

Critical behavior of the thermopower near the metal-insulator transition

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The diffusive behavior of the number-heat correlation function for an interacting electronic disordered system is determined at first order in the disorder strength. Singular corrections are found for the coefficient of the thermopower. The resulting scaling behavior in the various universality classes differs from that obtained in the noninteracting case.

The thermal properties of interacting electronic disordered systems near the metal-insulator transition have recently been the object of renewed attention.¹⁻⁷ In particular, the critical behavior of the specific heat has been established¹ in $2+\epsilon$ dimensions for various universality classes and the thermal conductivity has been shown^{2,3} to satisfy the Wiedemann-Franz law up to the metal-insulator transition. However, despite some theoretical efforts, the analysis of the coefficient Q of thermopower (that relates the voltage drop produced by a temperature gradient in open-circuit conditions) has been successfully settled only for noninteracting electrons.⁴⁻⁷ In this case different approaches agree in predicting a divergence of the ratio Q/T (T being the temperature) at the localization transition, namely,

$$\lim_{T \rightarrow 0} Q/T = (E_F - E_c)^{-1}, \quad (1)$$

where E_F is the Fermi energy and E_c is the localization threshold. While Eq. (1) can be readily understood in terms of exact relations for the kinetic coefficients that hold in the absence of the electron-electron interaction,⁸ its derivation in the context of the ϵ expansion for localization is far from trivial^{4,6} and requires a careful analysis of the energy dependence of diagrams with mixed heat and number (current or density) vertices.⁹ In particular, Castellani *et al.* derived⁶ Eq. (1) by evaluating the wave vector and frequency-dependent number-heat density response function $\chi_{nQ}(\mathbf{q}, \Omega)$ in the hydrodynamic regime for a noninteracting disordered system.

In this paper we extend the analysis of Ref. 6 to include the effect of the electron-electron interaction. Specifically, we evaluate $\chi_{nQ}(\mathbf{q}, \Omega)$ for a Coulomb gas in a random Gaussian potential to lowest order in the disorder strength $t = 1/[(2\pi)^2 N_0 D_0]$ (D_0 and N_0 being the values of the diffusion coefficient and of the density of states in the Born approximation), and to all order in the singlet and triplet scattering amplitudes Γ_s and Γ_t .¹⁰ The perturbative analysis is carried out in two dimensions where the combined effect of disorder and interaction leads to logarithmic contributions; the results are then discussed in the context of the renormalization-group approach at lowest order in $\epsilon = d - 2$. We find that

the ratio of the coefficient Q of the thermoelectric power and of the temperature T diverges at the metal-insulator transition less strongly than predicted by the noninteracting theory in the case of spin-flip or spin-orbit scattering. The divergence of Q/T is instead stronger in the nonmagnetic impurity case, while we recover the noninteracting result in the presence of an external magnetic field.

After this work was completed, we became aware of a paper by Hsu, Kapitulnik, and Yu¹¹ which investigates the thermopower of disordered interacting electronic systems and evaluates the thermoelectric coefficient via the number- and heat-current correlation functions. In contrast to our result, the logarithmic correction to Q found by Hsu, Kapitulnik, and Yu in two dimensions originates only from the corrections to the conductivity. A temperature-independent correction to Q is instead found, which would lead to a nonvanishing thermopower in the zero-temperature limit. We shall argue in the following on the source of this discrepancy and give support to our result.

We introduce the number-heat density response function

$$\chi_{nQ}(\mathbf{r} - \mathbf{r}', t - t') = -i\Theta(t - t') \langle \overline{[\rho(\mathbf{r}, t), K(\mathbf{r}', t')]} \rangle, \quad (2)$$

where ρ and K are the number and the grand-canonical Hamiltonian densities, respectively, and the overbar on the thermal average denotes a quenched impurity average. In a diffusing medium, the Fourier transform $\chi_{nQ}(\mathbf{q}, \Omega)$ is known to assume the structure⁶

$$\chi_{nQ}(\mathbf{q}, \Omega) = \frac{\chi_{nQ}^{\text{st}} D_n \mathbf{q}^2}{D_n \mathbf{q}^2 - i\Omega} + \frac{i\Omega \mathbf{q}^2 (L_{12} + D_n \chi_{nQ}^{\text{st}})}{(D_n \mathbf{q}^2 - i\Omega)(D_Q \mathbf{q}^2 - i\Omega)}, \quad (3)$$

