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Thermopower of single-channel disordered and chaotic conductors

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We show (analytically and by numerical simulation) that the zero-temperature limit of the distribution of the thermopower S of a one-dimensional disordered wire in the localized regime is a Lorentzian, with a disorder-independent width of $4\pi^3 k_B^2 T/3e\Delta$ (where T is the temperature and Δ the mean level spacing). Upon raising the temperature the distribution crosses over to an exponential form $\propto \exp(-2|S|eT/\Delta)$. We also consider the case of a chaotic quantum dot with two single channel ballistic point contacts. The distribution of S then has a cusp at $S = 0$ and a tail $\propto |S|^{-1-\beta} \ln |S|$ for large S (with $\beta = 1, 2$ depending on the presence or absence of time reversal symmetry).

Key words: thermo electric phenomena, localization, quantum chaos

1. Introduction

Thermo-electric transport properties of conductors probe the energy dependence of the scattering processes limiting conduction. At low temperatures and in small (mesoscopic) systems, elastic impurity scattering is the dominant scattering process. The energy dependence of the conductance is then a quantum interference effect [1]. The derivative dG/dE of the conductance with respect to the Fermi energy is measured by the thermopower S, defined as the ratio $-\Delta V/\Delta T$ of a (small) voltage and temperature difference applied over the sample at zero electric current. Experimental and theoretical studies of the thermopower exist for several mesoscopic devices. One finds a series of sharp peaks in the thermopower of quantum point contacts [2], aperiodic fluctuations in diffusive conductors [3], sawtooth oscillations in quantum dots in the Coulomb blockade regime [4], and Aharonov–Bohm oscillations in metal rings [5].

Here we study the statistical distribution of the thermopower in two different systems, not considered previously. A disordered wire in the localized regime and a chaotic quantum dot with ballistic point contacts. A single transmitted mode is assumed in both cases. In the disordered wire, conduction takes place by resonant tunnelling through localized states. The resonances are very narrow and appear at uncorrelated energies. The distributions of the thermopower and the conductance are both broad, but otherwise quite different: instead of the log normal distribution of the conductance [1] we find a Lorentzian distribution for the thermopower. In the quantum dot, the resonances are correlated and the widths are of the same order as the spacings. The correlations are described by random-matrix theory [6, 7], under the assumption that the classical dynamics in the dot is chaotic. The thermopower distribution in this case follows from the distribution of the time delay matrix found recently [8].

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The thermopower (at temperature T and Fermi energy E_F) is given by the Cutler–Mott formula [9, 10]

$$S = -\frac{1}{eT}\frac{\int dE\,(E-E_F)G(E)df/dE}{\int dE\,G(E)df/dE}, \tag{1}$$

where G is the zero-temperature conductance and f is the Fermi–Dirac distribution function. In the limit $T \to 0$ eqn (1) simplifies to

$$S = -\frac{\pi^2}{3}\frac{k_B^2 T}{eG}\frac{dG}{dE}, \tag{2}$$

where G and dG/dE are to be evaluated at $E = E_F$. We consider mainly the zero-temperature limit of the thermopower, by studying the dimensionless quantity

$$\sigma = \frac{\Delta}{2\pi G}\frac{dG}{dE}. \tag{3}$$

Here Δ is the mean level spacing near the Fermi energy. Since we are dealing with single-channel conduction, the conductance is related to the transmission probability $T(E)$ by the Landauer formula [1, 11]

$$G(E) = \frac{2e^2}{h}T(E). \tag{4}$$

The problem of the distribution of the thermopower is therefore a problem of the distribution of the logarithmic derivative of the transmission probability.

2. Disordered wire

In this section we study a disordered single-mode wire of length L much greater than the mean free path l. This is the localized regime. We compute the thermopower distribution in the zero-temperature limit. The analytical theory is tested by comparing with a numerical simulation. The effect of a finite temperature is considered at the end of the section. Electron–electron interactions play an important role in one-dimensional conduction, but we do not take these into account here.

