Vertex corrections to the mean-field electrical conductivity in disordered electron systems

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Abstract
The mean-field theory for noninteracting disordered electron systems is widely and successfully used to describe equilibrium properties of alloys over the whole range of disorder strengths. However, it fails to take into account the effects of quantum coherence and localizing backscattering effects when applied to transport phenomena. Vertex corrections due to multiple backscatterings may turn the electrical conductivity negative and make expansions around the mean field in strong disorder problematic. We show how to stabilize such an expansion with the inverse of the number of nearest neighbors on hypercubic lattices as a small parameter and how to include vertex corrections to the mean-field approximation in such a way that the conductivity remains non-negative in all disorder regimes.

1. Introduction
Fluctuations of the spatial distribution of the atomic potential give rise to the zero-temperature resistivity of crystalline solids. In order to study in detail the impact of fluctuations of the atomic potential on charge transport, it is appropriate to neglect all less important agents influencing the response of the electron gas to external electric perturbations and to investigate only scatterings of free electrons on random impurities. It is usual to study the effects of impurity scatterings on an Anderson model of disordered electrons [1] with a site-independent distribution of the atomic potential. A straightforward way to investigate this model is to use a perturbation (diagrammatic) expansion in the random potential. Nontrivial and physically interesting results can, however, be reached only via non-perturbative approaches. The most reliable non-perturbative method of describing the effects of disorder on one-electron functions is to use the mean-field, coherent-potential approximation (CPA) [2]. The coherent-potential approximation is nowadays considered as the archetype for mean-field theories of quantum disordered and interacting systems. Its generalized form [3] offers one possible interpretation of the equations of motion in the dynamical mean-field theory (DMFT) [4]. The CPA has proved reliable for producing an accurate equilibrium electronic structure of disordered systems [5] as well as transport properties of random alloys over a wide range of disorder strength [6]. However, it fails to account for inter-site quantum coherence and backscattering effects and it is essentially unable to go beyond the semi-classical description of transport properties qualitatively captured by the Boltzmann equation.

The coherent-potential approximations does not include vertex corrections to the one-electron (Drude-type) electrical conductivity [7]. In the simplest single-band tight-binding model the electrical conductivity at zero temperature in the \( \alpha \) direction can be represented in the CPA via the averaged one-electron propagator at the Fermi surface:

\[
\sigma^{(0)}_{\alpha\alpha} = \frac{e^2}{\pi N} \sum_{\mathbf{k}} |v_\alpha(k)|^2 |\text{Im}G^R(k)|^2
\]

where \( v_\alpha(k) = \frac{\partial \epsilon(k)}{\partial k_\alpha} \) is the electron group velocity in \( \alpha \) direction and superscript R denotes the retarded part of the averaged one-electron propagator. All the contributions to the
The vertex corrections to the zero-temperature conductivity then read \[12\]
\[\Delta \sigma_{\text{uv}} = \frac{e^2}{2\pi N^2} \sum_{kk} \int_0^{\infty} dq \left\{ G^R_{kk} \delta_{kk} |G^R_{k+iq}|^2 - \text{Re} \left[ G^R_{kk} \Gamma^{RR}_{kk} G^R_{k+iq} \right] \right\}. \tag{4}\]

We suppressed the bosonic momenton variable \( q = 0 \) and frequency \( \omega = 0 \) as we will do throughout the paper, when no confusion may arise, for variables whose values are set to zero.

Backscatters contribute to the vertex corrections with negative sign, that is, they restrict macroscopic charge diffusion, and in the strong-disorder limit they may lead to a diffusionless regime (Anderson localization). Close to the transition to the state with localized electrons, quantum interference becomes non-negligible and the vertex corrections may outweigh the Drude term if the vertex function is not appropriately renormalized \[13\]. Non-perturbative methods must be used to calculate transport properties near the mobility edge.

Most of the existing approaches to Anderson localization concentrate entirely on fluctuations in two-particle functions and their renormalization. Since the fluctuations of the self-energy are finite and do not affect the critical behavior at the mobility edge, they are completely neglected in these approaches \[14\]. If we want to determine transport properties over the whole range of the disorder strength and not only in the critical region of the Anderson localization transition, it is necessary to treat fluctuations in the one-electron and two-electron Green functions simultaneously. Normally such an approximation is offered by a mean-field approach, but the coherent-potential approximation does not cover spatial quantum interference. One has to go beyond the standard local mean-field approximation for the electrical conductivity.

A comprehensive mean-field solution is formally obtained from the limit to high spatial dimensions. Hence, a natural way to go beyond the mean-field approximation is to use expansion in the inverse of the spatial dimension of the regular lattice, which is equivalent to the inverse number of nearest neighbors on hypercubic lattices, as a small parameter. However, even systematic corrections to the Drude (mean-field) conductivity derived from the limit to high spatial dimensions may lead in three-dimensional models to negative values of the conductivity \[15, 16\]. One has to circumvent this deficiency. It is the aim of this paper to present a scheme for using the expansion around the mean-field vertex corrections may outweigh the Drude term if the vertex function is not appropriately renormalized \[13\]. Non-perturbative methods must be used to calculate transport properties near the mobility edge. Most of the existing approaches to Anderson localization concentrate entirely on fluctuations in two-particle functions and their renormalization. Since the fluctuations of the self-energy are finite and do not affect the critical behavior at the mobility edge, they are completely neglected in these approaches \[14\]. If we want to determine transport properties over the whole range of the disorder strength and not only in the critical region of the Anderson localization transition, it is necessary to treat fluctuations in the one-electron and two-electron Green functions simultaneously. Normally such an approximation is offered by a mean-field approach, but the coherent-potential approximation does not cover spatial quantum interference. One has to go beyond the standard local mean-field approximation for the electrical conductivity.

