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Energy diffusion in disordered electronic systems near the Anderson transition

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The problem of heat diffusion for a noninteracting electron gas scattered by random impurities is formulated in terms of a frequency- and wave-vector-dependent grand canonical energy-energy (heat-heat) correlation function $\chi_{KK}(\mathbf{q};\omega)$. Consistently with a Ward identity associated with the continuity equation for heat diffusion, we show that the heat-heat correlation function has the *same* critical diffusive behavior of the density-density correlation function. This result enables us, in particular, to predict that the electrical conductivity and the thermal conductivity (times the inverse temperature) of metals scale to zero in the same way near the Anderson transition.

I. INTRODUCTION

It is known that the electronic contribution to the specific heat (at constant volume and in the low-temperature limit) is not altered by the presence of disorder when the interaction among the electrons is neglected.[1] It is not *a priori* evident, however, whether this finding would remain true also for *dynamical* quantities related to the specific heat, such as the heat-diffusion coefficient and the thermal conductivity. The purpose of this paper is to characterize the behavior of the heat diffusion for a noninteracting electron gas scattered by random impurities by calculating the heat-heat correlation (response) function for small frequencies and wave vectors. It will be found from this analysis that the heat-heat correlation function exhibits the *same* critical diffusive behavior of the density-density correlation function.

We limit ourselves in this paper to consider a noninteracting electron gas, regarding it as a "reference system" which is worthwhile to study in itself before introducing interaction effects. The importance of obtaining theoretical predictions on the heat diffusion even in the absence of interactions (but beyond the weak-disorder limit) is evident when recalling that one of the most striking successes of the semiclassical Drude-Sommerfeld theory of metals has been the prediction of a universal *ratio* between electrical conductivity σ and thermal conductivity κ (Wiedemann-Franz law).[2] We shall verify as a by-product of our analysis that quantum-interference effects do not affect the validity of this law,[3] which can actually be extended near the Anderson transition, thereby predicting that σ and κ/T (T being the temperature) scale to zero in the same way near the localization transition. A short summary of this work has been already presented in Ref. 4.

We base our analysis of heat transport on the correlation-function method, which is appropriate to linear response. Linear-response theory to *thermal perturbations* is known, however, to be less cleancut than linear-response theory to mechanical perturbations (such as the coupling to an electromagnetic field) on which the more conventional analysis of number-density transport is based. For this reason, in the Appendix we recall the relevant Kubo-type expressions for heat transport driven by thermal perturbations and recast them in a form amenable to the application of standard diagrammatic techniques at finite temperatures. In particular, in order to obtain the above-mentioned generalization of the Wiedemann-Franz law, we shall express the thermal conductivity κ of Fourier's law in the form

$$\kappa = -\frac{1}{T}\lim_{\omega\to 0}\lim_{\mathbf{q}\to 0}\frac{\omega}{q^2}\mathrm{Im}[\chi_{KK}(\mathbf{q};\omega)] \; , \tag{1.1}$$

where $\chi_{KK}(\mathbf{q};\omega)$ is the space and time Fourier transform of the heat-heat correlation function[5]

$$\chi_{KK}(\mathbf{r}-\mathbf{r}';t-t') = \Theta(t-t')(-i)\langle[\mathcal{H}(\mathbf{r},t),\mathcal{H}(\mathbf{r}',t')]\rangle \tag{1.2}$$

with the grand canonical Hamiltonian density $\mathcal{H}(\mathbf{r},t)$ suitably defined from

$$K = H - \mu N = \int d\mathbf{r}\,\mathcal{H}(\mathbf{r}) \; . \tag{1.3}$$

In Eq. (1.2) the thermal average $\langle \cdots \rangle$ is taken at the equilibrium temperature T, the average over the impurity configurations is understood to be taken *after* the thermal average, and the time dependence is in the Heisenberg picture with the grand-canonical Hamiltonian (1.3) replacing the Hamiltonian H of the system (μ being the equilibrium chemical potential). $\chi_{KK}(\mathbf{q};\omega)$ fully describes the static and dynamical thermal properties of the system. In the following we shall concentrate on evaluating $\chi_{KK}(\mathbf{q};\omega)$ from a microscopic analysis for a noninteracting electron gas in the presence of disorder.

II. HEAT VERTEX FUNCTION FOR A DISORDERED ELECTRONIC SYSTEM IN THE ABSENCE OF INTERACTION

In this section we shall express the temperature function corresponding to (1.2) in the fixed impurities configuration in a form that allows averaging over the impurities configurations via standard diagrammatic methods. The vertex function which is introduced by the impurity average will then be analyzed in terms of a Ward identity associated with the continuity equation for heat diffusion.

A. Heat-heat correlation function in the fixed impurities configuration

The grand-canonical Hamiltonian for a system of noninteracting electrons can be expressed in the alternative forms

$$K=\int d\mathbf{x}\,\Psi^{\dagger}(\mathbf{x})[h(\mathbf{r})-\mu]\Psi(\mathbf{x})$$
$$=\int d\mathbf{x}\{[h(\mathbf{r})-\mu]\Psi^{\dagger}(\mathbf{x})\}\Psi(\mathbf{x})\;, \tag{2.1}$$

where $\mathbf{x}$ stands for the set of space ($\mathbf{r}$) and spin (ξ) labels, $\Psi(\mathbf{x})$ is a field operator, and $h(\mathbf{r})$ is the independent-particle Hamiltonian at given impurities configuration. For simplicity, we consider nonmagnetic impurities throughout. Equation (2.1) provides two different identifications of the grand-canonical Hamiltonian density via Eq. (1.3), the indeterminacy being connected with the fact that $\mathcal{K}(\mathbf{r})$ is not an observable.[6] This indeterminacy, however, is not relevant for macroscopic quantities such as the thermal conductivity and the heat-diffusion coefficient we are interested in. To preserve the hermiticity of the operator, we choose then to symmetrize $\mathcal{K}(\mathbf{r})$ by adding the two alternative forms (2.1).

