Letter

Second-order phase transitions and divergent linear response in dynamical mean-field theory

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Second-order phase transitions appear as a divergence in one of the linear response functions. For a system of correlated electrons, the relevant divergent response can and does involve many-particle observables, most famously the double occupancy. Generally, evaluating the linear response function of many-particle observables requires a many-particle generalization of the Bethe-Salpeter equation. However, here I show that the divergence of linear response functions in dynamical mean-field theory is governed by a *two*-particle Bethe-Salpeter equation, even for many-particle observables. The reason for this is that the divergence at the second-order phase transition is produced by the self-consistent feedback of the dynamical mean field.

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Electronic correlations lead to a plethora of phases, from metal-insulator transitions [1] and magnetism [2,3] to charge-density waves [3–5], Wigner crystals [6–8], phase separation [9], superconductivity [10,11], and orbital [12,13] and bond order [14,15]. Many of these phases are already present in variants of the Hubbard model [16,17]. Second-order phase transitions between these correlated phases at finite temperature are of special interest, since divergences occur in the correlation and response functions at these points, associated with the vanishing second derivative of the free-energy functional [18,19]. According to the fluctuation-dissipation theorem, the relevant correlation functions are many-particle observables of higher rank than the order parameter itself. For example, for a ferromagnetic or antiferromagnetic transition, the order parameter $\langle n_{i\sigma}\rangle$ is a single-particle operator, while the relevant correlation function $\langle n_{i\sigma}n_{j\sigma}\rangle$ is a two-particle operator.

Dynamical mean-field theory [20] (DMFT) is a hugely successful approximation for materials with correlated electrons [21], based on the theoretical [22] and experimental [23] observation that the electronic self-energy is often predominantly local. This assumption also leads to simplifications at the two-particle level [24–27], which have enabled the calculation of dynamical two-particle correlation functions [26,28–34] according to the Bethe-Salpeter equation. Thus, second-order phase transitions such as the metal-insulator transition can be analyzed at the two-particle level using the DMFT Bethe-Salpeter equation [18,19,35–41].

However, this analysis of the Bethe-Salpeter equation appears to be limited to the two-particle correlation functions and thus to single-particle order parameters. This excludes the most simple realization of the metal-insulator transition, where the double occupancy D and its response to a change in the Coulomb interaction strength dD/dU are the quantities of interest [35,41,42], so the order parameter is a two-particle operator and the divergent correlation-response function involves four-particle operators, whereas the compressibility $d\langle n\rangle/d\mu$ does not diverge at the critical point of the particle-hole symmetric Hubbard model [38,43,44].

More generally, considering the free energy as a function of μ, U, and possible other parameters, thermodynamic stability is a condition on the eigenvalues of the second derivative matrix of the free energy [41], which can be expressed in terms of mixed response functions such as $\partial D/\partial\mu|_U$. Finally, in multi-orbital systems, higher-order crystal field and magnetic order parameters [45–48] do not always have a representation as a single-particle observable, which follows from the addition rules for angular momentum in many-electron systems.

Thus, it is relevant to study the response of many-particle observables in correlated electron systems, especially with an eye on possible divergences. For the particular case of the double occupancy, Kowalski *et al.* [41] have used the Galitskii-Migdal formula to reduce the problem to single-particle objects, but a more general and systematic approach is clearly beneficial.

Here, I will show that in DMFT the linear response of many-particle correlation functions and especially their divergence is still governed by the usual, *two*-particle Bethe-Salpeter kernel. In fact, the many-particle order parameter and applied field only show up as "capping stones" at the end points of the two-particle Bethe-Salpeter equation. Thus, they do not generate the divergence at the second-order transition and their role is restricted to determining if the divergence is picked up in a particular response function. The reason for this remarkable simplification, from many-particle to two-particle physics, can be traced back to the particular form of the DMFT equations, where the self-consistent feedback of the dynamical mean field is responsible for the second-order phase transition [18,19,35,36]. On the other hand, going beyond linear response, the two-particle Bethe-Salpeter is no longer sufficient, as expected.