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resembles the construction of the self-consistent theory of Anderson localization of Vollhardt and Wölfle introducing a perturbation expansion for the current relaxation kernel, the inverse of the current response function [17].

The paper is organized as follows. We reformulate in section 2 the Kubo formula for the averaged electrical conductivity to a form where the strength of the disorder enters via the irreducible vertex from the Bethe–Salpeter equation in the electron–hole channel. In section 3 we calculate the leading-order contribution in the inverse lattice dimension to the irreducible electron–hole vertex and show how to asymptotically solve the Bethe–Salpeter equation in the low-energy region. The existence of the diffusion pole in the density-response function is discussed in section 4. Numerical results of this approximation on a cubic lattice for a binary alloy are presented in section 5. Conclusions are drawn in section 6.

2. An expression for the electrical conductivity derived from a symmetric Bethe–Salpeter equation

To derive a non-perturbative expression for the electrical conductivity we use a representation of the full two-particle vertex via a Bethe–Salpeter equation in the electron–hole channel. Using the allocation of variables of two-particle quantities from figure 1 and denoting the irreducible vertex in the electron–hole channel \( \Lambda \), we have

\[
\Gamma_{kk}^{ab}(q) = \Lambda_{kk}^{ab}(q) + \frac{1}{N} \sum_{k'} \Lambda_{kk'}^{ab}(q) G_{k}^{a} G_{k+q}^{b} \Gamma_{k'k}^{ab}(q). \tag{5}
\]

This Bethe–Salpeter equation can be extended to the full two-particle Green function by using the definition in equation (2). The two-particle Green function can then be determined from the electron–hole irreducible vertex as

\[
G_{k}^{ab}(q) = G_{k}^{a} G_{k+q}^{b} \times \left[ \delta(k - k') + \frac{1}{N} \sum_{k''} \Lambda_{kk''}^{ab}(q) G_{k''k}^{a}(q) \right]. \tag{6}
\]

This is an integral equation in momentum space with a kernel \( \Lambda_{kk}^{ab}(q) G_{k}^{a} G_{k+q}^{b} \) where the fermionic momenta \( k \) and \( k' \) are the active ones. This integral kernel is asymmetric in the active variables even for the difference momentum \( q = 0 \). We can, however, transform the above Bethe–Salpeter equation to a symmetric one, allowing for an easier diagonalization and non-perturbative solution. To do so, we redefine two-particle functions in momentum space by multiplying them from right and left by one-electron propagators:

\[
\hat{\Lambda}_{kk}^{ab}(q) = G_{k}^{a} \Lambda_{kk}^{ab}(q) G_{k+q}^{b}. \tag{7}
\]

The one-electron propagators are now absorbed in the rescaled vertex \( \hat{\Lambda} \) entering a symmetric Bethe–Salpeter equation for the rescaled full two-particle vertex:

\[
\hat{\Gamma}_{kk}^{ab}(q) = \hat{\Lambda}_{kk}^{ab}(q) + \frac{1}{N} \sum_{k'} \hat{\Lambda}_{kk'}^{ab}(q) \hat{\Gamma}_{k'k}^{ab}(q). \tag{8}
\]

We obtain analogously to this Bethe–Salpeter equation a symmetrized Bethe–Salpeter equation for the full two-particle Green function, the solution of which we formally represent as

\[
G_{k}^{ab}(q) = G_{k+q}^{b} \left[ 1 - \hat{\Lambda}^{ab}(q) \right]_{kk}^{-1} G_{k}^{a}. \tag{9}
\]

where \( \ast \) stands for the appropriate matrix multiplication in the electron–hole scattering channel used in equation (6).

This representation of the two-particle Green function can be used to derive a non-perturbative representation of the electrical conductivity that is free of the decomposition into the Drude term and vertex corrections. We obtain for the static optical conductivity at zero temperature

\[
\sigma_{ab} = \frac{e^2}{2\pi N^2} \sum_{kk} v_0(k) \left[ G_{k}^{A} \left[ 1 - \hat{\Lambda}^{RA}_{kk} \right]_{kk}^{-1} G_{k}^{R} - \text{Re}(G_{k}^{R} \left[ -\hat{\Lambda}^{RR}_{kk} \right]_{kk}^{-1} G_{k}^{R}) \right] \delta_{ab}. \tag{10}
\]

The expression for the electrical conductivity via the electron–hole irreducible vertex \( \hat{\Lambda} \) in equation (10) leads to non-negative results if the inverse operator on its right-hand side is correctly calculated or approximated. Its perturbation expansion, or separating out the even part of the inverse operator, leads to a decomposition of the conductivity into the Drude term (even contribution) and the vertex corrections (odd contribution). It is hence mandatory to use a non-perturbative evaluation or approximation for the inverse operator in equation (10) to guarantee non-negative results for all strengths of disorder.

