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Integrability of the diffusion pole in the diagrammatic description of noninteracting electrons in a random potential

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Abstract

We discuss restrictions on the existence of the diffusion pole in the translationally invariant diagrammatic treatment of disordered electron systems. We analyze Bethe–Salpeter equations for the two-particle vertex in the electron–hole and the electron–electron scattering channels and derive for systems with electron–hole symmetry a nonlinear integral equation that the two-particle irreducible vertices from both channels must obey. We use this equation and a parquet decomposition of the full vertex to set restrictions on an admissible form of the two-particle singularity induced by probability conservation. We find that such a singularity in two-particle functions can exist only if it is integrable, that is, only in the metallic phase in dimensions $d > 2$.

1. Introduction

Scattering of free charge carriers on impurities and lattice imperfections can lead at low temperatures to a metal–semiconductor transition. There are two qualitatively different scenarios how a metal can turn insulating due to excessive scatterings on impurities. In the first case the metal–insulator transition materializes in substitutional alloys when charge carriers are expelled from the Fermi surface and an energy gap develops. This transition, called a split band, is qualitatively well understood and quantitatively well modeled by a mean-field solution [1, 2]. The second type of a metal–insulator transition is much more complicated and up to now not completely understood. Electrons in a metal with random impurities can lose their ability to diffuse on macroscopic scales. Such a scenario was first suggested by Anderson [3] and is now called a Anderson localization transition.

One of the principal obstacles in understanding the Anderson localization transition is our inability to describe the vanishing of diffusion of electrons in random media analytically even in its simplest model version. Hence only approximate quantitative results are available both analytically and numerically. We have not yet succeeded in reconciling

results from analytic and numerical approaches. Analytic, mostly diagrammatic and field-theoretic approaches in the thermodynamic limit indicate that the critical behavior at the Anderson localization transition fits the one-parameter scaling scheme with a single correlation length controlling the long-range fluctuations [4, 5]. On the other hand, an increasing number of numerical studies of the Anderson localization transition in finite volumes suggest that, instead of homogeneous, translationally invariant parameters one has to take into consideration distributions of conductances or local particle densities [6, 7]. The two different methodological approaches, analytic and numerical, disagree not only on the number of relevant controlling parameters needed to understand Anderson localization but also on the critical behavior and the values of the critical exponents [8, 9]. Neither of these approaches is, however, absolutely conclusive in delivering ultimate answers.

In case of a disagreement between results from two rather well-established and otherwise reliable methods one has to revisit the assumptions under which either results were derived and to which restrictions they are subject. One of the most important features used in the description of the critical behavior of an Anderson localization transition

is a singular low-energy behavior of the density–density correlation function of disordered systems. This singularity has the form of a resolvent of a diffusion equation and is called the diffusion pole. The existence of the diffusion pole and a connection of the diffusion constant with the conductivity are consequences of conservation laws in random systems [10]. Conservation laws should be a firm part of any reliable theory. We, however, showed recently that an asymptotic solution of the Anderson model of noninteracting electrons in high spatial dimensions does not fully obey the conservation of probability [11]. We suggested a qualitative explanation for such an unexpected behavior but, more importantly, we amassed arguments that unrestricted compliance with the conservation law in random systems is in conflict with analyticity of the spectral function [12, 13]. Since a discussion about the form of the pole in the density response function is still ongoing [14, 15], we trace in this paper the origin of the diffusion pole and set exact restrictions on the form of the singularity in the two-particle vertex caused by conservation laws in the translationally invariant description of disordered systems. We first thoroughly analyze the assumptions used to derive the diffusion pole and then derive the most general admissible form of this singularity without referring or resorting to any specific approximation. We find that in electron–hole symmetric systems the diffusion pole must be integrable in momentum space.

2. Definitions and assumptions

We model the system of noninteracting electrons by a lattice gas described by an Anderson Hamiltonian [3]:

$$\hat{H} = \sum_{\mathbf{k}} |\mathbf{k}\rangle \epsilon(\mathbf{k}) \langle \mathbf{k}| + \sum_i |i\rangle V_i \langle i| \quad (1)$$

used to capture the impact of randomness on the electronic structure of metallic alloys as well as to understand the vanishing of diffusion in the limit of strong randomness. The first, homogeneous, part of this Hamiltonian is kinetic energy and is diagonalized in momentum space (Bloch waves). The second sum runs over lattice sites and describes a site-diagonal random potential. Values V_i at different positions are uncorrelated and follow a probability distribution $P(V_i)$. This term is diagonalized in the direct space by local Wannier states. The two operators do not commute, quantum fluctuations become important and the full Anderson Hamiltonian cannot be easily diagonalized. The only way to keep analytic control of the behavior of equilibrium states of the Anderson model is to go directly to the thermodynamic limit. Standardly it is approached by applying the ergodic theorem, that is, summation over lattice sites equals the configurational averaging.

Ergodicity itself, however, does not simplify the process of averaging over randomness. Another assumption must be adopted to master this problem. We assume that the thermodynamic limit can be performed independently term by term in the expansion in powers of the random potential. It means that we expect that the configurationally averaged perturbation expansion in the random potential converges for all quantities of interest.

The thermodynamic limit has an important simplifying consequence for macroscopic (averaged) quantities. The spectrum of a random Hamiltonian in the thermodynamic limit is invariant with respect to lattice translations. It means that operators \hat{H} and $\hat{T}_{\mathbf{R}} \hat{H} \hat{T}_{\mathbf{R}}^\dagger$, where $\hat{T}_{\mathbf{R}}$ is the operator of translation with a lattice vector \mathbf{R} , have an identical spectrum of eigenvalues with translationally shifted eigenvectors. A lattice translation by a vector \mathbf{R}_n applied to the Anderson Hamiltonian from equation (1) generates a new one, $\sum_{\mathbf{k}} |\mathbf{k}\rangle \epsilon(\mathbf{k}) \langle \mathbf{k}| + \sum_i |i + n\rangle V_i \langle i + n|$ having the same distribution of random energies. Unless we break translational symmetry in thermodynamic states, we are unable to distinguish translationally shifted Hamiltonians. We cannot, however, break translational invariance of the thermodynamic states arbitrarily, since their symmetry should be in agreement with the spatial distribution of the eigenstates of the Hamiltonian for the given configuration of the random potential. Since we do not know this spectrum, we must treat all lattice translations of the Hamiltonian as equivalent and instead of one configuration of the random potential we describe the whole class of translationally shifted equivalent Hamiltonians $\hat{T}_{\mathbf{R}} \hat{H} \hat{T}_{\mathbf{R}}^\dagger$. In this way we cannot distinguish directly between extended and localized eigenstates of the random potential, since the localized states are represented by a class of vectors differing by lattice translations.