2.1. Analytical theory

The localization length $\xi(E)$ (which is of order l and is defined by $\lim_{L\to\infty} L^{-1}\ln T(E) = -2/\xi(E)$) and the density of states $\rho(E)$ (per unit of length in the limit $L \to \infty$) are related by the Herbert–Jones–Thouless formula [12]

$$\frac{1}{\xi(E)} = \int dE'\rho(E')\ln|E-E'| + \text{constant}. \tag{5}$$

The additive constant is energy independent on the scale of the level spacing. Equation (5) follows from the Kramers–Kronig relation between the real and imaginary parts of the wavenumber (the real part determining ρ, the imaginary part ξ). Neglecting the width of the resonances in the large-L limit, the density of states $\rho(E) = L^{-1}\sum_i \delta(E-E_i)$ is a sum of delta functions, and thus

$$\sigma = -\frac{L\Delta}{\pi}\frac{d}{dE}\frac{1}{\xi(E)} = \frac{\Delta}{\pi}\sum_i \frac{1}{E_i - E_F}. \tag{6}$$

In the localized regime the energy levels E_i are uncorrelated, and we assume that they are uniformly distributed in a band of width B around E_F. To obtain the distribution of σ,

$$P(\sigma) = \prod_i \int_{-B/2}^{B/2}\frac{dE_i}{B}\,\delta\left(\sigma - \frac{\Delta}{\pi}\sum_j \frac{1}{E_j}\right), \tag{7}$$

we first compute the Fourier transform

$$P(k) = \int_{-\infty}^{\infty} d\sigma\, e^{ik\sigma} P(\sigma) = \left[\frac{1}{B}\int_{-B/2}^{B/2} dE\, e^{ik\Delta/\pi E}\right]^{B/\Delta} = e^{-|k|}, \tag{8}$$

where the limit $B/\Delta \to \infty$ is taken in the last step. Inverting the Fourier transform, we find that the thermopower distribution is a Lorentzian,

$$P(\sigma) = \frac{1/\pi}{1+\sigma^2}. \tag{9}$$

The 'full width at half maximum' of $P(\sigma)$ is equal to 2, hence it is equal to $4\pi^3 k_B^2 T/3e\Delta$ for $P(S)$. This width depends on the length L of the system (through $\Delta \propto 1/L$), but it does not depend on the mean free path l (as long as $l \ll L$, so that the system remains in the localized regime).

2.2. Numerical simulation

In order to check the analytical theory, we performed a numerical simulation using the tight-binding Hamiltonian

$$\mathcal{H} = -\frac{w}{2}\sum_j (c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}) + \sum_j V_j c_j^\dagger c_j. \tag{10}$$

The disordered wire was modelled by a chain of lattice constant a, with a random impurity potential V_j at each site drawn from a Gaussian distribution of mean zero and variance u^2. The localization length of the wire is given by $\xi = 2(a/u^2)(w^2 - E_F^2)$ [13]. We have chosen $u = 0.075\,w$, $E_F = -0.55\,w$, such that $\xi = 248\,a$, much smaller than $L = 8000\,a$. From the scattering matrix we obtained the conductance via the Landauer formula (4), and then the (dimensionless) thermopower via eqn (3) (with $\Delta = 3.3 \times 10^{-4}\,w$). The differentiation with respect to energy was carried out numerically, by repeating the calculation at two closely spaced values of E_F. As shown in Fig. 1, the agreement with the analytical result is good without any adjustable parameters.

2.3. Finite temperatures

Our derivation of the Lorentzian distribution of the thermopower holds if the temperature is so low that $k_B T$ is small compared to the typical width γ of the transmission resonances. What if $k_B T > \gamma$, but still $k_B T \ll \Delta$ (so that the discreteness of the spectrum remains resolved)? We will show that the distribution crosses over to an exponential, but in a highly nonuniform way.

Consider arbitrary γ and $k_B T$, both $\ll \Delta$. The Cutler–Mott formula (1) is dominated by two contributions, one from a peak in df/dE of width $k_B T$ around E_F and one from a peak in $G(E)$ of width γ_0 around E_0. Here γ_0 and E_0 are the width and position of the level closest to E_F. If $|E_F - E_0| \gg \max(k_B T, \gamma_0)$, the two peaks do not overlap and one can estimate the thermopower as

$$S = \frac{1}{eT}\left[\frac{\pi\gamma_0 (k_B T)^2}{3(E_F - E_0)^3} + \frac{E_F - E_0}{k_B T} e^{-|E_F - E_0|/k_B T}\right]\left[\frac{\gamma_0}{2\pi(E_F - E_0)^2} + \frac{1}{k_B T} e^{-|E_F - E_0|/k_B T}\right]^{-1}. \tag{11}$$

If $k_B T \ll \gamma_0$, the first terms in the numerator and denominator dominate over the second terms. This is the regime that the Lorentzian distribution (9) holds for all S.