To perform the average over the impurities configurations of the temperature function corresponding to (1.2), namely,

$$\chi_{KK}(\mathbf{r},\mathbf{r}';\tau-\tau')=-\langle T_{\tau}[\mathcal{K}'(\mathbf{r},\tau)\mathcal{K}'(\mathbf{r}',\tau')]\rangle\;, \tag{2.2}$$

where T_{τ} is the imaginary-time T-ordering operator and

$$\mathcal{K}'(\mathbf{r},\tau)=\mathcal{K}(\mathbf{r},\tau)-\langle\mathcal{K}(\mathbf{r})\rangle\;, \tag{2.3a}$$

$$\mathcal{K}(\mathbf{r},\tau)=\exp(K\tau)\mathcal{K}(\mathbf{r})\exp(-K\tau)\;, \tag{2.3b}$$

we exploit the Heisenberg equation of motion of the field operators $\Psi(\mathbf{x},\tau)$ and $\Psi^{\dagger}(\mathbf{x},\tau)$, and write[7]

$$\mathcal{K}(\mathbf{r},\tau)=\tfrac{1}{2}\left[(\partial_{\underline{\tau}}-\partial_{\tau})\sum_{\xi}\Psi^{\dagger}(\mathbf{x},\underline{\tau})\Psi(\mathbf{x},\tau)\right]_{\underline{\tau}=\tau}\;, \tag{2.4}$$

where we have set $\partial_{\tau}\equiv\partial/\partial\tau$. In this way the impurities' potential enters $\mathcal{K}(\mathbf{r},\tau)$ only through the time dependence of the field operators. The right-hand side of Eq. (2.2) can thus be expressed in terms of a two-particle Green's function by transferring the (imaginary) time derivatives of Eq. (2.4) outside the T_{τ}-ordering operator. We obtain

$$\begin{aligned}
&\langle T_{\tau}[\tfrac{1}{2}(\partial_{\underline{\tau}}-\partial_{\tau})\Psi^{\dagger}(\mathbf{x},\underline{\tau})\Psi(\mathbf{x},\tau)\tfrac{1}{2}(\partial_{\underline{\tau}'}-\partial_{\tau'})\Psi^{\dagger}(\mathbf{x}',\underline{\tau}')\Psi(\mathbf{x}',\tau')]_{\underline{\tau}=\tau^{+},\;\underline{\tau}'=\tau'^{+}}\rangle\\
&\quad=\tfrac{1}{2}(\partial_{\underline{\tau}}-\partial_{\tau})\tfrac{1}{2}(\partial_{\underline{\tau}'}-\partial_{\tau'})\langle T_{\tau}[\Psi(\mathbf{x},\tau)\Psi(\mathbf{x}',\tau')\Psi^{\dagger}(\mathbf{x}',\underline{\tau}')\Psi^{\dagger}(\mathbf{x},\underline{\tau})]\rangle_{\underline{\tau}=\tau^{+},\;\underline{\tau}'=\tau'^{+}}\\
&\quad\quad+\delta(\mathbf{x},\mathbf{x}')\delta(\tau-\tau'^{+})\tfrac{1}{2}[(\partial_{\underline{\tau}}-\partial_{\tau})\langle\Psi^{\dagger}(\mathbf{x},\underline{\tau})\Psi(\mathbf{x},\tau)\rangle]_{\underline{\tau}=\tau}\\
&\quad\quad-\tfrac{1}{4}\langle[\Psi^{\dagger}(\mathbf{x},\tau)\Psi(\mathbf{x}',\tau')(\partial_{\tau}-h(\mathbf{r})+\mu)\delta(\mathbf{x},\mathbf{x}')\delta(\tau-\underline{\tau}')\\
&\quad\quad\quad+\Psi^{\dagger}(\mathbf{x},\tau')\Psi(\mathbf{x},\tau)(\partial_{\tau'}-h(\mathbf{r}')+\mu)\delta(\mathbf{x},\mathbf{x}')\delta(\tau'-\underline{\tau})]_{\underline{\tau}=\tau^{+},\;\underline{\tau}'=\tau'^{+}}\rangle\;,
\end{aligned} \tag{2.5}$$

where $\tau^{+}=\tau+\eta$ ($\eta\rightarrow0^{+}$). Further manipulation of Eq. (2.5) rests on considering its space Fourier transform in the limit of small wave vectors, wherein an irrelevant term $O(q^{2})$ proportional to the number density will be neglected. With this provision and summing over the spin variables, we recast Eq. (2.5) in the compact form[8]

$$\begin{aligned}
\langle T_{\tau}[\mathcal{K}(\mathbf{r},\tau)\mathcal{K}(\mathbf{r}',\tau')]\rangle=&\tfrac{1}{2}(\partial_{\underline{\tau}}-\partial_{\tau})\tfrac{1}{2}(\partial_{\underline{\tau}'}-\partial_{\tau'})\\
&\times\sum_{\xi,\xi'}\langle[\Psi(\mathbf{x},\tau)\Psi(\mathbf{x}',\tau')\Psi^{\dagger}(\mathbf{x}',\underline{\tau}')\Psi^{\dagger}(\mathbf{x},\underline{\tau})]\rangle_{\underline{\tau}=\tau^{+},\;\underline{\tau}'=\tau'^{+}}+2\delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau'^{+})\langle\mathcal{K}(\mathbf{r})\rangle\;.
\end{aligned} \tag{2.6}$$

