Mean-field theories for disordered electrons: Diffusion pole and Anderson localization

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We discuss conditions to be put on mean-field-like theories to be able to describe fundamental physical phenomena in disordered electron systems. In particular, we investigate options for a consistent mean-field theory of electron localization and for a reliable description of transport properties. We argue that a mean-field theory for the Anderson localization transition must be electron-hole symmetric and self-consistent at the two-particle (vertex) level. We show that such a theory with local equations can be derived from the asymptotic limit to high spatial dimensions. The weight of the diffusion pole, i.e., the number of diffusive states at the Fermi energy, in this mean-field theory decreases with the increasing disorder strength and vanishes in the localized phase. Consequences of the disclosed behavior for our understanding of vanishing of electron diffusion are discussed.

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I. INTRODUCTION

Mean-field theories play an important role in the description of thermodynamic systems. They are intended and used as a first approximation offering a qualitative picture of the physics of the studied phenomena. The mean-field concept has developed from its initial intuitive ideas of van der Waals and Weiss through the Landau theory of critical phenomena to its present sophistication and systematics provided by the limit to infinite-dimensional lattice models. At present, a modern mean-field theory is no longer a weak-coupling approximate treatment neglecting spatial fluctuations. It represents a comprehensive theory providing a phase diagram in the whole range of the input parameters and simulating the exact behavior in specific limiting situations. Without a mean-field theory we are mostly unable to identify the relevant fluctuations, the mean values of which are reflected by thermodynamic (order) parameters. Mean-field theory is particularly important for critical phenomena with divergent correlation functions, where it allows us to handle singularities in a consistent and manageable way and to select the proper low-temperature phase, at least above the lower critical dimension.

Mean-field theories were primarily developed for collective phenomena in interacting systems. Nontrivial and sometimes not easily understandable effects are, however, also induced by randomness. Randomness, in connection with interaction or with quantum interference, can cause significant and sometimes even unexpected changes in the behavior of the system. Since mostly no exact solutions are available for disordered systems, a mean-field approximation has become one of the most powerful tools to handle fluctuations in the chemical composition of solids.

Milestones of a mean-field theory for disordered (noninteracting) electron systems were laid at the end of the 1960s and the beginning of the 1970s. The so-called coherent potential approximation (CPA) developed at that time is a self-consistent approximation describing rather accurately the electronic structure and thermodynamic properties of random alloys not only at the model level but also in realistic settings.[1] Later on, the CPA was shown to fit the modern definition of the mean-field theory as an exact solution of the model system in infinite spatial dimensions.[2,3]

The coherent potential approximation is nowadays considered as an archetype of mean-field theories of quantum disordered and interacting systems. Its generalized form[4] offers one possible interpretation of equations of motion in the dynamical mean-field theory (DMFT).[5] The CPA has proved reliable to produce an accurate equilibrium electronic structure of disordered systems[6] as well as transport properties of random alloys.[7] It, however, fails to account for intersite quantum coherence and backscattering effects. The CPA is essentially unable to go beyond the semiclassical description of transport properties qualitatively captured by the Boltzmann equation. This inability is due to the fact that the CPA does not include vertex corrections to the electrical conductivity independently of how strong the disorder may be.[8] The CPA is hence unsuitable for the description of one of the most prominent features of disordered systems, Anderson localization.

Anderson localization in disordered or amorphous solids takes place when there are available electronic states at the Fermi surface but no diffusion or charge transport at long distances is observed. Possibility of the absence of diffusion in impure metals and alloys was proposed by Anderson on a simple tight-binding model of disordered noninteracting electrons.[9] Since then, vanishing of diffusion, now called Anderson localization, has attracted much attention of both theorists and experimentalists.[10,11] In spite of a considerable portion of amassed experimental data, disclosed various specific and general aspects of the Anderson metal-insulator transition, and a number of theoretical and computational approaches so far developed we have not yet reached complete understanding of Anderson localization. Although many features of the critical behavior at the Anderson localization transition have been uncovered, the position of this disorder-driven metal-insulator transition within the standard classification scheme of phase transitions with control and order parameters has remained unclear. It has been mainly due to the nonexistence of an appropriate mean-field-like theory for this phenomenon.

The existing attempts to go beyond the single-site (mean-field) approximations for disordered systems based on cluster expansions have concentrated mostly on one-particle properties and momentum-dependent self-energy (coherent potential). Instead of individual sites, their clusters are self-consistently embedded in an average medium. Apart from the traveling-cluster approximation,[12,13] cluster expansions in the direct space fail to warrant global analytic properties of the self-energy, and hence spurious effects can emerge.[14,15] An alternative cluster expansion with discrete sets of available momenta was recently suggested so as analytic (Herglotz) properties of the resulting averaged propagators and the self-energy were guaranteed.[16] Cluster approximations, however, reduce spatial quantum coherence only to a discrete set of lattice sites or momenta. Such approximations then remain perturbative in the coherence range and cannot lead to Anderson localization for which we need long-range coherence with infinite-many backscattering or "crossed" diagrams.

Only very recently the present authors demonstrated that a mean-field-like solution for the Anderson metal-insulator transition can be derived from the asymptotic limit to high (but finite) spatial dimensions.[17] This solution is very close to the CPA in the resulting electronic structure. It shares the analytic properties of the CPA and reduces to it in infinite dimensions. It, however, differs from the CPA significantly in transport properties derived from two-particle functions. In addition to the one-electron self-consistency of the CPA, the mean-field theory is endowed with a two-particle self-consistency. That is, the two-particle irreducible vertices are determined from self-consistent nonlinear equations.

The mean-field-like theory for the disorder driven vanishing of diffusion of Ref. 17 shows some unexpected features. It contradicts the dogma that the weight of the diffusion pole, i.e., the number of diffusing particles, does not depend on the disorder strength. The weight of the diffusion pole is conserved only if all the states near the Fermi energy are finite combinations of Bloch waves for any configuration of the random potential. Or, equivalently, if a Ward identity between self-energy and the irreducible electron-hole vertex holds for all transfer energies.[18,19] We demonstrated in Ref. 20 that once the electron-hole irreducible vertex contains the so-called Cooper pole, the number of extended states at the Fermi level decreases with increasing the disorder strength. Hence, there is no chance for a theory with the Cooper pole to fully satisfy the Ward identity between the averaged one- and two-electron Green functions and to keep the number of diffusive states independent of the disorder strength.

The aim of this paper is to clarify the ambiguities connected with the mean-field concept applied to two-particle functions in disordered electron systems. We leave aside all interaction-driven phenomena and concentrate exclusively on the effects of randomness. We delimit the content and the range of validity of the two existing mean-field theories for the Anderson model of noninteracting electrons—the CPA and that of Ref. 17. The common ground for both theories is the limit to high spatial dimensions. We show that the ambiguity in the identification of the mean-field theory for two-particle functions results from two different ways how it can be derived: either via the generating local functional and Ward identities, or via a direct diagrammatic construction in high dimensions. The former construction, CPA, is suitable only for one-electron spectral and thermodynamic properties. Since the CPA lacks the electron-hole symmetry at the two-particle level, it becomes unreliable when applied to the calculation of transport properties in situations when localization effects are expected, e.g., near band edges. We demonstrate that the latter approach, when properly formulated, can lead to a theory being self-consistent and manifestly electron-hole symmetric at the one-particle level and as well at the two-particle level. The last two conditions are necessary ingredients for a theory being able to describe the Anderson localization transition.

The layout of the paper is as follows. In Sec. II we summarize basic properties of the CPA defined from the limit to infinite spatial dimensions. We show how the averaged grand potential is derived from the local one-particle propagator and the self-energy. The higher-order Green functions are then determined via local external perturbations. The mean-field theory with a two-particle self-consistency is constructed in Sec. III. First, inability of the CPA to reproduce the proper infinite-dimensional limit for two-particle Green functions is demonstrated. Then, using the parquet scheme and the electron-hole symmetry we derive a self-consistent (nonlinear) equation for the irreducible two-particle vertex. This equation is then solved at the mean-field level, i.e., in the leading nontrivial order of the high-dimensional limit. The explicit form of the diffusion pole in high spatial dimensions with its weight dependent on the disorder strength is finally obtained. Consequences of our findings for understanding of the disorder-driven vanishing of diffusion and Anderson localization are discussed in Sec. IV.

