

Density and current response functions in strongly disordered electron systems: diffusion, electrical conductivity and Einstein relation

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Abstract. We study noninteracting quantum charged particles (electron gas) subject to a strong random potential and perturbed by a weak classical electromagnetic field. We examine consequences of gauge invariance and charge conservation in the space of Bloch waves. We use two specific forms of the Ward identity between the one- and two-particle averaged Green functions to establish exact relations between the density and current response functions. In particular, we find precise conditions under which we can extract the current-current from the density-density correlation functions and *vice versa*. We use these results to prove a formula relating the density response and the electrical conductivity in strongly disordered systems. We introduce quantum diffusion as a response function that reduces to the diffusion constant in the static limit. We then derive Fick's law, a quantum version of the Einstein relation and prove the existence of the diffusion pole in the quasistatic limit of the zero-temperature electron-hole correlation function. We show that the electrical conductivity controls the long-range spatial fluctuations of the electron-hole correlation function only in the static limit.

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1 Introduction

Low-energy physics of equilibrium systems with weakly interacting electrons is well understood both qualitatively and quantitatively. The relevant information about the equilibrium system is contained in one- and two-particle Green functions, in particular in their behavior near the Fermi energy. A number of reliable approximate methods have been developed for the calculation of these functions. Among them, systematic renormalized perturbation expansions based on the many-body Feynman diagrammatic technique have proved most effective. When impurities or quenched configurational randomness are added we are still able to describe equilibrium properties of such systems quite reliably within diagrammatic schemes and a mean-field-type coherent-potential approximation (CPA) [1].

The situation gets less straightforward if we come out of equilibrium. This is the case when the system is disturbed by a time-dependent external force but does not manage to reach a new equilibrium within the relaxation times of the experimental setup. We then have to determine the response of the system to the external perturbation in order to obtain experimentally relevant data. We do not have at our disposal many established methods to calculate response functions. When the perturbation

is weak, which is the most common situation in practice, we can use the linear response theory to calculate effectively the response functions [2]. A fundamental tool for the calculation of the response functions within the linear-response theory is the Kubo formalism [3]. It determines how the response functions can be expressed in terms of two-particle Green (correlation) functions that are characteristics of the equilibrium state. Kubo formulas are means for the description of weakly nonequilibrium systems with equilibrium functions. Unlike the response functions, the equilibrium Green functions obey equations of motion and are suitable for developing systematic approximations within many-body diagrammatic techniques.

Kubo formalism, however, provides independent representations for different response functions that we have to approximate separately. The problem emerges with calculating different response functions *via* different Kubo formulas. We are generally unable to keep exact relations between response functions that may hold due to special symmetries of the system under investigation. The most pronounced case with “hidden” symmetries is the response to a weak electromagnetic perturbation where we have to satisfy gauge invariance together with charge and current conservations. Instantaneous field-dependent deviations of charge and current densities from their equilibrium values are described by density and current response

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functions. Within the linear-response theory these functions are obtained from Kubo formulas with density-density and current-current correlation functions, respectively. Although both correlation functions are derived from the same two-particle Green function, they are normally approximated independently according to the purpose they serve to.

When quantum coherence is negligible we can calculate transport properties from the coherent-potential approximation [1]. There is no contribution to the homogeneous current-current correlation function beyond the single electron-hole bubble in the single-band coherent-potential approximation [4]. Hence, most theories beyond the CPA, either on a model or a realistic level, use the Kubo formula for the electrical conductivity with the current-current correlation function to determine transport properties of disordered solids [5,6].

On the other hand, when quantum coherence effects are substantial and we expect the Anderson metal-insulator transition, the electrical conductivity is usually calculated from the electron-hole correlation function with the aid of the diffusion constant controlling its low-energy behavior near the diffusion pole [7,8]. The diffusion pole is crucial for scaling arguments and the renormalization group approach to Anderson localization [9].

There is a number of more or less heuristic arguments in the literature that relate the density response with the conductivity [10]. They are essentially derived from a semiclassical or equilibrium description of an electron gas exposed to an electromagnetic field. In weakly disordered quantum systems (described by continuum models) a relation between the density response and the conductivity can formally be derived as follows [10]. Gauge invariance is used to relate the external scalar potential with the electric field $\mathbf{E} = -\nabla\varphi$. The current density generated by the external field then is

$$\mathbf{j}(\mathbf{q}, \omega) = \boldsymbol{\sigma}(\mathbf{q}, \omega) \cdot \mathbf{E}(\mathbf{q}, \omega) = -i\boldsymbol{\sigma}(\mathbf{q}, \omega) \cdot \mathbf{q} \varphi(\mathbf{q}, \omega) \quad (1)$$

where $\boldsymbol{\sigma}(\mathbf{q}, \omega)$ denotes the tensor of the electrical conductivity. Charge conservation is expressed by a continuity equation. In equilibrium we can use its operator form being a consequence of Heisenberg equations of motion for the current and density operators. For Hamiltonians with quadratic dispersion relations we have

$$e\partial_t \hat{n}(\mathbf{x}, t) + \nabla \cdot \hat{\mathbf{j}}(\mathbf{x}, t) = 0. \quad (2)$$

Energy-momentum representation of the continuity equation in the ground-state solution is

$$-i\omega e\delta n(\mathbf{q}, \omega) + i\mathbf{q} \cdot \mathbf{j}(\mathbf{q}, \omega) = 0. \quad (3)$$

We have to use a density variation of the equilibrium density, *i.e.*, the externally induced density $\delta n(\mathbf{q}, \omega) = n(\mathbf{q}, \omega) - n_0$ in the continuity equation with averaged values of operators.

From the above equations and within the linear response $\delta n(\mathbf{q}, \omega) = -e\chi(\mathbf{q}, \omega)\varphi(\mathbf{q}, \omega)$ we obtain in the isotropic case

$$\sigma(\mathbf{q}, \omega) = \frac{-ie^2\omega}{q^2}\chi(\mathbf{q}, \omega). \quad (4)$$

The derived equality formally holds for complex functions without restrictions on momenta or frequencies. Frequencies can, in principle, be even complex. Relation (4) is often taken as granted for quantum systems in the whole range of the disorder strength and is used for the definition of the zero-temperature conductivity when describing the Anderson localization transition [7,8].

Although the above derivation of equation (4) may seem very general it suffers from a number of flaws. First, the operator continuity equation (2) cannot be directly used out of equilibrium. The nonequilibrium density and current operators no longer obey Heisenberg equations of motion with the perturbed Hamiltonian. The perturbation is decoupled from the equilibrium Hamiltonian and is treated in the linear-response theory only to linear order. Moreover, the conservation laws must be proved in the representation space of quantum states and for Green functions to be applicable for the response functions. We then need to prove completeness of the representation space and validity of the respective Ward identities. Second, strongly disordered electron systems can be described only by lattice models with nonquadratic dispersion relations. Continuity equation (2) is then to be modified beyond the hydrodynamic limit even in equilibrium. Hence, the above derivation of equation (4) cannot be fully trusted in quantitative studies of strongly disordered quantum systems with nonquadratic dispersion relations.

There is presently no reliable theory of strongly disordered electrons beyond the mean-field CPA. Since mean-field approximations do not include vertex corrections to the electrical conductivity, they are unsuitable for the investigation of localization effects in three spatial dimensions. Unlike low dimensions ($d \leq 2$), Anderson localization in $d = 3$ may occur only in strongly disordered systems. Anderson localization in bulk systems has not yet been understood or quantitatively described in a satisfactory manner. Its quantitative description demands bridging the gap between the mean-field (CPA) transport theory and theories for weakly and strongly localized electron states. It is clear that such an interpolating scheme should be based on advanced approximations for two-particle functions.

Recently, a diagrammatic method for summations of classes of two-particle diagrams has been proposed [11]. This theory has a potential to interpolate between the mean-field and localization theories provided exact relations between the density and current response functions have been established. Criteria for validity of relations between the density-density and the current-current correlation functions in approximate treatments of strongly disordered systems have not yet been set. When going beyond the CPA we have to establish such relations in the metallic regime of tight-binding models with extended electron states. Simultaneously, we have to formulate conditions under which the derived relations hold or may be broken.

The aim of this paper is threefold. First, we derive various relations between current-current, current-density, and density-density correlation functions for strongly

$$\chi(\mathbf{q}, \omega + i0^+) = \frac{1}{N^2} \sum_{\mathbf{kk}'} \int_{-\infty}^{\infty} \frac{dE}{2\pi i} \left\{ [f(E + \omega) - f(E)] G_{\mathbf{kk}'}^{AR}(E, E + \omega; \mathbf{q}) \right. \\ \left. + f(E) G_{\mathbf{kk}'}^{RR}(E, E + \omega; \mathbf{q}) - f(E + \omega) G_{\mathbf{kk}'}^{AA}(E, E + \omega; \mathbf{q}) \right\}. \quad (10)$$

disordered electrons described by Bloch waves. Second, we articulate conditions under which these relations hold or to which extent they may be broken in quantitative treatments. We show how the conductivity can be calculated in the hydrodynamic limit from the density response function and *vice versa*. Third, we introduce a generalization of diffusion *via* a quantum response function and derive a dynamical generalization of the Einstein relation between the diffusion constant and the electrical conductivity. We relate quantum diffusion with its classical counterpart and show that the long-range fluctuations of the electron-hole correlation function are controlled by the diffusion constant only in the static limit.

To reach this goal we use the Kubo formalism and averaged many-body Green functions in the space of Bloch waves. A weaker form of the continuity equation expressed in terms of one- and two-particle Green functions is shown to replace the operator identity. It is derived from equations of motion for Green functions and Ward identities assuming completeness of Bloch waves. We use two versions of the Ward identity due to Velický and Vollhardt and Wölfle. The former is nonperturbative but holds strictly only for the homogeneous case (zero transfer momentum). The latter identity holds for arbitrary transfer momenta but can be proved only perturbatively. Each Ward identity is used in a different manner to relate the conductivity with the density response.

The layout of the paper is as follows. In Section 2 we summarize the definitions and useful representations of the density and current response functions. In Section 3 we show how the current-current correlation function emerges from a momentum expansion of the density response function. Then in Section 4 we derive continuity equations expressed in Green functions and use them to show how the density response function can be revealed from the conductivity. Based on the derived relation between the density and current response function we introduce quantum diffusion in Section 5, reveal the diffusion pole in the quasistatic limit of the density response function and relate quantum diffusion to the electrical conductivity. In Section 6 we illustrate the generally derived results on an exactly solvable limit of infinite spatial dimensions. In the Appendix we discuss assumptions for and the range of validity of the Vollhardt-Wölfle-Ward identity used in the derivation of the continuity equation for Green functions.