We have verified that the well-known expression for the low-temperature specific heat C_V^0 (at constant volume) of a noninteracting electron gas in the absence of the impurities potential can be recovered from Eq. (2.6). Quite generally, we can in fact identify the specific heat with the "static" limit

$$C_V=-\frac{1}{T}\lim_{\mathbf{q}\rightarrow0}\lim_{\Omega_{\lambda}\rightarrow0}\chi_{KK}(\mathbf{q};\Omega_{\lambda})\;, \tag{2.7}$$

where $\Omega_{\lambda}=2\lambda\pi k_BT$ (λ an integer), by invoking the thermodynamic identity[9]

$$C_V=(Vk_BT^2)^{-1}\langle(H-\mu N-\langle(H-\mu N)\rangle)^2\rangle$$
$$-\frac{T}{V}\left[\left[\frac{\partial N}{\partial T}\right]_{V\mu}\right]^{2}\left[\left[\frac{\partial N}{\partial\mu}\right]_{VT}\right]^{-1} \tag{2.8}$$

(V being the volume occupied by the system) and noticing that the last term on the right-hand side of Eq. (2.8) can be neglected, being $O(T^3)$ at low temperatures. In the absence of disorder, Wick's theorem can be readily applied to the time-ordered product on the right-hand side of Eq. (2.6). After standard manipulations we then obtain, from Eq. (2.7),

$$C_V^0=(\pi^2/3)N_0k_B^2T \ , \tag{2.9}$$

N_0 being the single-particle density of states at the Fermi level (including spin degeneracy).

In the presence of disorder the electronic contribution to the specific heat maintains the above free-electron value (see Sec. III). This finding, in turn, is consistent with a Ward identity associated with local-energy conservation, to be discussed next.

B. The vertex function introduced by averaging over the impurities configurations and the associated Ward identity

Having expressed the heat-heat correlation function (2.2) by means of Eq. (2.6), the averaging over the impurities configurations of χ_{KK} proceeds in the standard way[10] since the impurities potential enters the right-hand side of Eq. (2.6) only through the (imaginary-) time dependence of the field operators. The averaging can then be described in terms of an effective scalar vertex function Γ. Before discussing, however, the relevant approximations for Γ, we examine a criterion to ensure that they are consistent with local energy conservation as expressed by the *continuity equation* between the grand-canonical Hamiltonian density and the heat-current operator

$$\partial_\tau \mathcal{K}(\mathbf{r},\tau)+\nabla\cdot\mathcal{J}_Q(\mathbf{r},\tau)=0 \ , \tag{2.10}$$

with $\mathcal{K}(\mathbf{r},\tau)$ given by Eq. (2.4) and

$$\mathcal{J}_Q(\mathbf{r},\tau)=(4m)^{-1}\left[(\partial_{\underline{\tau}}-\partial_\tau)(\nabla_{\underline{\mathbf{x}}}-\nabla_{\mathbf{r}})\times\sum_\xi \Psi^\dagger(\underline{\mathbf{x}},\underline{\tau})\Psi(\mathbf{x},\tau)\right]_{\underline{\mathbf{x}}=\mathbf{x},\ \underline{\tau}=\tau} \ . \tag{2.11}$$

Following the approach previously considered for the number- and spin-density correlation functions,[11] we implement the knowledge of Γ in terms of a Ward identity associated with Eq. (2.10). To this end, we consider the equation

$$\partial_{\tau_1}\overline{\langle T_\tau[\mathcal{K}'(\mathbf{r}_1,\tau_1)\Psi^\dagger(\mathbf{r}_{2'}\xi_2,\tau_{2'})\Psi(\mathbf{r}_2\xi_2,\tau_2)]\rangle}+\nabla_1\cdot\overline{\langle T_\tau[\mathcal{J}'_Q(\mathbf{r}_1,\tau_1)\Psi^\dagger(\mathbf{r}_{2'}\xi_2,\tau_{2'})\Psi(\mathbf{r}_2\xi_2,\tau_2)]\rangle}$$
$$=\delta(\mathbf{r}_1-\mathbf{r}_{2'})\delta(\tau_1-\tau_{2'})\partial_{\tau_1}G(\mathbf{r}_2-\mathbf{r}_1,\ \tau_2-\tau_1)+\delta(\mathbf{r}_1-\mathbf{r}_2)\delta(\tau_1-\tau_2)\partial_{\tau_1}G(\mathbf{r}_1-\mathbf{r}_{2'},\ \tau_1-\tau_{2'}) \ , \tag{2.12}$$

which can be established directly from the continuity equation (2.10). In Eq. (2.12) the prime over the operators (2.4) and (2.11) signifies that their equilibrium values have been subtracted as in Eq. (2.3a), the overbar denotes the average over the impurities configurations, and the G on the right-hand side are impurity-averaged single-particle Green's functions. Equation (2.12) as it stands holds within a term $O(q^2)$ in its Fourier transform. This term, albeit irrelevant in the limit $\mathbf{q}\to 0$ that we shall consider in practice for the Ward identity, has not been reported since it will cancel out in the final equation (2.16) below, which is thus exact.