II. THERMODYNAMIC MEAN-FIELD THEORY: ONE-PARTICLE SELF-CONSISTENCY

A. One-particle functions and generating functional

To construct a comprehensive mean-field theory for thermodynamic properties of a random system means to find an approximate representation in closed form for the grand potential averaged over random configurations

$$\Omega(\mu) = -\frac{1}{\beta}\left\langle \ln \mathrm{Tr} \exp\left\{-\beta\hat{H} + \beta\mu\hat{N}\right\}\right\rangle_{\mathrm{av}} \tag{1}$$

where μ is the chemical potential and $\hat{N}$ is the particle number operator. We will consider in this paper only a noninteracting lattice electron gas scattered on random impurities and described by the Anderson tight-binding Hamiltonian

$$\hat{H} = \sum_{\langle ij\rangle} t_{ij}\hat{c}_i^\dagger \hat{c}_j + \sum_i V_i \hat{c}_i^\dagger \hat{c}_i, \tag{2}$$

where V_i is a local, site-independent random potential.

It has become evident since the introduction of the concept of the limit to infinite spatial dimensions in quantum itinerant systems that a controllable comprehensive mean-field theory of itinerant models should be defined via this formal limit.[21] In high spatial dimensions the diagonal (local) and off-diagonal (nonlocal) elements of the one-particle

propagator separate from each other. The former are of order $O(d^0)$, while the latter vanish as $d^{-1/2}$, where d is the spatial dimension. The full one-particle propagator and the self-energy have the following high-dimensional asymptotics:

$$G = G^{\mathrm{diag}}[d^0] + G^{\mathrm{off}}[d^{-1/2}], \tag{3a}$$

$$\Sigma = \Sigma^{\mathrm{diag}}[d^0] + \Sigma^{\mathrm{off}}[d^{-3/2}]. \tag{3b}$$

We can classify contributions to the many-body perturbation expansion for the self-energy according to their high-dimensional asymptotic contribution and obtain in the leading order a local approximation for the irreducible part of the one-electron propagator. The interacting part of the thermodynamic potential in infinite spatial dimensions is then a functional of only G^{diag} and Σ^{diag}.[3]

In disordered systems the interparticle interaction is replaced by correlations between scatterings on impurities. The self-energy is here a coherent potential of an effective homogeneous (nonrandom) medium representing the effect of impurity scatterings on the motion of electrons. Since the scatterings are static, we can find an explicit representation of the averaged grand potential in infinite spatial dimensions. We can write

$$\Omega_\mu[\hat{G},\hat{\Sigma}] = F\{\hat{G}^{\mathrm{diag}-1} + \hat{\Sigma}^{\mathrm{diag}}\} - \frac{1}{\beta}\mathrm{Tr}\,\ln\hat{G}^{\mathrm{diag}} - \frac{1}{\beta}\mathrm{Tr}\,\ln(\hat{G}^{(0)-1} - \hat{\Sigma}^{\mathrm{diag}} + \mu) \tag{4a}$$

where we denoted

$$F\{\hat{X}\} = -\frac{1}{\beta}\langle \mathrm{Tr}\,\ln[\hat{X} - \hat{V}]\rangle_{\mathrm{av}} \tag{4b}$$

the local "interacting part" of the thermodynamic potential, in this case the effect of multiple scatterings.[4] The trace operator Tr extends over the lattice space as well as over the Matsubara frequencies. The only nonlocal contribution to the generating functional Ω_μ comes from the bare propagator $\hat{G}^{(0)}$. The site-diagonal (local) complex vectors $G_n^{\mathrm{diag}}(\mu)$ and $\Sigma_n^{\mathrm{diag}}(\mu)$ in fermionic Matsubara frequencies $(2n+1)\pi/\beta$ are variational parameters, the physical values of which are attained at stationarity points of the generating functional (4).

The defining equation for the local element of the averaged one-particle propagator is obtained from an equation $\delta\Omega_\mu/\delta\Sigma_n^{\mathrm{diag}}(\mu)=0$ and the self-energy is determined from $\delta\Omega_\mu/\delta G_n^{\mathrm{diag}}(\mu)=0$. After straightforward manipulations the two equations reduce to

$$1 = \left\langle \frac{1}{1 + [\Sigma_n(\mu) - V_i]G_n(\mu)} \right\rangle_{\mathrm{av}} \tag{5a}$$

and

$$G_n(\mu) = \frac{1}{N}\sum_{\mathbf{k}} G(\mathbf{k}, i\omega_n) = \int \frac{d\epsilon\rho(\epsilon)}{i\omega_n + \mu - \Sigma_n(\mu) - \epsilon}. \tag{5b}$$

We dropped the superscript diag in the local functions and introduced the electronic density of states $\rho(\epsilon)$. Due to the static character of the impurity scatterings the stationarity equations are diagonal in the Matsubara frequencies and can be solved for each frequency independently. Inserting the solution for all Matsubara frequencies to Eqs. (4) we obtain the equilibrium thermodynamic potential for noninteracting electrons scattered on random impurities. The equilibrium thermodynamics of the systems is then determined only by the local irreducible part of the averaged one-particle resolvent. This irreducible part is self-consistently determined from the Soven equation (5).

B. External sources and two-particle functions

Thermodynamics of disordered systems is not of much interest unless interparticle interactions are present. But even then the averaged thermodynamic potentials depend on only one-electron functions. One-electron functions, however, do not contain the complete information about the behavior of statistical ensembles, in particular of disordered systems. The equilibrium thermodynamic potentials do not contain sufficient information from which we could derive transport properties of the system and its response to weak external electromagnetic perturbations. To include the electrical conductivity into the mean-field description, the thermodynamic construction from the preceding section must be extended to include averaged two-particle propagators.

Averaged two-particle propagators in disordered systems contain at least two energy arguments (two in noninteracting and three in interacting systems). The best way to guarantee that one- and two-particle functions are approximated consistently within a single approximate scheme is to use the Baym-Kadanoff concept of external sources added to the equilibrium thermodynamic potential.[22] To introduce higher-order Green functions with several energies (chemical potentials) into the thermodynamic description we must replicate the original system so as for each energy we had an independent replica of the original system, that is, of creation and annihilation operators.

We replicate the creation and annihilation operators and introduce external perturbations into the thermodynamic description via a generalized grand potential of a ν-times replicated system $\Omega^\nu(E_1,E_2,\ldots,E_\nu;U)$ with ν chemical potentials $E_1,\ldots,E_\nu$. An external perturbation U is used to couple different replicas and to break the initial replica independence. We then can write

$$\Omega^\nu(E_1,E_2,\ldots,E_\nu;U) = -\frac{1}{\beta}\left\langle \ln \mathrm{Tr}\exp\left(-\beta\sum_{i,j=1}^{\nu}(\hat{H}_{AD}^{(i)}\delta_{ij} - E_i\hat{N}^{(i)}\delta_{ij} + \Delta\hat{H}^{(ij)})\right)\right\rangle_{\mathrm{av}}, \tag{6}$$

where we assigned to each replica characterized by energy (chemical potential) E_i a separate Hilbert space and denoted $\Delta\hat{H}^{(ij)} = \Sigma_{kl}U_{kl}^{(ij)}\hat{c}_k^{(i)\dagger}\hat{c}_l^{(j)}$ an external perturbation to be set zero at the end. Thermodynamic potential $\Omega^\nu(E_1,E_2,\ldots,E_\nu;U)$ is a generating functional for averaged products of Green functions up to the νth order. In practice, we will use linear-response theory with one- and two-particle Green functions, i.e., $\Omega^\nu(E_1,E_2,\ldots,E_\nu;U)$ is expanded up to U^2. Therefore it is sufficient to introduce only two replicas.

