

## Thermoelectric power in disordered electronic systems near the Anderson transition

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The number-density–heat-density correlation function  $\chi_{nQ}(\mathbf{q};\omega)$  for a noninteracting disordered electronic system, is evaluated at small wave vector and frequency by diagrammatic techniques and shown to meet its general hydrodynamic requirements. This analysis leads us to the conclusion that the ratio of the coefficient  $Q$  of thermoelectric power and of the temperature  $T$  diverges at the localization transition.

In this paper we evaluate the wave-vector- and frequency-dependent number-density–heat-density correlation function  $\chi_{nQ}(\mathbf{q};\omega)$  in the hydrodynamic limit for a noninteracting disordered electronic system, by using diagrammatic techniques. Standard scaling arguments allow us then to extend the results near the Anderson transition. Evaluation of the “mixed” correlation function  $\chi_{nQ}$  proves to be quite interesting, since it shows novel features (namely, the occurrence of a double pole) with respect to the well-studied number-density correlation function  $\chi_{nn}$ .<sup>1</sup> The present work completes the analysis of the thermal properties of noninteracting disordered electronic systems carried out in Ref. 2 via the evaluation of the heat-density correlation function  $\chi_{QQ}$ .

Our analysis enables us to predict the scaling behavior of the coefficient of thermoelectric power  $Q$  (that relates the voltage drop produced by a temperature gradient in open-circuit conditions<sup>3</sup>) near the Anderson transition. Our result for  $Q$  is, however, in contrast with a previous perturbation calculation<sup>4</sup> in the presence of nonmagnetic impurities, which led to a noncritical behavior for  $Q$ . Before embarking on the details of the perturbative analysis, it is thus worthwhile to give an alternative argument based on an exact expression for the transport coefficients provided by Chester and Thellung,<sup>5</sup> which yields quite generally the scaling behavior of  $Q$ . The following argument to predict the scaling behavior of  $Q$  parallels the derivation by Sivan and Imry within the context of a multichannel Landauer approach.<sup>6</sup>

For a system which can be described by a sum of one-particle Hamiltonians, it has been shown<sup>5</sup> that the kinetic coefficients  $L_{ij}$  can be cast in the form

$$L_{11} = - \int_{-\infty}^{+\infty} dE S(E) \frac{df(E)}{dE}, \quad (1a)$$

$$L_{12} = L_{21} = - \int_{-\infty}^{+\infty} dE (E - \mu) S(E) \frac{df(E)}{dE}, \quad (1b)$$

$$L_{22} = - \int_{-\infty}^{+\infty} dE (E - \mu)^2 S(E) \frac{df(E)}{dE}, \quad (1c)$$

where  $f(E) = \{1 + \exp[(E - \mu)/k_B T]\}^{-1}$  is the Fermi function,  $T$  is the temperature, and  $\mu$  is the chemical potential. In Eqs. (1) the function  $S(E)$  includes all system-dependent features through the density of states and the current matrix elements. The coefficients  $L_{ij}$

enter the linear equations for the number ( $j$ ) and heat ( $J_Q$ ) currents

$$\langle j \rangle = -L_{11} \nabla \mu - L_{12} T^{-1} \nabla T, \quad (2a)$$

$$\langle J_Q \rangle = -L_{21} \nabla \mu - L_{22} T^{-1} \nabla T \quad (2b)$$

set on by gradients of the thermodynamic parameters, and are related to the electrical conductivity  $\sigma = e^2 L_{11}$ , the thermal conductivity  $\kappa = (L_{11} L_{22} - L_{12}^2) (T L_{11})^{-1}$ , and the coefficient of thermoelectric power  $Q = L_{12} (e T L_{11})^{-1}$  ( $e$  being the electronic charge).