Consider a general Hubbard model of the form

$$H = \sum_{\text{sites } a,b} \sum_{\alpha\beta} t_{a\alpha,b\beta} c^\dagger_{a\alpha} c_{b\beta} + \sum_{\text{sites } a} H^{\text{local}}[\{c^\dagger_{a\alpha}, c_{a\beta}\}], \quad (1)$$

where a, b are sites in a lattice, α and β are orbital labels (which includes spin), $t_{a\alpha,b\beta}$ is the hopping, and H^{local} is a local Hamiltonian, which is a function of the creation and annihilation operators $c^\dagger_{a\alpha}, c_{a\beta}$ on that particular lattice site. The local Hamiltonian includes many-particle terms such as the Coulomb interaction $\frac{1}{2}\sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\gamma\delta} c^\dagger_\alpha c_\beta c^\dagger_\gamma c_\delta$. Here, $t_{a\alpha,b\beta}$ and H^{loc} are Hermitian. For a translationally invariant system, $t_{\mathbf{k},\alpha\beta}$ denotes the Fourier transform of $t_{a\alpha,b\beta}$ to momentum space. The model is considered at a finite temperature $T = 1/\beta$, and factors of T are suppressed in the equations for compactness.

In DMFT, this lattice Hamiltonian is replaced by an auxiliary impurity model with the same local Hamiltonian but with a dynamical hybridization function $\Delta_{\nu,\alpha\beta}$, where ν is a fermionic Matsubara frequency. This hybridization might be represented as an (infinite) discrete bath to obtain a Hamiltonian formulation of the impurity, or simply as an action in imaginary time. For now, a hybridization of the form $\Delta_{\tau-\tau',\alpha\beta} c^\dagger_\alpha(\tau) c_\beta(\tau')$ is used, where Δ_ν has been Fourier transformed to imaginary time. The generalization to Nambu space for superconducting phases is discussed at the end. Given a hybridization $\Delta_{\nu,\alpha\beta}$, the auxiliary impurity model can be solved numerically [49] and its time-ordered expectation values are denoted by $\langle\cdot\rangle$. In particular, DMFT works with the imaginary-time single-particle Green's function $g_{\alpha\beta}(\tau) = \langle c_\alpha(\tau) c^\dagger_\beta\rangle$ and its Fourier transform to Matsubara frequency $g_{\nu,\alpha\beta}$. In the following, $t_{\mathbf{k}}$, Δ_ν, and g_ν are considered as matrices in orbital space, and $\cdot^{-1}$ denotes the matrix inverse in this space.

The DMFT loop is closed by a prescription to find the hybridization Δ_ν, the dynamical mean field, which is given by a set of self-consistency conditions,

$$\forall_\nu : \; 0 \stackrel{!}{=} f_\nu(\Delta_\nu, g_\nu) = g_\nu - \int d\mathbf{k} \left[g_\nu^{-1} + \Delta_\nu - t_{\mathbf{k}}\right]^{-1}. \quad (2)$$

Here, $\int d\mathbf{k} = 1/N_k \sum_{\mathbf{k}}$ denotes taking the momentum average, i.e., the local part. Equation (2) is a coupled set of equations because the solution of the auxiliary impurity model g_ν implicitly depends on $\Delta_{\nu'}$ also for $\nu \neq \nu'$.

Linear response of local observables. Linear response considers the change of the expectation value of an operator $\hat{B}$ to a small perturbation $H \to H - A\hat{X}$ of the Hamiltonian, where A is the magnitude of the perturbation and A and $\hat{X}$ are called conjugate variables. Two examples introduced above are the density of orbital α, $\hat{n}_\alpha = c^\dagger_\alpha c_\alpha$, and the double occupancy on orbital α, $\hat{D}_\alpha = c^\dagger_{\alpha\uparrow} c_{\alpha\uparrow} c^\dagger_{\alpha\downarrow} c_{\alpha\downarrow}$, which are conjugate to the chemical potential μ and Hubbard interaction U acting on that orbital, respectively.