The natural basis for translationally invariant quantities is formed by Bloch waves labeled by quasimomenta. We generically denote \mathbf{k}, \mathbf{q} as fermionic and bosonic (transferred) momenta, respectively. The fundamental building blocks of the translationally invariant description of disordered electrons are averaged one- and two-particle resolvents $G(\mathbf{k}, z)$ and $G_{\mathbf{kk}'}^{(2)}(z_+, z_-; \mathbf{q})$, where $z_+ = E + \omega + i\eta$ and $z_- = E - i\eta$ are complex energies with E standing for the Fermi energy, ω for the bosonic transfer frequency (energy) and η is a (infinitesimally) small damping (convergence) factor. We adopt the electron–hole representation for the two-particle Green function with \mathbf{k} and \mathbf{k}' for incoming and outgoing electron momenta. The bosonic momentum \mathbf{q} measures the difference between the incoming momenta of the electron and the hole. Energies of the electron and the hole z_+, z_- in systems with noninteracting particles are external parameters.

The averaged one-electron resolvent in disordered systems can be represented as in many-body theories via an irreducible vertex—the self-energy $\Sigma(\mathbf{k}, z)$. We can write a Dyson equation for it:

$$\left\langle \left\langle \mathbf{k} \left| \frac{1}{z\hat{1} - \hat{H}} \right| \mathbf{k}' \right\rangle \right\rangle_{\text{av}} = \frac{\delta(\mathbf{k} - \mathbf{k}')}{z - \epsilon(\mathbf{k}) - \Sigma(\mathbf{k}, z)}. \quad (2)$$

The self-energy $\Sigma(\mathbf{k}, z)$ stands for the impact of scatterings of the electron on random impurities. Knowledge of the self-energy is then sufficient to determine the energy spectrum, spectral density and, in general, all aspects of propagation of single particles in disordered media.

The two-particle resolvent $G^{(2)}$ can then be represented via a two-particle vertex Γ defined from an equation:

$$G_{\mathbf{kk}'}^{(2)}(z_+, z_-; \mathbf{q}) = \left\langle \left\langle \mathbf{q} + \mathbf{k}, \mathbf{k} \left| \frac{1}{z_+ - \hat{H}} \otimes \frac{1}{z_- - \hat{H}} \right| \mathbf{k}', \mathbf{q} + \mathbf{k}' \right\rangle \right\rangle_{\text{av}}$$

$$\begin{aligned} &\equiv \left\langle \left\langle \mathbf{k} \left| \frac{1}{z_+ - \hat{H}} \right| \mathbf{k}' \right\rangle \left\langle \mathbf{q} + \mathbf{k}' \left| \frac{1}{z_- - \hat{H}} \right| \mathbf{q} + \mathbf{k} \right\rangle \right\rangle_{\text{av}} \\ &= G(\mathbf{k}, z_+) G(\mathbf{q} + \mathbf{k}, z_-) [\delta(\mathbf{k} - \mathbf{k}') \\ &\quad + \Gamma_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q}) G(\mathbf{k}', z_+) G(\mathbf{q} + \mathbf{k}', z_-)] \end{aligned} \quad (3)$$

where \otimes denotes the direct product of operators. The two-particle vertex represents a disorder-induced correlation between simultaneous propagation of two quasiparticles. Analogously to the self-energy it measures the net impact of elastic scatterings on the random potential.

The two-particle vertex Γ can be further simplified by introducing an irreducible vertex Λ playing the role of a two-particle self-energy. The irreducible and the full vertex are connected by a Bethe–Salpeter equation. Unlike the one-particle irreducibility, the two-particle irreducibility is ambiguous [16]. There are two types of two-particle irreducibility in systems with elastic scatterings only, electron–hole and electron–electron. They are characterized by different Bethe–Salpeter equations. The Bethe–Salpeter equation in the electron–hole scattering channel then is

$$\begin{aligned} \Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) &= \Lambda_{\mathbf{k}\mathbf{k}'}^{\text{eh}}(\mathbf{q}) \\ &\quad + \frac{1}{N} \sum_{\mathbf{k}''} \Lambda_{\mathbf{k}\mathbf{k}''}^{\text{eh}}(\mathbf{q}) G_+(\mathbf{k}'') G_-(\mathbf{q} + \mathbf{k}'') \Gamma_{\mathbf{k}''\mathbf{k}'}(\mathbf{q}). \end{aligned} \quad (4a)$$

We suppressed the frequency variables in equation (4a), since they are not dynamical ones. They can be easily deduced from the one-electron propagators $G_{\pm}(\mathbf{k}) = G^{\text{R,A}}(\mathbf{k}) \equiv G(\mathbf{k}, z_{\pm})$ used there.

The other nonequivalent representation of the two-particle vertex is obtained if we sum explicitly multiple scatterings of two electrons (holes). The alternative Bethe–Salpeter equation then is [16]

$$\begin{aligned} \Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) &= \Lambda_{\mathbf{k}\mathbf{k}'}^{\text{ee}}(\mathbf{q}) + \frac{1}{N} \sum_{\mathbf{k}''} \Lambda_{\mathbf{k}\mathbf{k}''}^{\text{ee}}(\mathbf{q} + \mathbf{k}' - \mathbf{k}'') \\ &\quad \times G_+(\mathbf{k}'') G_-(\mathbf{q} + \mathbf{k} + \mathbf{k}' - \mathbf{k}'') \Gamma_{\mathbf{k}''\mathbf{k}'}(\mathbf{q} + \mathbf{k} - \mathbf{k}''). \end{aligned} \quad (4b)$$

We introduced an irreducible vertex in the electron–electron scattering channel Λ^{ee} . Irreducible vertices Λ^{eh} and Λ^{ee} do not include isolated pair electron–hole and electron–electron scatterings, respectively.