The Sommerfeld expansion can be used to obtain the low-temperature leading contributions to  $L_{ij}$ ,

$$L_{11} = S(\mu), \quad (3a)$$

$$L_{12} = (\pi^2/3) k_B^2 T^2 \left[ \frac{dS(E)}{dE} \right]_{E=\mu}, \quad (3b)$$

$$L_{22} = (\pi^2/3) k_B^2 T^2 S(\mu), \quad (3c)$$

which are valid irrespective of the amount of disorder. Equations (3) are suitable to relate the critical behavior of  $\sigma$ ,  $\kappa$ , and  $Q$  near the Anderson transition. In fact, from the knowledge of the power-law behavior of the electrical conductivity near the Anderson transition, namely,

$$S(\mu) = \sigma(\mu)/e^2 \sim (\mu - E_c)^s, \quad (4)$$

where  $\mu - E_c$  is the difference between the Fermi energy and the mobility edge  $E_c$  and  $s$  is the conductivity exponent,<sup>1</sup> we can obtain both the Wiedemann-Franz law<sup>5</sup> in the form  $\kappa/T \sim (\mu - E_c)^s$  as  $T \rightarrow 0$ ,<sup>2</sup> as well as the asymptotic behavior of  $L_{12}$ ,

$$L_{12} \sim T^2 (\mu - E_c)^{s-1}. \quad (5)$$

For the coefficient of thermoelectric power we then find

$$Q \sim T \left[ \frac{dS(E)}{dE} \right]_{E=\mu} S(\mu)^{-1} \sim T (\mu - E_c)^{-1}; \quad (6)$$

that is,  $Q/T$  diverges at the localization threshold.<sup>6</sup> In the presence of nonmagnetic impurities the exponent  $s$  is given by  $s = 1 + O(\epsilon^4)$  with  $\epsilon = d - 2$  ( $d$  being the dimensionality).<sup>1,7</sup> At the same order,  $L_{12} \sim T^2$  is thus unaffected by the localization transition. In the presence

of magnetic impurities, on the other hand,  $s$  equals  $\frac{1}{2}$  at two-loop order,<sup>1</sup> which yields  $L_{12} \sim T(\mu - E_c)^{-1/2}$ .

Ting, Houghton, and Senna,<sup>4</sup> by taking into account the quantum interference in two dimensions due to the effect of nonmagnetic impurities at the one-loop approximation, found the same logarithmically singular contribution to  $\sigma$  and  $L_{12}$ , thereby suggesting the same exponentiation for these two quantities and  $Q/T = \text{const}$  at the transition. We believe that the results (5) and (6) are instead correct since, in the presence of nonmagnetic impurities, the one-loop contribution to  $\sigma(E)$  is independent of  $E$  and thus does not contribute to  $L_{12}$  according to Eq. (3b).<sup>8</sup> This conclusion is supported by the following perturbative analysis.

$L_{12}$  can be obtained by calculating either the current-current or the density-density correlation functions. We prefer to adopt the latter approach since it allows for a systematic use of Ward identities and for a direct com-

parison with the analysis of the nonlinear  $\sigma$  model.  $L_{12}$  will thus be obtained as the "rapid" limit

$$L_{12} = - \lim_{\omega \rightarrow 0} \lim_{q \rightarrow 0} \left[ \frac{\omega}{q^2} \text{Im}[\chi_{nQ}(\mathbf{q}; \omega)] \right]. \quad (7)$$

Here  $\chi_{nQ}(\mathbf{q}; \omega)$  is the Fourier transform of the number-density-heat-density correlation function<sup>9</sup>

$$\chi_{nQ}(\mathbf{r} - \mathbf{r}'; t - t') = -i\theta(t - t') \overline{[\rho(\mathbf{r}, t), \mathcal{H}(\mathbf{r}', t')]} , \quad (8)$$

where  $\rho$  and  $\mathcal{H}$  are the number and grand-canonical Hamiltonian densities, respectively,<sup>2</sup> and the overbar on the thermal average denotes a quenched impurity average. Specifically, we consider an on-site impurity potential  $u(\mathbf{r})$  with Gaussian distribution  $\overline{u(\mathbf{r})u(\mathbf{r}')} = u^2 \delta(\mathbf{r} - \mathbf{r}')$ .