In fact we are interested only in corrections to the products of the averaged one-particle propagators expressed via vertex functions. The two-particle vertex Γ is defined from the two-particle resolvent $G^{(2)}$ in momentum representation as

$$G^{(2)}_{\mathbf{k}\mathbf{k}'}(z_1,z_2;\mathbf{q}) = G(\mathbf{k},z_1)G(\mathbf{k}+\mathbf{q},z_2)[\delta(\mathbf{k}-\mathbf{k}') + \Gamma_{\mathbf{k}\mathbf{k}'}(z_1,z_2;\mathbf{q})G(\mathbf{k}',z_1)G(\mathbf{k}'+\mathbf{q},z_2)]. \tag{7}$$

The external disturbance U mixes different replicas and propagators in the replicated space are matrices in the replica indexes. Since we are interested only in the averaged two-particle functions, we can resort to two energies and to a two-by-two matrix propagator

$$\hat{G}^{-1}(\mathbf{k}_1,z_1,\mathbf{k}_2,z_2;U) = (\hat{G}^{(0)})^{-1} + \hat{U} - \hat{\Sigma} = \begin{pmatrix} z_1 - \epsilon(\mathbf{k}_1) - \Sigma_{11}(U) & U - \Sigma_{12}(U) \\ U - \Sigma_{21}(U) & z_2 - \epsilon(\mathbf{k}_2) - \Sigma_{22}(U) \end{pmatrix}, \tag{8}$$

where $\epsilon(\mathbf{k})$ is the lattice dispersion relation and the self-energy elements Σ_{ij} generally depend on both energies z_1, z_2. The matrix $\hat{G}$ represents the averaged resolvent that is to be used in the grand potential $\Omega^2(E_1,E_2;U)$ from Eq. (6). It is now a straightforward task to derive a matrix Soven equation generalizing Eq. (5a). We obtain

$$\hat{G}(z_1,z_2;U) = \langle[\hat{G}^{-1}(z_1,z_2;U) + \hat{\Sigma}(z_1,z_2;U) - \hat{V}_i]^{-1}\rangle_{\mathrm{av}}, \tag{9}$$

where $\hat{G}(z_1,z_2;U) = N^{-2}\Sigma_{\mathbf{k}_1\mathbf{k}_2}\hat{G}(\mathbf{k}_1,z_1,\mathbf{k}_2,z_2;U)$ is the local element of the matrix one-particle propagator. Inversions in Eq. (9) have matrix character in the replica space. The diagonal elements of the matrix equation (9) determine the one-particle propagators for energies z_1 and z_2. The off-diagonal elements, proportional to the perturbation U, determine the local two-particle resolvent that is defined as the coefficient at the linear term in the expansion of the local matrix propagator $\hat{G}(z_1,z_2;U)$ in the external perturbation U. The local two-particle Green function can be represented with the aid of the irreducible vertex (two-particle self-energy) λ via a Bethe-Salpeter equation. We find from Eq. (9) that the Bethe-Salpeter equation in the mean-field approximation reduces to an algebraic one

$$\gamma(z_1,z_2) = \frac{\lambda(z_1,z_2)}{1-\lambda(z_1,z_2)G(z_1)G(z_2)}, \tag{10}$$

where γ is the local part of the two-particle vertex Γ. The irreducible vertex λ in equilibrium ($U=0$) determined via Eq. (10) obeys an equation

$$\lambda(z_1,z_2) = \left.\frac{\delta\Sigma_U(z_1,z_2)}{\delta G_U(z_1,z_2)}\right|_{U=0} = \frac{1}{G(z_1)G(z_2)}\left(1 - \left\langle \frac{1}{1+[\Sigma(z_1)-V_i]G(z_1)}\frac{1}{1+[\Sigma(z_2)-V_i]G(z_2)}\right\rangle_{\mathrm{av}}^{-1}\right). \tag{11}$$

We can easily verify that this equation coincides with the CPA solution for the irreducible vertex $\lambda(z_1,z_2)$.[8]

There is no ambiguity in the mean-field construction of local one- and two-particle functions. But a mean-field treatment has a physical relevance only if it is able to produce nonlocal correlation functions, the long-range fluctuations of which may significantly influence the thermodynamic and dynamical behavior. There is not, however, a unique way how to generate the two-particle vertex with nonlocal contributions within the local mean-field approach. The simplest and most straightforward way is to use the Bethe-Salpeter equation with the CPA irreducible vertex λ, Eq. (10), and to replace the local propagators with the full nonlocal one-electron propagators $G(\mathbf{k},z)$. Such a Bethe-Salpeter equation remains algebraic in momentum representation and results in a two-particle vertex with only one transfer momentum. We obtain

$$\Gamma^{\pm}(z_1,z_2;\mathbf{q}^{\pm}) = \frac{\lambda(z_1,z_2)}{1-\lambda(z_1,z_2)\chi^{\pm}(z_1,z_2;\mathbf{q}^{\pm})}, \tag{12}$$

where we denoted the two-particle bubble

$$\chi^{\pm}(z_1,z_2;\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}} G(\mathbf{k},z_1)G(\mathbf{q}\pm\mathbf{k},z_2). \tag{13}$$

The ambiguity in this definition of the full mean-field vertex is in the type of nonlocal multiple scatterings we include into the Bethe-Salpeter equation. They are here denoted by the superscript $\pm$. The plus sign corresponds to multiple scatterings of electron-hole pairs, while the minus sign to electron-electron pairs. In case of elastic scatterings the electron-hole and electron-electron bubbles produce numerically the same number. However, the difference between the two types of pair scatterings lies in the respective transfer momentum $\mathbf{q}^{\pm}$. Using the notation for momenta in the two-particle resolvent from Eq. (7) we have $\mathbf{q}^{+}=\mathbf{q}$ and $\mathbf{q}^{-}=\mathbf{q}+\mathbf{k}+\mathbf{k}'$.

This ambiguity in the definition of the mean-field two-particle vertex is not usually acknowledged in the literature, since the electron-hole scattering channel, relevant for the electrical conductivity, is preferred and directly derived from the Baym-Kadanoff approach.[8] However, when the mean-field theory is viewed upon as the limit to infinite spatial dimensions, both electron-hole and electron-electron multiple scatterings possess the same high-dimensional

asymptotics.[23] *A priori*, neither electron-hole nor electron-electron multiple scatterings should be discarded. The appropriate form of the vertex is then selected by the physical quantities in which it appears, such as is the case of the electrical conductivity.

Incapability of the thermodynamic mean-field theory to determine uniquely the nonlocal part of the two-particle vertex results from the degeneracy of the local theory with elastic scatterings only (noninteracting systems). Multiple single-site scatterings, the only ones relevant in the mean-field approach, are unable to distinguish between electrons and holes. Only if we include explicitly scatterings on distinct lattice sites we are able to distinguish between electrons and holes. Hence, the standard thermodynamic mean-field theory of quantum itinerant systems uniquely defines only the local two-particle vertex, while it remains ambiguous in the determination of the full nonlocal two-particle vertex.

III. MEAN-FIELD THEORY FOR VERTEX FUNCTIONS: TWO-PARTICLE SELF-CONSISTENCY

A. Nonlocal contributions to the vertex function

A rather inaccurate way to the momentum-dependent two-particle vertex is not the only imperfection of the thermodynamic mean-field theory. This theory completely fails to account for backscattering effects, vertex corrections to the electrical conductivity, and the Anderson metal-insulator transition. All these effects are induced by strong nonlocal quantum coherence and spatial correlations reflected in the momentum behavior of the two-particle (vertex) functions. To capture these phenomena we must go beyond a perturbative description and to employ a self-consistent scheme for the (irreducible) vertex functions. The best local approximation for the irreducible vertex, CPA, is non-self-consistent at the two-particle level. We hence must go beyond the CPA and include nonlocal (long-range) contributions to the vertex function in a nonperturbative manner. Thereby a question arises whether we are able to reach a reasonably simple approximation with a two-particle self-consistency that could be called a mean-field theory. It is clear that such a theory must be momentum dependent, but the momentum dependence should be reduced to a necessary minimum. We will demonstrate in the next sections that the desired momentum dependence can be very effectively reduced by the asymptotic limit to high spatial dimensions.