We now turn to the regime $k_B T > \gamma_0$. The first terms dominate if $|E_F - E_0| \gg k_B T \ln k_B T/\gamma_0$. Hence $P(S)$ is a Lorentzian for $|S| \ll (k_B/e)(\ln k_B T/\gamma_0)^{-1}$. The logarithm of $k_B T/\gamma_0$ can be quite large, because the width of the levels is exponentially small in the system size, $\gamma \sim e^{-L/\xi}$. The Lorentzian persists in an

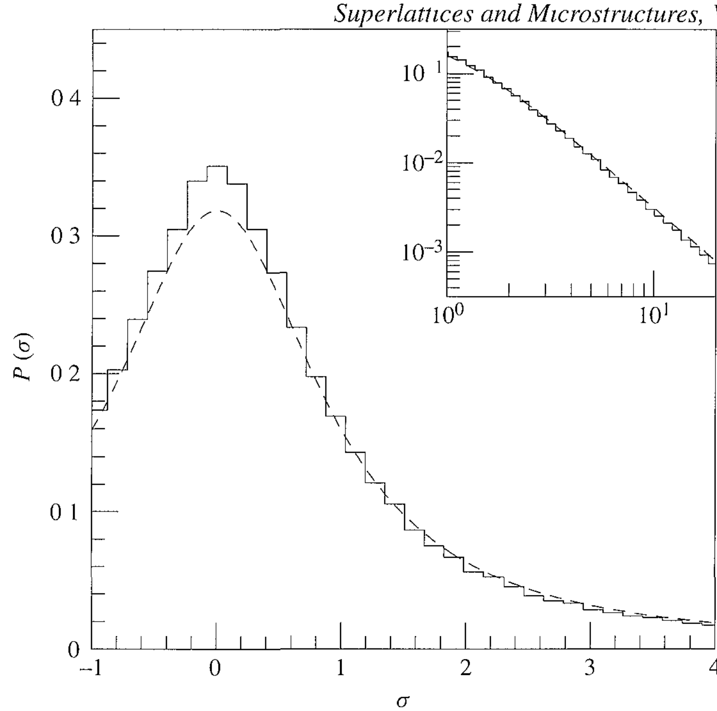

Fig. 1. Distribution of the dimensionless thermopower $\sigma = (\Delta/2\pi)d \ln T(E)/dE$ for a one dimensional wire in the localized regime The histogram is obtained from a numerical simulation for a sample length $L = 32\ 3\ \xi$ The dashed curve is the Lorentzian (9) being the analytical result for $L \gg \xi$ The inset shows the algebraic tail of the distribution on a logarithmic scale The thermopower S in the zero temperature limit is related to σ by $S = -(2\pi^3/3)(k_B^2 T/e\Delta)\sigma$

interval larger than its width, provided $k_B T < \Delta(\ln k_B T/\gamma_0)^{-1}$ The second terms in eqn (11) dominate if $k_B T \ll |E_F - E_0| \ll k_B T \ln k_B T/\gamma_0$ In this case the thermopower is simply $S = (E_F - E_0)/eT$, with exponential distribution

$$P(S) = \frac{eT}{\Delta} e^{\ 2|S|eT/\Delta} \tag{12}$$

The distribution (12) follows because the energy levels are uncorrelated, so that the spacing $|E_F - E_0|$ has an exponential distribution with a mean of $\Delta/2$