3. Expansion around the mean field

The representation from equation (10) offers a way to calculate the electrical conductivity non-perturbatively without the necessity to decompose it into the mean-field one-electron contribution and the two-particle vertex corrections. To guarantee non-negative results for the conductivity, one has to resolve the inverse in momentum space non-perturbatively. It would be ideal to diagonalize the irreducible vertex exactly. This is, however, possible only numerically in a discretized space with only a few points in the Brillouin zone. To allow for an analytic expression for inversion of the operator in equation (10), we use the asymptotic limit to high spatial dimensions and consider explicitly only the leading-order correction in the inverse lattice dimension \( d^{-1} \) to the irreducible vertex \( \Lambda \). It is just the ladder of multiple scatterings in the electron–electron channel [16].

3.1. The non-local electron–hole irreducible vertex, from high spatial dimensions

A small parameter for the expansion around the mean-field approximation, which is the exact solution for \( d = \infty \), is the off-diagonal mean-field Green function that can be represented in momentum space as

\[
\tilde{G}(k, \xi) = \frac{1}{\xi - \epsilon(k)} - \int \frac{d\rho(\epsilon)}{\xi - \epsilon}. \tag{11}
\]
with $\zeta = z - \Sigma(z)$, where $\Sigma(z)$ is the mean-field self-energy. The mean-field approximation is consistent only when the one-electron Green function is everywhere replaced by its local element. This applies in particular to two-particle quantities. The only consistent and unambiguous two-particle vertex within the mean-field approximation is the local one

$$\gamma^{ab} = \frac{\lambda^{ab}}{1 - \lambda^{ab} G^a G^b} \tag{12}$$

where we used the two-particle irreducible vertex $\lambda$. It is related to the one-electron self-energy via a Ward identity [7, 18]. The Ward identity is channel dependent. We have in the electron–hole and electron–electron channels [19]

$$\chi^{RA} = \frac{\text{Im} G^{R}}{\text{Im} G^{A}} = \frac{1}{\chi^{RA}(0)} \tag{13a}$$

$$\chi^{RR} = \frac{\Sigma^R}{G^R} = \frac{Z^R}{\chi^{RR}(0)} \tag{13b}$$

where we denoted $\Sigma^R = \partial \Sigma^R(\omega)/\partial \omega|_{\omega = 0}$, $G^R = \partial G^R(\omega)/\partial \omega|_{\omega = 0}$, and $Z^R = \Sigma^R/(\Sigma^R - 1)$. We also related the irreducible vertices to the homogeneous part of the non-local two-particle bubble, a convolution of two one-electron propagators:

$$\chi(\zeta, \zeta'; q) = N^{-1} \sum_k G(k, \zeta) G(k + q, \zeta'). \tag{14}$$

This bubble is non-local even in the mean-field limit ($d = \infty$).

On trying to extend the mean-field approximation also to the non-local two-particle functions, the results are no longer consistent, since the non-local vertex derived with the aid of the Ward identity, used in the CPA, does not cover all the non-vanishing contributions to two-particle functions for $d = \infty$. This ambiguity is a consequence of the fact that two (linear) operations do not commute, namely taking the (functional) derivative of the Green functions with respect to external sources and taking the limit $d \to \infty$ [20]. If we introduce the off-diagonal (non-local) part of the two-particle bubble

$$\tilde{\chi}^{ab}(q) = N^{-1} \sum_k \tilde{G}^{a}(k) \tilde{G}^{b}(k + q) = \chi^{ab}(q) - G^{a} G^{b}, \tag{15}$$

we can represent the leading non-local vertex correction to the local mean-field vertex in the form [15, 16]

$$\Gamma_{kk'}(\zeta_+, \zeta_-; q) = \gamma(\zeta_+, \zeta_-) + \lambda(\zeta_+, \zeta_-) \times \left[ \frac{\gamma'(\zeta_+, \zeta_-) \tilde{\chi}(\zeta_+, \zeta_-; q)}{1 - \lambda(\zeta_+, \zeta_-) \chi(\zeta_+, \zeta_-; q)} + \frac{\gamma'(\zeta_+, \zeta_-) \tilde{\chi}(\zeta_+, \zeta_-; q + k + k')}{1 - \lambda(\zeta_+, \zeta_-) \chi(\zeta_+, \zeta_-; q + k + k')} \right]. \tag{16}$$

The full momentum-dependent mean-field vertex, standardly derived via the local Ward identity, consists of only the first two terms on the right-hand side of equation (16), independent of the fermionic momenta $k$ and $k'$. For symmetry reasons they do not affect the electrical conductivity. It is the third term that generates the leading-order vertex corrections to the electrical conductivity and is responsible for the so-called weak localization [21].

To avoid addition of the vertex corrections to the mean-field conductivity, we use the Bethe–Salpeter equation (10) and express the conductivity via the electron–hole irreducible vertex $\tilde{A}$. Since we expand around the mean-field solution, we must use a modified Bethe–Salpeter equation suppressing multiple scatterings on the same site so as to avoid double counting of scattering effects. We denote the modified irreducible vertex as $\tilde{A}$. A modified Bethe–Salpeter equation for the full vertex reads [22, 23]

$$\tilde{\gamma}^{ab}(z_+, z_-; q) = \tilde{A}_{kk'}(z_+, z_-; q) + \frac{1}{N} \sum_{q'} \tilde{A}_{kk'}(z_+, z_-; q') \times \tilde{G}_+(k') \tilde{G}_-(k' + q) \Gamma_{k'k'}(z_+, z_-; q). \tag{17}$$