where D_n and D_Q are the number (charge) and heat diffusion coefficients and $\chi_{nQ}^{\text{st}} = -T \partial n / \partial T$ is a thermodynamic derivative, n being the electron density. L_{12} is the kinetic coefficient which enters the linear equations for the number and heat currents and determines the coefficient of the thermopower according to the expression

$$Q = eL_{12} / (T\sigma), \quad (4)$$

σ being the electric conductivity. From Eq. (3), L_{12} can be obtained as the "rapid" limit

$$L_{12} = - \lim_{\Omega \rightarrow 0} \lim_{q \rightarrow 0} \{ (\Omega/q^2) \text{Im}[\chi_{nQ}(\mathbf{q}, \Omega)] \}. \quad (5)$$

L_{12} could alternatively be derived from the heat-number current response function; however, we prefer to evaluate L_{12} from Eq. (5) because in the presence of interaction it is far simpler to deal with the energy density vertex than with the corresponding current vertex. Moreover, the perturbative expression of χ_{nQ} can be readily checked by a systematic use of Ward identities.

By using the equation of motion for the fermion operator $\psi(\mathbf{r}, t)$ in the Heisenberg representation, the two-body interaction term of $K(\mathbf{r}, t)$ can be manipulated to express $K(\mathbf{r}, t)$ itself in a more tractable bilinear form:

$$K(\mathbf{r}, t) = \frac{1}{2} \sum_{\sigma} \psi^{\dagger}(\mathbf{r}, t) \left[i \frac{\partial}{\partial t} + H_0(\mathbf{r}) \right] \psi(\mathbf{r}, t), \quad (6)$$

where $H_0(\mathbf{r}) = -\nabla^2/2 + u(\mathbf{r}) - \mu$ is the single-particle Hamiltonian. In Eq. (6), $u(\mathbf{r})$ is a random Gaussian potential with variance $u(\mathbf{r})u(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')/(2\pi\tau_0 N_0)$ (τ_0 being the scattering time in the Born approximation) and μ is the chemical potential. In the Matsubara formalism, Eq. (2) reduces to the following time-ordered product in the imaginary time τ :

$$\begin{aligned} \chi_{nQ}(\mathbf{r} - \mathbf{r}', \tau - \tau') &= - \frac{1}{2} \left[- \frac{\partial}{\partial \tau} + H_0(\mathbf{r}) \right] \\ &\times \langle T_{\tau} \psi^{\dagger}(\mathbf{r}, \bar{\tau}) \psi(\mathbf{r}, \tau) \\ &\times \psi^{\dagger}(\mathbf{r}', \tau') \psi(\mathbf{r}', \tau') \rangle_{\bar{\tau} = \tau^+} \\ &- \frac{1}{2} \delta(\mathbf{r} - \mathbf{r}') \delta(\tau - \tau') \langle \rho \rangle, \end{aligned} \quad (7)$$

where the last term originates by commuting the time derivative in K with the time-ordering operator and the connected part is understood in the first term.

A main difficulty in evaluating Eq. (7) stems from the explicit presence of the random potential in the heat vertex outside the T_{τ} product. To overcome this problem one needs to introduce two types of vertices.³ The first one, denoted by a circle, represents $-\partial/\partial\tau$ ($i\varepsilon_n$ in the Fourier space). The second one, denoted by a dot with a slash on the outgoing Green's function, replaces this function with the factor $-\frac{1}{2}\delta(\mathbf{r} - \mathbf{r}')$. This is because the action of the full heat vertex operator on the exact noninteracting Green's function gives

$$\frac{1}{2} [i\varepsilon_n + H_0(\mathbf{r})] G(\mathbf{r}, \mathbf{r}'; i\varepsilon_n) = i\varepsilon_n G(\mathbf{r}, \mathbf{r}'; i\varepsilon_n) - \frac{1}{2} \delta(\mathbf{r} - \mathbf{r}').$$

Once the random potential has been eliminated in this way from the external vertex, Eq. (7) can be evaluated according to standard impurity average techniques.