2 Density and current response functions in disordered systems

The simplest description of the electron motion in impure, weakly correlated metals is provided by a tight-binding

Anderson model. It assumes noninteracting spinless electrons moving in a random, site-diagonal potential V_i . Its Hamiltonian reads

$$\hat{H}_{AD} = \sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j + \sum_i V_i c_i^\dagger c_i. \quad (5)$$

The values of the random potential V_i are site-independent and obey a disorder distribution $\rho(V)$. Functions depending on the random potential V_i are averaged as

$$\langle X(V_i) \rangle_{av} = \int_{-\infty}^{\infty} dV_i \rho(V_i) X(V_i). \quad (6)$$

The averaged two-particle propagator (resolvent) is defined as an averaged product of one-particle propagators

$$G_{ij,kl}^{(2)}(z_1, z_2) = \left\langle \left[z_1 \hat{1} - \hat{t} - \hat{V} \right]_{ij}^{-1} \left[z_2 \hat{1} - \hat{t} - \hat{V} \right]_{kl}^{-1} \right\rangle_{av}. \quad (7)$$

The Fourier transform to momentum space is not uniquely defined, since due to momentum conservation we have only three independent momenta. For our purposes we choose the following notation and definition of the Fourier transform

$$G_{\mathbf{kk}'}^{(2)}(z_1, z_2; \mathbf{q}) = \frac{1}{N} \sum_{ijkl} e^{-i(\mathbf{k}+\mathbf{q}/2)\mathbf{R}_i} e^{i(\mathbf{k}'+\mathbf{q}/2)\mathbf{R}_j} \\ \times e^{-i(\mathbf{k}'-\mathbf{q}/2)\mathbf{R}_k} e^{i(\mathbf{k}-\mathbf{q}/2)\mathbf{R}_l} G_{ij,kl}^{(2)}(z_1, z_2). \quad (8)$$

The density response function is determined from the following thermodynamic representation of the Kubo formula [13]

$$\chi(\mathbf{q}, i\nu_m) = -\frac{1}{N^2} \sum_{\mathbf{kk}'} k_B T \sum_{n=-\infty}^{\infty} G_{\mathbf{kk}'}^{(2)}(i\omega_n, i\omega_n + i\nu_m; \mathbf{q}). \quad (9)$$

Here $\omega_n = (2n + 1)\pi T$ are fermionic and $\nu_m = 2m\pi T$ bosonic Matsubara frequencies at temperature T . Due to the analytic properties of the two-particle Green function we can perform analytic continuation from imaginary Matsubara to real frequencies using contour integrals. Only the contribution along the real axis survives and we obtain

see equation (10) above.

We have used the following definition

$$G_{\mathbf{kk}'}^{AR}(E, E + \omega; \mathbf{q}) = G_{\mathbf{kk}'}^{(2)}(E - i0^+, E + \omega + i0^+; \mathbf{q})$$

$$\begin{aligned} \sigma_{\alpha\alpha}(\mathbf{q}, \omega) = & -\frac{e^2}{4} \frac{1}{N^2} \sum_{\mathbf{k}, \mathbf{k}'} [v_\alpha(\mathbf{k} + \mathbf{q}/2) - v_\alpha(-\mathbf{k} + \mathbf{q}/2)] [v_\alpha(\mathbf{k}' + \mathbf{q}/2) - v_\alpha(-\mathbf{k}' + \mathbf{q}/2)] \\ & \times \int_{-\infty}^{\infty} \frac{dE}{2\pi\omega} \left\{ [f(E + \omega) - f(E)] G_{\mathbf{k}\mathbf{k}'}^{AR}(E, E + \omega; \mathbf{q}) + f(E) G_{\mathbf{k}\mathbf{k}'}^{RR}(E, E + \omega; \mathbf{q}) \right. \\ & \left. - f(E + \omega) G_{\mathbf{k}\mathbf{k}'}^{AA}(E, E + \omega; \mathbf{q}) - f(E) [G_{\mathbf{k}\mathbf{k}'}^{RR}(E, E; \mathbf{q}) - G_{\mathbf{k}\mathbf{k}'}^{AA}(E, E; \mathbf{q})] \right\}. \quad (15) \end{aligned}$$

and analogously for the functions G^{RR} and G^{AA} , where both energies are from the upper and lower complex energy half-plane, respectively. We have denoted the Fermi function $f(E) = [1 + \exp\{\beta(E - \mu)\}]^{-1}$ with the chemical potential μ .

The two-particle Green function is generally determined from a two-particle irreducible vertex and a Bethe-Salpeter equation. The former is known only approximately, except for special limits. Some specific elements of the full two-particle Green function can, however, be evaluated without knowing the two-particle irreducible vertex. They can be directly related to the one-particle Green function. This is enabled by Ward identities. A Ward identity relating the averaged one- and two-particle Green functions reads

$$\frac{1}{N} \sum_{\mathbf{k}'} G_{\mathbf{k}\mathbf{k}'}^{(2)}(z_1, z_2; \mathbf{0}) = \frac{1}{z_2 - z_1} [G(\mathbf{k}, z_1) - G(\mathbf{k}, z_2)], \quad (11)$$

and was proved for the first time within the coherent-potential approximation by Velický [4]. It is a nonperturbative identity valid quite generally beyond the CPA. It reflects probability conservation in the space of Bloch waves and is a consequence of completeness of extended states [11]. Completeness of Bloch waves cannot, however, be proved in the thermodynamic limit and must be assumed. As a consequence of this identity we obtain vanishing of the density response function for a homogeneous global perturbation, *i.e.*, for $\mathbf{q} = 0$. Using (11) in (10) we easily find

$$\begin{aligned} \chi(\mathbf{0}, \omega + i0^+) = & \frac{1}{\omega} \int_{-\infty}^{\infty} \frac{dE}{2\pi i} \left\{ f(E + \omega) [G^A(E + \omega) \right. \\ & \left. - G^R(E + \omega)] - f(E) [G^A(E) - G^R(E)] \right\} = 0. \quad (12) \end{aligned}$$

Another situation where we do not need to know the two-particle irreducible vertex is the static limit, $\omega = 0$. First, the static density response function is real and reads

$$\chi(\mathbf{q}, 0) = \frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'} \int_{-\infty}^{\infty} \frac{dE}{\pi} f(E) \Im G_{\mathbf{k}\mathbf{k}'}^{RR}(E, E; \mathbf{q}) \quad (13a)$$

that in the limit $\mathbf{q} \rightarrow 0$ goes over to

$$\chi(\mathbf{0}, 0) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\partial f(\omega)}{\partial \omega} \Im G^R(\omega) \xrightarrow{T \rightarrow 0} n_F \quad (13b)$$

with n_F being the density of states at the Fermi level and $G^R(\omega) = N^{-1} \sum_{\mathbf{q}} G^R(\mathbf{q}, \omega)$. Note that equations (13) hold only in the limit $\omega/q \rightarrow 0$. In the inverse case,

$q/\omega \rightarrow 0$, equation (12) applies. Non-commutativity of the limits $\omega \rightarrow 0$ and $q \rightarrow 0$ indicates that the point $q = 0, \omega = 0$ is not analytic in the same manner as in the Fermi liquid theory [14].

The current-current correlation function $\Pi_{\alpha\beta}(\mathbf{q}, t)$ determines the current $\mathbf{j}(\mathbf{q}, t)$ in the system perturbed by an external vector potential $\mathbf{A}(\mathbf{q}, t)$. The tensor of the electrical conductivity $\sigma_{\alpha\beta}(\mathbf{q}, t)$ determines the current response to an external electric field. It can be obtained from the current response function by using a relation $\mathbf{E}(\mathbf{x}, t) = -\dot{\mathbf{A}}(\mathbf{x}, t)$. In the Fourier representation we obtain [15]

$$\sigma_{\alpha\beta}(\mathbf{q}, \omega_+) = \frac{i}{\omega} [\Pi_{\alpha\beta}(\mathbf{q}, \omega_+) - \Pi_{\alpha\beta}(\mathbf{q}, 0)], \quad (14)$$

where $\omega_+ = \omega + i0^+$. The compensation term $\Pi_{\alpha\beta}(\mathbf{q}, 0)$ on the right-hand side of equation (14) is real and has been introduced to warrant finiteness of the complex conductivity. This additive term is not generated from the Kubo formula with a commutator of current operators. It originates from gauge invariance of the electron gas in an external electromagnetic field [16]. According to equation (14) there is no current in the system with a static vector potential and the static (complex) conductivity can be defined only *via* a dynamical one from the limit $\omega \rightarrow 0$.

Unlike the density response function the current response function cannot be simplified in any limit. To determine the conductivity from equation (14) we have to know the two-particle irreducible vertex. The current response function alike the density response function is a complex quantity with the same analytic properties. The parallel components are of interest for us. We have for real frequencies

see equation (15) above.

We have denoted the group velocity $v_\alpha(\mathbf{k}) = \hbar^{-1} \partial / \partial k_\alpha \epsilon(\mathbf{k})$, where $\epsilon(\mathbf{k})$ is the dispersion relation of the underlying lattice.

3 Dynamical conductivity calculated from density response

In this section we show how the dynamical conductivity can be obtained from the long-range behavior of the density response (hydrodynamic limit of small transfer momenta). To this purpose we use the Velický-Ward identity, equation (11). It enables us to evaluate averaged matrix elements of the two-particle Green function with zero

$$\begin{aligned}
I_2(z_+, z_-, \mathbf{q}) = & \text{Tr} \left\{ \widehat{G}(z_+) \widehat{G}(z_-) + \widehat{G}(z_+) [\Delta_1 \widehat{t} + \Delta_2 \widehat{t}] \widehat{G}(z_+) \widehat{G}(z_-) \right. \\
& - \widehat{G}(z_+) \widehat{G}(z_-) [\Delta_1 \widehat{t} - \Delta_2 \widehat{t}] \widehat{G}(z_-) - \widehat{G}(z_+) \Delta_1 \widehat{t} \widehat{G}(z_+) \widehat{G}(z_-) \Delta_1 \widehat{t} \widehat{G}(z_-) \\
& \left. + \widehat{G}(z_+) [\Delta_1 \widehat{t} \widehat{G}(z_+) \Delta_1 \widehat{t} \widehat{G}(z_+) + \widehat{G}(z_-) \Delta_1 \widehat{t} \widehat{G}(z_-) \widehat{\Delta}_1 \widehat{t}] \widehat{G}(z_-) \right\}. \quad (19)
\end{aligned}$$