As in these examples, and in the spirit of dynamical mean-field theory, I focus here on homogeneous local perturbations, i.e., $\hat{X} = \sum_{\text{sites } i} \hat{X}_i[\{c^\dagger_{i\alpha}, c_{i\beta}\}]$, where $\hat{X}_i$ is a local operator on site i of arbitrary order. Similarly, only site-local observables $\hat{B}$ are considered. In that case, in DMFT, it makes sense to identify [50] the expectation value of the impurity model as the relevant quantity, i.e., $\langle B\rangle = \frac{1}{N_\#}\sum_{\text{sites } i}\langle B_i\rangle = \langle B\rangle^{\text{imp}}$, which can be measured in the impurity solver. For the linear response to the homogeneous field A, the resulting linear change to a local observable B is the same on all sites, i.e., it is a $\mathbf{q}=\mathbf{0}$ response. More generally [51], it is also possible to consider how $\langle B_b\rangle$ depends on $\hat{A}_a$ for any pair of sites a, b, and the corresponding $\mathbf{q}$-dependent response function in momentum space. Similarly, since the perturbation is constant in time, the linear response is also assumed to be time independent and the response function has $\omega = 0$. The linear response formalism assumes that no spontaneous symmetry breaking in space or time takes place in response to the field, but second-order phase transitions are visible as a divergent linear response. For single-particle operators $A\hat{X}$ and $\hat{B}$, the DMFT linear response is given by the well-known Bethe-Salpeter equation [20]. Here, I show that the approach which was previously used to prove the thermodynamic consistency [52] of the DMFT compressibility can also be used to express the linear response of many-particle observerables in simple terms.

Derivation. For a local (i.e., impurity) expectation value $\langle B\rangle$, a change in the parameter A of the local Hamiltonian will lead to both direct changes and indirect changes via the DMFT self-consistent field Δ,

$$\frac{d\langle B\rangle}{dA} = \left.\frac{\partial\langle B\rangle}{\partial A}\right|_\Delta + \sum_{\nu'} \left.\frac{\partial\langle B\rangle}{\partial\Delta_{\nu'}}\right|_A \frac{\partial\Delta_{\nu'}}{\partial A}. \quad (3)$$

This requires the calculation of the change of Δ with respect to A, which can be determined from the fact that the DMFT self-consistency equation has to be satisfied both before and after applying the field. Restating the DMFT self-consistency, Eq. (2), in terms of g^{-1} instead of g will lead to more compact equations in the end [53]:

$$f(g^{-1}[\Delta[A], A], \Delta[A]) = (g^{-1})^{-1} - \int d\mathbf{k} (g^{-1} + \Delta - t_{\mathbf{k}})^{-1}. \quad (4)$$

Here, the square brackets denote that the mean-field Δ depends on A and the inverse of the local Green's function g^{-1} depends on A both directly and via $\Delta[A]$. f is diagonal in ν, so the ν labels are suppressed to keep the notation compact.

As stated before, the objects g^{-1}, Δ, $t_{\mathbf{k}}$ are matrices in orbital space. The derivative of one of these matrices with respect to another matrix is a rank-4 tensor in orbital space. Furthermore, g and Δ carry a single fermionic frequency, so the derivative $\partial g^{-1}/\partial\Delta$ has two fermionic frequencies, i.e., it is a matrix. It will make sense to interpret these rank-4 orbital tensors as matrices (rank-2 tensors) in a space of orbital pairs, keeping the additional matrix structure in frequency space as well. In this pair space, the usual single-frequency rank-2 orbital objects are vectors. For the matrix inverse in this pair space, the notation $\cdot^{\neg 1}$ is used, while $\cdot^{-1}$ is reserved for the original orbital space. For matrix derivatives, there is the useful identity $\partial(M^{-1})/\partial x = -M^{-1}(\partial M/\partial x)M^{-1}$.