The best way to construct a mean-field-like approximation for momentum-dependent functions is to build up the theory within a self-consistent expansion around the CPA. If we denote the local CPA one-particle propagator $G^{\mathrm{loc}}(z) = N^{-1}\Sigma_{\mathbf{k}} G^{\mathrm{CPA}}(\mathbf{k},z)$, the small parameter controlling the expansion around the CPA is a perturbed propagator $\overline{G}(\mathbf{k},z) = G(\mathbf{k},z) - G^{\mathrm{loc}}(z)$, where $G(\mathbf{k},z)$ is the full one-electron propagator. The CPA propagator G^{loc} contains the local self-energy $\Sigma^{\mathrm{loc}}(z)$ from Eq. (5a), while the full one a self-energy $\Sigma(\mathbf{k},z)$ that is to be determined later from a Dyson equation. We apply the expansion around the CPA to two-particle functions, where the one-particle propagators will be treated as external functions. It means, that we first disregard the consistency between the one- and two-particle functions. This consistency will be restored later via Ward identities once a suitable approximation for the vertex functions has been accomplished.

We can classify *nonlocal* contributions to the two-particle vertex by the type of a correlated two-particle propagation. We either simultaneously propagate an electron and a hole or two electrons (holes). Diagrammatically it means that we connect *spatially distinct* two-particle scattering events with antiparallel or parallel pairs of one-particle propagators. Multiple scatterings of pairs of the same type define a channel of a two-particle irreducibility. We call a diagram two-particle irreducible if it cannot be split into separate parts by cutting simultaneously either an electron-hole or an electron-electron pair of propagators. The two definitions of the two-particle irreducibility lead to topologically nonequivalent irreducible functions and to different Bethe-Salpeter equations for the full vertex. In each Bethe-Salpeter equation the two-particle functions are interconnected via one-particle propagators in a different manner. We can generically represent the channel-dependent Bethe-Salpeter equations as

$$\Gamma_{\mathbf{k}\mathbf{k}'}(z_+,z_-;\mathbf{q}) = \overline{\Lambda}^{\alpha}_{\mathbf{k}\mathbf{k}'}(z_+,z_-;\mathbf{q}) + [\overline{\Lambda}^{\alpha}\overline{GG} \odot \Gamma]_{\mathbf{k}\mathbf{k}'}(z_+,z_-;\mathbf{q}). \tag{14}$$

We used the symbol $\odot$ for the channel-dependent multiplication of the two-particle functions represented by specific momentum convolutions. Here $\overline{\Lambda}^{\alpha}$ is the irreducible vertex in the α-channel.

We will specify the momentum convolutions in the generic Bethe-Salpeter equation (14) for electron-hole and electron-electron multiple scatterings only. There is also a third two-particle channel, the so-called vertical channel with one-particle self-correlating scatterings.[24] These scatterings are, however, unimportant for the phenomenon of Anderson localization, since the corresponding two-particle propagator does not contain the diffusion pole.

Using the notation from Eq. (7) for the momentum dependence of the two-particle functions we can write explicitly the Bethe-Salpeter equation in the electron-hole channel with barred functions as

$$\begin{aligned}\Gamma_{\mathbf{k}\mathbf{k}'}(z_+,z_-;\mathbf{q}) &= \overline{\Lambda}^{eh}_{\mathbf{k}\mathbf{k}'}(z_+,z_-;\mathbf{q}) \\ &\quad + \frac{1}{N}\sum_{\mathbf{k}''} \overline{\Lambda}^{eh}_{\mathbf{k}\mathbf{k}''}(z_+,z_-;\mathbf{q})\overline{G}_+(\mathbf{k}'')\overline{G}_-(\mathbf{k}''+\mathbf{q}) \\ &\quad \times \Gamma_{\mathbf{k}''\mathbf{k}'}(z_+,z_-;\mathbf{q}).\end{aligned} \tag{15a}$$

The Bethe-Salpeter equation with the electron-electron multiple scatterings then analogously reads

$$\begin{aligned}\Gamma_{\mathbf{k}\mathbf{k}'}(z_+,z_-;\mathbf{q}) &= \overline{\Lambda}^{ee}_{\mathbf{k}\mathbf{k}'}(z_+,z_-;\mathbf{q}) \\ &\quad + \frac{1}{N}\sum_{\mathbf{k}''} \overline{\Lambda}^{ee}_{\mathbf{k}\mathbf{k}''}(z_+,z_-;\mathbf{q}+\mathbf{k}'-\mathbf{k}'')\overline{G}_+(\mathbf{k}'') \\ &\quad \times \overline{G}_-(\mathbf{Q}-\mathbf{k}'')\Gamma_{\mathbf{k}''\mathbf{k}'}(z_+,z_-;\mathbf{q}+\mathbf{k}-\mathbf{k}''),\end{aligned} \tag{15b}$$

where we denoted $\mathbf{Q}=\mathbf{q}+\mathbf{k}+\mathbf{k}'$ the transfer momentum between the two electrons of the scattered correlated pair. In these equations we abbreviated $\overline{G}(\mathbf{k},z_\pm)\to\overline{G}_\pm(\mathbf{k})$.

Equations (15) constitute the fundamental building blocks for the construction of systematic approximations for the two-particle vertex. They are analogues of the Dyson equation and enable us to determine the full vertex from irreducible vertices. We hence can apply the perturbation (diagrammatic) expansion to the two-particle irreducible vertices, i.e., two-particle self-energies. As a first step toward a mean-field-like theory for these vertices we must maximally simplify the momentum dependence of the vertex functions, but still staying beyond the local CPA. This will be achieved by the asymptotic limit to high (finite) spatial dimensions.

B. Asymptotic limit to high lattice dimensions

Bethe-Salpeter equations (15) use only off-diagonal one-particle propagators and hence are suitable for performing the limit to high spatial dimensions. We use the hypercubic lattice that has a straightforward high-dimensional limit. The one-electron propagator $\overline{G}$ has the following asymptotics:

$$\overline{G}(\mathbf{k},z) \doteq \frac{t}{\sqrt{d}}\sum_{\nu=1}^{d}\cos(k_\nu)\int\frac{d\epsilon\rho(\epsilon)}{[z-\Sigma(z)-\epsilon]^2}, \qquad (16)$$

where $\Sigma(z)$ is the CPA ($d=\infty$) self-energy.[25]

The irreducible two-particle vertices must collapse to local quantities in the limit to infinite dimensions. Since the Bethe-Salpeter equations (15) use only the off-diagonal propagators vanishing in the limit $d=\infty$, both vertices $\overline{\Lambda}^{eh}$ and $\overline{\Lambda}^{ee}$ must coincide with the full local two-particle CPA vertex in $d=\infty$. We hence have

$$\overline{\Lambda}^{eh}_{\mathbf{kk}'}(z_+,z_-;\mathbf{q}) = \overline{\Lambda}^{ee}_{\mathbf{kk}'}(z_+,z_-;\mathbf{q}) = \gamma(z_+,z_-). \qquad (17)$$

We further denote $\overline{\chi}(z_+,z_-;\mathbf{q})=\chi(z_+,z_-;\mathbf{q})-G_+G_-$ with $\chi(z_+,z_-;\mathbf{q})=\chi^+(z_+,z_-;\mathbf{q})$, $G_+=G^{\mathrm{loc}}(z_+)$, and $G_-=G^{\mathrm{loc}}(z_-)$. If we take into account only the electron-hole and electron-electron multiple scatterings we can represent the leading asymptotics of the full two-particle vertex in high dimensions as follows:

$$\Gamma_{\mathbf{kk}'}(z_+,z_-;\mathbf{q}) \doteq \gamma(z_+,z_-) + \lambda(z_+,z_-) \times\left(\frac{\gamma(z_+,z_-)\overline{\chi}(z_+,z_-;\mathbf{q})}{1-\lambda(z_+,z_-)\chi(z_+,z_-;\mathbf{q})} + \frac{\gamma(z_+,z_-)\overline{\chi}(z_+,z_-;\mathbf{Q})}{1-\lambda(z_+,z_-)\chi(z_+,z_-;\mathbf{Q})}\right). \qquad (18)$$

The standard nonlocal CPA vertex can be recovered from the above expression if we neglect the contribution from the electron-electron multiple scatterings, the second term in the brackets on the right-hand side (rhs) of Eq. (18). There is, however, no reason for this neglect, since both terms within the brackets on the rhs of Eq. (18) produce the same asymptotic behavior in powers of the inverse dimension, $O(d^{-1})$. Their only difference is in the momentum dependence.

