Asymptotic limit of high spatial dimensions and thermodynamic consistence

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The question of thermodynamic consistence and Φ-derivability of the asymptotic limit of high spatial dimensions for quantum itinerant models is addressed. It is shown that although the irreducible \( n \)-particle Green functions are local, reducible vertex functions retain different momentum dependence. As a consequence, the vertex corrections to conductivity do not generally vanish in the mean-field limit. The mean-field theory is a Φ-derivable approximation only if regular nonlocal or anomalous local external sources are admitted.

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The Baym and Kadanoff concept of thermodynamic consistence and conserving character of approximations is derived from an observation that knowing a thermodynamic potential as a functional of external disturbances we can reconstruct thermally averaged values of any observable \( \mathcal{Q} \). The most transparent way to guarantee thermodynamic consistence is to find a generating Luttinger-Ward functional \( \Phi(G, J) \) depending on the fully renormalized one-particle propagator \( G_j \) in the presence of a set of external disturbances \( J_\alpha \). Functional derivatives of the generating functional with respect to \( G \) lead to irreducible functions, while functional derivatives with respect to the external sources \( J_\alpha \) to reducible ones \( \Sigma \). The \( n \)-th orders of the derivatives generate \( n \)-particle functions, either irreducible or reducible. This definition of higher-order Green functions guarantees a conserving character of the approximation. But it may be in conflict with criteria for selecting Feynman diagrams contributing to the \( n \)-particle Green functions in special limits such as the mean-field theory. It is defined as an exact solution in infinite spatial dimensions.

Selection of relevant diagrams in high spatial dimensions is determined by a scaling of nonlocal terms in lattice Hamiltonians. It can, from principal reasons, be made only within a perturbation expansion. In lattice models of correlated and/or disordered electrons one can conclude from finiteness of the energy density on a collapse of diagrams to a single site, or on irrelevance of momentum conservation at internal vertices. The one-electron self-energy gets local in infinite spatial dimensions and can be generated from a Luttinger-Ward functional depending on only local elements of the full one-particle propagator. Such a functional, or its Legendre transform was constructed for Hubbard-like models without and with chemical randomness.

As far as we are interested only in the dynamics of one-particle quantities, we can completely neglect the off-diagonal elements of the propagator.

The limit of high spatial dimensions has an asymptotic character, i.e., leading orders in the small parameter \( d^{-1} \) are to be kept for each quantity. The off-diagonal elements of the one-particle propagator scale on a hypercubic lattice as \( d^{-|i-j|/2} \), where \(|i-j|\) the lattice distance between sites \( i \) and \( j \). The off-diagonal elements are essential for susceptibilities deciding about the existence of solutions with a long-range order.

To prove a long-range order we have to evaluate two-particle susceptibilities (correlation functions) at fixed momenta. The collapse of diagrams in the mean-field limit is well defined in the lattice space but the corresponding reduction in the momentum dependence of two-particle Green functions, depending generally on three momenta, is less evident. Particularly, if the limit \( d \to \infty \) is used within the Baym and Kadanoff conserving scheme, the locality in two-particle functions is still understood controversially.

It is the aim of this Letter to address the problem of compatibility of the high-dimensional asymptotics with the Baym concept of Φ-derivability of all Green functions. We show that all nonperturbative irreducible vertex functions are local and can be generated from the Luttinger-Ward functional via derivatives w.r.t. local propagators. Reducible \( n \)-particle Green functions are generally nonlocal, but the nonlocality is perturbative. They can be derived from the generating functional if we either keep the external sources nonlocal or allow for local anomalous perturbations that do not conserve charge or spin.

We can construct the limit to infinite lattice dimensions within the Baym and Kadanoff scheme. We start with a general model the partition function of which can be represented via a functional integral

\[
Z \{J; G^{(0)}\} = \int \mathcal{D}\varphi\mathcal{D}\varphi^* \exp \left\{ -\varphi^* \eta G^{(0)-1} \varphi + \varphi^* J \varphi + U [\varphi^*, \varphi] \right\}
\]

where, for the sake of simplicity, we suppressed all decoration indices for the lattice and internal degrees of freedom. All the interaction is contained in a local functional \( U \), \( J \) stands for external sources, and \( \eta = \pm 1 \) for bosons, fermions, respectively.