A scalar and a vector vertex function can be introduced by analogy with the scalar and vector couplings to an electromagnetic field.[12] Accordingly, we define

$$\tfrac{1}{2}(\partial_{\tau_{1'}}-\partial_{\tau_1})\left(\overline{\langle T_\tau[\Psi^\dagger(1')\Psi(1)\Psi^\dagger(2')\Psi(2)]\rangle}-\overline{\langle T_\tau[\Psi^\dagger(1')\Psi(1)]\rangle\langle T_\tau[\Psi^\dagger(2')\Psi(2)]\rangle}\right)_{1'=1^+}=\int d33'\,G(2,3)\Gamma(3,3';1)G(3',2') \tag{2.13a}$$

and

$$\tfrac{1}{2}(\partial_{\tau_{1'}}-\partial_{\tau_1})(1/2m)(\nabla_{1'}-\nabla_1)\left(\overline{\langle T_\tau[\Psi^\dagger(1')\Psi(1)\Psi^\dagger(2')\Psi(2)]\rangle}\right.$$
$$\left.-\overline{\langle T_\tau[\Psi^\dagger(1')\Psi(1)]\rangle\langle T_\tau[\Psi^\dagger(2')\Psi(2)]\rangle}\right)_{1'=1^+}=\int d33'\,G(2,3)\boldsymbol{\Gamma}(3,3';1)G(3',2') \ , \tag{2.13b}$$

where 1,2,... stand for the set of space, spin, and imaginary-time variables, 1^+ signifies that τ_1 is augmented by a positive infinitesimal, and the integration over the time variables on the right-hand side of Eqs. (2.13) is restricted between 0 and $(k_BT)^{-1}$.

In particular, in the absence of disorder, Eq. (2.13a) provides the bare vertex

$$\Gamma^0(3,3';1)=-\tfrac{1}{2}[(\partial_{\tau_{1'}}-\partial_{\tau_1})\delta(1,3')\delta(1',3)]_{1'=1^+} \ , \tag{2.14}$$

which, introducing the Fourier representation for the vertex functions with entries specified in Fig. 1(a) becomes

$$\Gamma^0(\mathbf{Q},\mathbf{q};\omega_n,\omega_{n'})=(2i)^{-1}(\omega_n+\omega_{n'}) \ . \tag{2.15}$$

By expressing the T_τ products appearing in Eq. (2.12) in terms of Eqs. (2.13) we obtain eventually the desired Ward identity

$$\int d33'\,G(2,3)[\partial_{\tau_1}\boldsymbol{\Gamma}(3,3';1)+\boldsymbol{\nabla}_1\cdot\boldsymbol{\Gamma}(3,3';1)]G(3',2')=\tfrac{1}{2}(\partial_{\tau_{1'}}-\partial_{\tau_1})[\delta(1,2')G(2,1')-\delta(2,1')G(1,2')]_{1'=1^+}\ , \qquad (2.16)$$

whose frequency-momentum representation reads

$$G(\mathbf{Q}+\mathbf{q}/2;\omega_n)[(\omega_n-\omega_{n'})\Gamma(\mathbf{Q},\mathbf{q};\omega_n,\omega_{n'})-\mathbf{q}\cdot\boldsymbol{\Gamma}(\mathbf{Q},\mathbf{q};\omega_n,\omega_{n'})]G(\mathbf{Q}-\mathbf{q}/2;\omega_{n'})$$
$$=[G(\mathbf{Q}+\mathbf{q}/2;\omega_n)-G(\mathbf{Q}-\mathbf{q}/2;\omega_{n'})](\omega_n+\omega_{n'})/2\ . \qquad (2.17)$$

Apart from the factor (2.15) on its right-hand side, Eq. (2.17) retains the same structure of the more familiar Ward identity associated with the continuity equation for the number density, the bare number vertex being unity.

III. DIFFUSIVE FORM OF THE HEAT-HEAT CORRELATION FUNCTION AND THE WIEDEMANN-FRANZ LAW

In this section we shall determine the critical behavior of the heat-heat correlation function by expressing it in terms of the scalar vertex function Γ introduced above and retaining the dominant approximation for Γ that is consistent with the identity (2.17). This analysis will eventually yield the generalization of the Wiedemann-Franz law anticipated in the Introduction.

By inserting Eq. (2.13a) in Eq. (2.6) we can express the Fourier transform of the temperature function corresponding to (1.2) as follows:

$$\chi_{KK}(\mathbf{q};\Omega_\lambda)=-\int_0^{(k_BT)^{-1}}d(\tau_1-\tau_2)e^{i\Omega_\lambda(\tau_1-\tau_2)}\int \mathbf{d}(\mathbf{r}_1-\mathbf{r}_2)e^{-i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)}$$
$$\times\sum_{\xi_1,\xi_2}\Big[\int d33'\,\tfrac{1}{2}[G(2,3)\partial_{\tau_2}G(3',2^+)$$
$$-G(3',2^+)\partial_{\tau_2}G(2,3)]\Gamma(3,3';1)+2\delta(1^+,2)\langle\mathcal{K}(1)\rangle\Big]$$
$$=-2k_BT\sum_{n=-\infty}^{+\infty}e^{i\omega_n\eta}\int\frac{\mathbf{dQ}}{(2\pi)^d}[(i/2)(2\omega_n+\Omega_\lambda)G(\mathbf{Q}-\mathbf{q}/2;\omega_n)G(\mathbf{Q}+\mathbf{q}/2;\omega_n+\Omega_\lambda)$$
$$\times\Gamma(\mathbf{Q},\mathbf{q};\omega_n,\,\omega_n+\Omega_\lambda)+2i\omega_nG(\mathbf{Q};\omega_n)]\ , \qquad (3.1)$$