We separate $\chi_{nQ}(\mathbf{q}, \Omega)$ into a static part χ_{nQ}^{st} which is nonvanishing in the limit $\Omega \rightarrow 0$ and a dynamic part χ_{nQ}^{dyn} . In the evaluation of χ_{nQ}^{st} , we use the thermodynamic identity

$$\chi_{nQ}^{\text{st}} = T \frac{\partial^2 F}{\partial \mu \partial T}, \quad (8)$$

where F is the thermodynamic potential per unit volume. Near two dimensions and at first order in t , $F(T) - F(0)$ is conveniently written^{1,12} as $-Z(\pi^2/3)T^2 N_0$, where Z is the temperature (frequency) renormalization factor given by $Z = 1 + \delta Z$ with

$$\delta Z = t(N_0 \Gamma_s + 3N_0 \Gamma_t) \ln T \tau. \quad (9)$$

The derivative with respect to μ in Eq. (8) requires us to analyze the dependence of the bare density of states N_0 (and of the parameters D_0 and τ_0 entering δZ) on the single-particle energy E . It is in fact easy to show that the derivative with respect to μ amounts to taking $\partial/\partial E|_{E=\mu}$ times a Fermi-liquid factor $Z_1 = 1 - 2N_0 \Gamma_s$.¹³ Both N_0 and τ_0 have a weak dependence on E : One gets $E \partial N_0 / \partial E \sim -N_0 / (E \tau_0)$ and $E \partial \tau_0 / \partial E \sim \tau_0 / (E \tau_0)$. A stronger dependence results instead for the bare diffusion coefficient $D_0 = (2/d)E \tau_0$: $E \partial D_0 / \partial E = D_0$.

By inserting Eq. (9) into Eq. (8) and retaining the leading contributions in $1/(\mu \tau_0)$, we get

$$\begin{aligned} \chi_{nQ}^{\text{st}} &= -(2\pi^2/3)T^2(N'_0 Z + N_0 Z') Z_1 \\ &= -[(2\pi^2/3)T^2 N'_0 + T c_v^0 Z'] Z_1 \\ &\simeq -[(2\pi^2/3)T^2 N'_0 - T c_v^0 \delta Z / \mu] Z_1, \end{aligned} \quad (10)$$

where $c_v^0 = (2\pi^2/3)T N_0$ is the bare specific heat and we have set $Z' = \partial Z / \partial E \approx (1/t)(\partial t / \partial E) \delta Z$ with $\partial t / \partial E \simeq -t/E$ since the main dependence of t on E arises from the bare diffusion coefficient.

At first order in t , the contributions to the dynamic part originate from the diagrams shown in Figs. 1-3. The vertex corrections of Fig. 1 give

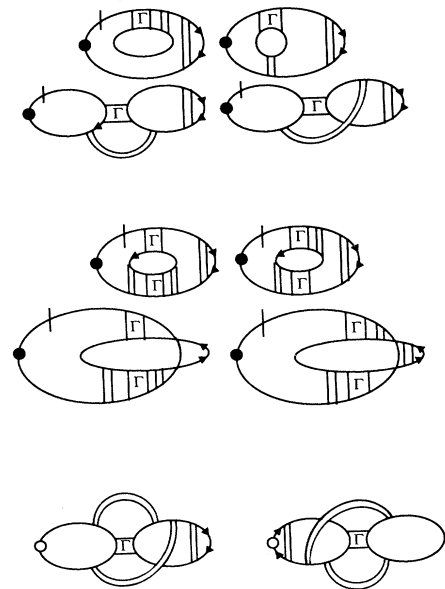


FIG. 1. Vertex corrections contributing to χ_{nQ}^{dyn} . Here and in Figs. 2 and 3, a static or a dynamic amplitude (Ref. 10) insertion is understood whenever appropriate.

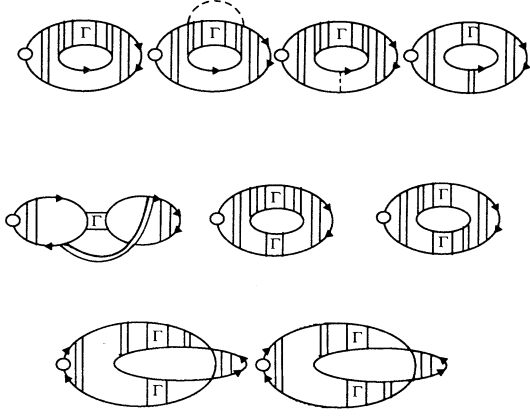


FIG. 2. Ladder and amplitude corrections contributing to χ_{nQ}^{dyn} .