3. Diffusion pole and electron–hole symmetry

Noninteracting particles scattered on impurities are marked by a diffusion pole. The low-energy limit of a special matrix element of the two-particle resolvent, electron–hole correlation function, has the following asymptotics for $q \rightarrow 0$ and $\omega/q \rightarrow 0$:

$$\begin{aligned} \Phi_E^{\text{RA}}(\mathbf{q}, \omega) &= \frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'} G_{\mathbf{k}\mathbf{k}'}^{\text{RA}}(E + \omega, E; \mathbf{q}) \\ &\doteq \frac{2\pi n_{\text{F}}}{-i\omega + D(\omega)q^2} + O(q^0, \omega^0) \end{aligned} \quad (5)$$

where n_{F} is the density of one-particle states at the Fermi level [10]. We used an abbreviation for the energy arguments $G_{\mathbf{k}\mathbf{k}'}^{\text{RA}}(E + \omega, E; \mathbf{q}) \equiv G_{\mathbf{k}\mathbf{k}'}^{(2)}(E + \omega + i0^+, E - i0^+; \mathbf{q})$. The low-energy electron–hole correlation function becomes a propagator of a diffusion equation with a dynamical diffusion

constant $D(\omega)$. The dynamical form of the diffusion constant is introduced so that both possible mobility regimes in disordered systems, metallic and localized, can be covered by this form of singularity. If $D(0) = D > 0$ then we are in the metallic, diffusive regime and if $\lim_{\omega \rightarrow 0} D(\omega)/(-i\omega) = \xi^2 > 0$ we are in the localized, diffusionless regime. This singularity with a dynamical diffusion constant $D(\omega)$ is generally called a diffusion pole. Its origin is in probability conservation leading to a diffusive behavior in the metallic phase. It is called the diffusion or Berezinski pole also in the localized phase with $D(0) = 0$ even though it generates no diffusion [17–19].

This form of a low-energy singularity is not evident and to prove it one has to use Ward identities connecting one- and two-particle averaged functions. Ward identities reflect conservation laws. In disordered noninteracting systems we have probability (mass or charge) conservation. It is mathematically equivalent to completeness of the Hilbert space of Bloch waves. First the Ward identity due to charge conservation was derived for disordered systems within the mean-field approximation by Velický [20] and later extended beyond this approximation in [16]. It is a consequence of an operator identity

$$\frac{1}{z_+ - \hat{H}} \frac{1}{z_- - \hat{H}} = \frac{1}{z_- - z_+} \left[\frac{1}{z_+ - \hat{H}} - \frac{1}{z_- - \hat{H}} \right] \quad (6)$$

where the multiplication is the standard operator (matrix) one. This identity holds for any one-particle Hamiltonian. In the thermodynamic limit we must, however, average this identity and the averaging procedure need not conserve all its aspects when projected onto translationally invariant states [12]. When using the above identity in the evaluation of the homogeneous part of the electron–hole correlation function, that is $q = 0$, we obtain

$$\Phi_E^{\text{RA}}(\mathbf{0}, \omega) \doteq \frac{2\pi n_{\text{F}}}{-i\omega}. \quad (7)$$

No spatial fluctuations ($q \neq 0$) of the correlation function in the low-frequency limit can be deduced from the Velický–Ward identity. To derive the spatial behavior of the diffusion pole in equation (5) one has to resort to another relation introduced by Vollhardt and Wölfle [21]. It utilizes the Dyson and a Bethe–Salpeter equation, equation (2) and equation (4a), and relates the one- and two-particle irreducible functions Σ and Λ^{eh} , respectively. It is

$$\begin{aligned} \Sigma^{\text{R}}(\mathbf{q} + \mathbf{k}, E + \omega) - \Sigma^{\text{A}}(\mathbf{k}, E) &= \frac{1}{N} \sum_{\mathbf{k}'} \Lambda_{\mathbf{k}\mathbf{k}'}^{\text{RA}}(E + \omega, E; \mathbf{q}) \\ &\quad \times [G^{\text{R}}(\mathbf{q} + \mathbf{k}', E + \omega) - G^{\text{A}}(\mathbf{k}', E)] \end{aligned} \quad (8)$$

and was proved diagrammatically (perturbatively). Using the Bethe–Salpeter equation one can show that in the homogeneous limit $q = 0$ this identity reflects the continuity equation and hence is equivalent to the Velický–Ward identity. Equation (8) together with the Bethe–Salpeter equation in the electron–hole channel are then used to show that the long-distance fluctuations of the low-energy limit of the electron–hole correlation function are controlled by a dynamical diffusion constant $D(\omega)$ [10]. Note that identity (7) holds for both pure and random systems, while equation (8) is nontrivial

only for disordered systems. The actual form of the diffusion pole, that is, the singularity from equation (5) is physically relevant only for a spatially fluctuating regime with $q \rightarrow 0$. The purely homogeneous case itself, $q = 0$ as in equation (7), may be a singular point and need not be pertinent for the form of spatial fluctuations with $q > 0$. This holds for both diffusive, $D(0) = D > 0$, and diffusionless, $D(0) = 0$, regimes. We need Bethe–Salpeter equations to assess properly the long-range spatial correlation of the propagation of two quasiparticles ($q > 0$) expressed by the low-energy limit of the electron–hole correlation function in equation (5).

Another important feature of noninteracting electrons on a bipartite lattice without external magnetic field and spin–orbit coupling is the electron–hole symmetry. It consists of simultaneous time inversion and charge conjugation. Finally, it is equivalent in the thermodynamic limit to reversing the direction of the particle propagation, that is $\mathbf{k} \rightarrow -\mathbf{k}$. The electron and the hole interchange their roles. The electron–hole invariance for the one-particle propagator then means $G(\mathbf{k}, z) = G(-\mathbf{k}, z)$. Electron–hole transformation leads to nontrivial symmetries when applied onto one of the fermion propagators in two-particle functions. It can be represented either by reversing the electron line leading to a transformation $\mathbf{k} \rightarrow -\mathbf{k}', \mathbf{k}' \rightarrow -\mathbf{k}, \mathbf{q} \rightarrow \mathbf{Q}$ or by reversing the hole propagator $\mathbf{k} \rightarrow \mathbf{k}, \mathbf{k}' \rightarrow \mathbf{k}', \mathbf{q} \rightarrow -\mathbf{Q}$. We denoted $\mathbf{Q} = \mathbf{q} + \mathbf{k} + \mathbf{k}'$. We then obtain two symmetry relations for the full two-particle vertex:

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \Gamma_{-\mathbf{k}'-\mathbf{k}}(\mathbf{Q}) = \Gamma_{\mathbf{k}\mathbf{k}'}(-\mathbf{Q}). \quad (9a)$$

The two-particle irreducible vertices are not invariant with respect to the electron–hole transformation, since the electron–hole vertex is transformed onto the electron–electron one and vice versa. We then have the following electron–hole symmetry relations:

$$\Lambda_{\mathbf{k}\mathbf{k}'}^{\text{ee}}(\mathbf{q}) = \Lambda_{-\mathbf{k}'-\mathbf{k}}^{\text{eh}}(\mathbf{Q}) = \Lambda_{\mathbf{k}\mathbf{k}'}^{\text{eh}}(-\mathbf{Q}). \quad (9b)$$

These relations say that the Bethe–Salpeter equation (4a) transforms upon interchanging an electron by a hole in one particle line onto the Bethe–Salpeter equation (4b) and vice versa. When the invariance with respect to the electron–hole transformation is applied to the two-particle resolvent we obtain

$$G_{\mathbf{k}\mathbf{k}'}^{\text{RA}}(E + \omega, E; \mathbf{q}) = G_{\mathbf{k}\mathbf{k}'}^{\text{RA}}(E + \omega, E; -\mathbf{q} - \mathbf{k} - \mathbf{k}'). \quad (10)$$

Since the two-particle resolvent contains the diffusion pole for $\omega, \mathbf{q}^2 \rightarrow 0$, the same singularity must emerge with equal weight also in the limit $\omega, (\mathbf{k} + \mathbf{k}' + \mathbf{q})^2 \rightarrow 0$.