$$\begin{aligned}
\text{Tr} \left\{ \widehat{G}(z_+) \left[(\Delta_1 \widehat{t} + \Delta_2 \widehat{t}) \widehat{G}(z_-) - \widehat{G}(z_+) (\Delta_1 \widehat{t} - \Delta_2 \widehat{t}) \right] \widehat{G}(z_-) \right\} = \\
\frac{1}{z_+ - z_-} \left\{ \text{Tr} \left[\left(\widehat{G}'(z_+) + \widehat{G}'(z_-) \right) \Delta_1 \widehat{t} \right] + \text{Tr} \left[\left(\widehat{G}'(z_+) - \widehat{G}'(z_-) \right) \Delta_2 \widehat{t} \right] \right. \\
\left. - \frac{2}{z_+ - z_-} \text{Tr} \left[\Delta_1 \widehat{t} \left(\widehat{G}(z_+) - \widehat{G}(z_-) \right) \right] \right\}, \quad (20a)
\end{aligned}$$

$$\begin{aligned}
\text{Tr} \left\{ \widehat{G}(z_+) \Delta_1 \widehat{t} \widehat{G}(z_+) \widehat{G}(z_-) \Delta_1 \widehat{t} \widehat{G}(z_-) \right\} = \frac{1}{(z_+ - z_-)^2} \left\{ \text{Tr} \left[\widehat{G}(z_+) \Delta_1 \widehat{t} \widehat{G}(z_+) \Delta_1 \widehat{t} \right] \right. \\
\left. + \text{Tr} \left[\widehat{G}(z_-) \widehat{\Delta}_1 \widehat{t} \widehat{G}(z_-) \Delta_1 \widehat{t} \right] - 2 \text{Tr} \left[\widehat{G}(z_+) \Delta_1 \widehat{t} \widehat{G}(z_-) \Delta_1 \widehat{t} \right] \right\}, \quad (20b)
\end{aligned}$$

$$\begin{aligned}
\text{Tr} \left\{ \widehat{G}(z_+) \left[\Delta_1 \widehat{t} \widehat{G}(z_+) \Delta_1 \widehat{t} \widehat{G}(z_+) + \widehat{G}(z_-) \Delta_1 \widehat{t} \widehat{G}(z_-) \Delta_1 \widehat{t} \right] \widehat{G}(z_-) \right\} = \\
\frac{1}{z_+ - z_-} \left\{ \text{Tr} \left[\widehat{G}'(z_+) \Delta_1 \widehat{t} \widehat{G}(z_+) \Delta_1 \widehat{t} \right] - \text{Tr} \left[\widehat{G}'(z_-) \Delta_1 \widehat{t} \widehat{G}(z_-) \Delta_1 \widehat{t} \right] \right. \\
\left. - \frac{1}{z_+ - z_-} \text{Tr} \left[\left(\widehat{G}(z_+) - \widehat{G}(z_-) \right) \Delta_1 \widehat{t} \left(\widehat{G}(z_+) - \widehat{G}(z_-) \right) \Delta_1 \widehat{t} \right] \right\}. \quad (20c)
\end{aligned}$$

transfer momentum in terms of the one-particle propagator. Zero transfer momentum is a severe restriction on the applicability and utilization of this Ward identity. Physically we are interested in the hydrodynamic limit, *i.e.*, the asymptotics $q \rightarrow 0$. We are unable to extend identity (11) beyond the homogeneous case. However, if we assume analyticity of the asymptotics $q \rightarrow 0$, we can use momentum q as an expansion parameter and investigate the hydrodynamic limit perturbatively. The hydrodynamic limit is analytic if frequency $\omega \neq 0$, *i.e.*, we are in the regime $q/\omega \ll 1$. We then can expand the density response function in powers of momentum q .

We define two configuration-dependent resolvent operators

$$\widehat{G}_\pm(z) = \left[z_\pm \widehat{1} - \widehat{t} \mp \Delta_1 \widehat{t} - \Delta_2 \widehat{t} - \widehat{V} \right]^{-1} \quad (16)$$

where $\Delta_1 \widehat{t} \pm \Delta_2 \widehat{t}$ is a difference in the dispersion relation of the two resolvents and is defined *via* its matrix elements $\langle \mathbf{k} | \Delta_1 \widehat{t} | \mathbf{k}' \rangle = \delta(\mathbf{k}' - \mathbf{k}) \mathbf{v}(\mathbf{k}) \cdot \mathbf{q} / 2$, $\langle \mathbf{k} | \Delta_2 \widehat{t} | \mathbf{k}' \rangle = \delta(\mathbf{k}' - \mathbf{k}) (\mathbf{q} \cdot \nabla_{\mathbf{k}})^2 \epsilon(\mathbf{k}) / 8$. We are interested in the following function of two energies

$$I(z_+, z_-, \mathbf{q}) = \frac{1}{N} \text{Tr} \left[\widehat{G}_+(z_+) \widehat{G}_-(z_-) \right] \quad (17)$$

that can be, after averaging over the configurations of the random potential, expressed *via* the two-particle Green function

$$\langle I(z_+, z_-, \mathbf{q}) \rangle_{av} = \frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'} G_{\mathbf{k}\mathbf{k}'}^{(2)}(z_+, z_-, \mathbf{q}). \quad (18)$$

We assume that the expansion in the operators $\Delta_{1,2} \widehat{t}$ commutes with the configurational averaging. We first expand the quantity I and then average the series term by term. It is sufficient for our purposes to expand only to second order in momentum \mathbf{q} . This precision determines the leading small-momentum behavior.

Expanding quantity I in $\Delta_{1,2} \widehat{t}$ we have to keep the order of operators in the products, since $\Delta_{1,2} \widehat{t}$ and the resolvent $\widehat{G}(z)$ do not commute. The expansion to second order reads

see equation (19) above.

Each direct product of the resolvent operators $\widehat{G}(z_\pm) \widehat{G}(z_\mp)$ can be simplified using identity (11). Doing this consequently we end up with a sum of products of two resolvents. We have three different terms to analyze:

see equations (20) above.

We insert equations (20) into expansion (19) and average over the configurations of the random potential V_i . To recover the density response function we have to limit the complex energies to the real axis from above or below with which we distinguish the causality. We define correlation functions that can be represented as traces of the averaged two-particle Green function

$$\Phi_E^{ab}(\mathbf{q}, \omega) = \frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'} G_{\mathbf{k}\mathbf{k}'}^{ab}(E, E + \omega; \mathbf{q}), \quad (21)$$

$$\begin{aligned}
\Phi_E^{AR}(\mathbf{q}, \omega) - \Phi_E^{AR}(\mathbf{0}, \omega) = & -\frac{1}{2\omega} \left[\langle \partial_E (G^R(E + \omega) + G^A(E)) \mathbf{q} \cdot \mathbf{v} \rangle \right] \\
& + \frac{1}{8\omega} \left[\langle \partial_E (G^R(E + \omega) - G^A(E)) (\mathbf{q} \cdot \nabla)^2 \epsilon \rangle \right] + \frac{1}{\omega^2} \left[\langle (G^R(E + \omega) - G^A(E)) \mathbf{q} \cdot \mathbf{v} \rangle \right] \\
& - \frac{1}{4\omega N^2} \sum_{\mathbf{k}\mathbf{k}'} \mathbf{q} \cdot \mathbf{v}(\mathbf{k}) \mathbf{q} \cdot \mathbf{v}(\mathbf{k}') \left\{ \partial_\epsilon \left[G_{\mathbf{k}\mathbf{k}'}^{AA}(E + \epsilon, E; \mathbf{0}) - G_{\mathbf{k}\mathbf{k}'}^{RR}(E + \omega, E + \omega + \epsilon; \mathbf{0}) \right]_{\epsilon=0} \right. \\
& \left. + \frac{2}{\omega} \left[G_{\mathbf{k}\mathbf{k}'}^{AA}(E, E; \mathbf{0}) + G_{\mathbf{k}\mathbf{k}'}^{RR}(E + \omega, E + \omega; \mathbf{0}) - 2G_{\mathbf{k}\mathbf{k}'}^{AR}(E, E + \omega; \mathbf{0}) \right] \right\} \quad (22a)
\end{aligned}$$

and analogously of the electron-electron (Φ^{RR}) and hole-hole (Φ^{AA}) ones that can be written generically as

$$\begin{aligned}
\Phi_E^{aa}(\mathbf{q}, \omega) - \Phi_E^{aa}(\mathbf{0}, \omega) = & -\frac{1}{2\omega} \left[\langle \partial_E (G^a(E + \omega) + G^a(E)) \mathbf{q} \cdot \mathbf{v} \rangle \right] \\
& + \frac{1}{8\omega} \left[\langle \partial_E (G^a(E + \omega) - G^a(E)) (\mathbf{q} \cdot \nabla)^2 \epsilon \rangle \right] + \frac{1}{\omega^2} \left[\langle (G^a(E + \omega) - G^a(E)) \mathbf{q} \cdot \mathbf{v} \rangle \right] \\
& - \frac{1}{4\omega N^2} \sum_{\mathbf{k}\mathbf{k}'} \mathbf{q} \cdot \mathbf{v}(\mathbf{k}) \mathbf{q} \cdot \mathbf{v}(\mathbf{k}') \left\{ \partial_\epsilon \left[G_{\mathbf{k}\mathbf{k}'}^{aa}(E + \epsilon, E; \mathbf{0}) - G_{\mathbf{k}\mathbf{k}'}^{aa}(E + \omega, E + \omega + \epsilon; \mathbf{0}) \right]_{\epsilon=0} \right. \\
& \left. + \frac{2}{\omega} \left[G_{\mathbf{k}\mathbf{k}'}^{aa}(E, E; \mathbf{0}) + G_{\mathbf{k}\mathbf{k}'}^{aa}(E + \omega, E + \omega; \mathbf{0}) - 2G_{\mathbf{k}\mathbf{k}'}^{aa}(E, E + \omega; \mathbf{0}) \right] \right\} . \quad (22b)
\end{aligned}$$

where a, b stand for A (advanced), R (retarded), depending on whether the imaginary part of the corresponding frequency argument is positive or negative. We then can represent the leading asymptotics of the averaged electron-hole correlation function for small momenta \mathbf{q}

see equations (22) above.

In the above equations we have used angular brackets to denote summation over fermionic momenta from the first Brillouin zone, that is

$$\langle G(\omega) f_{\mathbf{q}} \rangle = \frac{1}{N} \sum_{\mathbf{k}} G(\mathbf{k}, \omega) f_{\mathbf{q}}(\mathbf{k}) . \quad (23)$$

Note that only the term with ω^{-2} from the electron-hole correlation function diverges in the limit $\omega \rightarrow 0$ while the electron-electron and hole-hole functions remain finite. This is a manifestation of the diffusion pole missing in the latter two correlation functions.