The Fourier transform of the temperature function corresponding to (8) can be written as<sup>2</sup>

$$\chi_{nQ}(\mathbf{q}; \Omega_\lambda) = -V^{-1} \int d\mathbf{r} \int d\mathbf{r}' e^{-i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} k_B T \sum_{n=-\infty}^{+\infty} [2\delta(\mathbf{r} - \mathbf{r}') \overline{G(\mathbf{r}, \mathbf{r}; \omega_n)} - i(2\omega_n + \Omega_\lambda) \overline{G(\mathbf{r}, \mathbf{r}'; \omega_n + \Omega_\lambda) G(\mathbf{r}', \mathbf{r}; \omega_n)}] , \quad (9)$$

where  $V$  is the volume occupied by the system,  $\omega_n$  and  $\Omega_\lambda$  are fermionic and bosonic Matsubara frequencies, respectively, and  $G(\mathbf{r}, \mathbf{r}'; \omega_n) = [i\omega_n - h_0(\mathbf{r})]^{-1} \delta(\mathbf{r} - \mathbf{r}')$  is the temperature single-particle Green's function associated with the one-particle Hamiltonian  $h_0(\mathbf{r}) = -\nabla^2/2m + u(\mathbf{r}) - \mu$  (at fixed configuration of disorder). Upon taking the analytic continuation of Eq. (9) to the upper side of the real frequency axis and transforming the sum over the fermionic frequencies  $\omega_n$  into an integral along the real axis,  $\chi_{nQ}(\mathbf{q}; \omega)$  for small values of  $\mathbf{q}$  and  $\omega$  is naturally partitioned into a "static" part (that survives in the limit  $\omega \rightarrow 0$ ) and a "dynamic" part:

$$\chi_{nQ}(\mathbf{q}; \omega) = \chi_{nQ}^{\text{st}} + \chi_{nQ}^{\text{dyn}}(\mathbf{q}; \omega) , \quad (10a)$$

where

$$\chi_{nQ}^{\text{st}} = \int_{-\infty}^{+\infty} dE (E - \mu) \overline{v}(E) \frac{df(E)}{dE} = -T \left[ \frac{\partial n}{\partial T} \right]_{\mu} \quad (10b)$$

is a thermodynamic derivative, and ( $\omega \rightarrow 0$ )

$$\chi_{nQ}^{\text{dyn}}(\mathbf{q}; \omega) = (i\omega/\pi V) \int_{-\infty}^{+\infty} dE (E - \mu) \frac{df(E)}{dE} \int d\mathbf{r} \int d\mathbf{r}' e^{-i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} \overline{G_R(\mathbf{r}, \mathbf{r}'; E - \mu + \omega) G_A(\mathbf{r}', \mathbf{r}; E - \mu)} . \quad (10c)$$

In the static part (10b) we have used the identity

$$\frac{dG_{R(A)}(\mathbf{r}, \mathbf{r}; E)}{dE} = - \int d\mathbf{r}' G_{R(A)}(\mathbf{r}, \mathbf{r}'; E) G_{R(A)}(\mathbf{r}', \mathbf{r}; E) \quad (11)$$

that holds for the retarded (advanced) single-particle Green's function

$$G_{R(A)}(\mathbf{r}, \mathbf{r}'; E) = [E \pm i\delta - h_0(\mathbf{r})]^{-1} \delta(\mathbf{r} - \mathbf{r}') \quad (\delta \rightarrow 0^+) ,$$

and introduced the average single-particle density of states (including spin degeneracy)

$$\overline{v}(E) = -(2/\pi) \text{Im}[\overline{G_R}(\mathbf{r}, \mathbf{r}; E - \mu)] . \quad (12)$$