The uncorrelated propagation of electrons in a random potential is regular and the diffusion pole must emerge in the vertex function Γ . Taking into account the electron–hole invariance we can single out the singular parts of the electron–hole symmetric two-particle vertex and obtain

$$\Gamma_{\mathbf{k}\mathbf{k}'}^{\text{RA}}(\mathbf{q}, \omega) = \gamma_{\mathbf{k}\mathbf{k}'}^{\text{RA}}(\mathbf{q}, \omega) + \frac{\varphi_{\mathbf{k}\mathbf{k}'}^{\text{RA}}}{-i\omega + D(\omega)\mathbf{q}^2} + \frac{\varphi_{\mathbf{k}\mathbf{k}'}^{\text{RA}}}{-i\omega + D(\omega)(\mathbf{q} + \mathbf{k} + \mathbf{k}')^2}. \quad (11)$$

The reduced vertex γ^{RA} has a marginal and thermodynamically irrelevant singularity for $\omega \rightarrow 0$ at $k = k' = q = 0$. It can, nevertheless, display another singular behavior in fermionic variables \mathbf{k}, \mathbf{k}' that is not derivable from the diffusion pole. Such a singularity must not, however, affect the form of the diffusion pole in the electron–hole correlation function for $q \rightarrow 0$. The second term on the right-hand side of equation (11) dominates in the leading order of the limit $q \rightarrow 0, \omega \rightarrow 0$ while the third one is in the limit $\mathbf{q} + \mathbf{k} + \mathbf{k}' \rightarrow 0, \omega \rightarrow 0$.

Equation (11) is the most general form of the two-particle vertex reproducing the diffusion pole in the correlation function Φ . The singularity for $\mathbf{q} \rightarrow 0$ is the diffusion pole while the other for $\mathbf{q} + \mathbf{k} + \mathbf{k}' \rightarrow 0$ is called the Cooper pole and is caused by multiple electron–electron scatterings. To conform this representation with equation (7) we have to satisfy a normalization condition that in the metallic phase ($D(0) > 0$) is

$$\frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'} |G_+(\mathbf{k})|^2 \varphi_{\mathbf{k}\mathbf{k}'}^{\text{RA}} |G_+(\mathbf{k}')|^2 = 2\pi n_{\text{F}}. \quad (12)$$

4. Parquet equations with electron–hole symmetry

The full two-particle vertex can be decomposed apart from Bethe–Salpeter equations by means of the so-called parquet equation that can be represented in various equivalent ways [16]:

$$\begin{aligned} \Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) &= \Lambda_{\mathbf{k}\mathbf{k}'}^{\text{ee}}(\mathbf{q}) + \mathcal{K}_{\mathbf{k}\mathbf{k}'}^{\text{ee}}(\mathbf{q}) = \Lambda_{\mathbf{k}\mathbf{k}'}^{\text{eh}}(\mathbf{q}) + \mathcal{K}_{\mathbf{k}\mathbf{k}'}^{\text{eh}}(\mathbf{q}) \\ &= \mathcal{K}_{\mathbf{k}\mathbf{k}'}^{\text{eh}}(\mathbf{q}) + \mathcal{K}_{\mathbf{k}\mathbf{k}'}^{\text{ee}}(\mathbf{q}) + \mathcal{I}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) \\ &= \Lambda_{\mathbf{k}\mathbf{k}'}^{\text{ee}}(\mathbf{q}) + \Lambda_{\mathbf{k}\mathbf{k}'}^{\text{eh}}(\mathbf{q}) - \mathcal{I}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) \end{aligned} \quad (13)$$

where $\mathcal{K}_{\mathbf{k}\mathbf{k}'}^{\text{eh}}(\mathbf{q})$ and $\mathcal{K}_{\mathbf{k}\mathbf{k}'}^{\text{ee}}(\mathbf{q})$ are two-particle reducible vertices in the electron–hole and the electron–electron channel, respectively. We denoted $\mathcal{I} = \Lambda^{\text{eh}} \cap \Lambda^{\text{ee}}$ a two-particle fully irreducible vertex, that is, a vertex irreducible simultaneously for both the electron–hole and the electron–electron pair propagation (multiple scatterings).

The parquet equations hold generally for systems where the electron–hole and the electron–electron multiple scatterings are nonequivalent, that is, the corresponding two-particle irreducibilities are unambiguous and excluding definitions of diagrammatic contributions. The concept of the parquet theory based on nonequivalence of two-particle irreducibility can at best be understood in terms of sets of diagrams where the addition of functions is represented by a union of sets of diagrams the functions stand for. Nonequivalence of the electron–hole and the electron–electron multiple scatterings means $\mathcal{K}^{\text{ee}} \cap \mathcal{K}^{\text{eh}} = \emptyset$. We trivially have in each α -channel $\Lambda^\alpha \cap \mathcal{K}^\alpha = \emptyset$. Further on, we have $\Lambda^{\text{eh}} = \Lambda^{\text{eh}} \cap \Gamma = (\Lambda^{\text{eh}} \cap \Lambda^{\text{ee}}) \cup (\Lambda^{\text{eh}} \cap \mathcal{K}^{\text{ee}}) \subset \mathcal{I} \cup \mathcal{K}^{\text{ee}}$. On the other hand, $\mathcal{K}^{\text{ee}} = \mathcal{K}^{\text{ee}} \cap \Gamma = (\mathcal{K}^{\text{ee}} \cap \Lambda^{\text{eh}}) \cup (\mathcal{K}^{\text{ee}} \cap \mathcal{K}^{\text{eh}}) = \mathcal{K}^{\text{ee}} \cap \Lambda^{\text{eh}}$. Hence $\mathcal{K}^{\text{ee}} \subset \Lambda^{\text{eh}}$. Combining the above two relations we obtain $\Lambda^{\text{eh}} = \mathcal{I} \cup \mathcal{K}^{\text{ee}}$ from which we reach the parquet representations via irreducible or reducible vertices in equation (13), $\Lambda^{\text{eh}} \cup \Lambda^{\text{ee}} \setminus \mathcal{I} = \mathcal{I} \cup \mathcal{K}^{\text{ee}} \cup \mathcal{K}^{\text{eh}} = \Gamma$.

