competition between localization due to the Coulomb interaction $U$ and delocalization due to the dispersion $t$. We use $i$ to label the sites on the periodic lattice and $k$ to label the corresponding momentum. The model is given by the Hamiltonian

$$H = -\sum_{k,\sigma} t_{k} c_{k\sigma}^{\dagger} c_{k\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow},$$

where $c_{k\sigma}^{\dagger}$ is the creation operator for a fermion with momentum $k$ and spin $\sigma = \uparrow, \downarrow$ and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ is the number operator of electrons with spin $\sigma$ on site $i$.

We consider this model in the grand-canonical ensemble at temperature $T$ and chemical potential $\mu$. A central object of interest is the (one-particle) Green’s function $G_{k,\nu,\sigma} = -\langle c_{i\sigma}^{\dagger} c_{i\sigma} \rangle_{k,\nu}$ in the Matsubara formalism, where $\nu = \pi T(2n + 1)$, with $n \in \mathbb{Z}$ the fermionic Matsubara frequencies. For compactness, we assume paramagnetism and drop the spin labels, derivations with all spin labels can be found in the supplemental material. Dyson’s equation relates $G$ to the non-interacting ($U = 0$) Green’s function $G_{0}$, as $G_{k,\nu,\sigma} = (G_{0})^{-1}_{k,\nu} - \Sigma_{k,\nu,\sigma}$, thereby defining the self-energy $\Sigma$.

The Dynamical Mean-Field Theory [11, 12] (DMFT) provides an approximate solution to this model by setting $\Sigma_{k,\nu} = \Sigma_{k,\nu}^{\text{AIM}}$, where AIM stands for an auxiliary impurity model consisting of a single interacting site in a self-consistently determined bath. For the present discussion, it is sufficient to state that the auxiliary impurity model serves as a tool to evaluate the functional relation $\Sigma[g]$ between the Green’s function $g$ and the self-energy $\Sigma$ of the AIM (in practice, we use the ALPS [53] CTQMC [39] solver of Ref. [54] with improved estimators [55]). This auxiliary impurity model is defined by the self-consistency equation

$$g_{\nu} = \sum_{k} G_{k,\nu}[g] = \sum_{k} \frac{1}{(G_{0})^{-1}_{k,\nu} - \Sigma_{\nu}[g]} \equiv f[g], \quad (2)$$

where from now on $\sum_{k} \equiv \frac{1}{N} \sum_{k \in BZ}$ denotes the momentum average over the Brillouin Zone. The square brackets denote functional relations, i.e., $\Sigma_{\nu}$ depends on $g_{\nu}$, even when $\nu \neq \nu'$.

In this work, we consider the two-dimensional square lattice Hubbard model, $t_{k} = -2t(\cos k_{x} + \cos k_{y})$ at half-filling. The energy scale is set by $4t = 1$. The half-filled model is particle-hole symmetric, which leads to $\text{Re} g_{\sigma} = 0$ and $\text{Re} \Sigma_{\nu} = U/2$. In other words, only the imaginary parts of both quantities are of interest, which simplifies the analysis.

**Fixed point equation**: A DMFT solution is a fixed point $f[g^{*}] = g^{*}$ of Eq. (2). One way to search for solutions of such a self-consistency equation is iteratively, i.e., $g^{(n+1)} = f[g^{(n)}]$. An important question is if this iterative scheme converges to the fixed point $g^{*}$ if one starts the iteration close to $g^{*}$. In that case, the fixed point is called attractive. The textbook analysis, based on a linear expansion of $f$ around the fixed point, shows that $g^{*}$ is attractive if and only if all eigenvalues of the Jacobian $J_{\nu\nu'} = (\delta f/\delta g_{\nu'})|_{g^{*}}$ have magnitude smaller than 1. For DMFT, the Jacobian can be evaluated explicitly in Matsubara space by using that $f[g]$ depends on $g$ only via $\Sigma$,