To satisfy the self-consistency condition after the infinitesimal change in the external field A,

$$\forall_\nu:\ 0=\frac{df_\nu}{dA}=\left.\frac{\partial f_\nu}{\partial\Delta_\nu}\right|_{g^{-1}}\frac{\partial\Delta_\nu}{\partial A}+\sum_{\nu'}\left.\frac{\partial f_\nu}{\partial g_\nu^{-1}}\right|_{\Delta}\frac{\partial g_\nu^{-1}}{\partial\Delta_{\nu'}}\frac{\partial\Delta_{\nu'}}{\partial A}+\left.\frac{\partial f_\nu}{\partial g_\nu^{-1}}\right|_{\Delta}\left.\frac{\partial g_\nu^{-1}}{\partial A}\right|_{\Delta}, \tag{5}$$

$$\forall_\nu:\ 0=\left.\frac{\partial f_\nu}{\partial\Delta_\nu}\right|_{g^{-1}}\frac{\partial\Delta_\nu}{\partial A}+\sum_{\nu'}\frac{\partial f_\nu}{\partial g_\nu^{-1}}\left(-\delta_{\nu\nu'}\hat{1}-\frac{\partial\Sigma_\nu}{\partial\Delta_{\nu'}}\right)\frac{\partial\Delta_{\nu'}}{\partial A}-\left.\frac{\partial f_\nu}{\partial g_\nu^{-1}}\right|_{\Delta}\left.\frac{\partial\Sigma_\nu}{\partial A}\right|_{\Delta}. \tag{6}$$

Here, $g_\nu^{-1}=i\nu-\Delta_\nu-\Sigma_\nu$ acts as the definition of the impurity self-energy Σ. The relevant partial derivatives of the self-consistency condition are

$$\begin{aligned}\left.\frac{\partial f}{\partial\Delta}\right|_{g^{-1}}&=\int d\mathbf{k}[g^{-1}+\Delta-t_\mathbf{k}]^{-1}\frac{\partial\Delta}{\partial\Delta}[g^{-1}+\Delta-t_\mathbf{k}]^{-1}\\&=\int d\mathbf{k}\,G_\mathbf{k}G_\mathbf{k}\equiv\chi^{0,\mathrm{lat}},\end{aligned} \tag{7}$$

$$\begin{aligned}\left.\frac{\partial f}{\partial g^{-1}}\right|_{\Delta}&=-(g^{-1})^{-1}\frac{\partial g^{-1}}{\partial g^{-1}}(g^{-1})^{-1}\\&\quad+\int d\mathbf{k}[g^{-1}+\Delta-t_\mathbf{k}]^{-1}\frac{\partial g^{-1}}{\partial g^{-1}}[g^{-1}+\Delta-t_\mathbf{k}]^{-1}\\&=\int d\mathbf{k}\,G_\mathbf{k}G_\mathbf{k}-gg\equiv\chi^{0,\mathrm{lat}}-\chi^{0,\mathrm{imp}}\equiv\tilde{\chi}^0,\end{aligned} \tag{8}$$

where so-called bubbles of Green's functions are denoted as χ^0, and these are rank-4 tensors in orbital space. They are diagonal in frequency, since f depends on g and Δ at the same frequency only. Seen as a bubble, both propagators have the same frequency because the $\omega=0$ response is being considered. In particular, $\chi^{0,\mathrm{lat}}$ is the bubble of lattice Green's functions (at $q=0$, $\omega=0$), $\chi^{0,\mathrm{imp}}$ is the impurity bubble (also at $\omega=0$), and $\tilde{\chi}^0$ is their difference, the nonlocal part of the bubble. The only term connecting different Matsubara frequencies, $\partial\Sigma/\partial\Delta$ is related to the impurity vertex [19] F,

$$\frac{\partial\Sigma_\nu}{\partial\Delta_{\nu'}}\equiv F_{\nu\nu'}g_{\nu'}g_{\nu'}=F\chi^{0,\mathrm{imp}}. \tag{9}$$

Note that both F and $\chi^{0,\mathrm{imp}}$ are rank-4 tensors in orbital space, so they are matrices in pair space and their product is the matrix product in pair space, i.e., another rank-4 tensors in orbital space. Diagrammatically, this corresponds to contracting two legs of both objects.