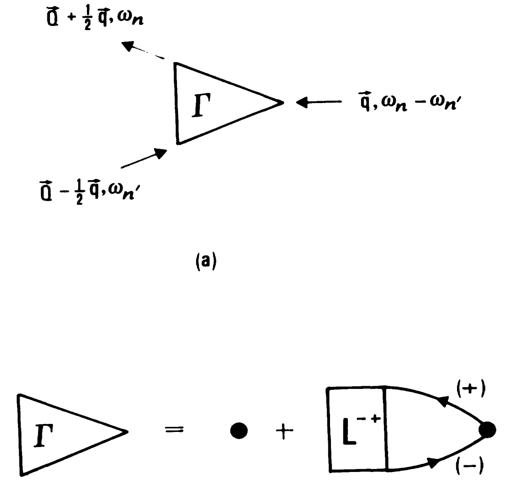

FIG. 1. (a) Entries for the frequency-momentum representation of the vertex functions; (b) skeleton structure for the scalar vertex function Γ. The solid circle represents the bare vertex function (2.15) and the single-particle lines are labeled by (+) and (−) to indicate the value of $\mathrm{sgn}(\omega_n)$ in Eq. (3.2).

where $\Omega_\lambda=2\lambda\pi k_BT$ (λ an integer), d is the space dimension of the system, and small values of $\mathbf{q}$ and Ω_λ are understood consistently with the hydrodynamic limit we are interested in. In Eq. (3.1) the scalar vertex function Γ contains all effects of averaging over the disorder that are not included in the averaged single-particle Green's functions, which (to leading order) are given by[13]

$$G(\mathbf{k};\omega_n)=[i\omega_n-(\epsilon_\mathbf{k}-\mu)+(i/2\tau_0)\mathrm{sgn}(\omega_n)]^{-1}\ , \qquad (3.2)$$

τ_0 being the scattering lifetime. To obtain Γ, the bare vertex (2.15) is dressed by disorder as depicted in the skeleton structure of Fig. 1(b), where, in the effective ladder,

$$L^{-+}(\mathbf{q};\Omega_\lambda)=\frac{1}{\pi N_0\tau_0^2}\,\frac{1}{|\Omega_\lambda|+D\mathbf{q}^2}\ , \qquad (3.3)$$

D is the renormalized diffusion coefficient that describes number-density transport and includes all quantum-interference effects. Thus, besides the ordinary Drude contribution ($2\tau_0\mu m^{-1}d^{-1}$), D also contains logarithmic corrections in two dimensions that drive the electronic system toward localization in $2+\varepsilon$ dimensions.[14] It may be verified that the skeleton structure of Fig. 1(b) with the choices (3.2) and (3.3) is consistent with the Ward identity (2.17) in the limit $\mathbf{q}\to 0$.

Explicit calculation of the right-hand side of Eq. (3.1) proceeds now by standard contour-integration techniques that transform the frequency sum into an integral over the real frequency axis. It is convenient to identity for the function $\chi_{KK}(\mathbf{q};\Omega_\lambda)$ a *static* and a *dynamic* contribution that have a finite and vanishing static limit, respectively.[11] The static contribution fully includes the second term within large parentheses on the right-hand side of Eq. (3.1), while the first term therein contributes to the static part only for $\Theta(\omega_n)\Theta(\omega_n+\Omega_\lambda)>0$ (Θ being the unit step function) with the vertex function assuming its bare value (2.15). The dynamic contribution to $\chi_{KK}(\mathbf{q};\Omega_\lambda)$ contains instead the effective ladder (3.3) since it originates from the first term within large parentheses on the right-hand side of Eq. (3.1) for $\Theta(\omega_n)\Theta(\omega_n+\Omega_\lambda)<0$. For the static contribution we obtain

$$\chi_{KK}^{(S)}(\mathbf{q};\Omega_\lambda)=-C_V^0T\ , \tag{3.4}$$

where C_V^0 is the free-electron value (2.9), apart from irrelevant terms $O(\Omega_\lambda)$ and $O(q^2)$. Some care should be exerted in deriving Eq. (3.4) since one can actually use the form (3.2) for the single-particle Green's function only in a small neighborhood of the origin ($|\omega_n|\ll\mu$). For larger values of ω the self-energy correction $-i(2\tau_0)^{-1}\operatorname{sgn}(\omega)$ should, in fact, be replaced by a more general expression that vanishes as $|\omega|\to\infty$.

The result (3.4) can be obtained from Eq. (3.1) in an alternative way that avoids these complications by calculating the dynamic contribution for $\mathbf{q}=0$ and small Ω_λ and recalling that, at any finite temperature,

$$\chi_{KK}(\mathbf{q}=0;\,\Omega_\lambda\neq0)=0\ . \tag{3.5}$$

The property (3.5) stems from the very definition of $\chi_{KK}(\mathbf{q};\omega)$ and corresponds physically to the energy conservation.[15] Without even resorting to the specific form (3.3) in the calculation of the dynamic contribution, we can make use of the Ward identity (2.17) with $\mathbf{q}=0$ and of Eq. (3.2) for small ω_n to obtain

$$\chi_{KK}^{(D)}(\mathbf{q};\Omega_\lambda)=C_V^0T \tag{3.6}$$

apart from a term $O(\Omega_\lambda)$. A combination of Eqs. (3.5) and (3.6) then reproduces Eq. (3.4).