The average of the product  $G_R G_A$  entering the dynamic part (10c) has been extensively considered in the literature.<sup>1</sup> Both a direct perturbative evaluation and the nonlinear  $\sigma$ -model analysis provide

$$V^{-1} \int d\mathbf{r} \int d\mathbf{r}' e^{-i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} \overline{G_R(\mathbf{r}, \mathbf{r}'; E - \mu + \omega) G_A(\mathbf{r}', \mathbf{r}; E - \mu)} = \frac{\pi \overline{v}(E)}{D(E)q^2 - i\omega} , \quad (13)$$

where  $D(E)$  is by definition the diffusion coefficient at energy  $E$  and is logarithmically singular as a function of  $\omega$  in two dimensions.<sup>10</sup>

Insertion of Eqs. (10b), (10c), and (13) into Eq. (10a) eventually yields

$$\chi_{nQ}(\mathbf{q};\omega) = \int_{-\infty}^{+\infty} dE (E - \mu) \frac{\bar{v}(E)D(E)\mathbf{q}^2}{D(E)\mathbf{q}^2 - i\omega} \frac{df(E)}{dE}, \quad (14)$$

which can be thought of as resulting from a superposition of diffusive modes at different energies. In the low-temperature limit the integral in Eq. (14) can be calculated by the Sommerfeld expansion, giving

$$\chi_{nQ}(\mathbf{q};\omega) = -(\pi^2/3)k_B^2 T^2 \frac{\mathbf{q}^2}{(D\mathbf{q}^2 - i\omega)^2} \times [\bar{v}'D^2\mathbf{q}^2 - i(\bar{v}'D + \bar{v}D')\omega], \quad (15)$$

where all quantities  $\bar{v}$ ,  $\bar{v}' = d\bar{v}(E)/dE$ ,  $D(E)$ , and  $D' = dD(E)/dE$  are evaluated at  $E = \mu$ . According to Eq. (15),  $\chi_{nQ}$  shows a double pole which is not present in either  $\chi_{nn}$  or  $\chi_{QQ}$ .<sup>1,2</sup> The form (15) is in agreement with the general hydrodynamic structure

$$\chi_{nQ}(\mathbf{q};\omega) = \mathbf{q}^2 \frac{D_n D_Q \chi_{nQ}^{\text{st}} \mathbf{q}^2 + iL_{12}\omega}{(D_n \mathbf{q}^2 - i\omega)(D_Q \mathbf{q}^2 - i\omega)}, \quad (16)$$

which can be obtained by the methods of Ref. 11.<sup>12</sup> In Eq. (16)  $D_n$  and  $D_Q$  are the number and heat diffusion coefficients, respectively, that are known to coincide with  $D$  for noninteracting disordered electrons.<sup>2</sup> Comparison of Eq. (15) with Eq. (16) then gives

$$\chi_{nQ}^{\text{st}} = -(\pi^2/3)k_B^2 T^2 \bar{v}', \quad (17a)$$

$$L_{12} = (\pi^2/3)k_B^2 T^2 \left[ \frac{d[\bar{v}(E)D(E)]}{dE} \right]_{E=\mu}, \quad (17b)$$

which are both correct in view of Eqs. (10b) and (7). Equation (17b) is then consistent with Eq. (3b) provided we identify<sup>13</sup>

$$S(E) = \bar{v}(E)D(E). \quad (18)$$

In the continuous model we are considering, to zero-loop order (i.e., when no quantum interference is present)  $S(E)$  is given by  $\sigma_0(E)/e^2 = \bar{v}(E)D_0(E)$  with diffusion coefficient  $D_0(E) = 2\tau(E)Em^{-1}d^{-1}$ .<sup>14</sup> Here  $\tau(E)$  is the scattering time in the Born approximation, which is specified by the consistency condition<sup>15</sup>

$$\pi\bar{v}(E)\tau(E)u^2 = 1. \quad (19)$$

Equation (17b) then gives

$$L_{12}^0 = (\pi^2/3)k_B^2 T^2 \bar{v}(\mu)D_0(\mu)\mu^{-1}$$

to this order.