The leading-order contribution to the off-diagonal part of the irreducible vertex in high spatial dimensions is just the last term on the right-hand side of equation (16). We then have

$$\tilde{A}_{kk'}^{ab}(q) = \gamma^{ab} \left[ 1 + \frac{\gamma^{a\beta} \tilde{G}_{k + k' + q}^{\beta}}{1 - \gamma^{a\beta} \tilde{G}_{k + k' + q}^{\beta}} \right]. \tag{18}$$

To calculate the conductivity with the aid of the vertex $\tilde{A}$ and a symmetrized Bethe–Salpeter equation, we redefine the two-electron Green function

$$\tilde{G}^{ab}_{kk'}(q) = G^b_{k + q} \delta(k - k') + G^a_{k, k'}^{ab}(q) \tilde{G}^{b}_{k + q} G^a_{k', k} \tag{19}$$

which does not change the long-range diffusive behavior of the full two-particle Green function. This constrained function can be represented as a solution of a symmetrized Bethe–Salpeter equation

$$\tilde{G}^{ab}_{kk'}(q) = G^b_{k + q} [1 - \tilde{A}_{kk'}^{ab}(q)]^{-1} G^a_{k, k'} \tag{20}$$

with a kernel that we denote for further calculations as $K^{-1} = 1 - \tilde{A}$. We use the constrained two-electron Green function $\tilde{G}$ in the calculation of the electrical conductivity. The result is not changed by this substitution. From the symmetrized Bethe–Salpeter equation (19), we obtain

$$\sigma_{ab\beta} = \frac{e^2}{2\pi N^2} \sum_{kk'} \nu_{ab}(k) \left[ G^a_{kk'} [1 - \tilde{A}_{kk'}^{ab} \Lambda^{-1} G^R_{kk'} - \text{Re}(G^R_{kk'} [1 - \tilde{A}_{kk'}]^{-1} G^R_{kk'} \nu_{ab}(k')). \tag{21}$$

The off-diagonal propagator $\tilde{G}$ is the fundamental parameter in the expansion around the mean-field limit. This makes this expansion consistent and, moreover, it makes the calculation of corrections to the mean-field result numerically more stable. It is preferable to use the full local mean-field vertex $\gamma^{ab}$ instead of the irreducible one, $\lambda^{ab}$. In all formulas of the expansion around the mean field, since the latter contains a pole in the RR (or AA) channel that is canceled in the former one. Note that the leading-order vertex correction calculated from an expansion of the right-hand side of equation (21) coincide with the leading corrections to the mean-field conductivity derived in [19].
The explicit representation for the integral kernel from equation (21) to be inverted is

\[ (K^{ab})^{-1}_{kk}(q) = (L^{ab})^{-1}_{kk}(q) - \gamma^{ab} \tilde{G}^{a}(k) \tilde{G}^{b}(k' + q) \]

\[ = \delta_{kk'} - \gamma^{ab} \tilde{G}^{a}(k') \tilde{G}^{b}(k' + q) \times S^{ab}(k + k' + q) - \gamma^{ab} \tilde{G}^{a}(k) \tilde{G}^{b}(k' + q) \]  

(22)

with \( k \) and \( k' \) as active variables. We used the notation

\[ S^{ab}(q) = \gamma^{ab} \tilde{\chi}^{ab}(q)/(1 - \gamma^{ab} \tilde{\chi}^{ab}(q)). \]  

(23)

One can attempt to invert the matrix from equation (22) exactly numerically, but this is a rather demanding task. Since we expect the mean-field conductivity to dominate in the metallic phase within the energy bands we can resort to an approximate matrix inversion so that non-negativity of the result is preserved and the bulk conductivity not significantly affected. For the metallic phase, we can use the dominance of the low-energy singularity of the diffusion pole and approximate non-perturbative analytic evaluation of the matrix \((K^{ab})^{-1}_{kk'}(q)\) on three-dimensional lattices.

3.2. The approximate analytic solution for the metallic phase

The dominant contribution to the irreducible vertex \( \tilde{\chi} \) from equation (18) comes, in the metallic phase, from the pole in \( S^{RA}(Q) \) for \( Q = 0 \). This means that we can single out fermionic momenta \( k, k' \) in the inversion, such that \( k + k' + q \approx 0 \). Then the pre-factor \( \tilde{G}_k \tilde{G}_{k'+q} \) at function \( S^{RA}(k+k'+q) \) in equation (22) becomes relevant only in the vicinity of the pole, that is for \( k + k' + q \approx 0 \). We further get rid of the dependence of the pre-factor on the fermionic variable in that we replace it by its average over the Brillouin zone, namely \( N^{-1} \sum_k \tilde{G}_k \tilde{G}_{-k} \). This simplification leads to the inverse of a reduced matrix

\[ L^{-1}_{kk'}(q) = \delta_{kk'} - \gamma \tilde{\chi}(0) S(k + k' + q). \]  

(24)

Although this approximation is justified for vertex \( \tilde{\chi}^{AR} \), since only the electron–hole channel contains the pole, we use it, for consistency, also for vertex \( \tilde{\chi}^{RR} \).