A renormalized perturbation theory is achieved if we replace the bare one-particle propagator \( G^{(0)} \) with \( G = (G^{-1} + \Sigma)^{-1} \). It is a straightforward task to write
down a generating functional for the renormalized perturbation theory. The grand potential contains the renormalized one-particle propagator $G$ and the self-energy $\Sigma$ as variational functions as follows

$$\Omega [J; G, \Sigma] = -\beta^{-1} \ln Z \left\{ 0; G^{-1} + \Sigma \right\} + \eta \beta^{-1} \text{tr} \ln G + \eta \beta^{-1} \text{tr} \ln \left[ G^{(0)-1} - \eta J - \Sigma \right].$$ (2)

The physical values of $G$ and $\Sigma$ are obtained from the equations $\delta \Phi / \delta \Sigma = 0$ and $\delta \Phi / \delta G = 0$, respectively. Note that $G$ and $\Sigma$ are Legendre conjugate variables.

Representation (1) holds in any dimension. In the limit $d \to \infty$ we have to separate site-diagonal and off-diagonal parts of $G$ and $\Sigma$. The electron systems show the following asymptotics in high dimensions

$$G = G^{\text{diag}}[\delta^0] + G^{\text{off}}[d^{-1}/2], \quad \Sigma = \Sigma^{\text{diag}}[\delta^0] + \Sigma^{\text{off}}[d^{-3}/2].$$ (3)

The grand potential in the limit $d = \infty$ is obtained if the off-diagonal parts $G^{\text{off}}$ and $\Sigma^{\text{off}}$ are completely neglected in (2). The nonlocal part of the grand potential is contained solely in the bare propagator $G^{(0)}$. Hence, all nonlocal quantities in the mean-field theory are treated perturbatively without renormalizations.

According to Baym and Kadanoff, $n$-particle Green functions can be generated via successive applications of functional derivatives w.r.t. the external source $J$. Local sources are dominant in $d = \infty$ and we have for one- and two-particle functions

$$G_{11'}[J] = -\beta \frac{\delta \Omega[J]}{\delta J_{11'}} = \langle \phi_{11'}^c \phi_{11'} \rangle_J, \quad L_{11', 22'} = \eta \frac{\delta G_{11'}}{\delta J_{22'}}$$ (4)

where $1 \equiv (R_1, t_1, \sigma_1, \ldots)$ denotes a set of degrees of freedom in the space-time representation. The bar indicates a coordinate of a complex-conjugate field and any decoration of the labeling index refers always to the undecorated lattice site.

We now find equations of motion for two-particle functions and an explicit representation for the two-particle vertex in $d = \infty$. As a first step we subtract the free two-particle propagation from $L_{11', 22'}$ and define a new vertex function

$$\Gamma_{11', 22'} = \sum_{1', 1''} G_{11', 1''}^{-1} G_{1'', 22'}^{-1} \left[ L_{1', 1'', 22''} - \eta G_{1', 22''} G_{22', 1''}^{-1} G_{2', 1''}^{-1} \right]$$ (5)

where the inversions use only the site-diagonal functions.

Analogously we define a local vertex $\gamma_{11', 1''}$ from an averaged cumulant two-particle function

$$\gamma_{11', 1''} = \eta \sum_{2, 2''} \delta_{R_1, R_2} G_{12}^{-1} G_{2', 2''}^{-1} \left( \langle \phi_{1, 2}^c \phi_{2', 2''} \phi_{1''} \phi_{2'} \rangle - \langle \phi_{1, 2}^c \phi_{2', 2''} \phi_{1''} \phi_{2'} \rangle - \eta \langle \phi_{1, 2}^c \phi_{2', 2''} \phi_{1''} \phi_{2'} \rangle G_{11', 22'}^{-1} G_{1', 22''}^{-1} \right).$$ (6)