One must be careful when using the parquet decomposition for noninteracting electrons with only elastic scatterings.

In this case multiple scatterings on a single site are identical for both channels. Hence, the two Bethe–Salpeter equations (4) are identical when the one-electron propagators are purely local. We then obtain $\Lambda^{\text{eh}} = \Lambda^{\text{ee}} = \mathcal{I}$. It means that irreducible and reducible local diagrams coincide and the concept of two-particle irreducibility becomes ambiguous. To amend this problem we introduce a stronger *full two-particle irreducibility* including also local scatterings where the electron and the hole are indistinguishable. We denote this vertex \mathcal{J} . The irreducible vertices \mathcal{I} , Λ^{eh} and Λ^{ee} for noninteracting electrons should be rewritten in equation (13) so that we replace vertex \mathcal{I} by vertex \mathcal{J} . We then have

$$\mathcal{I}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \mathcal{J}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) + \frac{\mathcal{J}^0 G_+ G_-}{1 - \mathcal{J}^0 G_+ G_-} \mathcal{J}^0, \quad (14a)$$

$$\Lambda_{\mathbf{k}\mathbf{k}'}^\alpha(\mathbf{q}) = \bar{\Lambda}_{\mathbf{k}\mathbf{k}'}^\alpha(\mathbf{q}) + \frac{\mathcal{J}^0 G_+ G_-}{1 - \mathcal{J}^0 G_+ G_-} \mathcal{J}^0 \quad (14b)$$

where $\mathcal{J}^0 = N^{-3} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \mathcal{J}_{\mathbf{k}\mathbf{k}'}(\mathbf{q})$ and $G_\pm = N^{-1} \sum_{\mathbf{k}} G_\pm(\mathbf{k})$ are the appropriate local (momentum independent) parts. Vertex $\bar{\Lambda}_{\mathbf{k}\mathbf{k}'}^\alpha(\mathbf{q})$ is irreducible in channel α but does not contain successive multiple scatterings on the same site. It is important that the fully irreducible vertex $\mathcal{J}_{\mathbf{k}\mathbf{k}'}(\mathbf{q})$ contains only cumulant averaged powers of the random potential on the same lattice site so that double counting is avoided.

We now use the symmetries from equation (9) to replace the two irreducible vertices by a single function. We define

$$\Lambda_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) \equiv \Lambda_{\mathbf{k}\mathbf{k}'}^{\text{ee}}(\mathbf{q}) = \Lambda_{\mathbf{k}\mathbf{k}'}^{\text{eh}}(-\mathbf{q} - \mathbf{k} - \mathbf{k}'). \quad (15)$$

We use this definition in the parquet equation (13) where we represent the full vertex by a solution of the Bethe–Salpeter equation (4a). We then obtain a fundamental equation for the irreducible vertex:

$$\begin{aligned} \Lambda_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) &= \mathcal{I}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) \\ &+ \frac{1}{N} \sum_{\mathbf{k}''} \Lambda_{\mathbf{k}\mathbf{k}''}(-\mathbf{q} - \mathbf{k} - \mathbf{k}'') G_+(\mathbf{k}'') G_-(\mathbf{q} + \mathbf{k}'') \\ &\times [\Lambda_{\mathbf{k}''\mathbf{k}'}(\mathbf{q}) + \Lambda_{\mathbf{k}''\mathbf{k}'}(-\mathbf{q} - \mathbf{k}'' - \mathbf{k}') - \mathcal{I}_{\mathbf{k}''\mathbf{k}'}(\mathbf{q})]. \end{aligned} \quad (16)$$

It is a nonlinear integral equation for vertex Λ from an input \mathcal{I} that may have multiple solutions. We choose the physical one by matching it to a perturbative solution reached by an iterative procedure with an auxiliary coupling constant λ and a starting condition $\Lambda^{(0)} = \lambda \mathcal{I}$. The iteration procedure for a fixed coupling constant λ is determined by a recursion formula

$$\begin{aligned} &\frac{1}{N} \sum_{\mathbf{k}''} [\delta_{\mathbf{k}''\mathbf{k}'} - \Lambda_{\mathbf{k}\mathbf{k}''}^{(n-1)}(-\mathbf{q} - \mathbf{k} - \mathbf{k}'') G_+(\mathbf{k}'') \\ &\times G_-(\mathbf{q} + \mathbf{k}'')] (\Lambda_{\mathbf{k}''\mathbf{k}'}^{(n)}(\mathbf{q}) - \lambda \mathcal{I}_{\mathbf{k}''\mathbf{k}'}(\mathbf{q})) \\ &= \frac{1}{N} \sum_{\mathbf{k}''} \Lambda_{\mathbf{k}\mathbf{k}''}^{(n-1)}(-\mathbf{q} - \mathbf{k} - \mathbf{k}'') G_+(\mathbf{k}'') \\ &\times G_-(\mathbf{q} + \mathbf{k}'') \Lambda_{\mathbf{k}''\mathbf{k}'}^{(n-1)}(-\mathbf{q} - \mathbf{k}'' - \mathbf{k}'). \end{aligned} \quad (17)$$

In this way vertex $\Lambda = \Lambda^{(\infty)}$ is completely determined from the input, the fully irreducible vertex $\lambda \mathcal{I}$. A physical solution for $\lambda = 1$ is reached only if the iteration procedure converges for $0 < \lambda \ll 1$ and the result can analytically be continued to $\lambda = 1$. This construction of the physical solution

corresponds to the linked-cluster expansion from many-particle physics [22]. The iteration scheme from equation (17) is the only available way to reach a physical solution and hence its convergence and analyticity are of principal importance for the diagrammatic description of disordered systems. Using equations (14) we can rewrite equation (16) to another one for the irreducible vertex $\bar{\Lambda}$ determined from \mathcal{J} . The latter vertex is the genuine independent input. Notice that in single-site theories with local one-electron propagators we obtain a solution to equation (17) to be $\bar{\Lambda} = \mathcal{J}^0$.

Equation (16) (alternatively equation (17)) is a fundamental equation of motion for the two-particle irreducible vertex, being electron–hole-symmetric. It is exact as far as we use the exact fully irreducible vertex \mathcal{I} . The corresponding full two-particle vertex obeys simultaneously both the Bethe–Salpeter equations in the electron–hole and the electron–electron channels, equations (4), if $\Lambda_{\mathbf{k}\mathbf{k}'}^{\text{eh}}(\mathbf{q}) \neq \Lambda_{\mathbf{k}\mathbf{k}'}^{\text{ee}}(\mathbf{q})$.