Different powers of momentum \mathbf{q} and frequency ω appear in equations (22). There is no restriction on validity of equations (22) in frequency but they hold only for small momenta, more precisely only perturbatively up to second order. Equations (22) establish relations between the density-density and the current-current correlation functions in the asymptotic limit $q \rightarrow 0$. Generally, however, these two functions are not directly proportional, since the right-hand sides of equations (22) contain one-particle contributions. They cancel each other if we combine the electron-hole with the electron-electron and the hole-hole correlation functions appropriately to build up the density response function.

For the isotropic situation we define in the hydrodynamic limit

$$g(\omega) = -i \lim_{q \rightarrow 0} \frac{\omega}{q^2} \chi(\mathbf{q}, \omega) . \quad (24a)$$

This quantity can be generalized to an anisotropic case as

$$g_{\alpha\beta}(\omega) = -i\omega \frac{\partial^2}{\partial q_\alpha \partial q_\beta} \chi(\mathbf{q}, \omega) \Big|_{q=0} . \quad (24b)$$

Function $g(\omega)$ measures the leading long-range correlations of the density response. Its real part can be identified with the diffusive conductivity or mobility of the system. It is now easy to find an explicit representation of this function using equations (22). All contributions except for the last terms on the right-hand sides of equations (22) cancel and we obtain equality $\sigma_{\alpha\alpha}(\mathbf{0}, \omega) = e^2 g_{\alpha\alpha}(\omega)$, being just equation (4) in the limit $\mathbf{q} = \mathbf{0}$. Note that in the course of the derivation we had to sum contributions from the electron-hole, electron-electron, and hole-hole correlation functions and to integrate over energies.

If we resort to the low-frequency limit $\omega \rightarrow 0$, the diffusion pole in the electron-hole correlation function dominates in the density response and we recover the conductivity directly from Φ^{AR} . It is interesting to note that in this static limit we derive the mobility (*dc*-conductivity) with contributions from G^{AR} and G^{RR} solely from the electron-hole correlation function Φ^{AR} .

4 Density response calculated from conductivity

We showed in the preceding section how the conductivity can be revealed from the small-momentum behavior of the density response. In this section we express the current-current correlation function in terms of the density-density correlation function. The aid we use for this task is a

$$G_{\mathbf{k}\mathbf{k}'}^{(2)}(z_+, z_-; \mathbf{q}) = G(\mathbf{k}_+, z_+)G(\mathbf{k}_-, z_-) \left[\delta(\mathbf{k} - \mathbf{k}') + \frac{1}{N} \sum_{\mathbf{k}''} \Lambda_{\mathbf{k}\mathbf{k}''}(z_+, z_-; \mathbf{q}) G_{\mathbf{k}''\mathbf{k}'}^{(2)}(z_+, z_-; \mathbf{q}) \right] \quad (26)$$

$$\begin{aligned} [\Delta_{\mathbf{q}}\epsilon(\mathbf{k}) - \Delta z] G_{\mathbf{k}\mathbf{k}'}^{(2)}(z_+, z_-; \mathbf{q}) &= \Delta_{\mathbf{q}} G(\mathbf{k}; z_+, z_-) \delta(\mathbf{k} - \mathbf{k}') + \frac{1}{N} \sum_{\mathbf{k}''} \Lambda_{\mathbf{k}\mathbf{k}''}(z_+, z_-; \mathbf{q}) \\ &\times \left[\Delta_{\mathbf{q}} G(\mathbf{k}; z_+, z_-) G_{\mathbf{k}''\mathbf{k}'}^{(2)}(z_+, z_-; \mathbf{q}) - G_{\mathbf{k}\mathbf{k}'}^{(2)}(z_+, z_-; \mathbf{q}) \Delta_{\mathbf{q}} G(\mathbf{k}''; z_+, z_-) \right]. \quad (29) \end{aligned}$$

continuity equation and another Ward identity

$$\begin{aligned} \Sigma(\mathbf{k}_+, z_+) - \Sigma(\mathbf{k}_-, z_-) &= \frac{1}{N} \sum_{\mathbf{k}'} \Lambda_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q}) \\ &\times [G(\mathbf{k}'_+, z_+) - G(\mathbf{k}'_-, z_-)] \quad (25) \end{aligned}$$

proved for retarded and advanced functions by Vollhardt and Wölfle in reference [17]. We have denoted $\mathbf{k}_{\pm} = \mathbf{k} \pm \mathbf{q}/2$. Note that identity (25) for $\mathbf{q} = \mathbf{0}$, $z_+ = E_F + i0^+$, $z_- = E_F - i0^+$ was already used in reference [18]. Identity (25) is related to equation (11), however, the two Ward identities are identical neither in the derivation nor in the applicability and validity domains. The former holds for nonzero transfer momentum \mathbf{q} , *i.e.*, for an inhomogeneous perturbation while the latter only for $q = 0$. On the other hand, we show in the appendix that equation (25), unlike equation (11), holds only perturbatively within an expansion in powers of the random potential. Hence, we can prove this identity for nonzero transfer momentum \mathbf{q} only by assuming that perturbation expansions for the self-energy Σ and simultaneously for the two-particle irreducible vertex Λ converge. It was shown earlier that in the homogeneous case, $q = 0$, the Vollhardt-Wölfle-Ward identity follows from the Velický-Ward one [11]. We stress that both variants of the Ward identity hold only if Bloch waves form a complete set of quantum states for lattice electrons subject to a random potential.

To derive a continuity equation for Green functions we start with an equation of motion for the two-particle Green function. It is a Bethe-Salpeter equation where the input is a two-particle irreducible vertex. We have three possibilities (topologically distinct scattering channels) how to construct a Bethe-Salpeter equation [11]. For our purposes the electron-hole channel is the most suitable one. The Bethe-Salpeter equation in momentum representation there reads

see equation (26) above

where $\Lambda_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q})$ is the two-particle irreducible vertex from the electron-hole channel. The one-electron propagators $G(\mathbf{k}_{\pm}, z_{\pm}) = [z_{\pm} - \Sigma(\mathbf{k} \pm \mathbf{q}/2, z_{\pm}) - \epsilon(\mathbf{k} \pm \mathbf{q}/2)]^{-1}$ are the averaged resolvents.

The product of the one-electron propagators from the right-hand side of equation (26) can be decomposed into

$$\begin{aligned} G(\mathbf{k}_+, z_+)G(\mathbf{k}_-, z_-) &= \\ &- \frac{\Delta_{\mathbf{q}} G(\mathbf{k}; z_+, z_-)}{\Delta z - \Delta_{\mathbf{q}} \Sigma(\mathbf{k}; z_+, z_-) - \Delta_{\mathbf{q}} \epsilon(\mathbf{k})} \quad (27) \end{aligned}$$

where we denoted

$$\Delta_{\mathbf{q}} \epsilon(\mathbf{k}) = \epsilon(\mathbf{k}_+) - \epsilon(\mathbf{k}_-), \quad (28a)$$

$$\Delta_{\mathbf{q}} G(\mathbf{k}; z_+, z_-) = G(\mathbf{k}_+, z_+) - G(\mathbf{k}_-, z_-). \quad (28b)$$

and analogously the difference $\Delta_{\mathbf{q}} \Sigma(\mathbf{k}; z_+, z_-)$. We multiply both sides of the Bethe-Salpeter equation (26) by the denominator from the right-hand side of equation (27) and assume validity of equation (25). We then obtain a “difference” equation of motion

see equation (29) above.

We now define correlation functions generalized to complex frequencies describing density-density and density-current correlations by summing over the fermionic momenta in equation (29)

$$\bar{\Phi}(z_1, z_2; \mathbf{q}) = \frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'} G_{\mathbf{k}\mathbf{k}'}^{(2)}(z_1, z_2; \mathbf{q}), \quad (30a)$$

$$\bar{\Phi}_{\epsilon}(z_1, z_2; \mathbf{q}) = \frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'} \Delta_{\mathbf{q}} \epsilon(\mathbf{k}) G_{\mathbf{k}\mathbf{k}'}^{(2)}(z_1, z_2; \mathbf{q}), \quad (30b)$$

$$\bar{\bar{\Phi}}_{\epsilon}(z_1, z_2; \mathbf{q}) = \frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'} G_{\mathbf{k}\mathbf{k}'}^{(2)}(z_1, z_2; \mathbf{q}) \Delta_{\mathbf{q}} \epsilon(\mathbf{k}'). \quad (30c)$$

The contributions from the two-particle irreducible vertex Λ in equation (29) cancel each other provided the two-particle irreducible vertex is symmetric, *i.e.*, $\Lambda_{\mathbf{k}\mathbf{k}'} = \Lambda_{\mathbf{k}'\mathbf{k}}$. If so, we end up with a continuity equation relating generalized density-density and density-current correlation functions

$$\begin{aligned} \bar{\Phi}_{\epsilon}(z_+, z_-; \mathbf{q}) - \Delta z \bar{\Phi}(z_+, z_-; \mathbf{q}) &= \\ &\frac{1}{N} \sum_{\mathbf{k}} \Delta_{\mathbf{q}} G(\mathbf{k}; z_+, z_-). \quad (31a) \end{aligned}$$

Another continuity equation can be derived by multiplying equation (29) with the energy difference and summing over the fermionic momenta. We obtain an equation relating generalized current-current and density-current correlation functions

$$\begin{aligned} \bar{\Phi}_{\epsilon\epsilon}(z_+, z_-; \mathbf{q}) - \Delta z \bar{\bar{\Phi}}_{\epsilon}(z_+, z_-; \mathbf{q}) &= \\ &\frac{1}{N} \sum_{\mathbf{k}} \Delta_{\mathbf{q}} G(\mathbf{k}; z_+, z_-) \Delta_{\mathbf{q}} \epsilon(\mathbf{k}). \quad (31b) \end{aligned}$$

$$\sigma_{\epsilon\epsilon}(\mathbf{q}, \omega) = -e^2 \int_{-\infty}^{\infty} \frac{dE}{2\pi\omega} \left\{ [f(E+\omega) - f(E)] \Phi_{\epsilon\epsilon}^{AR}(E, E+\omega; \mathbf{q}) + f(E) \Phi_{\epsilon\epsilon}^{RR}(E, E+\omega; \mathbf{q}) - f(E+\omega) \Phi_{\epsilon\epsilon}^{AA}(E, E+\omega; \mathbf{q}) - f(E) [\Phi_{\epsilon\epsilon}^{RR}(E, E; \mathbf{q}) - \Phi_{\epsilon\epsilon}^{AA}(E, E; \mathbf{q})] \right\}. \quad (36)$$

$$\sigma_{\epsilon\epsilon}(\mathbf{q}, \omega) + ie^2 \omega \chi(\mathbf{q}, \omega) = \frac{e^2}{\omega} \int_{-\infty}^{\infty} \frac{dE}{2\pi} f(E) \left[\Phi_{\epsilon\epsilon}^{RR}(E, E; \mathbf{q}) - \Phi_{\epsilon\epsilon}^{AA}(E, E; \mathbf{q}) \right] - \frac{ie^2}{\omega} \int_{-\infty}^{\infty} \frac{dE}{\pi} f(E) \frac{1}{N} \sum_{\mathbf{k}} \Delta_{\mathbf{q}} \epsilon(\mathbf{k}) \left[\Im G^R(\mathbf{k}_+, E) - \Im G^R(\mathbf{k}_-, E) \right] = 0. \quad (37)$$