The inverse of the matrix on the right-hand side of equation (24) can be explicitly evaluated by using a Fourier transformation diagonalizing convolutions (correlations) resulting from multiplication in the matrix inversion in momentum space. We introduce a Fourier transform in a \( d \)-dimensional momentum space as follows:

\[ f(x) = \int dq \, e^{i qx} f(q), \]

\[ f(q) = \int dx \, (2\pi)^d / \int dx \, e^{-i qx} f(x). \]

We can now explicitly represent matrices

\[ L^{ab}_{kk'}(q) = \int dx \, (2\pi)^d / \int dx \, e^{-i k x} \left[ \frac{e^{-i(k-k') x} + \gamma^{ab} \tilde{\chi}^{ab}(x) S^{ab}(-x) e^{-i(k+k'+q) x}}{1 - \gamma^{ab} \tilde{\chi}^{ab}(x) S^{ab}(x) S^{ab}(-x)} \right] \]  

(25)

and

\[ K^{ab}_{kk'} = L^{ab}_{kk'}(q) + \gamma^{ab} \left( \frac{\int dx \, \tilde{G}(x)}{2(2\pi)^d} \right)^2 \left[ \frac{e^{-i k x} + \gamma^{ab} \tilde{\chi}^{ab}(x) e^{-i(k+k'+q) x}}{1 - \gamma^{ab} \tilde{\chi}^{ab}(x) S^{ab}(x) S^{ab}(x)} \right] \int dy \, \tilde{G}(y) \]  

(26)

where we used the notation

\[ (G^{a} L^{ab} G^{b}) (q) = \frac{1}{N^2} \sum_{kk'} \tilde{G}^{a}_{k+q} L^{ab}_{kk'}(q) \tilde{G}^{b}_{k}. \]

(27)

We suppressed the frequency variables, whose (infinitesimal) imaginary parts are indicated by the superscripts.

We further introduce Fourier transforms of velocities:

\[ \tilde{v}^{\alpha}(x) = \int dk \, v^{\alpha}(k) \tilde{G}^{a}(k), \]

so as to reach a representation of the electrical conductivity containing the leading-order vertex corrections to the mean-field Drude conductivity in a form guaranteeing its non-negativity:

\[ \sigma = \frac{e^2}{2\pi} \int \frac{dx}{(2\pi)^d} \left[ \frac{\tilde{\chi}(x) \tilde{\chi}^{R}(x)}{1 + \gamma^{RA} \tilde{\chi}^{RA}(x) \tilde{S}^{R}(x)} - \text{Re} \left( \frac{\tilde{\chi}(x) \tilde{\chi}^{R}(x)}{1 + \gamma^{RR} \tilde{\chi}^{RR}(x) \tilde{S}^{R}(x)} \right) \right] \equiv \sigma^{AR} - \text{Re} \sigma^{RR} \]

(28)

Note that \( \tilde{\chi}(x) = -\tilde{\chi}(-x) \), while \( \tilde{S}(x) = \tilde{S}(-x) \). It is the first term on the right-hand side of equation (28) that is dominant within the band with non-zero imaginary part of the self-energy and \( \sigma^{RA} \geq |\sigma^{RR}| \geq 0 \).

The above approximation is consistent if \( (G^{a} G^{a} L^{RA} G^{R}) (q) \) remains positive for \( q = 0 \). It is fulfilled if a stability condition

\[ 2 \geq \int \frac{dq}{(2\pi)^d} \left( 1 - \gamma^{RA} \tilde{\chi}^{RA}(q) \right) \]  

(29)

satisfied. This poses a restriction on the disorder strength measured by the full local mean-field vertex \( \gamma \) for which this approximation is consistent and reliable.

4. The electron–hole correlation function and the diffusion pole

The proposed scheme for inverting the kernel in the Bethe–Salpeter equation in the metallic phase with the aid of an expansion around the mean field can also be used to determine the electron–hole correlation function. In a conserving solution this function displays a pole in the low-energy asymptotics. A relation (the Ward identity) between the electron–hole irreducible vertex and the self-energy must
then be satisfied. We show how to reach consistency between a non-local electron–hole irreducible vertex and the self-energy in the present approach.

We first redefine the electron–hole correlation function so as to keep its singular structure intact but make the explicit expression in the expansion around the mean-field limit as simple as possible. We hence use the off-diagonal one-electron propagators to define a constrained electron–hole correlation function:

$$
\tilde{\Phi}^R_E(q, \omega) = \frac{1}{N^2} \sum_{kk'} \tilde{G}^A_{k+q} \left[ 1 - \tilde{\Lambda}^R_E(q) \right]^{-1} \tilde{G}^R_{kk'}. \tag{30}
$$

As is well known, this function contains a (diffusion) pole when the Ward identity relation between the self-energy and the irreducible vertex is obeyed for all frequencies [11]. Its mean-field, local version is expressed in equation (13). The full, frequency-dependent Ward identity holds only in the mean-field limit. Once we go beyond this and introduce non-local corrections to the irreducible vertex, the full Ward identity is in conflict with analyticity of the self-energy and integrability of the diffusion pole [24, 25]. When we approximate the non-local part of the irreducible vertex from which we then determine the self-energy, the Ward identity can be obeyed only in the static limit, that is, for zero frequency difference between the electron and the hole. The exact low-energy asymptotics of the electron–hole correlation function with the static Ward identity reads [23]

$$
\tilde{\Phi}^R_E(q, \omega) \approx \frac{\tilde{\Phi}_0}{-i\Delta_{E}\omega + D^R_E(\omega)q^2}. \tag{31}
$$

where $\Delta_E \geq 1$ is a constant directly proportional to the disorder strength. This electron–hole correlation function contains the diffusion pole of order $\omega^{-1}$ for $q = 0$, but its weight decreases with increasing disorder strength and vanishes in the localized phase [23]. Physical consistency dictates that this low-energy behavior of the electron–hole correlation function be reproduced also in approximations.