5. Integrability of the diffusion pole

If we combine equation (15) and the parquet equation (13), where the electron–hole symmetry, equation (9), is used, we can represent the two-particle vertex Γ of noninteracting electrons in a random potential as

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \Lambda_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) + \Lambda_{\mathbf{k}\mathbf{k}'}(-\mathbf{q} - \mathbf{k} - \mathbf{k}') - \mathcal{I}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}). \quad (18)$$

This decomposition into irreducible vertices is exact if electrons and holes are distinguishable quasiparticles (electron–electron and electron–hole scattering diagrams are topologically distinct and contribute independently to two-particle functions), the system is electron–hole-symmetric and the two-particle fully irreducible vertex \mathcal{I} is known exactly.

The irreducible vertex Λ obeys equation (16) which replaces the Bethe–Salpeter equations for the full vertex Γ . Unlike Bethe–Salpeter equations, equation (16) is manifestly nonlinear and can pose a restriction on possible singularities in its solutions. We now demonstrate that, due to representation (18), the diffusion and Cooper poles from equation (11) may materialize in the full two-particle vertex Γ only if the diffusion pole is present in the irreducible vertex Λ .

We need not find the most general form of the low-energy ($\omega \rightarrow 0$) singularities compliant with equation (16) but rather check whether and when singularities from representation (11) can emerge in solutions of equation (16).

It appears that vertex $\Lambda_{\mathbf{k}\mathbf{k}'}(\mathbf{q})$ contains the diffusion pole of the full vertex Γ , $\Lambda_{\mathbf{k}\mathbf{k}'}^{\text{eh}}(\mathbf{q})$ the Cooper pole and the fully irreducible vertex $\mathcal{I}_{\mathbf{k}\mathbf{k}'}(\mathbf{q})$ is free of these poles. This fact follows from an alternative form of equation (16):

$$\begin{aligned} \Lambda_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) &= \mathcal{I}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) \\ &+ \frac{1}{N} \sum_{\mathbf{k}''} \Gamma_{\mathbf{k}\mathbf{k}''}(\mathbf{q}) G_+(\mathbf{k}'') G_-(\mathbf{q} + \mathbf{k}'') \Gamma_{\mathbf{k}''\mathbf{k}'}(\mathbf{q}) \\ &- \frac{1}{N} \sum_{\mathbf{k}''} [\Lambda_{\mathbf{k}\mathbf{k}''}(\mathbf{q}) - \mathcal{I}_{\mathbf{k}\mathbf{k}''}(\mathbf{q})] \\ &\times G_+(\mathbf{k}'') G_-(\mathbf{q} + \mathbf{k}'') \Gamma_{\mathbf{k}''\mathbf{k}'}(\mathbf{q}) \end{aligned} \quad (19)$$

where we used the fundamental parquet equation (13) to represent the integral kernel Λ . The electron–hole symmetry leads in the limit $q \rightarrow 0$ and $\omega \rightarrow 0$ to a representation of the complex conjugate of the full two-particle vertex:

$$\Gamma_{\mathbf{k}\mathbf{k}'}^{\text{RA}}(\mathbf{q}, \omega)^* = \Gamma_{\mathbf{k}'+\mathbf{q}, \mathbf{k}+\mathbf{q}}^{\text{RA}}(-\mathbf{q}, -\omega) \quad (20)$$

that we use to evaluate the convolution of the diffusion poles from the full vertex Γ in the first sum on the right-hand side of equation (19). We obtain for $\mathbf{k} = \mathbf{k}'$ in the leading order of $q \rightarrow 0$ and $\omega \rightarrow 0$:

$$\frac{1}{N} \sum_{\mathbf{k}''} \Gamma_{\mathbf{k}\mathbf{k}''}^{\text{RA}}(\mathbf{q}, \omega) G_+(\mathbf{k}'') G_-(\mathbf{q} + \mathbf{k}'') \Gamma_{\mathbf{k}'\mathbf{k}}^{\text{RA}}(\mathbf{q}, \omega) \xrightarrow{q \rightarrow 0, \omega \rightarrow 0} \frac{1}{N} \sum_{\mathbf{k}''} \frac{|\varphi_{\mathbf{k}'\mathbf{k}}^{\text{RA}} G_+(\mathbf{k}'')|^2}{\omega^2 + D(\omega)^2 q^4}.$$

This squared diffusion pole must be compensated by the second sum on the right-hand side of equation (19). It means that the diffusion pole must be completely contained in function $\Lambda_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) - \mathcal{I}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \mathcal{K}_{\mathbf{k}\mathbf{k}'}^{\text{eh}}(\mathbf{q})$. From the electron–hole symmetry we then obtain that the Cooper pole must completely be contained in the function $\mathcal{K}_{\mathbf{k}\mathbf{k}'}^{\text{ce}}(\mathbf{q})$. Consequently the sum of the diffusion and the Cooper pole from the full vertex $\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q})$ in equation (11) is already part of the function $\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) - \mathcal{I}_{\mathbf{k}\mathbf{k}'}(\mathbf{q})$. The fully irreducible vertex $\mathcal{I}_{\mathbf{k}\mathbf{k}'}(\mathbf{q})$ is hence free of the diffusion and Cooper poles.

We first prove integrability of the diffusion pole in the metallic phase with $D(0) = D > 0$. When inserting the singular part of the two-particle vertex due to the diffusion pole we obtain the leading singularity on the left-hand side of equation (17):

$$S_{\mathbf{k}\mathbf{k}'}^{\text{L}}(\mathbf{q}, \omega) = -\frac{1}{-i\omega + Dq^2} \times \frac{1}{N} \sum_{\mathbf{k}''} \frac{\varphi_{\mathbf{k}\mathbf{k}''}^{\text{RA}} \varphi_{\mathbf{k}''\mathbf{k}'}^{\text{RA}} G_+(\mathbf{k}'') G_-(\mathbf{q} + \mathbf{k}'')}{-i\omega + D(\mathbf{q} + \mathbf{k} + \mathbf{k}'')^2} \quad (21a)$$

and on its right-hand side

$$S_{\mathbf{k}\mathbf{k}'}^{\text{R}}(\mathbf{q}, \omega) = \frac{1}{N} \sum_{\mathbf{k}''} \frac{\varphi_{\mathbf{k}\mathbf{k}''}^{\text{RA}} \varphi_{\mathbf{k}''\mathbf{k}'}^{\text{RA}}}{-i\omega + D(\mathbf{q} + \mathbf{k} + \mathbf{k}'')^2} \times \frac{G_+(\mathbf{k}'') G_-(\mathbf{q} + \mathbf{k}'')}{-i\omega + D(\mathbf{q} + \mathbf{k}' + \mathbf{k}'')^2}. \quad (21b)$$