The limit to infinite spatial dimensions reduces the momentum dependence of two-particle functions but does not lead to a mean-field-like approximation for vertices. There is no self-consistency in the two-particle parameters and the local irreducible vertices are determined from the CPA. We hence cannot expect that this high-dimensional two-particle non-selfconsistent asymptotics would lead to major deviations from the CPA. The only significant change in the vertex function, Eq. (18), with respect to the CPA vertex from Eq. (12) is the existence of vertex corrections to the electrical conductivity in the form of *weak localization* properly described by multiple electron-electron scatterings (maximally crossed diagrams).

C. Parquet equations and electron-hole symmetry

To go significantly beyond the CPA predictions for transport properties and response functions we have to introduce a self-consistency that would extend also to the two-particle irreducible vertices. That is, the two-particle irreducible vertices $\overline{\Lambda}^{eh}$ and $\overline{\Lambda}^{ee}$ should be determined from nonlinear equations. This effect can be achieved by introducing the so-called *parquet equations*. The concept of parquet equations is based on the observation that two-particle reducible diagrams in one scattering channel are irreducible in the other *distinguishable* scattering channels. Parquet equations were introduced in many-body theories[26–28] but recently they were adjusted also to disordered systems.[24] The reducible diagrams from one channel can become irreducible in the other channels only if different channels are indeed distinguishable or nonequivalent. The idea of parquet equations cannot be applied to local propagators of noninteracting particles with indistinguishable electrons and holes, hence within the CPA. It, however, works very efficiently for nonlocal vertex functions in the Anderson model of disordered electrons.

If we again take into account only the electron-hole and the electron-electron scattering channels, we can write the basic parquet equation for the full two-particle vertex in high dimensions

$$\Gamma_{\mathbf{kk}'}(z_+,z_-;\mathbf{q}) = \overline{\Lambda}^{eh}_{\mathbf{kk}'}(z_+,z_-;\mathbf{q}) + \overline{\Lambda}^{ee}_{\mathbf{kk}'}(z_+,z_-;\mathbf{q}) - \gamma(z_+,z_-). \qquad (19)$$

Equation (19) tells us that the full vertex is decomposed into irreducible and reducible diagrams in the either scattering channel and that the reducible diagrams consist of only the irreducible diagrams from the other channel from which the completely irreducible vertex, i.e., the vertex irreducible in both channels, was subtracted. The limit to high lattice dimensions then determines the completely irreducible vertex to be the full local CPA ($d=\infty$) vertex γ.

Parquet equation (19) can now be used in the Bethe-Salpeter equations (15) to exclude the full vertex Γ from them. Thereby we reach a closed set of nonlinear integral equations for the irreducible vertices $\overline{\Lambda}^{eh}$ and $\overline{\Lambda}^{ee}$. This set of equations is generally not solvable without further approximations. To approximate the resulting parquet equations in a systematic and controlled way we again utilize the mean-field idea—limit to high dimensions. For two-particle func-

tions and parquet equations we must use this limit only in the asymptotic sense so as nonlocal fluctuations would not be lost completely.

One can make an important observation in high spatial dimensions. The off-diagonal one-particle propagators $\overline{G}$ behave in the leading asymptotic order as Gaussian random variables with respect to momentum summations.[17] Using representation (16) we can easily prove the following relations:

$$\frac{1}{N}\sum_{\mathbf{q}'}\overline{\chi}(\mathbf{q}'+\mathbf{q})\overline{G}_{\pm}(\mathbf{q}'+\mathbf{k}) \doteq \frac{Z}{4d}\overline{G}_{\pm}(\mathbf{q}-\mathbf{k}), \tag{20a}$$

$$\frac{1}{N}\sum_{\mathbf{q}}\overline{\chi}(\mathbf{q}+\mathbf{q}_1)\overline{\chi}(\mathbf{q}+\mathbf{q}_2) \doteq \frac{Z}{4d}\overline{\chi}(\mathbf{q}_1-\mathbf{q}_2), \tag{20b}$$

where we used abbreviations $Z=t^2\langle G_+^2\rangle\langle G_-^2\rangle$ with $\langle G_\pm^2\rangle = N^{-1}\Sigma_{\mathbf{k}}G_\pm(\mathbf{k})^2$. The equalities in Eq. (20) hold only within the leading asymptotic order $d\to\infty$. The functions $\overline{G}_\pm$ and $\overline{\chi}$ form a closed set of Gaussian random variables with respect to momentum convolutions. We hence can use Eqs. (20) to simplify the parquet equations for the irreducible vertices $\overline{\Lambda}^{eh}$ and $\overline{\Lambda}^{ee}$.

Before we attempt to resolve the parquet equations in high dimensions, we utilize the time-reversal invariance of the system. It is an important feature of electron systems without spin- and orbital-dependent scatterings. According to this invariance the physical (measurable) results should not depend on the orientation of propagators. We hence can write for one- and two-particle propagators

$$\overline{G}(\mathbf{k},z) = \overline{G}(-\mathbf{k},z), \tag{21a}$$

$$\Gamma_{\mathbf{k}\mathbf{k}'}(z_+,z_-;\mathbf{q}) = \Gamma_{\mathbf{k}\mathbf{k}'}(z_+,z_-;-\mathbf{Q}) = \Gamma_{-\mathbf{k}'-\mathbf{k}}(z_+,z_-;\mathbf{Q}). \tag{21b}$$

In case of the two-particle vertex, the time reversal was applied only to one fermion propagator. The time reversal leaves the full two-particle vertex invariant but it transforms the Bethe-Salpeter equation (15a) to Eq. (15b) and vice versa. It means that the irreducible vertices transform as follows:

$$\overline{\Lambda}^{ee}_{\mathbf{k}\mathbf{k}'}(z_+,z_-;\mathbf{q}) = \overline{\Lambda}^{eh}_{\mathbf{k}\mathbf{k}'}(z_+,z_-;-\mathbf{Q}) = \overline{\Lambda}^{eh}_{-\mathbf{k}'-\mathbf{k}}(z_+,z_-;\mathbf{Q}). \tag{21c}$$

The time-reversal (electron-hole) symmetry reduces the number of parquet equations to just one nonlinear integral equation for a single vertex that we define as $\overline{\Lambda}_{\mathbf{k}\mathbf{k}'}(z_+,z_-;\mathbf{q}) \equiv \overline{\Lambda}^{ee}_{\mathbf{k}\mathbf{k}'}(z_+,z_-;\mathbf{q}) = \overline{\Lambda}^{eh}_{\mathbf{k}\mathbf{k}'}(z_+,z_-;-\mathbf{Q})$. The resulting equation for this vertex reads

$$\overline{\Lambda}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \gamma + \frac{1}{N}\sum_{\mathbf{k}''}\overline{\Lambda}_{\mathbf{k}\mathbf{k}''}(-\mathbf{q}-\mathbf{k}-\mathbf{k}'')\overline{G}_+(\mathbf{k}'')\overline{G}_-(\mathbf{q}+\mathbf{k}'') \times\left[\overline{\Lambda}_{\mathbf{k}''\mathbf{k}'}(-\mathbf{q}-\mathbf{k}'-\mathbf{k}'') + \overline{\Lambda}_{\mathbf{k}''\mathbf{k}'}(\mathbf{q}) - \gamma\right]. \tag{22}$$

Equation (22) can now be simplified in high spatial dimensions by using the Gaussian summation rules, Eqs. (20). It is clear from these rules that the fermionic momenta from different two-particle functions must be summed independently in the leading asymptotic order. Any correlated momentum summation involving two different two-particle functions costs a factor $1/d$. Then only the conserved bosonic transfer momenta survive as in the case of the high-dimensional vertex from Eq. (18). We hence must sum both sides of Eq. (22) over incoming and outgoing fermionic momenta $\mathbf{k},\mathbf{k}'$ so as to extract the high-dimensional limit of the irreducible vertex $\overline{\Lambda}$. To reach an equation for the relevant variables we introduce

$$\overline{\Lambda}(\mathbf{q}) = \frac{1}{N^2}\sum_{\mathbf{k}\mathbf{k}'}\overline{\Lambda}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}). \tag{23a}$$