$$J_{\nu\nu'} = \sum_{k} \frac{\delta G_{k,\nu}}{\delta g_{\nu'}} = -\sum_{k} G_{k,\nu}^{2} \frac{\delta G_{k,\nu}^{-1}}{\delta g_{\nu'}} = \sum_{k} G_{k,\nu}^{2} \frac{\delta \Sigma_{\nu}}{\delta g_{\nu'}} = T \sum_{k} G_{k,\nu}^{2} \delta \Sigma_{\nu} = -\tilde{\chi}_{0}^{-1} \equiv \hat{B}. \quad (3)$$

The functional derivative $\delta \Sigma/\delta g$ is the irreducible vertex $\Gamma$ (times $T$), which is real for particle-hole symmetric systems [32], and we have introduced the notation $(\tilde{\chi}_{q}^{A})_{\nu\nu'} = -T \delta \nu' \sum_{k} G_{k,\nu} G_{k+q,\nu'}$ for the “bubble” of DMFT Green’s functions. The hat denotes a matrix in Matsubara space and, when possible, we will drop the matrix indices $\nu, \nu'$. In the last line, we recognize $\hat{B}$ —the Bethe-Salpeter kernel at $q = 0$ and $\omega = 0$ —a quantity that usually occurs in the calculation of linear response functions [12].

**Response functions**: Indeed, the DMFT recipe provided above not only allows us to determine the one-particle Green’s function $G$ for a given set of parameters $(U, \mu, T)$. On top of this, DMFT also describes how the system would (linearly) respond [12] to an external field with frequency $\omega$ and momentum $q$. We restrict our analysis to time-independent fields, $\omega = 0$. The response function $\chi_{q}$ is obtained from the Bethe-Salpeter equation
To determine the stability of this solution, we proceed with
\[
\frac{dn}{d\mu} = T^2 \sum_{\nu \nu'} (\hat{\chi}^{\text{DMFT}})_{\nu \nu'}.
\] (5)

The response in DMFT is thermodynamically consistent in the sense that this Bethe-Salpeter determination of \(dn/d\mu\) gives the same result as changing \(\mu\) explicitly and calculating the change \(n\) [56].

Landau theory: Following Landau, the free energy functional is the essential ingredient for understanding stable and unstable phases and hysteresis close to the critical point. Characteristic free energy curves are sketched in Fig. 1. The second derivative of the free energy determines if the stationary point is a local minimum (\(\delta^2 F > 0\), stable, denoted by triangles in Fig. 1) or a local maximum (\(\delta^2 F < 0\), unstable, denoted by a vertical bar). The critical point is where a stable point turns unstable, in other words, \(\delta^2 F = 0\) exactly at the critical point (purple curve in Fig. 1).

The Mott transition of DMFT has been studied using Landau theory [23, 57, 58]. Chitra and Kotliar [59] have shown a relation between the Bethe-Salpeter equation and the free energy functional. Here we rederive a similar equation using Potthoff’s self-energy functional [60] approach to DMFT. When evaluated at one of the fixed points, this functional is equal to the grand potential and thereby it provides direct access to information about thermodynamic stability [61].

The stationary point of the self-energy functional occurs when the first derivative is zero, resulting in the Dyson equation [60],
\[
\frac{1}{T} \frac{\delta \Omega[\Sigma]}{\delta \Sigma} = \frac{1}{G_0^{-1} - \Sigma} - G = 0.
\]

To determine the stability of this solution, we proceed with the second derivative (Hessian),
\[
\frac{1}{T} \frac{\delta^2 \Omega}{\delta \Sigma^2} = \frac{1}{G_0^{-1} - \Sigma} - \frac{\delta G}{\delta \Sigma} = G^2 - \frac{\delta \Sigma}{\delta G}^{-1},
\]
\[
(\frac{\delta^2 \Omega}{\delta (\Sigma)^2})^{-1} = \hat{\Gamma} \frac{\hat{1}}{1 - B},
\] (6)
where the stationary point (Dyson) equation was used.