Since the singular term from equation (21a) contains the complete form of the diffusion pole, the sum over momenta must not bring any new singular contribution in small frequencies and is of order $O(\omega^0)$. To assess the low-frequency behavior ($\omega \rightarrow 0$) of the sum over momenta we equal external fermionic momenta $\mathbf{k}' = \mathbf{k}$ and use an asymptotic representation for the contribution from the singular part of the integrands:

$$S_{\mathbf{k}\mathbf{k}}^{\text{L}}(\mathbf{q}, \omega) \doteq \frac{\varphi_{\mathbf{k}, -\mathbf{q}-\mathbf{k}}^{\text{RA}} \varphi_{-\mathbf{q}-\mathbf{k}, \mathbf{k}}^{\text{RA}} G^{\text{R}}(\mathbf{q} + \mathbf{k}) G^{\text{A}}(\mathbf{k})}{-i\omega + Dq^2} \times \frac{1}{N} \sum_{\mathbf{k}''}^{\kappa} \frac{1}{-i\omega + D(\mathbf{q} + \mathbf{k} + \mathbf{k}'')^2}, \quad (22a)$$

$$S_{\mathbf{k}\mathbf{k}}^{\text{R}}(\mathbf{q}, \omega) \doteq \varphi_{\mathbf{k}, -\mathbf{q}-\mathbf{k}}^{\text{RA}} \varphi_{-\mathbf{q}-\mathbf{k}, \mathbf{k}}^{\text{RA}} G^{\text{R}}(\mathbf{q} + \mathbf{k}) G^{\text{A}}(\mathbf{k}) \times \frac{1}{N} \sum_{\mathbf{k}''}^{\kappa} \frac{1}{[-i\omega + D(\mathbf{q} + \mathbf{k} + \mathbf{k}'')^2]^2} \quad (22b)$$

where κ is an appropriate momentum cutoff. The two expressions cannot be more divergent in the low-frequency limit as $(-i\omega)^{-1}$ for any value of the external momenta \mathbf{q} and \mathbf{k} . Due to the normalization condition, equation (12), we find for each vector \mathbf{k} a set (of measure one) of momenta \mathbf{q} so that $\varphi_{\mathbf{k}, -\mathbf{q}-\mathbf{k}}^{\text{RA}} \neq 0$. If the homogeneous case, $q = 0$, falls into this set then from equation (22a) we obtain integrability of the diffusion pole. If not, then for $\varphi_{\mathbf{k}, -\mathbf{q}-\mathbf{k}}^{\text{RA}} \neq 0$ we obtain $S_{\mathbf{k}\mathbf{k}}^{\text{L}}(\mathbf{q}, \omega) \propto (-i\omega)^{d/2-1}/(-i\omega + Dq^2)$ and $S_{\mathbf{k}\mathbf{k}}^{\text{R}}(\mathbf{q}, \omega) \propto (-i\omega)^{d/2-2}$. For low dimensions $d \leq 2$, both functions $S_{\mathbf{k}\mathbf{k}}^{\text{L}}(\mathbf{q}, \omega)$ and $S_{\mathbf{k}\mathbf{k}}^{\text{R}}(\mathbf{q}, \omega)$ have a stronger divergence than $(-i\omega)^{-1}$ (for $q = 0$) and equation (17) cannot be satisfied by any function $\Lambda_{\mathbf{k}\mathbf{k}}(\mathbf{q}, \omega)$. The diffusion pole can hence exist in the metallic phase only in dimensions $d > 2$.

In the localized phase we expect the following low-energy asymptotics ($q \rightarrow 0, \omega \rightarrow 0$) of the dynamical diffusion constant [18, 19]:

$$\xi^2 = \frac{D(\omega)}{-i\omega} > 0 \quad (23)$$

where ξ is a localization length. Using this asymptotics we can represent the singular part of the irreducible vertex Λ as follows:

$$\Lambda_{\mathbf{k}\mathbf{k}'}^{\text{sing}}(\mathbf{q}, \omega) \doteq \frac{\varphi_{\mathbf{k}\mathbf{k}'}}{-i\omega} \frac{1}{1 + \xi^2 \mathbf{q}^2}. \quad (24)$$

We utilize the electron–hole symmetry to evaluate the complex conjugate of the irreducible vertex Λ in the low-frequency $\omega \rightarrow 0$ and momentum $q \rightarrow 0$ limit:

$$\Lambda_{\mathbf{k}\mathbf{k}'}^{\text{RA}}(\mathbf{q}, \omega)^* = \Lambda_{-\mathbf{k}-\mathbf{q}, -\mathbf{k}'-\mathbf{q}}^{\text{RA}}(\mathbf{q}, -\omega) \quad (25)$$

and use it to derive a condition for the vanishing of quadratic singularity of order ω^{-2} on the right-hand side of equation (16). After substituting the representation of vertex Λ from equation (24) and setting $\mathbf{k}' = \mathbf{k}$ and $\mathbf{q} = 0$ in equation (16) we obtain

$$\frac{1}{N} \sum_{\mathbf{k}''} \left| \frac{\varphi_{\mathbf{k}\mathbf{k}''}^{\text{RA}} G_+(\mathbf{k}'')}{1 + \xi^2 (\mathbf{k} + \mathbf{k}'')^2} \right|^2 [2 + \xi^2 (\mathbf{k} + \mathbf{k}'')^2] = 0. \quad (26)$$

This condition can be fulfilled only if the irreducible vertex $\Lambda_{\mathbf{k}\mathbf{k}''}(\mathbf{q}, \omega)$ is free of the singularity due to the diffusion pole for $q \rightarrow 0$ and $\omega \rightarrow 0$, that is, $\varphi_{\mathbf{k}\mathbf{k}''}^{\text{RA}} = 0$ point-wise. The diffusion pole hence can exist nowhere in the localized phase.

6. Discussion and conclusions

The most severe consequence of integrability of the diffusion pole is nonexistence of the Berezinski pole in the localized phase in any dimension. It means that, when approaching the low-energy limit $q \rightarrow 0$ and $\omega/q \rightarrow 0$ in low dimensions ($d \leq 2$), we cannot meet the diffusion-pole-induced singularity. The localized phase must be reached in a non-critical or a less critical manner than that of the diffusion pole. It means that the homogeneous case $q = 0$ where the Velický–Ward identity, equation (7), holds is an isolated singular point with no relevance for spatial fluctuations with $q > 0$. Theories, such as the self-consistent theory of Anderson localization of Vollhardt and Wölfle [23], leading to solutions with a nonintegrable

diffusion pole are in conflict with the Bethe–Salpeter equation either in the electron–hole or in the electron–electron channel or with the electron–hole symmetry at the two-particle level.