Further on we have in the leading order

$$\frac{1}{N^2}\sum_{\mathbf{k}\mathbf{k}'}\overline{\Lambda}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}+\mathbf{k}+\mathbf{k}') = \frac{1}{N}\sum_{\mathbf{q}}\overline{\Lambda}(\mathbf{q}) = \overline{\Lambda}_0. \tag{23b}$$

Since the fermionic momenta from different two-particle functions are summed independently in high spatial dimensions, the parquet equation (22) reduces with the above definitions to

$$\overline{\Lambda}(\mathbf{q}) = \gamma + \overline{\Lambda}_0\frac{\overline{\Lambda}_0\overline{\chi}(\mathbf{q})}{1-\overline{\Lambda}_0\overline{\chi}(\mathbf{q})}. \tag{24a}$$

We see that the high-dimensional irreducible vertex is completely determined from a single local (mean-field) parameter $\overline{\Lambda}_0$ and the two-particle bubble $\overline{\chi}(\mathbf{q})$. Summing both sides of Eq. (24a) over momenta we obtain an equation for the local two-particle irreducible vertex

$$\overline{\Lambda}_0 = \gamma + \overline{\Lambda}_0^2\frac{1}{N}\sum_{\mathbf{q}}\frac{\overline{\chi}(\mathbf{q})}{1-\overline{\Lambda}_0\overline{\chi}(\mathbf{q})}. \tag{24b}$$

Knowing the local part of the two-particle irreducible vertex $\overline{\Lambda}_0$ we can reconstruct the full two-particle vertex in high spatial dimensions. We have

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \gamma + \Lambda_0\left(\frac{\overline{\Lambda}_0\overline{\chi}(\mathbf{q})}{1-\Lambda_0\chi(\mathbf{q})} + \frac{\overline{\Lambda}_0\overline{\chi}(\mathbf{k}+\mathbf{k}'+\mathbf{q})}{1-\Lambda_0\chi(\mathbf{k}+\mathbf{k}'+\mathbf{q})}\right), \tag{25}$$

where, in analogy to the non-self-consistent high dimensional vertex, Eq. (18), $\Lambda_0=\overline{\Lambda}_0/(1+\overline{\Lambda}_0G_+G_-)$ and $\overline{\chi}(\mathbf{q}) = \chi(\mathbf{q})-G_+G_-$.

Equations (23)–(25) form an approximation for two-particle functions with a single, local parameter determined self-consistently. Such an approximation is a self-consistent extension of the high-dimensional limit of the two-particle vertex, Eq. (18). We hence can call it a mean-field approximation for two-particle functions of noninteracting disordered electron systems. The self-consistently determined mean-field parameter $\overline{\Lambda}_0$ exactly reproduces the leading $1/d$ correction to the CPA irreducible vertex λ. The fundamental

self-consistent equation of this approximation, Eq. (24b), has a typical mean-field character. That is, it can be used in any dimension. The lattice structure enters the equation only through the momentum summation running over the first Brillouin zone. Notice, however, that we cannot reduce the momentum summation in two-particle functions to an integral over the density of states.

D. Self-energy and diffusion pole in high dimensions

The mean-field theory constructed in the preceding section is a self-consistent approximation for the two-particle vertex where one-particle propagators are assumed to be external functions. Such a situation cannot be the final stage of the theory, since due to conservation laws and thermodynamic consistency the one- and two-particle functions are correlated. Actually, the electron-hole irreducible vertex is connected with the self-energy for noninteracting disordered electrons via the Vollhardt-Wölfle Ward identity[18]

$$\Sigma^R(\mathbf{k},E+\omega)-\Sigma^A(\mathbf{k},E)=\frac{1}{N}\sum_{\mathbf{k}'}\Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E+\omega,E)\times\left[G^R(\mathbf{k}',E+\omega)-G^A(\mathbf{k}',E)\right]. \tag{26}$$

Here we denoted Σ^R,Σ^A the retarded and advanced self-energy and $\Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E+\omega,E)\equiv\Lambda^{eh}_{\mathbf{k}\mathbf{k}'}(E+\omega+i0^+,E-i0^+;\mathbf{0})$. Note that the irreducible vertex Λ in Eq. (26) does not have bar, i.e., it is defined via the Bethe-Salpeter equation with the full one-electron propagators G^R,G^A. The Ward identity says that if we modify the electron-hole irreducible vertex we must change adequately the one-electron self-energy and vice versa. We hence cannot approximate independently the irreducible vertex without changing appropriately the self-energy. If we have an analytic expression for the self-energy as a functional of the one-electron resolvent, we can use a differential form of the Ward identity (11) to determine the irreducible vertex. Then the vertex function is determined directly from the one-electron propagator. Such a construction of the irreducible vertex does not lead to bifurcation points and multiple solutions, i.e., to a phase transition, unless we find them in the self-energy itself. It is normally very difficult to determine bifurcation points in the self-energy that is a bounded function. It is more convenient to search for possible bifurcation points in two-particle functions that may display divergences.

It is clear that we need self-consistent equations for functions that could have multiple solutions. Such a self-consistent approximation for the irreducible vertex was achieved in the preceding section. A self-consistent equation for the irreducible vertex cannot be derived from a self-energy directly. To achieve consistency between the one- and two-particle functions in this case we must determine the self-energy as a functional of the irreducible vertex. This must be done in concord with the Ward identity (26).

The self-energy as a functional of the irreducible vertex is overdetermined from identity (26). We can nevertheless use the Vollhardt-Wölfle identity to determine the self-energy from the vertex function as suggested in Ref. 29 and used in the parquet approach from Ref. 24. We use only a specific element of the Vollhardt-Wölfle identity to determine the imaginary part of the self-energy. In the mean-field case, where the irreducible vertex is local, we can write a generalized CPA equation

$$\mathrm{Im}\,\Sigma^R(E)=\Lambda^{RA}_0(E,E)\mathrm{Im}\,G^R(E). \tag{27a}$$

Consistency, or negative definiteness of $\mathrm{Im}\,\Sigma^R$, demands that the local element of the irreducible vertex $\Lambda^{RA}_0(E,E)=N^{-2}\Sigma_{\mathbf{k}\mathbf{k}'}\Lambda_{\mathbf{k}\mathbf{k}'}(E+i0^+,E-i0^+;\mathbf{0})$, determined from the mean-field equation (24b), is positive.

We cannot find the real part of the self-energy directly from the irreducible vertex. Instead, we use causality of the self-energy and the Kramers-Kronig relation expressing the real part of an analytic function as a Hilbert transform of its imaginary part. We have

$$\mathrm{Re}\,\Sigma(E)=\Sigma_\infty+P\int_{-\infty}^{\infty}\frac{dE'}{\pi}\frac{\mathrm{Im}\,\Sigma^R(E')}{E'-E}. \tag{27b}$$

Equations (27) now determine the self-energy from the mean-field (local) irreducible vertex Λ_0. Notice, however, that to determine the self-energy at one frequency we must know the irreducible vertex in the whole frequency range. Equations (27) complete the mean-field theory for vertex functions, Eqs. (23) and Eqs. (24), and make it a consistent approximation with proper analytic properties of one- and two-particle Green functions.

The Vollhardt-Wölfle identity, its specific form from Eq. (27a), not only serves as a means for a consistent determination of a causal self-energy from a given irreducible vertex, but it is also indispensable for the existence of the diffusion pole in the electron-hole correlation function. We now show in what form the diffusion pole survives in the mean-field theory for vertex functions with the self-energy determined by Eqs. (27).

The electron-hole correlation function is defined from the averaged two-particle Green function as

$$\Phi^{RA}_E(\mathbf{q},\omega)=\frac{1}{N^2}\sum_{\mathbf{k}\mathbf{k}'}G^{(2)}_{\mathbf{k}\mathbf{k}'}(E+\omega+i0^+,E-i0^+;\mathbf{q}). \tag{28}$$

The two-particle Green function is evaluated with the full two-particle vertex via Eq. (7).