$$c_v^0 T \left[-i\Omega \frac{Z' - 2\xi'_0}{D_0 q^2 - i\Omega Z_1} Z_1 + i\Omega D'_0 \frac{(\delta Z - 2\delta\xi_0)q^2}{(D_0 q^2 - i\Omega)(D_0 q^2 - i\Omega Z_1)} Z_1 \right], \quad (11)$$

where $\delta\xi_0(\varepsilon)$ is the ordinary lowest-order correction to

$$c_v^0 T \left[-i\Omega \frac{2\xi'}{D_0 q^2 - i\Omega Z_1} Z_1 + 2\delta\xi \frac{i\Omega D'_0 q^2}{(D_0 q^2 - i\Omega)(D_0 q^2 - i\Omega Z_1)} + \frac{\Omega^2 Z_1 Z'}{(D_0 q^2 - i\Omega)(D_0 q^2 - i\Omega Z_1)} - \frac{\Omega^2 \delta Z Z_1 D'_0 q^2}{(D_0 q^2 - i\Omega)^2 (D_0 q^2 - i\Omega Z_1)} - i\Omega \delta D q^4 D'_0 Z_1 \left[\frac{1}{(D_0 q^2 - i\Omega)^2 (D_0 q^2 - i\Omega Z_1)} + \frac{1}{(D_0 q^2 - i\Omega)(D_0 q^2 - i\Omega Z_1)^2} \right] - \frac{1}{2} Z' Z_1 \frac{D_0 q^2 i\Omega}{(D_0 q^2 - i\Omega)(D_0 q^2 - i\Omega Z_1)} \right], \quad (12)$$

where δD is the lowest-order correction¹⁰ to the diffusion coefficient $D = D_0 + \delta D$. Recalling the expression for the effective ladder $L = \xi^2 / (-iZ\Omega + Dq^2)$, Eq. (12) shows that amplitude and Z corrections partially compensate each other, whereas the last term has the structure of a correction to the diffusion coefficient. The last term originates from the first three diagrams of Fig. 2 once the relevant Hikami vertex¹⁰ is fully expanded in terms of the energies carried by the fermion lines, in the form

$$2\pi N_0 \tau^4 \left\{ \left[D_0 \left[\varepsilon + \frac{\omega}{2} + \frac{\Omega}{2} \right] q^2 - i\Omega \right] + \left[D_0 \left[\varepsilon + \frac{3\Omega}{2} - \frac{\omega}{2} \right] k^2 - i\omega \right] + \frac{3}{2} i D'_0 q^2 D_0 k^2 \right\}, \quad (13a)$$

$$2\pi N_0 \tau^4 \left\{ \left[D_0 \left[\varepsilon + \frac{\Omega}{2} - \frac{\omega}{2} \right] q^2 - i\Omega \right] + \left[D_0 \left[\varepsilon - \frac{\Omega}{2} + \frac{\omega}{2} \right] k^2 - i\omega \right] - \frac{3}{2} i D'_0 q^2 D_0 k^2 \right\}, \quad (13b)$$

which appear in the electron and hole ladder corrections, respectively. We like to point out that the derivative of the standard log correction to D does not appear in Eq. (12) because δD is independent of ε at leading order (neglecting the energy dependence of the cutoff).

Adding to Eqs. (11) and (12) the corresponding bare contribution of Fig. 3(a), the resulting expression can be cast in the form

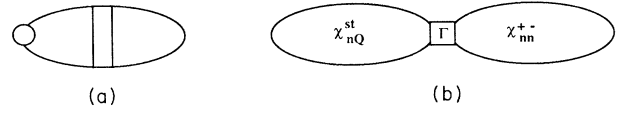


FIG. 3. Additional diagrams contributing to χ_{nQ}^{dyn} . (a) Zero-order term and (b) contribution from χ_{nQ}^{st} and χ_{nn}^{+-} .

the single-particle density of states¹⁰ $N(\varepsilon)$ with coupling parameters evaluated at the energy $E = \varepsilon + \mu$. In Eq. (11) and below, ε is set equal to zero after the derivative is carried out. We note that, at the same order and by fully taking into account the ε dependence of $\delta N(\varepsilon)$, we find $N(\varepsilon)/N_0 = \xi(\varepsilon) = \xi_0(\varepsilon) + Z'\varepsilon/2$. Equation (11) reflects the identities

$$\xi(\varepsilon)\Lambda_n(\varepsilon) = Z_1(1 + Z'\varepsilon) \quad \text{and} \quad \xi(\varepsilon)\Lambda_Q(\varepsilon) = Z(\varepsilon),$$

which generalize the identities derived for the density vertex Λ_n and the heat vertex Λ_Q in the context of the analysis of density-density correlation function¹⁰ and of the thermal conductivity.³