Equation (6) is a matrix equation in Matsubara space, \(\delta^2 \Omega/\delta (\Sigma)^2\) is the Hessian matrix, which is a real matrix in the case of particle-hole symmetry, and stability requires that all eigenvalues of the Hessian are positive. At the critical point, one eigenvalue of \(\delta^2 \Omega/\delta \Sigma^2\) is equal to zero, so Eq. (6) needs to have a divergent eigenvalue.

The same Bethe-Salpeter kernel \(\hat{B}\) has appeared three times in stability criteria: in the Jacobian of the fixed point equation; in the compressibility; and in the second derivative of the self-energy functional. The latter two relate to the stability of the physical solution, whereas the Jacobian determines the attractiveness of the fixed point in an iterative scheme. For DMFT, these two aspects are tied together by the same Bethe-Salpeter kernel \(\hat{B}\).

This allows us to create a unified picture of the hysteresis region of the particle-hole symmetric metal-insulator transition. At the critical end point \((U_c, T_c)\), the purple dot in Fig. 1, the two stable (triangles in Fig. 1) and the one unstable (vertical marks in Fig. 1) stationary points merge together. Therefore, the quadratic part of the free energy functional vanishes at this point (purple curve), which together with Eq. (6) means that the Bethe-Salpeter kernel \(\hat{B}\) has an eigenvector \(V\) with eigenvalue \(\lambda \rightarrow 1\) (Fig. 2) exactly at the critical end point. Since \(\hat{B}\) is equal to the Jacobian of the fixed point equation, the stable and unstable solutions correspond to attractive and repulsive fixed points, respectively [25].

Figure 3 shows the eigenvector \(V\) close to the critical end point. The physical meaning of this eigenvector is that it relates the three fixed points that exist at \(T < T_c\), as \(g_m(\nu) - g_u(\nu) \propto (T_c - T)^{\beta} V(\nu)\) and \(g_t(\nu) - g_u(\nu) \propto (T_c - T)^{\beta} V(\nu)\), where \(g_m, g_t\) and \(g_u\) are Green’s function at the metallic, insulating and unstable fixed points, respectively, and \(\beta\) is a critical exponent. This together with particle-hole symmetry \(g(\nu) = -g(-\nu)\) implies \(V(\nu) = -V(-\nu)\), i.e., the eigenvector \(V\) is antisymmetric [49]. As the difference between solutions, \(V\) provides the “order parameter”, similar to Kotliar’s [57] \(\delta \Delta_L\), in
The eigenvector $V$ corresponding to the leading eigenvalue $\lambda$ of the Bethe-Salpeter kernel, for $T$ just above $T_c$. As $U$ increases and the Mott transition is approached, the eigenvector localizes around $\nu = 0$ and $\lambda \to 1$. The eigenvector is normalized to $\sum_\nu |V(\nu)|^2 = 1$.

The compressibility stays finite as the Mott transition is approached. Right: The Hessian of $\partial^2 \Omega / \partial (i \Sigma)^2 |V\rangle$ vanishes as $U \to U_c$. As $\lambda$ approaches 1, the compressibility goes from a parabola to a double-well potential along the direction given by $V$. Figure 4 shows that the second derivative of the grand potential indeed vanishes as one gets close to the Mott transition.

The frequency structure of $V$, in Fig. 3, shows that the three solutions $g(\nu)$ differ only at low frequency, i.e., close to the Fermi level. This is in agreement with what is known qualitatively from investigations of the Density of States: the difference between the insulator and the metal is that the latter has a quasiparticle peak at the Fermi level. Astretsov et al. [63] used a single Matsubara frequency approximation to study the cuprates, our result here is a direct quantitative proof that this kind of approximation is justified at the critical end point of the Mott transition.