Inserting these results into Eq. (6) and using the pair-frequency space notation (i.e., bubbles and vertices are matrices, derivatives with respect to A are vectors) gives

$$\begin{aligned}0&=\sum_{\nu'}\left[\chi^{0,\mathrm{lat}}_{\nu\nu'}-\tilde{\chi}^0_{\nu\nu'}-\left(\tilde{\chi}^0\frac{\partial\Sigma}{\partial\Delta}\right)_{\nu\nu'}\right]\frac{\partial\Delta_{\nu'}}{\partial A}-\tilde{\chi}^0\frac{\partial\Sigma_\nu}{\partial A},\\0&=\sum_{\nu'}(\chi^{0,\mathrm{imp}}-\tilde{\chi}^0F\chi^{0,\mathrm{imp}})_{\nu\nu'}\frac{\partial\Delta_{\nu'}}{\partial A}-\tilde{\chi}^0\frac{\partial\Sigma_\nu}{\partial A}.\end{aligned} \tag{10}$$

Isolating $\partial\Delta/\partial A$ gives

$$(\chi^{0,\mathrm{imp}}-\tilde{\chi}^0F\chi^{0,\mathrm{imp}})\frac{\partial\Delta}{\partial A}=\tilde{\chi}^0\frac{\partial\Sigma}{\partial A}, \tag{11}$$

$$\frac{\partial\Delta}{\partial A}=(\chi^{0,\mathrm{imp}})^{\neg1}(\hat{1}-\tilde{\chi}^0F)^{\neg1}\tilde{\chi}^0\frac{\partial\Sigma}{\partial A}, \tag{12}$$

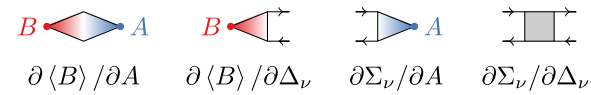
with $\hat{1}$ the unit matrix in pair-frequency space. Finally,

$$\frac{d\langle B\rangle}{dA}=\left.\frac{\partial\langle B\rangle}{\partial A}\right|_{\Delta}+\left.\frac{\partial\langle B\rangle}{\partial\Delta}\right|_{A}(\chi^{0,\mathrm{imp}})^{\neg1}(\hat{1}-\tilde{\chi}^0F)^{\neg1}\tilde{\chi}^0\frac{\partial\Sigma}{\partial A}. \tag{13}$$

Here, $\partial\Sigma/\partial A$ is the connected time-ordered correlator $\langle\mathcal{T}Acc^\dagger\rangle-\langle A\rangle\langle\mathcal{T}cc^\dagger\rangle$ with the fermionic legs amputated [54], while $\partial\langle B\rangle/\partial\Delta$ is the connected time-ordered correlator $\langle\mathcal{T}Bcc^\dagger\rangle-\langle B\rangle\langle\mathcal{T}cc^\dagger\rangle$ and $(\chi^{0,\mathrm{imp}})^{\neg1}$ corresponds to amputating both its fermionic legs. Both depend on a single fermionic frequency (and $\omega=0$). Finally, $\partial\langle B\rangle/\partial A$ is the connected time-ordered correlator $\langle\mathcal{T}BA\rangle-\langle B\rangle\langle A\rangle$. The ingredients of Eq. (13) are illustrated in Fig. 1, while Fig. 2 contains a diagrammatic representation of Eq. (13) itself, where the geometric series $(\hat{1}-\tilde{\chi}^0F)^{\neg1}$ has been expanded up to second order in the nonlocal Bethe-Salpeter kernel [19] $\tilde{\chi}^0F$.