For $\chi_{KK}^{(D)}(\mathbf{q};\Omega_\lambda)$, at finite values of $\mathbf{q}$ and $\Omega_\lambda>0$, we obtain

$$\begin{aligned}\chi_{KK}^{(D)}(\mathbf{q};\Omega_\lambda)&=-\frac{\Omega_\lambda}{\Omega_\lambda+D\mathbf{q}^2}2N_0\int_{-\infty}^{+\infty}dz\,z^2\frac{df(z)}{dz}\\&=C_V^0T\frac{\Omega_\lambda}{\Omega_\lambda+D\mathbf{q}^2}\ ,\end{aligned} \tag{3.7}$$

where $f(z)$ is the Fermi distribution function. Adding together the static (3.4) and dynamic (3.7) contributions eventually leads to the diffusive behavior

$$\chi_{KK}(\mathbf{q};\Omega_\lambda)=-C_V^0T\frac{D\mathbf{q}^2}{\Omega_\lambda+D\mathbf{q}^2}\ . \tag{3.8}$$

This result amounts to the statement that, in the absence of electron-electron interaction, the density and heat-diffusion coefficients coincide. Physically, particle number and energy diffuse at the same rate since there exists a single- (elastic) scattering process. A similar result is familiar in the kinetic theory of gases[16] and it is relevant that quantum-interference effects do not affect it.

Performing the analytic continuation of Eq. (3.8) to the upper side of the real frequency axis and entering the result into Eq. (1.1) for the thermal conductivity, we obtain the generalization of the Wiedemann-Franz law[3] near the Anderson transition in the form

$$\kappa=C_V^0D\ . \tag{3.9}$$

By recalling both the Einstein relation $\sigma=e^2N_0D$ (e being the electron charge) and the free-electron result (2.9), Eq. (3.9) asserts that the ratio κ/σ is a universal function of the temperature.[2] Moreover, since this function is not critically affected by varying the impurity concentration, Eq. (3.9) predicts that, near the electronic critical concentration n_c,

$$\lim_{T\to0}\frac{\kappa}{T}\sim(n-n_c)^s\ , \tag{3.10}$$

s being the same critical exponent of the electrical conductivity. Existing theories[17] provide the value $s=1$ in three dimensions for the case of nonmagnetic impurities. Regardless of the importance of including the electron-electron interaction in the transport process, Eq. (3.10) *per se* awaits experimental confirmation.

In conclusion, we have shown that the electronic heat diffusion in the presence of disorder (but in the absence of electron-electron interaction) has the same critical properties of the number-density diffusion, in agreement with a local Ward identity derived for the heat vertex. From this result it follows that the Wiedemann-Franz law extends its range of validity up to the localization transition. The present analysis, besides being relevant in itself, is a necessary preliminary step for including the electron-electron interaction in the study of the heat-transport properties of disordered electronic systems.

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APPENDIX: KUBO-TYPE EXPRESSIONS FOR ENERGY DIFFUSION DRIVEN BY THERMAL PERTURBATIONS

Linear-response theory to mechanical perturbations is relatively simple to describe since in this case one can define an interaction Hamiltonian between the system and an external agent. When the system is driven out of equilibrium by thermal perturbations, on the other hand, nonconservative forces come physically into play and the problem can hardly be treated within the Hamiltonian formalism.[18] In this case one has to rely on the existence of a *hydrodynamic limit* whereby the influence of a thermostat on the system can be characterized by a few parameters (such as the *local* temperature and chemical potential) *slowly* varying in space and time for a local thermodynamic equilibrium to be established in the conjugate variables (such as the energy and number density) at each stage of the transport process.

Alternative methods for nonequilibrium systems (such as the method of local integrals of motion[6] or the method of nonconservative forces[15]) lead to the following form of the nonequilibrium statistical operator:

$$\rho(t)=\frac{\exp\{-[A(t)+B(t)]\}}{\mathrm{Tr}(\exp\{-[A(t)+B(t)]\})}\ , \tag{A1}$$

where

$$A(t)=\int d\mathbf{r}\,\beta(\mathbf{r},t)\mathcal{H}(\mathbf{r})\ , \tag{A2}$$

$$B(t)=-\int_{-\infty}^{0}dt'\int d\mathbf{r}[\,\mathcal{J}_Q(\mathbf{r},t')\cdot\nabla\beta(\mathbf{r},t+t') +\mathcal{H}(\mathbf{r},t')\partial_{t'}\beta(\mathbf{r},t+t')]\ . \tag{A3}$$

In these expressions $\beta(\mathbf{r},t)$ is the local inverse temperature which may fluctuate both in space and time, $\mathcal{H}(\mathbf{r},t)$ is the grand-canonical Hamiltonian density which is suitably defined from Eq. (1.3), and $\mathcal{J}_Q(\mathbf{r},t)$ is the heat-current operator defined in terms of the energy and number-current operators[19]

$$\mathcal{J}_Q(\mathbf{r},t)=\mathcal{J}_H(\mathbf{r},t)-\mu\mathcal{J}(\mathbf{r},t)\ . \tag{A4}$$

The time dependence of the operators is understood in the Heisenberg picture with the grand-canonical Hamiltonian (1.3) replacing the Hamiltonian of the system. Notice that $\mathcal{H}(\mathbf{r},t)$ and $\mathcal{J}_Q(\mathbf{r},t)$ given by (A4) are mutually related by a local continuity equation and that in deriving Eqs. (A2) and (A3) the fluctuations of the chemical potential have been neglected.[20]