Combining the above two continuity equations we obtain the resulting relation between the generalized current-current and density-density correlation functions replacing the operator continuity equation (3)

$$\Phi_{\epsilon\epsilon}(z_+, z_-; \mathbf{q}) - (\Delta z)^2 \Phi(z_+, z_-; \mathbf{q}) = \frac{1}{N} \sum_{\mathbf{k}} \Delta_{\mathbf{q}} G(\mathbf{k}; z_+, z_-) [\Delta z + \Delta_{\mathbf{q}} \epsilon(\mathbf{k})]. \quad (31c)$$

Actually, the function $\Phi_{\epsilon\epsilon}$ is strictly speaking not the current-current correlation function. We used an energy difference $\Delta_{\mathbf{q}} \epsilon(\mathbf{k})$ from equation (28a) in this correlation function instead of momentum. Only in case of quadratic dispersion relation we have $\Delta_{\mathbf{q}} \epsilon(\mathbf{k}) = \hbar \mathbf{q} \cdot \mathbf{k} / m$ and the energy difference is proportional to the group velocity. Otherwise $\Phi_{\epsilon\epsilon}$ equals the current-current correlation function only in the small-momentum limit, $q \rightarrow 0$. We use

$$\Delta_{\mathbf{q}} \epsilon(\mathbf{k}) \approx \mathbf{q} \cdot \mathbf{v}(\mathbf{k}) \quad (32)$$

to convert the energy difference in the hydrodynamic limit to a multiple of the group velocity $\mathbf{v}(\mathbf{k})$ and denote

$$\Phi_{\alpha\beta}(z_+, z_-; \mathbf{q}) = \frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'} v^\alpha(\mathbf{k}) v^\beta(\mathbf{k}') G_{\mathbf{k}\mathbf{k}'}^{(2)}(z_+, z_-; \mathbf{q}). \quad (33)$$

With the aid of equation (33) we rewrite continuity equation (31c) to

$$\sum_{\alpha\beta} q^\alpha q^\beta \Phi_{\alpha\beta}(z_+, z_-; \mathbf{q}) - \sum_{\alpha} q^\alpha \langle v^\alpha \Delta_{\mathbf{q}} G(z_+, z_-) \rangle = \Delta z [\Delta z \Phi(z_+, z_-; \mathbf{q}) + \langle \Delta_{\mathbf{q}} G(z_+, z_-) \rangle] \quad (34)$$

where the angular brackets stand for the summation over fermionic momenta from the first Brillouin zone as defined in equation (23). In the isotropic case we obtain

$$\Phi_{\alpha\alpha}(z_+, z_-; \mathbf{q}) = \frac{1}{q^2} \mathbf{q} \cdot \langle \mathbf{v} \Delta_{\mathbf{q}} G(z_+, z_-) \rangle + \frac{\Delta z}{q^2} [\Delta z \Phi(z_+, z_-; \mathbf{q}) + \langle \Delta_{\mathbf{q}} G(z_+, z_-) \rangle]. \quad (35)$$

It is the most general relation between the current-current and the density-density correlation functions for arbitrary complex frequencies and non-zero momenta. It holds

for finite momenta as far as the dispersion law remains quadratic. Equation (35) for general dispersion relations is valid only in the hydrodynamic regime of small momenta.

To return to measurable quantities we limit the complex frequencies to the real axis. To derive exact relations we first define a generalization of the conductivity with the correlation functions $\Phi_{\epsilon\epsilon}^{ab}$:

see equation (36) above.

We use continuity equation (31c) to relate $\sigma_{\epsilon\epsilon}$ and χ and find

see equation (37) above.

Vanishing of the right-hand side in equation (37) can be explicitly manifested when continuity equation (31c) is applied to the two-particle correlation functions $\Phi_{\epsilon\epsilon}^{RR}$ and $\Phi_{\epsilon\epsilon}^{AA}$. The two terms on the right-hand side of equation (37) add to zero.

We can extract the electrical conductivity from $\sigma_{\epsilon\epsilon}(\mathbf{q}, \omega)$ in the limit $q \rightarrow 0$ by replacing $\Phi_{\epsilon\epsilon} = \sum_{\alpha} q_{\alpha}^2 \Phi_{\alpha\alpha}$ that leads to $\sigma_{\epsilon\epsilon}(\mathbf{q}, \omega) = \sum_{\alpha} q_{\alpha}^2 \sigma_{\alpha\alpha}(\mathbf{q}, \omega)$. In the isotropic case we then reveal equation (4) from equation (37). It is important to state that this proof of equation (4) is strongly based on the Ward identity (25) for nonzero momenta. The latter can be proved only perturbatively, see Appendix, and hence it is unclear whether equation (4) holds beyond the perturbative regime near the Anderson localization transition.

5 Diffusion, diffusion pole, and Einstein relation in quantum systems

In the preceding sections we proved validity of equation (4) for strongly disordered lattice systems in the hydrodynamic limit, $q \rightarrow 0$. It is a useful relation in particular in approximate theories. It enables us to approximate only either the density response or the conductivity and to determine the other one from equation (4). We can find another relation between the density response and the electron-hole correlation function and the conductivity when we resort to the quasistatic limit, $\omega \rightarrow 0$. In this limit the density response function is in the leading order determined by the electron-hole correlation function. Its

long-range fluctuations are then governed by a diffusion constant.

Diffusion, *i.e.*, the particle motion caused by inhomogeneities in the chemical potential, is in classical systems defined *via* Fick's law. It relates the static current with the negative gradient of the charge density *via* a diffusion constant [3, 13]. The diffusion constant introduced in this way has in classical physics an intuitive phenomenological character without a proper microscopic justification. This can come only from a quantum treatment. The study of diffusion in quantum disordered systems was launched by the seminal work of Anderson analyzing the destructive effects of quantum coherence on diffusion of disordered electrons [19]. Since then diffusion has become part of transport studies of disordered and interacting quantum itinerant systems [8, 12, 20]. However, even in these quantum approaches diffusion is introduced either *via* (self-consistent) perturbation expansions leading to the diffusion pole in the electron-hole correlation function or *via* the semiclassical limit where the electron-hole correlation function becomes a Green function of the classical diffusion equation [10].

Here we propose a nonperturbative way to define diffusion *via* a quantum response function. We define a new tensor $D_{\alpha\beta}(\mathbf{q}, \omega)$ so that the conductivity tensor and the density response are related as follows

$$\sigma_{\alpha\beta}(\mathbf{q}, \omega) = -e^2 D_{\alpha\beta}(\mathbf{q}, \omega) [\chi(\mathbf{q}, \omega) - \chi(\mathbf{q}, 0)]. \quad (38)$$

It is a formal definition of a tensor $D_{\alpha\beta}(\mathbf{q}, \omega)$ that we can call quantum diffusion "constant". We show in the following that this definition provides a suitable way to extend the notion of classical diffusion to quantum models enabling us to retain the Einstein relation between the conductivity and the diffusion constant and the role of the static diffusion constant at the diffusion pole of the electron-hole correlation function.

We first use equation (4) to exclude the density response $\chi(\mathbf{q}, \omega)$ from equation (38) and equation (13a) to determine $\chi(\mathbf{q}, 0)$. Doing so we obtain in the isotropic case

$$\left[1 + \frac{iq^2}{\omega} D(\mathbf{q}, \omega) \right] \sigma(\mathbf{q}, \omega) = e^2 D(\mathbf{q}, \omega) \int_{-\infty}^{\infty} \frac{dE}{\pi} f(E) \Im \Phi_E^{RR}(\mathbf{q}, 0). \quad (39)$$

If we define the homogeneous dynamical conductivity $\sigma(\omega) = \sigma(\mathbf{0}, \omega)$ (in the same way also the dynamical diffusion) and use the Velický-Ward identity (11) in the limiting case $z_1 - z_2 \rightarrow 0$ we obtain a dynamical generalization of the Einstein relation

$$\begin{aligned} \sigma(\omega) &= e^2 D(\omega) \int_{-\infty}^{\infty} \frac{dE}{\pi} f'(E) \Im G^R(E) \\ &= e^2 D(\omega) \left(\frac{\partial n}{\partial \mu} \right)_T \end{aligned} \quad (40a)$$

that at zero temperature reduces to

$$\sigma(\omega) = e^2 n_F D(\omega). \quad (40b)$$

A classical version of the static limit of this formula was proved by Einstein for the Brownian motion in a random medium [21] and later on it was re-derived in the framework of nonequilibrium statistical mechanics by Kubo [3]. Here we derived the Einstein relation for quantum response functions and showed that it is a consequence of gauge invariance expressed by equation (4).

We can use equation (40a) to derive Fick's law for the diffusion current. If the electron gas is perturbed by a static and slowly spatially varying scalar electric potential φ the new thermodynamic equilibrium will be fixed by an electrochemical potential $\xi = \mu + e\varphi$ (electron charge is $-e$). There are no currents in equilibrium, so the diffusion current $\mathbf{j}^{diff} \propto \nabla \xi$ must compensate the current due to the external electric field. With the aid of the static limit of equation (40a) we can then write for the diffusion current [22]

$$\begin{aligned} \mathbf{j}^{diff} &= \frac{1}{e} \mathbf{j} = -\frac{1}{e} \sigma \nabla \varphi \\ &= -D \left(\frac{\partial n}{\partial \mu} \right)_T \nabla (\mu + e\varphi) = -D \nabla n. \end{aligned} \quad (41)$$

We have denoted the static diffusion constant $D = D(0)$ and assumed that the charge density varies only due to the variation of the electrochemical potential. It is evident from this derivation that Fick's law holds only in the static limit and for slowly spatially varying charge density.

It has not yet become clear from the above reasoning how the isotropic diffusion function $D(\mathbf{q}, \omega)$ is related to the classical diffusion equation and to the diffusion pole in the electron-hole correlation function. The existence of the diffusion pole in quantum systems is usually deduced from the semiclassical limit and the diffusion equation. We can prove, however, the existence of the diffusion pole entirely from first quantum principles. We use equation (4) to exclude conductivity $\sigma(\mathbf{q}, \omega)$ from equation (38) and come to a representation for the density response

$$\chi(\mathbf{q}, \omega) = \frac{D(\mathbf{q}, \omega) \chi(\mathbf{q}, 0) q^2}{-i\omega + D(\mathbf{q}, \omega) q^2} \quad (42)$$

known from other treatments of diffusion [23]. Equation (42) holds for arbitrary frequencies and momenta within the range of quadratic dispersion relation.