At $T < T_c$ and $U_{c1} < U < U_{c2}$, the Bethe-Salpeter equation is convergent (and the iterative scheme is attractive) at both the metallic and the insulating solutions, $\lambda < 1$, and divergent (repulsive) at the unstable fixed point, $\lambda > 1$. Although both metallic and insulating solution are attractive fixed points, only one of them is the global minimum (e.g., green and orange curves in Fig. 1) of the free energy in most of the hysteresis region. Only at $U_c(T)$ (the blue line in Fig. 1), both solutions have exactly the same free energy, this is where the phase transition occurs. At $U_{c1}$ ($U_{c2}$) the unstable and insulating (metallic) fixed point merge, so that $\lambda = 1$ at this fixed point, but the metallic (insulating) solution, with $\lambda < 1$, is the global minimum of the free energy.

Kotliar et al. [64] predicted a compressibility divergence at the critical end point of the doping-driven Mott transition, $dn/d\mu \to \infty$. On first sight, our present eigenvalue analysis seems to imply the same here, since the BSE diverges. However, a divergence in the BSE can be canceled by an exact orthogonality [49, 64], and that is indeed what happens at particle-hole symmetry [52]. The eigenvector $V \propto g_m - g_i$ is antisymmetric in $\nu$ and therefore does not contribute to the sum in Eq. (5) [49, 52, 65], so that $dn/d\mu$, shown in Fig. 4, is finite (and small) at the critical end point. This is consistent with the absence of phase separation at particle-hole symmetry [24]. A finite compressibility combined with a divergence of the BSE is reminiscent of the zero temperature case where, in fact, the divergence of the BSE is required so that $dn/d\mu$ can vanish at the Mott transition [50]. In other words, both critical end points of the particle-hole symmetric Mott transition are characterized by a divergent BSE without a divergence in $dn/d\mu$.

The situation away from particle-hole symmetry is more complicated because of the complex-valuedness of the Green’s functions [52]. The antiferromagnetic transition in DMFT [16] — which occurs when the assumption of paramagnetism is lifted — can also be analyzed along the lines of the current work as a divergence of the BSE in the magnetic channel. An important open question is the generalization of our analysis to the instabilities found in multi-orbital Hund’s physics [66–73], and more generally to systems that show phase separation [24, 64, 74–82].

In conclusion, we identified the Bethe-Salpeter kernel with the Jacobian of the DMFT fixed point equation and with the curvature of the free energy functional. Near the critical end point of the finite temperature correlation-driven Mott transition the BSE diverges. The eigenvector corresponding to the divergence relates the insulating and metallic solutions that exist below the critical temperature. Particle-hole symmetry then implies that this eigenvector is antisymmetric and does not contribute to the compressibility [52], which remains finite.

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SUPPLEMENTAL MATERIAL: SIGN CONVENTION AND DETAILED DERIVATIONS

The literature contains different definitions of the vertex, especially concerning the sign. Here, we take as the fundamental equation

$$\Gamma_{\nu\nu'}^{\sigma\sigma'} \equiv \frac{1}{T} \frac{\delta \Sigma_{\nu\sigma}}{\delta g_{\nu'\sigma'}}. \quad (7)$$

It is instructive to apply this to the Hartree-Fock self-energy,

$$\Sigma_{\nu\sigma}^{\text{HF}} = UT \sum_{\nu',\sigma' \neq \sigma} g_{\nu',\sigma'}. \quad (8)$$

$$\Gamma_{\nu\nu'}^{\sigma\sigma'}(T) \equiv \frac{1}{T} \frac{\delta \Sigma_{\nu\sigma}}{\delta g_{\nu'\sigma'}} = U(1 - \delta_{\sigma\sigma'}), \quad (9)$$

$$\Gamma^{\uparrow\uparrow} = +U, \quad (10)$$

$$\Gamma^{\downarrow\downarrow} = 0, \quad (11)$$

$$\Gamma^{\uparrow\downarrow} = \Gamma^{\downarrow\uparrow} = -U, \quad (12)$$

$$\Gamma^{\text{ch}} \equiv \Gamma^{\uparrow\uparrow} + \Gamma^{\downarrow\downarrow} = +U. \quad (13)$$