Linear processes are consistent with the hydrodynamic limit insofar as the derivatives of the thermodynamic parameters are small. One can thus regard the operator $B(t)$ as aperturbation to $A(t)$ and expand $\rho(t)$ to lowest order in $B(t)$ in Eq. (A1), in the form[6]

$$\rho(t)\simeq\left[1-\int_0^1 d\tau[\,e^{-A(t)\tau}B(t)e^{A(t)\tau} -\langle e^{-A(t)\tau}B(t)e^{A(t)\tau}\rangle_L\,]\right]\rho_L(t)\ , \tag{A5}$$

where $\langle\ \cdots\ \rangle_L$ denotes the statistical average with the *local-equilibrium distribution*

$$\rho_L(t)=\frac{\exp[-A(t)]}{\mathrm{Tr}\{\exp[-A(t)]\}}\ . \tag{A6}$$

With the aid of the nonequilibrium statistical operator (A5) one can calculate the space- and time-dependent average value of the heat-current operator. The first term within large parentheses on the right-hand side of Eq. (A5) gives a vanishing contribution since the local-equilibrium distribution, although needed to define the local thermodynamic parameters, does not produce any transport flow. In the remaining terms one may further replace the statistical averages $\langle\ \cdots\ \rangle_L$ with the equilibrium averages $\langle\ \cdots\ \rangle$ by assuming that deviations from complete equilibrium are small, and write

$$\begin{aligned}\langle\mathcal{J}_Q(\mathbf{r};t)\rangle&\equiv\mathrm{Tr}[\rho(t)\mathcal{J}_Q(\mathbf{r})]\\&\simeq-\beta^{-1}\int_0^{\beta}d\tau\langle\mathcal{J}_Q(\mathbf{r})[\,e^{-K\tau}B(t)e^{K\tau}\\&\qquad-\langle e^{-K\tau}B(t)e^{K\tau}\rangle]\rangle\ ,\end{aligned} \tag{A7}$$

where β is the inverse equilibrium temperature. One may further show that in Eq. (A7) the term containing the time derivative of the local inverse temperature [cf. Eq. (A3)] can be neglected in the lowest significant order since it actually involves higher derivatives of the form $\partial_{t'}\nabla\beta(\mathbf{r},t')$.

The linear-response expression (A7) can be rewritten in terms of the more familiar retarded correlation functions by transforming the integration over imaginary time into an integration over real time.[21] In particular, by neglecting nonlocality and retardation effects, Eq. (A7) provides a microscopic derivation of Fourier's law,

$$\langle\mathcal{J}_Q(\mathbf{r};t)\rangle=-\kappa\nabla T(\mathbf{r},t)\ , \tag{A8}$$

where the thermal conductivity κ is given by

$$\begin{aligned}\kappa=&-\frac{1}{T}\lim_{\omega\to0}\lim_{\mathbf{q}\to0}\frac{1}{\omega}\\&\times\mathrm{Im}\left[\int_{-\infty}^{+\infty}dt'e^{i\omega(t-t')}\int d\mathbf{r}'\,e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}\right.\\&\left.\qquad\times\chi^{\alpha\alpha}_{\mathcal{J}_Q\mathcal{J}_Q}(\mathbf{r}-\mathbf{r}';t-t')\right]\ .\end{aligned} \tag{A9}$$

In this expression

$$\chi^{\alpha\alpha}_{\mathcal{J}_Q\mathcal{J}_Q}(\mathbf{r}-\mathbf{r}';t-t') =\Theta(t-t')(-i)\langle[\mathcal{J}^{\alpha}_Q(\mathbf{r},t),\mathcal{J}^{\alpha}_Q(\mathbf{r}',t')]\rangle \tag{A10}$$

is the diagonal component of the retarded heat-current correlation tensor, and we have taken advantage of homogeneity and isotropy that result after averaging over the impurity configurations. Notice that the "rapid" limit in Eq. (A9), which is required to obtain a nonvanishing value of the heat current,[18] corresponds to taking the adiabatic limit after the thermodynamic limit.[6]

In the theory of electrical transport one finds it sometimes convenient to express the current-current correlation function in terms of the associated density-density correlation function. A connection between these two correlation functions is straightforward to derive from the continuity equation essentially because the number-density operators at different space points commute. As this is not the case for the energy-density operators, the corresponding relation between the heat-current and the (grand-canonical) Hamiltonian density correlation functions is unavoidably more involved. Nevertheless, these additional complications are unnecessary as far as the rapid limit in Eq. (A9) is concerned since one can prove that, in the small-$\mathbf{q}$ limit, the *imaginary* parts of any associated current-current and density-density correlation functions are proportional, provided a continuity equation holds.[21] We may thus rewrite the thermal conductivity κ in the alternative form (1.1) of the text.

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[1] Proper account of the interaction produces instead relevant corrections which are logarithmically singular as the temperature goes to zero in two dimensions: B. L. Altshuler, A. G. Aronov, and A. Yu. Zyuzin, Zh. Eksp. Teor. Fiz. **84**, 1525 (1983) [Sov. Phys.—JETP **57**, 889 (1983)].

[2] See, e.g., N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders College, Philadelphia, 1976).

[3] G. V. Chester and A. Thellung [Proc. Phys. Soc. London **77**, 1005 (1961)] have proven from quite general arguments that the Wiedemann-Franz law holds for arbitrarily strong (elastic) scattering by the impurities. In this respect their result is more exhaustive than ours, which rests on diagrammatic (perturbative) methods. Our analysis, however, enables us in addition to study separately the *dynamical* regression of spontaneous equilibrium fluctuations of number and energy densities.