Second-order phase transitions. Looking at Eq. (13), none of the impurity correlation functions can be responsible for the divergence, since the impurity model is a finite system at finite temperature, whose expectation values are smooth functions of the model parameters. Instead, the inversion in Eq. (13) is the origin of divergences [19]. Exactly at the critical point, one of the eigenvalues of the nonlocal Bethe-Salpeter kernel $\tilde{\chi}^0F$ is equal to 1, so the inverse in Eq. (13) is divergent, and the associated eigenvector V describes the order parameter of the transition. This can be seen as a matrix generalization of the Stoner criterion, where $\tilde{\chi}^0$ describes how many electronic fluctuations are available while F is the effective interaction between correlated electrons.

In the pair-frequency space view, the second term in Eq. (13) is a scalar product of the form vector-matrix-vector. The matrix which is inverted in Eq. (13) is independent of A and B, i.e., it is always a *two*-particle kernel, even when A and B are many-particle operators, and a single eigenvector V describes the divergent linear response of any observables with respect to any applied field. The overlap between the eigenvector V and the two capping vertices $\partial\langle B\rangle/\partial\Delta$ and $\partial\Sigma/\partial A$ determines if a particular response function $d\langle B\rangle/dA$



$\partial\langle B\rangle/\partial A$ $\partial\langle B\rangle/\partial\Delta_\nu$ $\partial\Sigma_\nu/\partial A$ $\partial\Sigma_\nu/\partial\Delta_{\nu'}$

FIG. 1. Diagrammatic representation of contributors to the response. The black lines with arrows indicate fermionic propagators. Note that some of the fermionic propagators are amputated and some are not (see main text for definitions). The operators A and B are denoted by small blue and red dots, respectively.

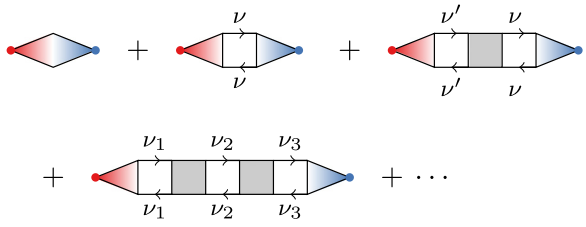


FIG. 2. Diagrammatic representation of the linear response. The geometric series is shown up to second order, higher-order terms have additional vertices, and particle-hole propagators inserted. Lines with arrows represent the nonlocal propagator $\tilde{G}$, and a pair of these lines represents a nonlocal bubble $\tilde{\chi}^0$.

is divergent at the critical point. In particular, symmetry can lead to vanishing overlap, thereby avoiding a divergent response.

The Supplemental Material [55] shows the antiferromagnetic transition [56,57] as an example, where the linear response with respect to the staggered field ($A = h_{\mathrm{AF}}$) is divergent at $U = U_c$ while the linear response with respect to the interaction strength ($A = U$) is not. The reason is that for the antiferromagnetic transition, the relevant eigenvector V is spin antisymmetric and thus has nonzero overlap with $\partial\Sigma/\partial h$ which is also spin antisymmetric, but zero overlap with $\partial\Sigma/\partial U$ which is spin symmetric.

Another example is the metal-insulator transition in the particle-hole symmetric Hubbard model, where at the critical point $d\langle D\rangle/dU$ is divergent [41,42] but $d\langle n\rangle/d\mu$ is not [43] because of frequency symmetry [19,38,44]: The eigenvector V is frequency antisymmetric while $\partial\Sigma/\partial\mu$ and $\partial\langle n\rangle/\partial\Delta$ are frequency symmetric at particle-hole symmetry [58], so their overlap with V is zero. Below the critical temperature, the resulting hysteresis region has three coexisting solutions (two stable) with different values of $\langle D\rangle$, but a single value of $\langle n\rangle$.