The ladder and amplitude corrections of Fig. 2 lead instead to

$$-i\Omega c_v^0 T \frac{\partial}{\partial \varepsilon} \left[\frac{\xi^2(\varepsilon)\Lambda_n(\varepsilon)\Lambda_Q(\varepsilon)}{D(\varepsilon)q^2 - i\Omega Z(\varepsilon)} \right] \frac{Dq^2 - i\Omega Z}{Dq^2 - i\Omega Z_1} = -i\Omega c_v^0 T \frac{\partial}{\partial \varepsilon} \left[\frac{Z(\varepsilon) + \varepsilon Z'}{D(\varepsilon)q^2 - i\Omega Z(\varepsilon)} \right] \frac{Dq^2 - i\Omega Z}{Dq^2 - i\Omega Z_1} Z_1, \quad (14)$$

where the wave-function renormalization $\delta\xi$ has disappeared and where $D(\epsilon) = D_0 + \delta D + D_0(Z'/2)\epsilon$ identifies the full energy dependence of the diffusion coefficient.

A final contribution to χ_{nQ}^{dyn} derives by taking into account that the $+$ -density-density correlation¹⁰ χ_{nn}^{+-} can be diagrammatically connected to the heat static part [see Fig. 3(b)] to give $\chi_{nQ}^{\text{st}}(Z_1 - 1)i\Omega/(D\mathbf{q}^2 - i\Omega Z_1)$. By adding all contributions we eventually get

$$\begin{aligned} \chi_{nQ}(\mathbf{q}, \Omega) &= -c_v^0 T \frac{\partial}{\partial \epsilon} \left[\frac{(1 + Z'\epsilon)D(\epsilon)\mathbf{q}^2}{D(\epsilon)\mathbf{q}^2 - i\Omega Z(\epsilon)} \right] \\ &\quad \times \frac{D\mathbf{q}^2 - i\Omega Z}{D\mathbf{q}^2 - i\Omega Z_1} Z_1 \\ &= -c_v^0 T \frac{\partial}{\partial \epsilon} \left[\frac{Z(\epsilon)D_Q(\epsilon)\mathbf{q}^2}{D_Q(\epsilon)\mathbf{q}^2 - i\Omega} \right] \frac{D_Q\mathbf{q}^2 - i\Omega}{D_n\mathbf{q}^2 - i\Omega}, \end{aligned} \quad (15)$$

where $D_n = D/Z_1$. The last expression can be shown to coincide with χ_{nQ} obtained from the solution of the Landau Boltzmann equation for quasiparticles^{3,14} with diffusion coefficient $D_{QP}(\epsilon) = D_Q(\epsilon) = D(\epsilon)/Z(\epsilon)$. By carrying out the derivatives in Eq. (15), we recover the general form of Eq. (3), with the kinetic coefficient L_{12} given by

$$L_{12} = L_{12}^0(1 + \delta Z/2), \quad L_{12}^0 = (2\pi^2/3)T^2 N_0 D_0 / \mu. \quad (16)$$

This result contrasts with the analysis carried out in Ref. 11, where no logarithmic correction to L_{12} is found in two dimensions. A more divergent contribution $\delta L_{12}/L_{12}^0 \sim 1/T$ is instead obtained in Ref. 11. However, the authors have missed a term for η_{11}^p (in their notation) which exactly cancels the $1/T$ contribution from η_{11}^q . The reason is that in evaluating integrals of the type $\int d\mathbf{p}' p'^2 G_-^2 G_+$, they retain only the term $2i\mu\tau^2(2\pi N_0)$ and overlook the presence of the term $-2(1/2\tau)\tau^2(2\pi N_0)$ originating from the value of ξ_p at the pole of the Green's function. As to the disagreement on the logarithmic correction, we suggest that this disagreement arises from the fact that Hsu, Kapitulnik, and Yu consider the expansion of the single-particle Green's functions only to first order in their arguments. We found, in fact, it necessary to expand the single-particle Green's functions to third order in their arguments in order to obtain the singular correction $\sim \delta Z/2$ in our Eq. (16). On the other hand, the recovering of the structure given in Eq. (3) is far from trivial and makes us confident on the validity of our perturbative analysis.