In the presence of nonmagnetic impurities, the one-loop correction to  $S(E)$  (which leads to the Anderson localization) is given by  $\delta S(E) = (2\pi^2)^{-1} \ln[\omega\tau(E)]$  which shows only an irrelevant dependence on  $E$  [via  $\tau(E)$ ] since the prefactor is constant. No logarithmic contribution is thus present in  $L_{12}$ . This result is consistent, at the order here considered, with the scaling behavior (5) with  $s = 1$ .

In the presence of magnetic impurities, on the other hand, the first correction in the  $2 + \epsilon$  expansion gives  $\delta S(E) = e^2 [4\pi^4 \sigma_0(E)]^{-1} \ln[\omega\tau(E)]$  with a prefactor that depends explicitly on  $E$  via  $\sigma_0(E)$ .<sup>1,16</sup>  $L_{12}$  acquires thus a logarithmic correction:

$$L_{12} = L_{12}^0 \{1 - e^4 [2\pi^2 \sigma_0(\mu)]^{-2} \ln[\omega\tau(\mu)]\}. \quad (20)$$

At the fixed-point value for the dimensionless conductance  $e^2/(2\pi^2 \sigma^*) = (\epsilon/2)^{1/2}$ , upon exponentiation of the expression (20) for  $L_{12}$  we obtain the scaling behavior

$$L_{12} T^{-2} \sim \omega^{-\epsilon/2} \sim \xi^\epsilon \sim (\mu - E_c)^{-\nu\epsilon}, \quad (21)$$

where we have introduced the localization length  $\xi \sim (\mu - E_c)^{-\nu}$  with exponent  $\nu = (2\epsilon)^{-1}$  in the present case. Agreement with Eq. (5) is thus recovered in both cases.

It is worthwhile at this point to try a comparison of these results with experiments. To our knowledge, the available experimental data on thermal power are on palladium, palladium-gold,<sup>17</sup> and bismuth<sup>18</sup> thin films, where, owing to their two-dimensional character, the localization transition should not occur. In these cases a comparison with the predictions of the theory can then possibly be made in the weak-localization regime only, where the same logarithmic increase of the resistivity should be observed for the thermal power in the absence of magnetic effects. The available data in the literature are not detailed enough in this region to allow for a comparison with the theory. Experiments in three-dimensional systems would provide further useful information near the transition. One should, however, be aware of the fact that it might be necessary to extend the theory to include the electron-electron interaction, especially when a spin-orbit coupling is present as in the materials thus far considered.

In conclusion, we have presented a perturbative calculation for the number-density-heat-density correlation function of a noninteracting disordered electronic system, and derived from it both the hydrodynamic expression for this function and the scaling behavior of the coefficients of thermoelectric power near the Anderson transition.

*Note added in proof.* After submission of this paper, we became aware of the work by V. V. Afonin, Yu. M. Gal'perin, and V. L. Gurevich, Zh. Eksp. Teor. Fiz. **87**, 335 (1984) [Sov. Phys.—JETP **60**, 194 (1984)], where the incorrect result of Ref. 4 was questioned and corrected in agreement with our result.

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<sup>1</sup>See, e.g., *Anderson Localization*, edited by Y. Nagaoka and H. Fukuyama (Springer-Verlag, New York, 1982).

<sup>2</sup>C. Castellani, C. Di Castro, and G. Strinati, *Europhys. Lett.* **4**, 91 (1987); G. Strinati and C. Castellani, *Phys. Rev. B* **36**, 2270 (1987).

<sup>3</sup>See, e.g., N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders College, Philadelphia, 1976), Chap. 13.

<sup>4</sup>C. S. Ting, A. Houghton, and J. R. Senna, *Phys. Rev. B* **25**, 1439 (1982).