The electron–hole correlation function in this approximation has an explicit representation

$$
\tilde{\Phi}^R_E(q) = \frac{\langle \tilde{G}^A L^R G^R \rangle(q)}{1 - \gamma^R \langle \tilde{G}^A L^R G^R \rangle(q)}. \tag{32}
$$

In an approximation with a non-local irreducible vertex we must go beyond the local mean-field self-energy to guarantee the low-energy asymptotics of equation (31). To make the proposed approximation consistent with the diffusion pole, we have to correct the one-electron self-energy appropriately. We can use the static (zero-frequency) Ward identity, which complies with this type of approximation, to determine the imaginary part of the self-energy from the irreducible vertex:

$$
\text{Im} \Sigma^R(k) = \frac{1}{N} \sum_{kk'} \tilde{\Lambda}^R_{kk'} \text{Im} \tilde{G}^R_{kk}. \tag{33}
$$

where both the two-particle irreducible vertex and the averaged one-electron propagator are unrestricted. The real part of the self-energy is then calculated from the Kramers–Kronig relation [23].

This way of making the approximation with a non-local irreducible vertex compatible with the diffusion pole in the electron–hole correlation function is rather tedious and numerically demanding. Non-local parts in momenta for different frequencies of the self-energy are interconnected and must be determined simultaneously. There is, however, a more effective way to ensure a qualitatively correct low-energy asymptotics of the function $\tilde{\Phi}^R_E(q)$ from equation (32). Instead of correcting the self-energy, we can rescale the local static vertex by a positive constant such that the diffusion pole in function $\tilde{\Phi}^R_E(q)$ is guaranteed with the local mean-field self-energy. For this purpose we introduce a positive number $0 \leq \phi \leq 1$ with which we rescale the static part of the mean-field vertex

$$
\gamma^R \longrightarrow \phi \gamma^R. \tag{34}
$$

in equation (22). Note that vertex $\gamma$ is not rescaled in the definition of function $\tilde{S}(q)$ in equation (23), since it is consistently defined within the mean-field approximation. The scaling parameter is determined so that the denominator vanishes in the static and homogeneous limit. That is

$$
1 = \phi \gamma^R \langle \tilde{G}^A L^R G^R \rangle. \tag{35}
$$

It is easy to rewrite this equation as a more explicit one:

$$
\phi = \frac{\langle \tilde{G}^A \tilde{G}^R \rangle}{\langle \tilde{G}^A L^R G^R \rangle} = \frac{\int \frac{dx}{(2\pi)^d} \tilde{G}^R(x) \tilde{G}^\Lambda(x)}{\int \frac{dx}{(2\pi)^d} \frac{1}{1 - \phi \gamma^R \langle \tilde{G}^A L^R G^R \rangle(x)}}, \tag{36}
$$

whose solution can be straightforwardly found numerically. The introduced static scaling factor effectively decreases the disorder strength and prevents the system from undergoing the Anderson localization transition to a phase without macroscopic diffusion. This simplified approach with only multiple scatterings in the leading order of the inverse lattice dimension leads to weak localization but does not take into account higher-order corrections and spatial coherence of electron scatterings on random impurities beyond maximally crossed diagrams. Hence, the present approximation leads to an Anderson insulator with vanishing diffusion for dimension $d = 1, 2$, but to reach the Anderson localization transition for $d > 2$ we have to introduce a self-consistent renormalization of the irreducible vertex $\tilde{\Lambda}$ [22, 23]. Nevertheless, the proposed approximation with non-local vertex corrections to the two-particle irreducible vertex does not result in unphysical behavior for any dimension or disorder strength.

With the diffusion pole in the electron–hole correlation function we can determine its low-energy behavior expressed in terms of the constants $A_E$ and $D^R_E$. They are

$$
A_E = -i\phi \frac{\partial}{\partial \omega} \left[ \gamma^R(E + \omega) \left( \tilde{G}^\Lambda(E) \times \tilde{L}^R(E + \omega) \right) \right]_{\omega=0} \tag{37a}
$$
The small imaginary part of the energy for regularizing density of states on the disorder strength is plotted in figure 2. We use the mean-field approximation (CPA) for the self-energy and the one-electron Green function. We use elliptic integrals to calculate integrals with the density of states on the disorder strength. The dependence of the density of states of a simple cubic lattice [26]. The site-independent distribution of the random potential is \( \rho(V) = (1 - c)\delta(V - \Delta/2) + c\delta(V + \Delta/2) \). We use the mean-field approximation (CPA) for the self-energy and the one-electron Green function. We use elliptic integrals to calculate integrals with the density of states of a simple cubic lattice [26]. The dependence of the density of states on the disorder strength is plotted in figure 2.

The small imaginary part of the energy for regularizing integrals along the real axis was chosen as \( \eta = 10^{-8} \).

We need direct momentum integration to calculate two-particle properties in this approximation. We use the standard technique [27] to discretize the irreducible Brillouin zone of the simple cubic lattice with \( 8^3 - 24 \) mesh points according to the precision needed. All calculations were performed at zero temperature for a simple cubic lattice and a symmetric \( (c = 1/2) \) binary alloy with a split-band limit for \( \Delta_c = \sqrt{6} \) at which the imaginary part of the self-energy diverges.