The above perturbative result for L_{12} in $d=2$ allows us to obtain the scaling behavior of L_{12} (and of coefficient Q of the thermopower) at lowest order in $\epsilon = d - 2$, provided we make the assumption that L_{12} is a scaling quantity. This assumption is strongly supported by the analysis of the noninteracting case where the perturbative log correction to L_{12} does in fact lead to the same scaling behavior which can be inferred from the exact relations of Ref. 8. We thus exponentiate the log terms of Eqs. (16) and (9) to get

$$L_{12} = \sqrt{Z} L_{12}^0. \quad (17)$$

Strictly speaking, Eq. (17) is valid only to lowest order in

ϵ in the particle-hole channel model¹⁰ we have been considering; however, we suggest that Eq. (17) has a more general validity and we shall use it to state that L_{12} scales as \sqrt{Z} in the various universality classes.

To this end we first recall that when magnetic impurities, external magnetic fields, or spin-orbit coupling are present, a metal-insulator transition is obtained at a finite fixed-point value $t^* \sim \epsilon$. The conductivity then scales as $\sigma \sim (\delta n)^\mu \sim (T)^{\epsilon/x_T}$, where δn is the deviation from the critical density and $\mu = \epsilon\nu$ (ν being the index of the correlation length which at one loop is given by $\nu = 1/\epsilon$). x_T is the temperature critical index which is related to that of Z by the scaling law¹

$$x_Z + x_T = 2 + x_\sigma = d. \quad (18)$$

Using Eq. (17), we obtain for the coefficient of the thermopower

$$Q/T = eL_{12}/(\sigma T^2) \sim (\delta n)^{x_Z\nu/2-\mu} \sim T^{(x_Z/2-\epsilon)/(d-x_Z)}. \quad (19)$$

At lowest order in ϵ , $x_Z = \epsilon/2$ for magnetic impurities, $x_Z = \epsilon$ in the spin-orbit case, and $x_Z = 0$ in the presence of a magnetic field.^{1,10}

In the nonmagnetic impurity case, on the other hand, $t^* = 0$ and the conductivity remains finite, while Z diverges with $x_Z = -3\epsilon$.^{1,10} In this case we obtain, at order ϵ ,

$$Q/T \sim (\delta n)^{x_Z\nu/2} \sim T^{(x_Z/2)/(2-x_Z)}, \quad (20)$$

where again $\nu = 1/\epsilon$ and Eq. (18) has been used with d replaced by 2.

It was suggested in Ref. 14 that the fixed-point behavior at $t^* = 0$ could be modified by higher-order contributions in ϵ to allow for a vanishing conductivity $\sigma \sim (\delta n)^{\nu\Theta}$. In that case Eq. (20) would accordingly change into

$$Q/T = (\delta n)^{(x_Z/2-\Theta)\nu} \sim T^{(x_Z/2-\Theta)/(2+\Theta-x_Z)}, \quad (21)$$

where now x_Z should consistently include higher-order corrections. It is, however, worth noticing that Belitz and Kirkpatrick¹⁵ have recently argued that the fixed point discussed in Ref. 14 would be unstable with respect to higher-order terms and would only describe a crossover region with $\Theta = 0$ to any order in ϵ .

We comment finally on the experimental situation. Although there has been an increasing number of reported measurements on the thermopower in disordered systems,¹⁶⁻¹⁹ very few works have addressed the problem of determining the diffusion corrections to L_{12} . It is worth pointing out that it might be difficult to verify experimentally the theoretical predictions since phonon effects can dominate the behavior of the thermal power at (intermediate) low temperature, thereby overshadowing the diffusion effects.^{18,19} Measurements¹⁹ in strong magnetic fields, on the other hand, select the electronic diffusion contributions to Q and may hopefully reveal an anomalous behavior of L_{12} at sufficiently low temperature. Specifically, in the weak localization regime, the magnetic field cuts off two-thirds of the triplet contribution to Z for Zeeman splitting frequencies larger than the spin-orbit or spin-flip scattering rate;²⁰ an additional dependence of Q on the field would possibly appear similar in origin to the positive magnetoresistance.

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