This representation directly indicates a singularity in the $\omega \rightarrow 0, q \rightarrow 0$ limit of the density response. Since the order of the limits is relevant for the result, we have to specify it explicitly. To single out the singular contribution in the density response function we have to choose $\omega/q \ll 1$.

We find from equation (10)

$$\chi(\mathbf{q}, \omega) = \chi(\mathbf{q}, 0) + \frac{i\omega}{2\pi} (\Phi_{E_F}^{AR}(\mathbf{q}, \omega) + O(q^0)) + O(\omega). \quad (43)$$

Using this asymptotics in equation (42) we obtain an explicit manifestation of the diffusion pole in the zero-temperature electron-hole correlation function

$$\Phi_{E_F}^{AR}(\mathbf{q}, \omega) \approx \frac{2\pi n_F}{-i\omega + Dq^2} \quad (44)$$

$$\lambda(z_+, z_-) = \frac{1}{G(z_+)G(z_-)} \left[1 - \left\langle \frac{1}{1 + (\Sigma(z_+) - V_i)G(z_+)} \frac{1}{1 + (\Sigma(z_-) - V_i)G(z_-)} \right\rangle_{av}^{-1} \right] = \frac{\Sigma(z_+) - \Sigma(z_-)}{G(z_+) - G(z_-)} = \frac{\Delta\Sigma}{\Delta G}. \quad (47b)$$

representing the singular part of the electron-hole correlation function. We identified the static diffusion constant with $D = \lim_{q \rightarrow 0} D(\mathbf{q}, 0)$. Representation (44) was derived for zero temperature in the asymptotic limit $q \rightarrow 0, \omega \rightarrow 0$ with the restriction $\omega/q \ll 1$.

To extend it to the opposite limit, $q/\omega \ll 1$, we have to show that the diffusion function $D(\mathbf{q}, \omega)$ is analytic in the limit $q \rightarrow 0, \omega \rightarrow 0$. It is not a priori clear that the diffusion constant in equation (44) equals the diffusion constant obtained from the inverse order of limits $D = \lim_{\omega \rightarrow 0} \lim_{q \rightarrow 0} D(\mathbf{q}, \omega)$ used in Fick's law, equation (41). The quantum diffusion function $D(\mathbf{q}, \omega)$, however, was introduced in such a way that the limits $\omega \rightarrow 0$ and $q \rightarrow 0$ can be interchanged and we have only one definition for the static diffusion constant from the density response function

$$D = \frac{i}{2} \frac{\lim_{\omega \rightarrow 0} \nabla_q^2 \chi(\mathbf{q}, \omega)|_{q=0}}{\lim_{q \rightarrow 0} \partial_\omega \chi(\mathbf{q}, \omega)|_{\omega=0}} = \frac{2\pi n_F}{\lim_{q \rightarrow 0} q^2 \Phi^{AR}(\mathbf{q}, 0)}. \quad (45)$$

The first equality in equation (45) holds quite generally while the second one only at zero temperature. Note that representation (44) holds only at zero temperature for small momenta and in the quasistatic limit $\omega \rightarrow 0$.

We proved in equation (44) that quantum diffusion introduced *via* a response function in equation (38) reduces in the static and homogeneous limit to the diffusion constant. It determines the long-range fluctuations of the electron-hole correlation function and hence in the semiclassical limit also the diffusive behavior in the diffusion equation. However, only the static diffusion constant D enters the denominator of the electron-hole correlation function. The same holds for the diffusion current and Fick's law in equation (41). A dynamical generalization of the diffusion constant from the electron-hole correlation function to a frequency-dependent quantity *via*

$$n_F \tilde{D}(\omega) = \frac{\omega^2}{4\pi} \nabla_q^2 \Phi_{E_F}^{AR}(\mathbf{q}, \omega)|_{q=0}, \quad (46)$$

cannot be linked to the frequency dependent conductivity. Such a dynamical diffusion is nevertheless often used in the literature as a replacement for the dynamical conductivity in quantitative treatments of Anderson localization [7]. Beware that the dynamical diffusion defined in equation (46) no longer fulfills the Einstein relation and hence deviates from the dynamical conductivity calculated from the Kubo formula with the current-current correlation function. We show explicitly in the next section that in an exactly solvable mean-field limit the left-hand side of equation (46), if related to the conductivity *via* the Einstein relation equation, (40b), differs at finite frequencies

from the conductivity obtained from the direct Kubo formula.

6 Infinite-dimensional model: Explicit exact solution

We derived exact relations between density and current correlation functions for a lattice electron gas in a random potential. We now demonstrate the generally derived formulas explicitly on an exactly solvable limit of infinite spatial dimensions. This limit serves as a mathematical tool for the definition of a mean-field theory not only for classical spin systems but also for itinerant disordered and interacting models [24–26]. In case of the Anderson model of disordered electrons the mean-field theory, *i.e.*, the limit of infinite spatial dimensions, equals the coherent potential approximation. We hence resort in this section to this solution.

Equation determining the local self-energy in the coherent-potential approximation is Soven's equation that can be written as [11]

$$G(z) = \left\langle [G^{-1}(z) + \Sigma(z) - V_i]^{-1} \right\rangle_{av} \quad (47a)$$

where $G(z) = N^{-1} \sum_{\mathbf{k}} G(\mathbf{k}, z)$. The two-particle irreducible vertex then is

see equation (47b) above.

The second equality in equation (47b) is the Velický-Ward identity.

It is straightforward to find an explicit form of the two-particle Green function in the coherent-potential approximation

$$G_{\mathbf{k}\mathbf{k}'}^{(2)}(z_+, z_-; \mathbf{q}) = G_+(\mathbf{k})G_-(\mathbf{k}) \left[\delta(\mathbf{k} - \mathbf{k}') + \frac{\lambda(z_+, z_-)G_+(\mathbf{k}')G_-(\mathbf{k}')}{1 - \lambda(z_+, z_-)\langle G_+G_- \rangle} \right] \quad (48)$$

where $G_{\pm}(\mathbf{k}) = G(\mathbf{k} \pm \mathbf{q}/2, z_{\pm})$ and $\langle G_+G_- \rangle = N^{-1} \sum_{\mathbf{k}} G_+(\mathbf{k})G_-(\mathbf{k})$.

Using the two-particle Green function, equation (48), we easily obtain explicit representations for the density-density and density-current correlation functions

$$\Phi(z_+, z_-; \mathbf{q}) = \frac{\langle G_+G_- \rangle}{1 - \lambda(z_+, z_-)\langle G_+G_- \rangle}, \quad (49a)$$

$$\Phi_{\epsilon}(z_+, z_-; \mathbf{q}) = \frac{\langle \Delta_{\mathbf{q}} \epsilon G_+G_- \rangle}{1 - \lambda(z_+, z_-)\langle G_+G_- \rangle}. \quad (49b)$$

We now insert equations (49) together with the explicit representation for the two-particle Green function, equation (48), into the right-hand side of equation (31a) and find

$$\begin{aligned} \Phi_\epsilon(z_+, z_-; \mathbf{q}) - \Delta z \Phi(z_+, z_-; \mathbf{q}) = \\ \frac{\left\langle (\Delta_{\mathbf{q}}\epsilon - \Delta z) \frac{\Delta_{\mathbf{q}}G}{\Delta_{\mathbf{q}}\epsilon - \Delta z - \Delta\Sigma} \right\rangle}{1 - \lambda(z_+, z_-)\langle G_+G_- \rangle} \\ = \frac{\langle \Delta G \rangle - \Delta\Sigma\langle G_+G_- \rangle}{1 - \lambda(z_+, z_-)\langle G_+G_- \rangle} = \langle \Delta G \rangle. \end{aligned} \quad (50)$$

That is, continuity equation (31a) is fulfilled. Analogously we can explicitly verify equations (31b) and (31c). Actually, validity of continuity equations (31) follows from the Velický-Ward identity, since the two-particle irreducible vertex $\lambda(z_+, z_-)$ is momentum independent. In such a case the Vollhardt-Wölfle and the Velický identities are fully equivalent.

As next we show that the *dc*-conductivity in the coherent-potential approximation can be calculated using the diffusion constant D from equation (44). To this purpose we need to evaluate $\nabla_{\mathbf{q}}^2\langle G_+G_- \rangle$ at zero transfer frequency $\omega = 0$. We have

$$\begin{aligned} \nabla_{\mathbf{q}}^2\langle G_+G_- \rangle &= \frac{1}{2}\nabla_{\mathbf{q}}\langle (G_-\nabla_{\mathbf{k}}G_+ - G_+\nabla_{\mathbf{k}}G_-) \rangle \\ &= \frac{1}{4}\langle G_-\nabla_{\mathbf{k}}^2G_+ + G_+\nabla_{\mathbf{k}}^2G_- - 2\nabla_{\mathbf{k}}G_+\nabla_{\mathbf{k}}G_- \rangle \\ &= -\langle \nabla_{\mathbf{k}}G_+\nabla_{\mathbf{k}}G_- \rangle \end{aligned} \quad (51)$$

where in the last equality we used integration per parts in momentum space. We utilize this result and equation (11) to obtain the electron-hole correlation function

$$\Phi(\mathbf{q}, \Delta z) = -\frac{\Delta G}{\Delta z - \frac{1}{2}\frac{\Delta\Sigma}{\Delta\Sigma - \Delta z}\frac{\langle v_{\mathbf{k}}^2(\Delta G)^2 \rangle}{\Delta G}q^2}, \quad (52)$$

that in the low-energy limit reduces for real frequencies to

$$\Phi^{AR}(\mathbf{q}, \omega) = \frac{2\pi n_F}{-i\omega + \sigma^{CPA}q^2/e^2n_F} \quad (53)$$

proving the Einstein relation for the *dc*-conductivity σ^{CPA} of the coherent-potential approximation. It is evident from equation (52) that the frequency-dependent coefficient in the denominator of the electron-hole correlation function does not equal the dynamical diffusion from equation (40b). To show this explicitly we use definition (46) and compare the result with the real-part of the conductivity at zero temperature given by

$$\begin{aligned} \Re\sigma_{\alpha\alpha}(\omega) &= e^2 \int_{E_F-\omega}^{E_F} \frac{dE}{2\pi\omega} [\Re\Phi_{\alpha\alpha}^{AR}(E, E+\omega; \mathbf{0}) \\ &- \Re\Phi_{\alpha\alpha}^{RR}(E, E+\omega; \mathbf{0})] = \sigma_{\alpha\alpha}^{AR}(\omega) + \sigma_{\alpha\alpha}^{RR}(\omega). \end{aligned} \quad (54a)$$