We use the above definitions in the mean-field limit of the generating functional (2) with inhomogeneous but local one-particle functions to find an explicit form of a two-particle function $\delta \Sigma_{11', 22'}$ needed for the evaluation of $L_{11', 22'}$. If we switch from $L$ to $\Gamma$ we finally obtain a Bethe-Salpeter integral equation of motion

$$\sum_{3, 3'} \left\{ \delta_{3, 1} \delta_{3', 1'} - \eta \sum_{1', 1''} \gamma_{11', 1''} G_{11', 1''}^{\text{off}} G_{11', 1''}^{\text{off}} \right\} \Gamma_{33', 22'} = \delta_{R_1, R_2} \gamma_{11', 22'}.$$ (7)

This form of the Bethe-Salpeter equation is natural for the mean-field limit, since it separates diagonal and off-diagonal propagators. The former are contained nonperturbatively in the local vertex $\gamma$ while the latter participate only via two-particle bubbles forming the nonlocal part of the vertex $\Gamma$.

We can further introduce a two-particle irreducible vertex that we denote $\Lambda$. This function enables us to replace in (7) the off-diagonal one-particle propagators with the unrestricted ones. A new equation of motion with the two-particle irreducible vertex reads

$$\sum_{3, 3'} \left\{ \delta_{3, 1} \delta_{3', 1'} - \eta \sum_{1', 1''} \Lambda_{11', 1''} G_{11', 1''}^{\text{off}} G_{11', 1''}^{\text{off}} \right\} \Gamma_{33', 22'} = \delta_{R_1, R_2} \Lambda_{11', 22'}.$$ (8)

This form of the Bethe-Salpeter equation is common in general treatments without the collapse of diagrams. In the mean-field limit, $d = \infty$, the irreducible vertex $\Lambda$ is the same for $\gamma$ as well as for $\Gamma$.

The irreducible vertex function is related to the self-energy via a generalized Ward identity

$$\Lambda_{11', 22'} = \delta_{R_1, R_2} \frac{\delta \Sigma_{11', 22'}}{\delta G_{22'}}$$ (9)

following directly from the above derivation. Since the irreducible vertex functions appear in integral kernels of the Bethe-Salpeter equations of motion for higher-order Green functions, they get local in the lattice space in the mean-field limit and hence independent of momenta in spatially homogeneous solutions. Variations at fixed momenta as used in [8,10] loose their meaning where off-diagonal elements in the lattice space are treated perturbatively. Nonlocal corrections to the irreducible vertex functions are negligible in leading order of $d \to \infty$.

The above derivation of the two-particle vertex function within the Baym and Kadanoff conserving scheme is a generalization of the Brandt and Mielisch construction of charge susceptibilities in the Falicov-Kimball model [8]. The review on the $d = \infty$ approach [8] uses, however, a different construction of two-particle functions. The question is whether the two constructions lead to the same vertex function. In other words, does $\Gamma_{11', 22'}$
contain all leading $d^{-1}$ contributions to the two-particle vertex?

It is undisputable that maximally two different lattice sites are relevant for two-particle functions in $d = \infty$. Two-particle Green functions have four end points. We generally have three possibilities how to select couples of end points from the same lattice site, Fig. 1.

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Attaching end points of two-particle functions to lattice sites determines multiple repetition of nonlocal two-particle bubbles in the Bethe-Salpeter equations for two-particle reducible functions. Each choice in Fig. 1 is of the same order in the parameter $d^{-1}$ and represents a different two-particle reducibility. The first choice, resulting from the above Baym and Kadanoff construction, leads to the so-called interaction two-particle channel of a chain of spin-triplet polarization bubbles screening the bare interaction. The second type of nonlocality in the two-particle function induces electron-hole, and the last one then electron-electron (spin-singlet) multiple scatterings.

We use the three ways of constructing nonlocal two-particle functions and define three types of multiplication of the off-diagonal bubbles and the local vertex in the Bethe-Salpeter equation.