Nonexistence of the Berezinski pole in the diagrammatic description of the localized phase has an important consequence on the relevance of criteria determining the diffusionless regime. We cannot use the averaged inverse participation number [8] in the translationally invariant description, since it vanishes in both the delocalized as well in the localized phase. Using equation (23) we obtain

$$P_E^{-1} \propto \frac{1}{N} \sum_{\mathbf{q}} \lim_{\omega \rightarrow 0} (-i\omega) \Phi_E^{\text{RA}}(\mathbf{q}, \omega) = 0$$

even in the localized phase, since the weight of the low-energy singularity of the electron–hole correlation function Φ^{RA} vanishes there. In a sense this conclusion is not surprising. The inverse participation number measures a portion of the lattice space where the amplitude of the wavefunction of the electron differs measurably from zero, that is $|\Psi_i|^2 \gg N^{-1}$. In a translationally invariant description of the diagrammatic theory in the thermodynamic limit we do not have appropriate tools to discriminate or prefer locally restricted areas. This may happen only for finite lattices with fixed configurations of the random potential breaking the global translational symmetry of the infinite volume. In fact, it has been known for a long time that the averaged inverse participation number is not a good criterion for the determination of the absence of diffusion [8].

Numerical simulations are performed on finite lattices and they seem to confirm the existence of the diffusion pole with the weight one near the metal–insulator transition [24, 25] as well as in the localized phase [15]. However, numerical simulations can be performed only on rather small lattices where one cannot effectively reach the diffusive regime $q \rightarrow 0$ with $\omega/q \rightarrow 0$. Numerical studies in [24, 25] calculate the electron–hole correlation function of a model for the quantum Hall effect, that is in an external magnetic field without the electron–hole symmetry. The numerical analysis in [15] investigates the limit $\omega \rightarrow 0$ with $q/\omega \rightarrow 0$ and not $\omega/q \rightarrow 0$. As we know [10], the two limits do not commute and the former has no relevance for the existence of the diffusion pole. The numerically observed $1/\omega$ behavior reflects only the Velický identity (7) valid for any configuration of the random potential.

Studies of Anderson localization on finite lattices never restore full translational symmetry of the thermodynamic limit. Eigenvalues of the random Hamiltonian with localized eigenstates are degenerate. As discussed in the Introduction, homogeneous shifts of configurations of the random potential by lattice vectors do not change the spectrum of the underlying Hamiltonian. If the extent of a localized eigenstate is L lattice sites then the corresponding eigenenergy is approximately N/L times degenerate, that is the dimension of the subspace of the corresponding eigenvalue is N/L . Each eigenvector from this subspace corresponds to a different configuration of the random potential. After configurational averaging the weight of the localized eigenvectors is L/N , vanishing in the thermodynamic limit. A truly reliable comparison of numerical results with those from the diagrammatic approach

can be made only if the translational symmetry in the numerical calculations is fully restored, that is when

$$\sum_{i,j} e^{i\mathbf{q}\cdot(\mathbf{R}_i+\mathbf{R}_j)} G_{ij,ji}^{\text{RA}} = 0$$

for each momentum $q \neq 0$ from the first Brillouin zone.

Integrability of singularities in two-particle vertices poses no restriction on the weight of the diffusion pole in the metallic phase in dimensions $d > 2$. The localized phase in $d > 2$ is, however, different. There the widely accepted form of the diffusion pole becomes momentum-independent due to vanishing of the diffusion constant $D(\omega) \sim \omega$ and hence nonintegrable. The fundamental equation (16) for the irreducible vertex Λ cannot lead to a two-particle vertex with such a singularity. If the diffusion pole in $d > 2$ survives in the metallic phase unchanged, with weight one, till the Anderson metal–insulator transition, there must be a jump at the transition point at which the diffusion pole abruptly ceases to exist.

Last but not least, we obtain as a consequence of equation (16) that the two-particle vertex $\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q})$ in the metallic phase of the most interesting spatial dimensions $2 < d < 4$ contains, apart from the diffusion and the Cooper pole, also another low-energy singularity for $\omega \rightarrow 0$ and $|\mathbf{k} - \mathbf{k}'| \rightarrow 0$. We found that $S_{\mathbf{k}\mathbf{k}'}^{\text{R}}(\mathbf{0}, \omega) \doteq (-i\omega)^{d/2-2}$ in $d < 4$ and hence a new singularity in vertex $\Lambda_{\mathbf{k}\mathbf{k}'}^{\text{RA}}(\mathbf{q}, \omega)$ emerges for $\mathbf{k} - \mathbf{k}' \rightarrow 0$. Due to the normalization condition, equation (12), it must be integrable, which is the case for $d > 2$. This new singularity is compatible with the decomposition from equation (11) of the two-particle vertex Γ into singularities caused by the diffusion pole. The existence of a new singularity makes either the weight of the diffusion pole $\varphi_{\mathbf{k}\mathbf{k}'}^{\text{RA}}$ or the reduced vertex $\gamma_{\mathbf{k}\mathbf{k}'}^{\text{RA}}(\mathbf{q}, \omega)$ or both singular with an integrable singularity. A new singularity in the two-particle vertex indicates that the averaged two-particle functions in spatial dimensions $2 < d < 4$ behave qualitatively differently and have a richer analytic structure from those in higher dimensions. How far this singularity influences the macroscopic behavior and transport properties of disordered systems and, in particular, criticality of the Anderson localization transition remains to be investigated.

To conclude, we proved in this paper that the diffusion pole with a dynamical diffusion constant $D(\omega)$ can exist in the two-particle vertex of models of noninteracting electrons in a random potential invariant with respect to the electron–hole transformation only in the metallic phase. That is, the static diffusion constant is positive, $D(0) = D > 0$, and the lattice dimension $d > 2$. An equation of motion for two-particle irreducible vertices prevents the existence of the diffusion pole with a linearly vanishing diffusion constant $D(\omega) \sim \omega$ in the localized phase. The existing translationally invariant descriptions of electrons in a random potential predicting the existence of such a pole in the localized phase should hence be revisited. In view of our result, it seems very difficult, if not impossible, to build up a consistent analytic theory of Anderson localization with a pole in the localized phase induced by probability conservation.

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