<sup>5</sup>G. V. Chester and A. Thellung, *Proc. Phys. Soc. London* **77**, 1005 (1961).

<sup>6</sup>U. Sivan and Y. Imry, *Phys. Rev. B* **33**, 551 (1986).

<sup>7</sup>S. Hikami, *Nucl. Phys.* **B215**, [FS7], 555 (1983).

<sup>8</sup>In Ref. 4  $L_{12}$  has been calculated at one-loop order via the heat-current vertex. In doing so, it seems that the dependence on  $E$  of only the vertex and of the Green's functions has been included. One needs instead to take into account also the dependence on  $E$  of the diffusion coefficient entering the Cooper propagator, as will be shown below. When this is consistently done, the logarithmic correction does not contribute to  $L_{12}$ .

<sup>9</sup>We set  $\hbar=1$  throughout.

<sup>10</sup>In the perturbative analysis of the number- ( $\chi_{nn}$ ) and heat- ( $\chi_{QQ}$ ) density correlation functions, the value of  $E$  is set equal to the chemical potential  $\mu$  owing to the presence of the factor  $df(E)/dE$  which is even in  $E-\mu$  and sharply peaked about  $\mu$  in the low-temperature limit. For the mixed correlation function  $\chi_{nQ}$ , on the other hand, the presence of the factor  $E-\mu$  in the integral over  $E$  in Eq. (10c) requires us to consider the explicit  $E$  dependence at the right-hand side of Eq. (13). In this context, we have to mention that the average density of states  $\bar{\nu}(E)$  differs, in general, from the free-electron density of states  $\nu(E)$  (which is constant in two dimensions), although this difference is usually neglected. At the same level of approximation, a ladder summation should

be considered for the average of the products  $G_R G_R$  and  $G_A G_A$  as well as for the Hikami vertex, in order to be consistent with conservation criteria.

<sup>11</sup>L. P. Kadanoff and P. C. Martin, *Ann. Phys. (N.Y.)* **24**, 419 (1963).

<sup>12</sup>Higher-order terms in the Sommerfeld expansion of the right-hand side of Eq. (14) do not match the hydrodynamic form (16), as they derive from diffusion modes at higher energy  $E$  that would require longer times for the local thermodynamic equilibrium to be established.

<sup>13</sup>An expression of the type (14) can also be derived for the number- ( $\chi_{nn}$ ) and heat- ( $\chi_{QQ}$ ) density correlation functions,<sup>1,2</sup> with the factor  $(E-\mu)$  raised to the power 0 and 2 in the two cases, respectively. Akin to Eq. (7), from the "rapid" limits of these expressions one can then obtain all kinetic coefficients (1) with  $S(E)$  given by Eq. (18).

<sup>14</sup>We have found a slight difference [of the order  $E^{-1}\tau(E)^{-1}$ , where  $\tau(E)$  is the scattering time evaluated via Eq. (19) below] in the definition of the zero-loop contribution to  $D(E)$ , depending on the way the momentum integrals over products of Green's functions of the diagrammatic structure were calculated. However, this does not affect our results since it only modifies the value of  $\sigma_0(E)$  which will consistently appear in the higher-order terms.

<sup>15</sup>A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1963), Sec. 39. Recall that Eq. (19) holds in the neighborhood of the Fermi surface which needs only be considered in the low-temperature limit.

<sup>16</sup>Recall that  $\sigma_0(E)$  includes the spin degeneracy.

<sup>17</sup>M. J. Burns, W. C. McGinnis, R. W. Simon, G. Deutscher, and P. M. Chaikin, *Phys. Rev. Lett.* **47**, 1620 (1981); M. J. Burns and P. M. Chaikin, *Phys. Rev. B* **27**, 5924 (1983).

<sup>18</sup>J. J. Lin, J. L. Cohn, and C. Uher, in *Proceedings of the University of Tokyo International Symposium on Anderson Localization*, Tokyo, 1987 (unpublished).