The three functions $\kappa^\alpha$ form three integral kernels of the Bethe-Salpeter equations for three vertex functions $\Gamma^\alpha$. We hence have three different nonlocal vertex functions being of the same order in the small parameter $d^{-1}$. These functions differ in their nonlocal parts and reduce to the same vertex $\gamma$ when all four end points are from the same site. The full vertex function is then a sum of the solutions to the three Bethe-Salpeter equations from which the local vertex $\gamma$ must be twice subtracted.

It is more instructive to give an explicit representation for the full two-particle vertex function in the Fourier representation with fermionic $k = (\mathbf{k}, i\omega_n)$ and bosonic $q = (\mathbf{q}, i\nu_m)$ four-momenta. The three contributions to the full vertex function in $k$-space are obtained by Fourier transforming (8). Two-particle bubbles

$$\chi_{,\sigma}\sigma'(\mathbf{q}, i\omega_n, i\omega_{n'}) = \frac{1}{N} \sum_\mathbf{k} G_\sigma(\mathbf{k}, i\omega_n)G_{\sigma'}(\mathbf{q} \pm \mathbf{k}, i\omega_{n'})$$

(11)

carry the surviving momentum dependence of the two-particle functions in the infinite-dimensional limit. We have an explicit representation (8) for a hypercubic lattice with the nearest-neighbor hopping $t = 1/\sqrt{d}$

$$\chi_{\sigma,\sigma'}(\mathbf{q}, i\omega_n, i\omega_{n'}) = -\text{sign}(\omega_n\omega_{n'}) \left\{ \int_0^\infty d\lambda \lambda^\alpha \theta(\omega_n)\theta(\lambda'\omega_{n'}) \exp \left\{ i(\lambda x_\sigma(i\omega_n) + \lambda' x_{\sigma'}(i\omega_{n'})) \right\} \right\}$$

(12)

with $x_\sigma(z) = z + \mu + \sigma B - \Sigma_\sigma(z)$ and $X(\mathbf{q}) = d^{-1} \sum_{\nu=1}^d \cos(q_\nu)$. The last quantity, measuring nonlocality in infinite dimensions, behaves as a Gaussian random variable with variance $d^{-1}$ when summed over momenta. The local bubble, entering the local vertex $\gamma$, is a product of local propagators and equals $\chi$ with $X = 0$.

To clarify the meaning of different four-momenta in the vertex functions we introduce a generic notation shown in Fig. 1. The full vertex function in leading asymptotic $d^{-1}$ order in the absence of external sources $J_\alpha$ reads in this notation

$$\Gamma_{\sigma,\sigma'}(\mathbf{k}, i\omega_n; \mathbf{k}', i\omega_{n'}; \mathbf{q}, i\nu_m) = \Gamma_{\sigma,\sigma'}^{U}(\mathbf{q}; i\omega_n, i\omega_{n'}; i\nu_m) + \Gamma_{\sigma,\sigma'}^{eh}(\mathbf{k} + \mathbf{q}; i\omega_n, i\omega_{n'}; i\nu_m) - \gamma_{\sigma,\sigma'}(i\omega_n, i\omega_{n'}; i\nu_m) + \Gamma_{\sigma,\sigma'}^{ee}(\mathbf{k} - \mathbf{q}; i\omega_n, i\omega_{n'}; i\nu_m) - \gamma_{\sigma,\sigma'}(i\omega_n, i\omega_{n'}; i\nu_m)$$

(13)

where the each momentum-dependent contribution is determined from a separate Bethe-Salpeter equation with the appropriate multiplication from (10). Each of the nonlocal terms in (13) depends only on one transfer momentum reflecting the fact that maximally two different lattice sites are relevant. However, because of different ways to connect the end points in the two-particle vertex, the full function depends on all three independent momenta. We have $\gamma(\ldots) = N^{-1} \sum_\mathbf{q} \Gamma^\alpha(\mathbf{q}; \ldots)$ for all channels $\alpha = U, eh, ee$. 