[4] C. Castellani, C. Di Castro, and G. Strinati, Europhys. Lett. (in press).

[5] We set $\hbar=1$ throughout.

[6] D. N. Zubarev, *Non-Equilibrium Statistical Thermodynamics* (Consultants Bureau, New York, 1974), Chap. IV.

[7] Cf., e.g., A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971), Chaps. 7 and 9.

[8] In the presence of the electron-electron interaction it is no longer possible to express χ_{KK} in terms of time-derivative operators only. We obtain instead with the same provision that has led to Eq. (2.6):

$$\begin{aligned}\chi_{KK}(\mathbf{r}_1,\mathbf{r}_2;\tau_1-\tau_2)\\ =(\tfrac{1}{4})^2\sum_{\xi_1,\xi_2}&[(\partial_{\tau_{1'}}+h(\mathbf{r}_{1'})-\mu)+(-\partial_{\tau_1}+h(\mathbf{r}_1)-\mu)]\\ &\times[(\partial_{\tau_{2'}}+h(\mathbf{r}_{2'})-\mu)+(-\partial_{\tau_2}+h(\mathbf{r}_2)-\mu)]\\ &\times(-\langle T_\tau[\Psi(1)\Psi(2)\Psi^\dagger(2')\Psi^\dagger(1')]\rangle\\ &\quad+\langle T_\tau[\Psi(1)\Psi^\dagger(1')]\rangle\\ &\quad\times\langle T_\tau[\Psi(2)\Psi^\dagger(2')]\rangle)_{1'=1^+,\,2'=2^+}\\ -\delta(\tau_1-\tau_{2^+})\delta(\mathbf{r}_1-\mathbf{r}_2)(\langle\mathcal{K}\rangle+\tfrac{1}{2}\langle\mathcal{K}_{\text{int}}\rangle)\ ,\end{aligned}$$

$\langle\mathcal{K}_{\text{int}}\rangle$ being the averaged interaction energy per unit volume. This remark casts some doubts on previous results on the theory of thermoelectric power which were obtained using the independent-particle heat-current vertex (2.11) below: C. S. Ting, A. Houghton, and J. R. Senna, Phys. Rev. B **25**, 1439 (1982).

[9] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon, London, 1959), Chap. 11.

[10] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, NJ, 1963), Sec. 39.

[11] C. Castellani, C. Di Castro, G. Forgacs, and E. Tabet, J. Phys. C **16**, 159 (1983); Nucl. Phys. **B225**, 441 (1983); C. Castellani, C. Di Castro, P. A. Lee, M. Ma, S. Sorella, and E. Tabet, Phys. Rev. B **33**, 6169 (1986).

[12] J. R. Schrieffer, *Theory of Superconductivity* (Benjamin, New York, 1964), Sec. 8-5.

[13] Equation (3.2) is valid to leading order in $(\tau_0\mu)^{-1}$. Corrections to this equation are not singular even in two dimensions. Since we are interested in the critical behavior of $\chi_{KK}(\mathbf{q};\omega)$ near the Anderson transition, we shall consistently not consider these irrelevant finite corrections.

[14] L. P. Gor'kov, A. I. Larkin, and D. E. Khmel'niskii, Pis'ma Zh. Eksp. Teor. Fiz. **30**, 248 (1979) [JETP Lett. **30**, 228 (1979)]; *Anderson Localization,* edited by Y. Nagaoka and H. Fukuyama (Springer, New York, 1982).

[15] For a review, see, e.g., J. A. McLennan, Adv. Chem. Phys. **5**, 261 (1963).

[16] See, e.g., U. Fano and L. Fano, *Physics of Atoms and Molecules* (University of Chicago Press, Chicago, 1972), Sec. 1-2. One of us (G.S.) is indebted to Professor U. Fano for bringing this point to his attention.

[17] E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979); F. J. Wegner, Z. Phys. B **35**, 207 (1979); K. B. Efetov, A. I. Larkin, and D. E. Kheml'nitskii, Zh. Eksp. Teor. Fiz. **79**, 1120 (1980) [Sov. Phys.—JETP **52**, 568 (1980)]; S. Hikami, A. I. Larkin, and Y. Nagaoka, Prog. Theor. Phys. **63**, 707 (1980); A. J. McKane and M. Stone, Ann. Phys. (N.Y.) **131**, 36 (1981). See also the review in Ref. 14.

[18] J. M. Luttinger [Phys. Rev. **135**, A1505 (1964)] has provided a mechanical treatment of heat transport in the static case by introducing a fictitious gravitational field to produce a nonuniform temperature. Although in this way there still remains the problem of associating a suitable gravitational field to the actual temperature fluctuations, one can nonetheless obtain the correct expressions for the thermal coefficients.

[19] The subtraction of the term $\mu\mathcal{I}(\mathbf{r})$ in the definition of the heat current (A4) corresponds physically to the fact that transport of electrons in states above (below) the Fermi surface increases (decreases) the local temperature. Cf. P. L. Taylor, *A Quantum Approach to the Solid State* (Prentice-Hall, Englewood Cliffs, NJ, 1970), Sec. 7-6.

[20] Neglecting the fluctuations of the chemical potential is well justified at low temperature for an electronic system in the limit of weak disorder (cf. the derivation of the Wiedemann-Franz law given in Ref. 2). We assume here that this approximation is also valid in the limit of strong disorder we are interested in.

[21] See, e.g., L. P. Kadanoff and P. C. Martin, Ann. Phys. (N.Y.) **24**, 419 (1963).