We first compare the results for the electrical conductivity calculated from different mean-field approaches with vertex corrections. In particular, we compare the approximate zero-temperature conductivity from equation (28) with that from the Drude formula, equation (1), and with the conductivity including vertex corrections from equation (4) using the vertex function from the high-dimensional asymptotics, equation (16). We plotted in figure 3 the behavior of these conductivities near the internal band edge (split band). We set the electron charge as \( e = 1 \). We can see that before the split-band limit is reached, the effect of the disorder becomes so strong that the vertex corrections, when added linearly, outweigh the Drude term and turn the full conductivity negative. The non-perturbative inclusion of vertex corrections from equation (28) remains, however, positive up to the band edge. The expected transition to the localized phase near the split-band edge, as discussed above, cannot be described within this simple approximation. Deeper within the band, the two approximate formulas for conductivity coincide, since the relative weight of the vertex corrections is small. Note that the stability condition, equation (29), is fulfilled everywhere in the metallic phase.

The ratio of the modulus of the vertex correction and the Drude conductivity is shown figure 4. We plotted the leading-order vertex correction derived from conductivity \( \sigma_A \) from formula (28), that is \( \Delta \sigma_A = \sigma_A - \sigma^{(0)} \). We added for comparison the leading-order \( 1/d \) correction \( \Delta \sigma_\infty \) from [19] and \( \sigma_{MF} \), a mean-field conductivity with the vertex correction from [16] where the momentum integration was evaluated in high spatial dimensions. The approximation from [16] is similar to that in the non-perturbative approach of this paper and was derived for the same purpose: to produce non-negative conductivity in an expansion around the mean field. The latter, unlike the present form, completely eliminates the divergence in the electron–hole vertex function significantly influencing the conductivity in low spatial dimensions. We can see that the first two ratios coincide quite well, but the third, from [16], shows a different trend to the first two. Its relative weight decreases when approaching the split-band limit. Moreover, it displays a spurious peak which is a consequence of using the local irreducible CPA vertex \( \lambda \).
in the expansion around the mean-field solution. On rewriting the expansion in terms of the full local CPA vertex \( \gamma \), this peak vanishes. This peak is reminiscent of a singularity in the irreducible vertex \( \lambda^{RR} \) for \( \Delta \approx 1.5883 \) which is, however, compensated in the full vertex \( \gamma^{RR} \). This fact gives evidence that one has to use the full local vertex in the expansion around the mean field using the off-diagonal one-electron propagator as a small parameter. Otherwise we have no guarantee that the singularity from \( \lambda^{RR} \) is fully compensated.

The pole in the electron–hole scattering channel played an important role in the derivation of the non-perturbative expression for the conductivity with vertex corrections, equation (28). We assumed that the low-energy asymptotics of this pole makes a dominant contribution to the conductivity, due to which we could replace a product of two off-diagonal one-electron propagators by its average over the Brillouin zone. In figure 5 we compared the vertex correction from equation (28) with its second-order expansion in \( \gamma \) (the first order vanishes), \( \Delta \sigma_0 \), and the exact first-order vertex correction from equation (4), \( \Delta \sigma_1 \). The latter two do not differ much in the strong-disorder limit, near the split-band transition where the vertex correction is comparable to the Drude term. For weak disorder, where the influence of the pole in function \( S(q) \) is smaller, the approximate non-perturbative and perturbative vertex corrections are almost equal. The impact of the vertex correction on the total conductivity is, however, negligible there.

The primary objective of the present construction was to rewrite and evaluate the Kubo formula for the conductivity in such a way that two-particle vertex corrections to the one-electron Drude contribution never turn the total conductivity negative. The approximate construction determines the averaged full two-particle vertex and hence can be used for a construction of all averaged one-particle and two-particle quantities. One such function of importance is the electron–hole correlation function \( \Phi^{RA} \). It is singular in the low-energy limit if the Ward identity is obeyed on a finite frequency interval around zero. Then also an Einstein relation couples the zero-temperature conductivity with the diffusion constant, \( \sigma = e^2\rho_F D \). As we argued, the validity of the full-scale Ward identity cannot be reached in theories distinguishing electron–electron and electron–hole scatterings. We can only guarantee the validity of the Ward identity in the static limit \( \omega \to 0 \). We introduced a reduction factor \( \phi \) with which we secured the existence of the diffusion pole in the electron–hole correlation function with the local, mean-field self-energy. We plotted in figure 6 this factor together with the weight of the diffusive (extended) states, \( A^{-1} \). The reduction factor \( \phi \) does not differ much from unity even in the strong-disorder limit. The corrections to the self-energy induced by non-locality of the irreducible electron–hole vertex that had to be included in a fully self-consistent approach are hence not of principal relevance. As expected, the weight of the extended states vanishes at the split-band limit \( A^{-1} = 0 \).

The conductivity \( \sigma_A \) is compared with conductivities determined from the Einstein relation with the diffusion constants \( D^0 \) and \( D = D^0/A \) in figure 7. We can see that in the strong-disorder limit the conductivity from the renormalized diffusion constant \( D \) matches the approximated one from the Kubo formula, while the conductivity from the bare diffusion constant \( D^0 \) is quite off for all disorder strengths.
Figure 7. Conductivity and bare ($D^0$) and renormalized ($D = D^0/A$) diffusion constants multiplied by the density of states at the Fermi energy $\rho_F$.

Note that $D^0 > 0$ at the split-band limit. Conductivities $\sigma_A$ and $\rho_F D^0/\Delta$ are distinct for intermediate disorder strengths, but not significantly. In the weak-disorder limit, all three quantities share the same asymptotics.