3
To construct a Luttinger-Ward functional $\Phi$ generating higher-order functions of the mean-field theory, we have to account properly for the off-diagonal propagators. Unlike the diagonal elements, suffering no restriction in $d = \infty$, the off-diagonal propagators contribute only under favorable circumstances, i.e., when properly combined with summations over neighboring sites. That is why the off-diagonal elements appear in a perturbative manner in the mean-field limit. However, going to higher-order Green functions we have to take into account higher powers of the off-diagonal elements. The two-particle functions are generally of order $d^{-1}$. They can be generated via functional derivatives of the local, but inhomogeneous self-energy, or by derivatives of the nonlocal self-energy w.r.t. nonlocal sources or the off-diagonal propagator. The leading order of the nonlocal part of the self-energy is $d^{-3/2}$ and of the off-diagonal propagator $d^{-1/2}$. Hence, a functional derivative $\delta \Gamma_{\text{off}} / \delta G_{12} \propto d^{-1}$ contributes in leading order to the two-particle vertex. To turn the mean-field theory a $\Phi$-derivable approximation, we have to consider nonlocal external sources $J_{\text{off}}$ connecting fluctuating fields at different lattice sites. The two-particle functions not derivable with local external sources can then be generated via nonlocal derivatives

$$L_{11',22'}^{\text{ch}} = \frac{\delta G_{12}}{\delta J_{12'}^{\text{off}}} \quad L_{11',22'}^{\text{ee}} = \frac{\delta G_{12}}{\delta J_{12'}^{\text{off}}}.$$ (14)

Generally, $n$-particle functions demand to keep nonlocal sources in $\Phi$ up to the $n$th power. Once we introduce nonlocal external sources into $\Phi$, we have to expand all quantities, including the one-particle propagator and the self-energy appearing in $\Phi$ in powers of $J_{\text{off}}$.

This perturbative construction with off-diagonal external sources is applicable only in the high-temperature phase. At low temperatures, each constituent of the two-particle vertex function (13) controls a different type of fluctuations that may cause phase transitions. A singularity in the function $\Gamma^U$ signals a longitudinal, in $\Gamma^{\text{ch}}$ a transversal (magnetic) order, and a singularity in $\Gamma^{\text{ee}}$ indicates a superconducting instability. Neglecting any of the components of the full vertex function means suppressing potentially relevant fluctuations.

The latter two transitions give rise to anomalous Green functions in the ordered phase. To describe these phases correctly we have to introduce anomalous (complex) local sources into the partition sum connecting, in a hermitian manner, $\varphi_i^{\dagger} \varphi_j$ for the transversal order and $\varphi_i^{\dagger} \varphi_j$ in the superconducting phase (12). These anomalous perturbations induce local anomalous propagators and self-energies as variational functions in the generating functional (13). The mean-field Luttinger-Ward functional, that is able to generate the complete leading asymptotics of higher-order Green functions and to describe all low-temperature phases, must contain either regular (of density type) nonlocal, or anomalous (complex) but local external sources and their conjugate variational functions. However, only local variational functions and order parameters are treated nonperturbatively in $d = \infty$.

The newly derived vertex function (13) contains the full momentum dependence and fulfills all the symmetry transformations of the exact solution. It means that the current-current correlation function and consequently the electrical conductivity do have nontrivial vertex corrections contrary to general expectations (14,7). It is only the function $\Gamma^{\text{ch}}$ that looses vertex corrections to the conductivity due to the symmetry. The other two, explicitly depending on $q$, correct the conductivity of a single particle-hole bubble in high dimensions.

To conclude, we showed how to construct a generating functional for the mean-field theory with the correct asymptotics of higher-order Green and correlation functions. The mean-field theory as a complete solution in $d = \infty$ is a $\Phi$-derivable theory if either regular nonlocal or anomalous local sources are introduced. Only then we are sure to generate the complete leading asymptotics of higher-order vertex functions and to describe all possible low-temperature phases. However, the full higher-order vertex functions in $d = \infty$ cannot be generated from single equations or directly via functional derivatives from the Luttinger-Ward functional as in the exact theory.

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