In other words, $\Gamma > 0$ signals repulsion in that channel. We define the bubble $X$ and generalized susceptibility $\chi$ so that both are positive, after being summed over Matsubara frequencies,

$$X_{\nu\nu',\sigma\sigma'} = -T \delta_{\nu\nu'} \delta_{\sigma\sigma'} \sum_{k} G_{\nu\sigma,k} G_{\nu',\sigma,k}. \quad (14)$$

$$\chi_{\nu,\sigma}^{\text{DMFT}} = \frac{1}{1 + XT}. \quad (15)$$

Expanding the denominator to first order shows that if $U > 0$ ($\Gamma^{\text{ch}} > 0$), then $\chi < X$, a repulsive interaction suppresses the corresponding susceptibility. Our sign convention for $\Gamma$ is opposite to Georges et al. [12], who use $\chi_{\nu,\sigma}^{\text{DMFT}} = 1/(1 - X\Gamma)\dot{X}$. Based on the denominator of the Bethe-Salpeter equation, we define the Bethe-Salpeter kernel $\mathcal{B}$ as

$$\dot{\mathcal{B}} = -\dot{X} \mathcal{B}, \quad (16)$$

so that an eigenvalue of $+1$ corresponds to the divergence of the Bethe-Salpeter equation.

With spin and Matsubara labels, the Jacobian reads

$$J_{\nu\nu',\sigma\sigma'} = \frac{\partial f_{\nu\sigma}}{\partial g_{\nu'\sigma'}} = \sum_{k} \delta G_{k,\nu\sigma} \delta g_{\nu'\sigma'}. \quad (17)$$

$$= -\sum_{k} G_{k,\nu\sigma}^{2} \frac{\delta G_{k,\nu'\sigma'}}{\delta g_{\nu'\sigma'}} = +\sum_{k} G_{k,\nu'\sigma'}^{2} \frac{\delta G_{k,\nu\sigma}}{\delta g_{\nu'\sigma'}} = +T \sum_{k} G_{k,\nu'\sigma'}^{2} \Gamma_{\nu\nu'}^{\sigma'}. \quad (18)$$

$$= -\dot{\mathcal{X}}_{\nu\nu',\sigma\sigma'} \Gamma_{\nu\nu'}^{\sigma'}. \quad (18)$$

$$\mathcal{B} = \dot{\mathcal{B}}. \quad (19)$$

If we consider paramagnetic solutions, $g_{\sigma} = g_{\sigma'} = g$ change in the same way and we get

$$\frac{\partial f_{\nu,\sigma'}}{\partial g_{\nu}} = \frac{\partial f_{\nu,\uparrow}}{\partial g_{\uparrow}} + \frac{\partial f_{\nu,\downarrow}}{\partial g_{\downarrow}} = \mathcal{B}^{\uparrow} + \mathcal{B}^{\downarrow} = \mathcal{B}^{\text{ch}}, \quad (19)$$
i.e., for paramagnetic solutions only the charge channel of the Bethe-Salpeter kernel is relevant.