From Eq. (27a) and from $\chi^{RA}(\mathbf{0})=\mathrm{Im}\,G^R/\mathrm{Im}\,\Sigma^R$ we obtain that both the denominators in the high-dimensional limit of the two-particle vertex Γ^{RA} vanish at zero transfer momenta. Hence, the mean-field approximation for vertex functions contains the diffusion pole in the electron-hole channel (first term in the brackets on the rhs of Eq. (25)) and the Cooper pole in the electron-electron channel (second term). Only the diffusion pole survives as a singularity in the electron-hole correlation function, Eq. (28).

To derive the low-energy behavior of the electron-hole correlation function we denote

$$A_E=1+2i\,\mathrm{Im}\,G^R(E)\left.\frac{\partial\Lambda^{RA}_0(E+\omega,E)}{\partial\omega}\right|_{\omega=0} \tag{29a}$$

and

$$D_E^0(\omega) = 2\,\mathrm{Im}\,\Sigma^R(E)\Lambda_0^{RA}(E+\omega,E)\left.\frac{\partial\chi^{RA}(\mathbf{q})}{\partial(q^2)}\right|_{q=0}. \tag{29b}$$

With these two definitions we find the high-dimensional asymptotics of the low-energy limit of the electron-hole correlation function at zero temperature to be

$$\Phi_E^{RA}(\mathbf{q},\omega) \approx \frac{2\pi n_E}{-iA_E\omega + D_E^0(\omega)\mathbf{q}^2}, \tag{30}$$

where n_E is the density of states at the Fermi energy E.

The low-energy asymptotics of the electron-hole correlation function serves as an important tool for testing consistency of approximations. We find from gauge invariance and the (unrestricted) Ward identity (26) that the electron-hole correlation function should display the diffusion pole in form of Eq. (30) with $A_E=1$ for arbitrary disorder strength. It then means that the low-energy behavior of the electron-hole correlation function is controlled by a single parameter, the bare dynamical diffusion constant $D_E^0(\omega)$.[18,19] However, we already found in Ref. 17 that the constant A_E increases with the disorder strength and becomes infinite at the Anderson localization transition. The disorder dependent weight of the diffusion pole n_E/A_E is the central unexpected feature of the mean-field theory for vertex functions. This mean-field approximation obeys the Vollhardt-Wölfle identity only in the limit to zero frequency, Eq. (27a), and not for finite energy differences. We found a consistent explanation for the decrease of the weight of the diffusion pole with increasing disorder strength.[20] The weight of the diffusion pole, n_E/A_E, expresses a portion of extended (diffusive) states from all available states at the Fermi energy determined by the density of states calculated from the one-electron Green function, $n_E=-\mathrm{Im}\,G^R(E)/\pi$.

The dependence of the weight of the diffusion pole on the disorder strength found in the mean-field theory for averaged two-particle functions could be an artifact of this specific approximation. We could still hope that the full exact solution recovers the invariant weight of the diffusion pole expected from the unrestricted conservation laws for averaged Green functions. Based only on approximation-free arguments we found that the Vollhardt-Wölfle identity (26) for finite frequencies ω cannot be fulfilled in any finite dimension if the electron-hole irreducible vertex Λ^{eh} contains the Cooper pole. Enforcing the full form of the Vollhardt-Wölfle identity together with the Cooper pole in the electron-hole irreducible vertex inevitably leads to a self-energy being a nonanalytic function of its energy argument for almost all Fermi energies within the energy bands.[30,31] In our mean-field approach the analytic properties of the self-energy are determined by positivity of the vertex function $\Lambda_0^{RA}(E,E)$ and Kramers-Kronig relation, Eq. (27b). The form of the two-particle vertex $\Lambda_0^{RA}(E,E)$ is fixed by its high-dimensional asymptotics. This asymptotics and analytic properties of the self-energy force deviations from the Vollhardt-Wölfle Ward identity. It hence seems that the high-dimensional behavior of the two-particle vertex and the disorder-dependent weight of the diffusion pole, disclosed by the asymptotic mean-field solution, are generic features of the Anderson model of disordered electrons. At least for theories that can be analytically continued from the limit to high spatial dimensions.

IV. DISCUSSION AND CONCLUSIONS

We presented in this paper two ways how to reach mean-field-like approximations for noninteracting disordered electron systems. The first one, being the standard thermodynamic mean-field theory known from many-body systems, uses the limit to infinite spatial dimensions applied to the generating, configurationally averaged thermodynamic potential. The limit to infinite spatial dimensions enables one to separate the diagonal and off-diagonal elements of the one-particle propagator and its self-energy and to find an explicit representation for the generating functional. The local one-particle functions from the generating functional serve as generalized variational parameters, the physical values of which are determined from stationarity equations for the generating functional. The higher-order Green and vertex functions are determined from responses of the system to *local* external perturbations. In this way the construction of a mean-field approximation is consistent and unambiguous in the determination of one-particle functions as they are the only ones entering the generating functional. The higher-order Green functions are defined uniquely only in their local parts.

The nonlocal parts of two-particle Green functions are no longer determined from the local thermodynamic theory uniquely. We can either use the standard construction of Baym and Kadanoff or we can directly apply the asymptotic limit to infinite spatial dimensions to two-particle functions. The outcome of these two constructions is not identical. In the former way we miss some of the leading-order (maximally crossed) diagrams and lose the electron-hole symmetry at the two-particle level. These deficiencies severely discredit reliability of the thermodynamic mean-field theory in the calculation of spatial coherence and transport properties of disordered systems. To overcome these drawbacks we proposed another route toward a mean-field-like approximation for vertex functions based on a direct analysis of two-particle functions in high spatial dimensions.

The incapability of the thermodynamic mean-field theory to correctly describe nonlocal correlations in two-particle functions is caused by the degeneracy of local theories with elastic scatterings. Static local approximations are unable to distinguish between electrons and holes. Only quantum dynamics or multiple scatterings on spatially distinct impurities can discern the motion of an electron from the motion of a hole. The distinguishability of electrons and holes is of principal importance for encountering backscattering effects and for a two-particle self-consistency used in the construction of a mean-field theory for vertex functions.

A mean-field approximation for vertex functions in disordered electron systems was constructed from the *asymptotic* limit to high spatial dimensions, where, unlike the thermodynamic mean field, the lattice dimension is high but finite. Alike the strict limit $d=\infty$, the asymptotic behavior in high

dimensions leads to significant simplifications in momentum convolutions that enable us to reduce the approximation to a mean-field-like one with a local generator determined from a self-consistent equation. We applied the asymptotic limit directly within a diagrammatic expansion around the CPA for two-particle functions. The basic ingredients for the construction were parquet equations for the two-particle irreducible vertices from the electron-hole and the electron-electron scattering channels. Using the electron-hole symmetry at the two-particle level and the asymptotic limit to high dimensions we succeeded in producing a self-consistent approximation for the local part of the electron-hole irreducible vertex. It is a self-consistent $1/d$ extension of the CPA irreducible vertex. The mean-field theory for vertex functions then determines in a unique way the full two-particle vertex that correctly reproduces the limit to infinite dimensions with the electron-hole symmetry at both one- and two-particle levels.

The mean-field theory for vertex functions is an approximation for two-particle functions. The one-electron functions, used as an input for the two-particle equations, are then calculated from the vertex function via a specific form of the Vollhardt-Wölfle Ward identity and the Kramers-Kronig relation. With this extension of the theory to one-particle functions we accomplished an approximate description of disordered systems fulfilling all consistency conditions on one- and two-particle functions.

The most important achievement of this mean-field theory is its ability to describe the disorder-induced vanishing of diffusion, that is, the Anderson localization transition. This theory succeeded for the first time to bridge qualitatively correctly the weak and the strong disorder limits and to cover the split-band limit as well as vanishing of diffusion. The other existing approaches have concentrated on only one of the two phenomena. They either miss the two-particle self-consistency or do not consistently match the one- and two-particle functions.