A binary alloy does not allow for increasing the disorder strength in the metallic phase to an arbitrary value due to the split-band limit. To see that the present construction with the expansion around the mean-field electron–hole irreducible vertex works also in the strong-disorder limit, we use a box distribution for the local random potential described by a distribution function

$$
\rho(V) = \frac{1}{\Delta} \Theta \left( \frac{\Delta}{2} - V^2 \right).
$$

We plotted in figure 8 the conductivity $\sigma_A$ from equation (28) as a function of the disorder strength $\Delta$ of the box distribution function from equation (38) and compared it with the conductivity $\sigma_0$ with the direct vertex correction and the Drude conductivity $\sigma^{(0)}$. As expected, conductivity $\sigma_0$ goes through zero at $\Delta \approx 8.71$, while the conductivity with vertex corrections added to the electron–hole irreducible vertex remains non-zero for all interaction strengths. As we already discussed, the approximation with only the leading-order vertex corrections cannot be used to describe the Anderson metal–insulator transition for which self-consistency at the two-particle level must be introduced. We further compared in figure 9 the calculated conductivity with the conductivities calculated from the Einstein formula with the bare and renormalized diffusion constants, $D^0$ and $D$, respectively. The same trend as for the binary alloy can be observed: that conductivities $\sigma_A$ and $\rho_F D$ asymptotically coalesce in the limit of strong disorder.

6. Conclusions

We presented in this paper a scheme for treating consistently vertex corrections to the mean-field, Drude conductivity. The idea of this construction is to use an expansion in the inverse lattice dimension, that amounts to an expansion in the off-diagonal one-electron mean-field propagator, not directly for the conductivity but rather for the irreducible electron–hole vertex. The latter vertex is then used as an integral kernel of a Bethe–Salpeter equation determining the conductivity. A proper non-perturbative solution of the Bethe–Salpeter equation then guarantees non-negativity of the conductivity over the whole range of the disorder strength. Such an approach makes a perturbation expansion around the mean field meaningful not only for the one-electron quantities but also for the two-electron functions.

We explicitly expanded in this paper the electron–hole irreducible vertex only in first order in the inverse lattice dimension. That is, we summed a series of multiple electron–electron scatterings that were of the same order in the expansion parameter. This sum is known to be responsible for weak localization. We further used dominance of the contribution from the diffusion pole in momentum convolutions to solve the Bethe–Salpeter equation for the electrical conductivity. We derived an explicit representation for the electrical conductivity, equation (28), that remains non-negative irrespective of how strong the disorder is. We explicitly demonstrated that the resulting
expression for the electrical conductivity leads to reliable results within the energy bands with non-zero density of states. The first-order approximation which we used in this paper is insufficient for describing the Anderson metal–insulator transition on three-dimensional lattices, but it treats weak localization correctly and leads to an insulating solution with zero electrical conductivity in dimensions $d = 1, 2$ for all disorder strengths.

Although the approximation used in this paper does not lead to the Anderson metal–insulator transition, it offers a scheme for building up a renormalized perturbation expansion for two-particle vertices controlled by a small parameter, the inverse of the number of nearest neighbors or the spatial lattice dimensionality. When an appropriate two-particle self-consistency is introduced, e.g. via the parquet approach, vertices of two types emerge: ones corresponding to the metallic phase with diffusive behavior for weak disorder and ones with a vanishing diffusion constant for strong disorder [28]. The description of the Anderson transition between the metallic and insulating solutions within this construction differs from other approaches e.g. Efetov’s supersymmetry approach within an effective medium approximation [29]. The most significant difference lies in the way in which the disorder-induced fluctuations of one-electron functions are taken into account when two-particle response functions are calculated. The Efetov approach, as well as theories based on nonlinear $\sigma$-models, completely decouple one-electron functions from the two-particle ones so as to restrict the description to just universal critical properties, assumed to be independent of model differences on small length scales. The only parameter from one-electron quantities entering the two-particle correlation functions in Efetov’s approach is the imaginary part of the self-energy at the Fermi surface, representing the strength of disorder. Our approach is less universal and attempts to treat fluctuations in one-electron and two-electron functions on the same footing. Our approach hence does not allow for using simplifications and scalings of the long-wavelength approach of Efetov and going that deep into the critical region. On the other hand, our approach offers the possibility of checking the scaling assumptions and for studying whether and under which conditions the universal scaling regime of two-particle functions near the Anderson localization transition emerges.

An important constraint of approximations with non-local two-particle vertices is compatibility with the one-electron self-energy. This can be achieved via a static Ward identity. We reached consistency in the approximation with only the leading-order vertex corrections by a rescaling of the local mean-field vertex $\gamma$ by a multiplication factor $\phi$ determined self-consistently. This scaling effectively reduces the disorder strength, but allows us to work with the mean-field local self-energy, which simplifies the calculations tremendously. This rescaling works well inside the energy bands, but it is then less accurate at band edges where one expects Lifshitz tails. One has to use the Ward identity with a non-local self-energy to obtain a more detailed picture of the band edges for finite-dimensional lattices.

The proposed construction of the electrical conductivity can be used to extend systematically the standard mean-field one-electron approximation by including two-particle vertex corrections to the electrical conductivity in such a way that the latter remains non-negative and no fundamental physical law is broken. The approximate construction in its lowest order is simple enough to find application also in the calculation of transport properties of real disordered materials beyond the model level presented here.

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