We separated contributions to the conductivity from the electron-hole and electron-electron current-current correlation functions, σ^{AR} , σ^{RR} . It is useful to introduce also a

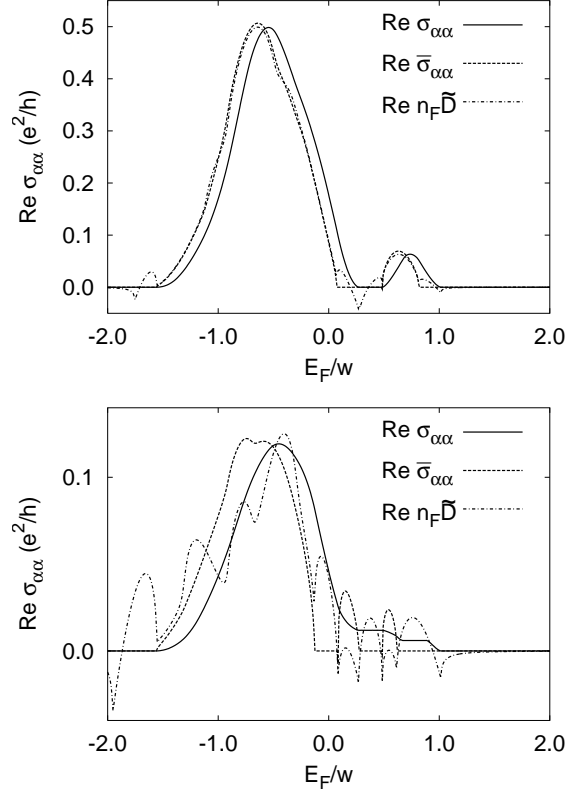


Fig. 1. Dynamical conductivities defined in three different manners, equations (46, 54) for a binary alloy on a simple cubic lattice with the random potential $V_i = \pm 0.6w$, weighted with $x = 0.1$ and $1 - x$, respectively. Frequency is $\omega = 0.2w$ in the upper pane and $\omega = 0.4w$ in the lower pane. Here w is the energy half-bandwidth.

simplified asymptotic form of the low-frequency conductivity

$$\Re\bar{\sigma}_{\alpha\alpha}(\omega) = e^2 \frac{1}{2\pi} [\Re\Phi_{\alpha\alpha}^{AR}(E_F - \omega, E_F; \mathbf{0}) - \Re\Phi_{\alpha\alpha}^{RR}(E_F - \omega, E_F; \mathbf{0})] \quad (54b)$$

where the integrand in the energy integral is replaced by its initial value. This representation is asymptotically exact in the limit $\omega \rightarrow 0$ for smooth current-current correlation functions $\Phi_{\alpha\alpha}$ near the Fermi energy E_F and carries the same frequency dependence as the diffusion constant $\tilde{D}(\omega)$ defined in equation (46).

For the numerical calculations we use a binary alloy with two values of the random potential $V_i = \pm\Delta$ weighted with probability x and $1 - x$. Figure 1 shows the two dynamical conductivities and the diffusion constant from equation (46) on a simple cubic lattice with parameters $x = 0.1$, $\Delta = 0.6w$ for frequencies $\omega = 0.2w$ and $\omega = 0.4w$ with w being the half-bandwidth. Note that the split-band value of the disorder strength is $\Delta_c \approx 0.4w$. Although the three quantities differ for low frequencies only slightly inside the band, they behave differently near the band edges and for higher frequencies. In particular,

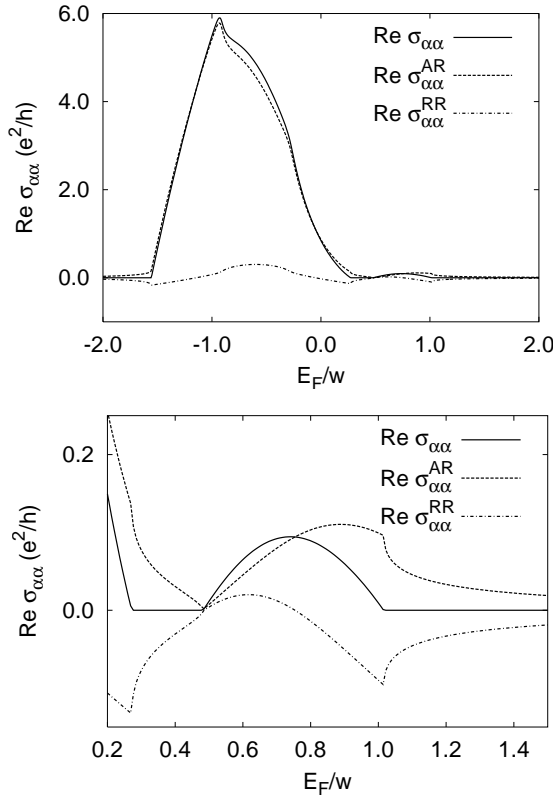


Fig. 2. Weight of contributions to the full conductivity from the electron-hole and electron-electron parts in the static case, $\omega = 0$. The setting is the same as in Figure 1. The lower pane shows the details of the satellite (split-off) band.

the diffusion constant shows anomalous behavior when the Fermi energy approaches the band edges. The compensating terms from the electron-electron (density-density) correlation function get relevant there. Anomalous behavior of the diffusion constant is more transparent for higher frequencies (lower pane). We cannot evidently rely on $n_F \tilde{D}(\omega)$ as a good approximation to the conductivity for finite frequencies except for Fermi energies deep inside the energy band. The smoothening impact of the integral over frequencies on the behavior of the dynamical conductivity gets clear from our numerical results.

Recently a discussion was renewed about the proportion of contributions to the Kubo formula for the electrical conductivity from the electron-hole and electron-electron current-current correlation functions, σ^{AR} and σ^{RR} in equation (54a), respectively [27]. In Figure 2 these contributions are compared for the same setting of the binary alloy on a simple cubic lattice for $\omega = 0$. The contribution from σ^{AR} dominates inside the band far from the band edges. Outside the central band and in the satellite impurity band the importance of the compensating effects of σ^{RR} is evident. The situation worsens when we go over to the dynamical conductivity, Figure 3. We can see that there is no region where the electron-hole contribution would dominate or approximate the full conductivity reliably. It is important to note that the

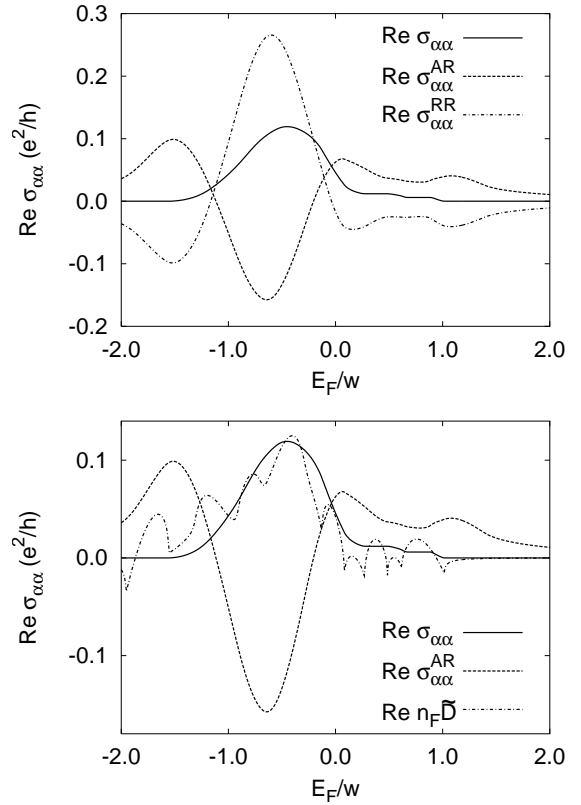


Fig. 3. Electron-hole and electron-electron contributions to the conductivity at $\omega = 0.4w$. The lower pane shows differences between the conductivity obtained from the diffusion constant \tilde{D} and σ^{AR} .

conductivity σ^{AR} differs from the (dynamical) diffusion constant defined from the electron-hole density-density correlation function, equation (46). The latter contains both terms, σ^{AR} and σ^{RR} even in the static limit. The difference is evident in Figure 3. The conductivity calculated from $\tilde{D}(\omega)$ is much closer to the full electrical conductivity than σ^{AR} . With increasing frequency the role of the term σ^{RR} increases. We hence cannot interchange contributions to the electrical conductivity from the electron-hole density-density correlation function $\Phi^{AR}(\mathbf{q}, \omega)$ (its leading q -dependent term) and the conductivity $\sigma^{AR}(\mathbf{q}, \omega)$. The former is generally a better approximation than the latter except for Fermi energies near the band edges and in band tails where both the approximations equally fail.

7 Discussion and conclusions

We showed in this paper that a number of general relations between density-density, density-current and current-current correlation functions hold in the hydrodynamic limit. With the aid of these relations we proved that equivalence between the electrical conductivity and the density response, equation (4), is a consequence of gauge invariance in the quantum space of Bloch waves. We further generalized this relation beyond the hydrodynamic limit

of strongly disordered electron systems, equation (37). We introduced a response function $D_{\alpha\beta}(\mathbf{q}, \omega)$ that we identified with quantum diffusion. We showed that quantum diffusion defined in this manner fulfills in the homogeneous case ($q = 0$) the Einstein relation between the electrical conductivity and the diffusion constant. The static limit ($\omega = 0$) of the diffusion constant then enters Fick's law and the classical diffusion equation. We demonstrated that only the *static* diffusion constant enters the electron-hole correlation function where it controls its long-range fluctuations in the quasistatic limit. There is no extension of the diffusion constant from a dynamical, inhomogeneous electron-hole correlation function that would equal the dynamical electrical conductivity from the Kubo formula.

The electrical conductivity can be calculated from the density response and *vice versa* only if Ward identities are fulfilled. We used two, not fully equivalent, types of the Ward identity for noninteracting electrons in a random potential. They both are generally a consequence of completeness of Bloch waves and reflect probability conservation in the space of extended waves. They can be proved only if perturbation expansion in the strength of the random potential for the irreducible two-particle vertex converges and results in an analytic function. The Velický-Ward identity, equation (11), holds only for the homogeneous case, *i.e.*, zero transfer momentum in the two-particle Green function. To be of use in the calculation of the conductivity we had to assume analyticity of the hydrodynamic limit for all frequencies and to use the transfer momentum as an expansion parameter. On the other hand, the Vollhardt-Wölfle-Ward identity, equation (25), holds for arbitrary transfer momenta in the two-particle function, but it can be proved only *via* a perturbation (diagrammatic) expansion for the two-particle vertex function. Moreover, to warrant this identity we are not allowed to sum selected classes of relevant diagrams. A single relevant diagram for the two-particle irreducible vertex of order n produces $n - 1$ irrelevant diagrams as can be seen from the proof of the Ward identity. Selection of relevant diagrams may be, however, dictated by the existence of a singularity in the two-particle function or by analyticity (causality) of the theory. There is hence no generally valid argument that the Ward identities and consequently the relation between the conductivity and the density response hold beyond the perturbative regime near the Anderson localization transition.