The consistency between the one-electron self-energy and the electron-hole irreducible vertex is essential for credibility of approximate treatments of the Anderson metal-insulator transition. Only with this relation correctly taken into account we obtain the proper form of the diffusion pole and electron diffusion on long distances. In this respect the mean-field theory for vertex functions leads, surprisingly against the common expectations, to a nonconserving weight of the diffusion pole and its dependence on the disorder strength. The thermodynamic mean-field theory and all other approaches to the Anderson localization transition assume or use the unrestricted form of the Ward identity (26) being a consequence of conservation of the norm of the wave function for all configurations of the random potential. We argued already earlier that the Hilbert space of Bloch waves is incomplete in the sense that it does not encompass the eigenstates of all configurations of the random potential. At a given energy we observe even in the metallic regime macroscopically relevant numbers of configurations with localized states.[20]

Vanishing of the diffusion pole at the Anderson metal-insulator transition and in the localized phase modifies the existing picture of the critical behavior for vanishing of diffusion. In the standard approaches, such as the nonlinear sigma model or the Vollhardt-Wölfle self-consistent approximation, the dynamical diffusion constant is the only parameter controlling the low-energy behavior of the electron-hole correlation function. In our mean-field theory we have apart from the diffusion constant also the weight of the diffusion pole that significantly influences the description of long-range correlations and diffusion. In the critical region, however, only the constant $A_E \to \infty$ from Eq. (29a) is relevant and all critical scales can be derived from it. For instance the renormalized diffusion constant $D_E = D_E^0/A_E$ vanishes at the localization transition with the diverging parameter A_E, etc. It means that the mean-field description of the Anderson localization transition is compatible with a one-parameter scaling theory.

Although the one-parameter scaling holds for the Anderson localization transition, two relevant parameters in the critical region, n_E/A_E and D_E^0/A_E, nevertheless lead to a modification of the critical behavior deduced from the field-theoretic approaches. The two parameters stand for two quantities influencing the electrical conductivity. The former expresses the number of extended states at the Fermi energy E and the latter the averaged velocity of the diffusive particles. Both quantities go simultaneously to zero at the Anderson metal-insulator transition. It is straightforward to verify that the mean-field theory for vertex functions predicts that $A_E \sim |\lambda_c - \lambda|^{-1/2}$, where λ is the bare disorder strength and λ_c its critical value. Having two vanishing parameters we have to distinguish two types of the critical behavior. First, we have properties of individual electrons. One of them is diffusion as seen from the semiclassical diffusion equation. This is quantitatively described by the renormalized diffusion constant $D_E \sim |\lambda_c - \lambda|^{1/2}$. Second, we have statistical values describing the disordered sample as a whole. Among them the averaged conductivity is the most interesting one. It is proportional to the product of the number of available diffusive states and the renormalized diffusion constant, so that we have $\sigma \sim n_E D_E^0/A_E^2 \sim |\lambda_c - \lambda|^1$. Notice, however, that there is not a direct relation between the diffusion constant and the conductivity calculated from the Kubo formula, since due to deviations from the Ward identity, the Einstein relation does not hold. Finally we can also deduce the critical exponent for the localization length in the localized phase. Its square is inversely proportional to the order parameter, being the imaginary part of the local irreducible vertex $\mathrm{Im}\,\Lambda^{RA}(E+0^+,E) \sim |\lambda - \lambda_c|^{1/2}$. We hence obtain $\xi \sim |\lambda - \lambda_c|^{-1/4}$. The critical exponent for the conductivity equals the mean-field exponent from the Vollhardt-Wölfle theory but the critical exponent for the localization length is one-half of their value. We remind that the critical behavior obtained from the mean-field theory for vertex functions holds only for dimensions $d > d_u = 4$. We expect corrections to the mean-field critical behavior in lower dimensions.

To conclude, we demonstrated that to reach a reliable quantitative description of the Anderson localization transition one must sum up self-consistently nonlocal contributions to the electron-hole and the electron-electron irreducible vertex functions. It can be achieved in a mean-field manner via the asymptotic limit to high spatial dimensions leading to a self-consistent extension of the CPA local vertex.

The most important conclusion of this mean-field theory of Anderson localization is that the weight of the diffusion pole is not conserved and that the diffusion pole is absent in the localized phase. The decreasing weight of the diffusion pole with the increasing disorder strength is a consequence of incompleteness of the Hilbert space of Bloch waves. At any Fermi energy there are macroscopically relevant numbers of configurations with localized as well as with delocalized states. The number of configurations with extended states decreases with increasing the disorder strength and vanishes at the localization transition. This feature can essentially be checked by other, e.g., numerical means. Due to the disorder-dependent weight of the diffusion pole the Einstein relation does not hold and we have to distinguish individual and statistical transport properties of disordered systems. One should have this in mind when calculating the critical behavior of the Anderson localization transition.

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[1] R. J. Elliot, J. A. Krumhansl, and P. L. Leath, Rev. Mod. Phys. **46**, 465 (1974).
[2] R. Vlaming and D. Vollhardt, Phys. Rev. B **45**, 4637 (1992).
[3] V. Janiš and D. Vollhardt, Phys. Rev. B **46**, 15712 (1992).
[4] V. Janiš, Phys. Rev. B **40**, 11331 (1989).
[5] V. Janiš, Z. Phys. B: Condens. Matterr **83**, 227 (1991).
[6] A. Gonis, *Green Functions for Ordered and Disordered Systems* (North-Holland, Amsterdam, 1992).
[7] P. Weinberger, Phys. Rep. **377**, 281 (2003).
[8] B. Velický, Phys. Rev. **184**, 614 (1969).
[9] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).
[10] P. A. Lee and R. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).
[11] B. Kramer and A. MacKinnon, Rep. Prog. Phys. **56**, 1469 (1993).
[12] R. Mills and P. Ratanavararaksa, Phys. Rev. B **18**, 5291 (1978).
[13] T. Kaplan, P. L. Leath, L. J. Gray, and H. W. Diehl, Phys. Rev. B **21**, 4230 (1980).
[14] V. Čápek, Phys. Status Solidi B **52**, 399 (1972).
[15] W. H. Butler and B. G. Nickel, Phys. Rev. Lett. **30**, 373 (1973).
[16] M. Jarrell and H. R. Krishnamurthy, Phys. Rev. B **63**, 125102 (2001).
[17] V. Janiš and J. Kolorenč, Phys. Rev. B **71**, 033103 (2005).
[18] D. Vollhardt and P. Wölfle, Phys. Rev. B **22**, 4666 (1980); D. Vollhardt and P. Wölfle, in *Electronic Phase Transitions*, edited by W. Hanke and Yu. V. Kopaev (Elsevier Science Publishers B. V., Amsterdam, 1992).
[19] V. Janiš, J. Kolorenč, and V. Špička, Eur. Phys. J. B **35**, 77 (2003).
[20] V. Janiš and J. Kolorenč, Phys. Status Solidi B **241**, 2032 (2004).
[21] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
[22] G. Baym and L. P. Kadanoff, Phys. Rev. **124**, 287 (1961); G. Baym, *ibid.* **127**, 1391 (1962).
[23] V. Janiš, Phys. Rev. Lett. **83**, 2781 (1999).
[24] V. Janiš, Phys. Rev. B **64**, 115115 (2001).
[25] E. Müller-Hartmann, Z. Phys. B: Condens. Matterr **74**, 507 (1989).
[26] C. De Dominicis, J. Math. Phys. **3**, 983 (1962); **4**, 255 (1963); C. De Dominicis and P. C. Martin, *ibid.* **5**, 14 (1964); **5**, 31 (1964).
[27] A. D. Jackson, A. Lande, and R. A. Smith, Phys. Rep. **86**, 55 (1982).
[28] N. E. Bickers and S. R. White, Phys. Rev. B **43**, 8044 (1991); N. E. Bickers, Int. J. Mod. Phys. B **5**, 253 (1991).
[29] S. V. Maleev and B. P. Toperverg, Zh. Eksp. Teor. Fiz. **69**, 1440 (1975) [Sov. Phys. JETP **42**, 734 (1975)].
[30] V. Janiš and J. Kolorenč, Mod. Phys. Lett. B **18**, 1051 (2004).
[31] V. Janiš and J. Kolorenč, cond-mat/0407618 (unpublished).