Physically, the reason for any divergence in DMFT is a runaway self-consistent response of Δ to an external perturbation, and the self-consistency equation governing Δ only involves single-particle operators. In linear response, taking first derivatives thus leads to two-particle correlations only, explaining why the two-particle kernel is sufficient.

On the other hand, the first nonlinear response, $d^2\langle B\rangle/dA_1dA_2$, requires a three-particle equivalent of the Bethe-Salpeter equation. It enters through the derivative $\partial^2\Delta/\partial A_1\partial A_2$, which can be isolated from a three-particle equivalent of Eq. (5). This equation will contain a three-particle impurity vertex $\partial^2 g^{-1}/\partial\Delta^2$. Subsequent higher orders require Bethe-Salpeter equations of higher and higher order.

Superconductivity. Superconductivity can be described in DMFT and its cluster extensions using the Nambu formulation [59–62], where the dynamical mean field also has anomalous components of the form $\Delta^{\mathrm{an.}}(c^\dagger c^\dagger + cc)$, which leads to anomalous components in g and in all vertices. To find instabilities towards a superconducting phase, it is necessary to take these anomalous processes into account in the Bethe-Salpeter equation, even in the normal phase, where it corresponds to the particle-particle channel of the nonlocal Bethe-Salpeter equation (see Refs. [63,64] for a recent discussion). For this situation, the present derivation can be generalized by incorporating a Nambu index into the orbital label, which leads to a treatment of the particle-particle and particle-hole channels on equal footing. Diagrammatically, propagators and capping vertices with two incoming or outgoing fermions are then allowed. With this generalization, the conclusions about the nature of second-order transitions in DMFT hold, since the necessary ingredient is that the dynamical mean-field couples to precisely two fermionic operators, regardless of their Nambu index.

Extensions. The so-called extended DMFT [65–69] (EDMFT) and its generalizations [58,70–73] introduce additional dynamical mean fields which couple to densities or other composite operators instead of individual fermionic operators, e.g., a term $\Lambda(\tau-\tau')n(\tau)n(\tau')$ in the impurity model. This $\Lambda(\omega)$ is determined using a many-particle self-consistency condition similar to Eq. (2), whose variation automatically generates many-particle vertices even when single-particle observables such as $dn/d\mu$ are considered [52]. Thus, the two-particle Bethe-Salpeter kernel is generally insufficient to identify second-order transitions in these extensions of DMFT.

Locality. The approach presented here is restricted to perturbations and operators which are impurity local and spatially homogeneous, $\mathbf{q}=\mathbf{0}$. The generalization to commensurate $\mathbf{q}\neq\mathbf{0}$ is straightforward [51,55]. On the other hand, an extension to nonlocal operators, e.g., the linear response to changes in $t_{\mathbf{k}}$ or the identification of bond ordering, requires more work. In the same vein, the response to changes in temperature changes the Matsubara frequencies themselves, which requires an extension of the current formalism.

In conclusion, I have shown that the linear response in dynamical mean-field theory is mainly governed by the two-particle Bethe-Salpeter equation, even when many-particle observables are considered. In fact, the specific form of the applied perturbation and the studied observable only appears as capping vertices at the two ends of the Bethe-Salpeter ladder. This generalizes previous formulas for the (density, double occupancy)-(μ, U) response matrix [41] to arbitrary local observables and perturbations. The DMFT linear response functions are equivalent to second derivatives of the free energy [18,29,41], so this result shows that any DMFT second-order phase transition or thermodynamic instability must appear in the nonlocal Bethe-Salpeter kernel. Furthermore, the spatial structure of the equation is entirely captured by the nonlocal Bethe-Salpeter kernel, so all divergent response functions have the same correlation length close to the phase transition.

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