Quantum diffusion was defined as a special combination of the conductivity and the density response function, equation (38). We chose such an extension of the diffusion constant so that we could keep the Einstein relation between the optical conductivity and the homogeneous diffusion. We explicitly demonstrated that it is only the static diffusion constant D that enters the electron-hole correlation function where it controls its long-range fluctuations near the diffusion pole. A dynamical extension of the diffusion constant defined from the dynamical electron-hole correlation function does not obey the Einstein relation and hence is no longer related to the dynamical conduc-

tivity calculated from the Kubo formula. This conclusion has not been realized in the existing literature.

To conclude, we showed that gauge invariance in the space of Bloch waves of extended electrons in a random potential responding to an electromagnetic perturbation holds within linear-response theory if Ward identities (11) and (25) are fulfilled. In this case an (approximate) averaged two-particle Green function generates density and current response functions consistent in the hydrodynamic limit with relation (4). Or, what is more important, we can safely apply the approximate two-particle Green function only in either Kubo formula and use equation (4) to determine the other response function. We explicitly demonstrated that Ward identities can be proved only in the “diffusive” regime characterized by convergence of the perturbation expansion for the two-particle irreducible vertex and by analyticity of the hydrodynamic limit for all frequencies. A necessary condition for validity of Ward identities is completeness of extended Bloch waves. This cannot be generally proved in the thermodynamic limit of random systems and must be assumed. Completeness of extended Bloch waves means that there are no bound localized states in the system. We, however, know that in solutions with weakly or strongly localized electrons a singularity in the electron-hole irreducible vertex emerges and Bloch waves need not span the entire space of quantum states. One has to bear this aspect in mind when interpolating between the diffusive and localized regimes.

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Appendix A: Proof and validity of the Vollhardt-Wölfle-Ward identity

The Vollhardt-Wölfle-Ward identity (25) is a primary tool for proving the continuity equations relating the current and density correlation functions. Understanding its proof and the domain of its validity is hence very important. The original proof of Vollhardt and Wölfle [17] is restricted to real frequencies with different small imaginary parts only. However, it is valid for arbitrary complex frequencies. To demonstrate this we summarize the principal assumptions and steps of its proof from which we conclude on the domain of validity of equation (25).

First, we have to assume that the self-energy Σ is a functional of the full one-electron propagator G

$$\Sigma(\mathbf{p}, z) = \Sigma[G](\mathbf{p}, z) \quad (\text{A.1})$$

so that the perturbation expansion in the random potential consists of irreducible diagrams only. We consider here only noninteracting electrons in a random potential although the reasoning can be extended to correlated

$$\begin{aligned} \Sigma(\mathbf{p}, z) = \langle V \rangle_{av} + \sum_{n=1}^{\infty} \sum_{k=1}^{[(n+1)/2]} \sum_{j_1, \dots, j_k=1}^{n+1} \sum_{l_1, \dots, l_k} \frac{1}{l_1! \dots l_k!} \delta(l_1 + \dots + l_k - n - 1) \langle V_{j_1}^{l_1} \rangle_c \dots \langle V_{j_k}^{l_k} \rangle_c \\ \sum_{\mathbf{R}_1, \dots, \mathbf{R}_{n+1}} \sum_{\mathcal{P}\{i_1, \dots, i_{n+1}\}} \delta_{j_1, i_1} \dots \delta_{j_1, i_1} \delta_{j_2, i_{1+1}} \dots \delta_{j_k, i_{n+1}} \\ \frac{1}{N^n} \sum_{\mathbf{p}_1, \dots, \mathbf{p}_n} e^{i\mathbf{R}_{i_1}(\mathbf{p}-\mathbf{p}_1)} e^{i\mathbf{R}_{i_2}(\mathbf{p}_1-\mathbf{p}_2)} e^{i\mathbf{R}_{i_{n+1}}(\mathbf{p}_n-\mathbf{p})} G(\mathbf{p}_1, z) \dots G(\mathbf{p}_n, z) \end{aligned} \quad (\text{A.2})$$

$$\Delta\Sigma(\mathbf{p}) = \Sigma_+(\mathbf{p}) - \Sigma_-(\mathbf{p}) = \sum_{n=1}^{\infty} \frac{1}{N^n} \sum_{\mathbf{p}_1, \dots, \mathbf{p}_n} \sum_{\mathcal{D}_n} X_{\mathcal{D}_n}(V; \mathbf{p}, \mathbf{p}_1, \dots, \mathbf{p}_n) [G_+(\mathbf{p}_1) \dots G_+(\mathbf{p}_n) - G_-(\mathbf{p}_1) \dots G_-(\mathbf{p}_n)]. \quad (\text{A.5})$$

$$G_+(\mathbf{p}_1) \dots G_+(\mathbf{p}_n) - G_-(\mathbf{p}_1) \dots G_-(\mathbf{p}_n) = \sum_{i=1}^n G_+(\mathbf{p}_1) \dots G_+(\mathbf{p}_{i-1}) \times \Delta G(\mathbf{p}_i) G_-(\mathbf{p}_{i+1}) \dots G_-(\mathbf{p}_n) \quad (\text{A.6})$$

electrons as well. Perturbation expansion of the self-energy $\Sigma(\mathbf{p}, z)$ in the random potential reads

see equation (A.2) above

where $[x]$ is the integer part of x , $\mathcal{P}\{i_1, \dots, i_{n+1}\}$ denotes a permutation of the indices $\{1, 2, \dots, n+1\}$, and the angular brackets stand for cumulant averages defined from

$$\langle \exp V \rangle_{av} = \exp \left\{ \sum_{n=1}^{\infty} \frac{1}{n!} \langle V^n \rangle_c \right\}. \quad (\text{A.3})$$

Only the momentum variables and momentum-dependent functions are of importance. We denote \mathcal{D}_n the sum of all diagrams with n internal fermionic lines with momenta $\mathbf{p}_1, \dots, \mathbf{p}_n$. Then representation (A.2) can be simplified to

$$\begin{aligned} \Sigma(\mathbf{p}, z) = \langle V \rangle_{av} + \sum_{n=1}^{\infty} \frac{1}{N^n} \\ \times \sum_{\mathbf{p}_1, \dots, \mathbf{p}_n} \sum_{\mathcal{D}_n} X_{\mathcal{D}_n}(V; \mathbf{p}, \mathbf{p}_1, \dots, \mathbf{p}_n) G(\mathbf{p}_1, z) \dots G(\mathbf{p}_n, z). \end{aligned} \quad (\text{A.4})$$

We use notation $G_{\pm}(\mathbf{p}) = G(\mathbf{p} \pm \mathbf{q}/2, z_{\pm})$ and $\Sigma_{\pm}(\mathbf{p}) = \Sigma(\mathbf{p} \pm \mathbf{q}/2, z_{\pm})$ and apply expansion (A.4) for the self-energy difference. We obtain

see equation (A.5) above.

The difference of the products of one-electron propagators can further be rewritten to a sum

see equation (A.6) above

where left (right) to the difference $\Delta G(\mathbf{p}_i)$ only $G_+(\mathbf{p}_j)$ ($G_-(\mathbf{p}_j)$) appear. We sum all diagrams for the fixed difference of the one-electron propagators, being now two-particle irreducible diagrams from the electron-hole channel. We then come to a new representation

$$\Delta\Sigma(\mathbf{p}) = \sum_{n=1}^{\infty} \sum_{i=1}^n \frac{1}{N} \sum_{\mathbf{p}_1} \Lambda_{\mathbf{p}\mathbf{p}_i}^{(i, n-i)}(z_+, z_-; \mathbf{q}) \Delta G(\mathbf{p}_i) \quad (\text{A.7})$$

where $\Lambda_{\mathbf{p}\mathbf{p}_i}^{(n, i)}(z_+, z_-; \mathbf{q})$ is a sum of two-particle irreducible diagrams with n internal one-electron lines of which i lines carry energy z_+ and $n-i$ lines energy z_- .

Last but very important step in the proof of identity (25) is an assumption that removing the difference ΔG from equation (A.7) and fixing the internal variable $\mathbf{p}_i = \mathbf{p}'$ does not change summability of the perturbation expansion. If so, we can write

$$\Lambda_{\mathbf{p}\mathbf{p}'}(z_+, z_-; \mathbf{q}) = \sum_{n=1}^{\infty} \sum_{i=1}^n \Lambda_{\mathbf{p}\mathbf{p}'}^{(i, n-i)}(z_+, z_-; \mathbf{q}). \quad (\text{A.8})$$

The equality holds if and only if the perturbation expansion in the random potential for the two-particle irreducible vertex $\Lambda_{\mathbf{p}\mathbf{p}'}(z_+, z_-; \mathbf{q})$ converges point-wise for the chosen values of independent variables $z_+, z_-, \mathbf{p}, \mathbf{p}', \mathbf{q}$. This is a rather severe restriction on applicability of the Ward identity (25). It says that the Ward identity is valid only in cases where no selective rules for sums of two-particle irreducible diagrams apply, *i.e.*, all classes of diagrams are equally important. This happens when the irreducible two-particle vertex is regular (bounded). However, physically the most interesting situation occurs when due to backscatterings a Cooper pole appears in the irreducible vertex Λ . Thanks to this pole only a class of relevant (crossed electron-hole) diagrams determines the low-energy behavior of the two-particle vertex. In the asymptotic region of the Cooper pole in the electron-hole irreducible vertex, the Ward identity (25) *cannot be proved*. In fact it gets violated whenever we take into account a selected series of diagrams dictated by causality of the approximation or leading to a divergence and we have to consider a nonperturbative solution for the two-particle irreducible vertex. Each selected (relevant) diagram of order n from the formal expansion of the singular two-particle vertex generates in the Ward identity $n-1$ irrelevant diagrams to complete the sum from the right-hand side of equation (A.6) so that the self-energy difference can be represented *via* the vertex Λ . The irrelevant diagrams

are neglected in approximations with selected dominant classes of diagrams violating then identity (25). Hence, summability of the perturbation expansion for the two-particle irreducible vertex is an additive assumption in the proof of the Ward identity (25). There is no nonperturbative proof of this identity except for the homogeneous case, $q = 0$, where it is a consequence of the Velický-Ward identity (11).

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