The second derivative of the free energy functional is

\[
\frac{1}{T} \frac{\delta^2 \Omega}{\delta \Sigma_{\nu \sigma} \delta \Sigma_{\nu' \sigma'}} = \frac{\delta_{\nu \nu'} \delta_{\sigma \sigma'}}{\left(G_0^{-1}\right)_{\nu \sigma} - \Sigma_{\nu \sigma}} - \frac{\delta G_{\nu \sigma}}{\delta \Sigma_{\nu \sigma}} \delta_{\Sigma_{\nu \sigma}} \delta_{\Sigma_{\nu' \sigma'}} = \frac{\delta_{\nu \nu'} \delta_{\sigma \sigma'}}{G_{\nu \sigma}^2 - \Sigma_{\nu \sigma}} - \left(\delta G_{\nu \sigma} \delta_{\Sigma_{\nu \sigma}} \delta_{\Sigma_{\nu' \sigma'}}\right)^{-1} \nonumber
\]

\[
= -\frac{1}{T} \left( \hat{X}_{\nu \nu', \sigma \sigma'} + \left(\hat{\Gamma}_{\nu \nu'}\right)^{-1}_{\sigma \sigma'} \right). \quad (20)
\]

As with the Jacobian, the restriction to paramagnetic solutions selects the charge channel of \( \Gamma \) and \( \mathcal{B} \).

Although \( \Sigma \) is generally a complex function, at particle-hole symmetry, \( \Sigma \) is purely imaginary (modulo the constant Hartree contribution), so it is sufficient to look at \( \delta^2 \Omega / \delta (i \Sigma)^2 \). On the right-hand side, \( \hat{\Gamma} \) and \( \hat{X} \) are real matrices and therefore \( \Omega \) is a real function. Because of this, it makes sense to talk about minima and maxima and not just about stationary points.

At the critical point, one eigenvalue of the Hessian \( \delta^2 \Omega / \delta \Sigma^2 \) changes sign, the corresponding eigenvector determines the unstable direction of the free energy landscape. In general, there is no reason for the Hessian and the Bethe-Salpeter kernel to have the same eigenbasis, since Eq. (21) is a matrix equation. However, it is easy to show that exactly at the critical point, the eigenvector \( V \) with \( \hat{B}V = V \) is also a left eigenvector of the Hessian with eigenvalue 0:

\[
\langle V | \delta^2 \Omega / \delta \Sigma^2 = -(\hat{1} - \hat{B}) \hat{\Gamma}^{-1} = -\langle V | 0 \hat{\Gamma}^{-1} = \langle V | 0.
\]

The Hessian is symmetric, so any left eigenvector is also a right eigenvector. Finally, the inverse matrix and the original matrix have the same eigenvectors.

The combination shown in Fig. 4,

\[
\langle V | \delta^2 \Omega / \delta (i \Sigma)^2 | V \rangle = (\lambda - 1) \langle V | \hat{\Gamma}^{-1} | V \rangle, \quad (22)
\]

with \( V \) the leading Bethe-Salpeter eigenvector, approaches the relevant eigenvalue of the Hessian as one goes towards the critical point. Note that the eigenvector \( V \) is only determined up to a scale factor, the results shown in Fig. 4 use \( \sum_{\nu} |V(\nu)|^2 = 1 \), as in Fig. 3).

Formally, the self-energy functional and the grand potential only coincide at the stationary point(s). In a Landau theory analysis of the critical region, three stationary points are close together, with a free energy landscape described by lowest-order polynomials (up to \( \phi^4 \)). Since the grand potential \( \Phi \) and the functional \( \Omega \) are equal at all stationary points, and the stationary points move arbitrarily close together as the critical end point is approached, local minima in the grand potential will correspond to local minima in \( \Omega \). Furthermore, the density is fixed at particle-hole symmetry, so the grand potential (given here by \( \Omega \)) is equal to the free energy, modulo a constant shift.

To summarize, the three central equations read,

\[
\hat{J} = \hat{B}, \quad (23)
\]

\[
\hat{\chi} = \hat{\Gamma} \frac{\hat{1}}{1 - \hat{B}} \hat{\chi}, \quad (24)
\]

\[
\left( \frac{\delta^2 \Omega}{\delta (i \Sigma)^2} \right)^{-1} = \hat{\Gamma} \frac{\hat{1}}{1 - \hat{B}}. \quad (25)
\]