We conclude that the thermopower distribution for $\gamma < k_B T \ll \Delta$ contains both Lorentzian and exponential contributions The peak region $|S| \ll (k_B/e)\,(\ln k_B T/\gamma)^{-1}$ is the Lorentzian (9) The intermediate region $(k_B/e)\,(\ln k_B T/\gamma)^{-1} \ll |S| \ll (k_B/e) \ln k_B T/\gamma$ is the exponential (12) The far tails $|S| \gg (k_B/e) \ln k_B T/\gamma$ cannot be explained by eqn (11) With increasing temperature, the Lorentzian peak region shrinks, and ultimately the exponential region starts right at $S = 0$ This applies to the temperature range $\Delta\,(\ln k_B T/\gamma)^{-1} < k_B T \ll \Delta$

To illustrate these various regimes, we computed $P(S)$ numerically from eqn (1) We took the density of states

$$\rho(E) = L^{-1} \sum_i \frac{\gamma_i/2\pi}{(E - E_i)^2 + \gamma_i^2/4}, \tag{13}$$

so that the conductance according to eqn (5) has the energy dependence

$$G(E) \propto \prod_i \left[(E - E_i)^2 + \gamma_i^2/4\right]^{-1} \tag{14}$$

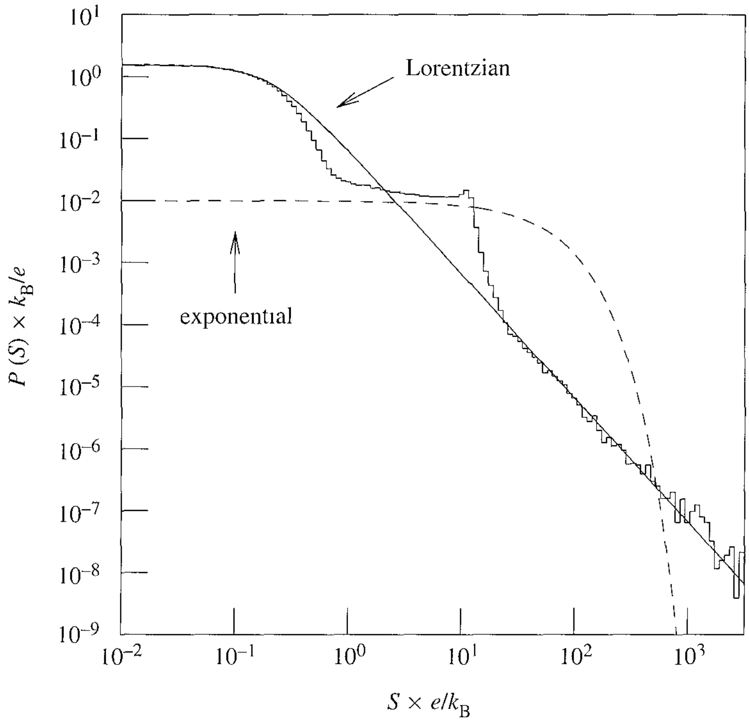

Fig. 2. Thermopower distribution of a one-dimensional wire in the localized regime at finite temperature The histogram is obtained from eqns (1) and (14), by numerical integration for a set of randomly chosen energy levels E_i, all having the same width $\gamma_i = \gamma = 10^{-6}\Delta$ The temperature is $k_BT/\Delta = 0.01$, such that $\gamma \ll k_BT \ll \Delta$ The distribution follows the Lorentzian (9) (solid curve) for small and large S, but it follows the exponential (12) (dashed curve) in an intermediate region

The levels E_i were chosen uniformly and independently (mean spacing Δ), but the fluctuations of the widths γ_i were ignored ($\gamma_i \equiv \gamma$ for all i). Such fluctuations are irrelevant in the low-temperature limit $k_BT \ll \gamma$, but not for $\gamma < k_BT \ll \Delta$. We believe that ignoring fluctuations in γ_i should still be a reasonable approximation, because γ_0 appears only in logarithms. The resulting $P(S)$ is plotted in Fig. 2. We see the expected crossover from a Lorentzian to an exponential. The exponential region appears as a plateau. Beyond the exponential region, the distribution appears to return to the Lorentzian form. We have no explanation for this far tail.

3. Chaotic quantum dot

In this section we consider a chaotic quantum dot with single-channel ballistic point contacts (see Fig. 3, inset). Because there are no tunnel barriers in the point contacts, the effects of the Coulomb blockade are small and here we ignore them altogether. For this system, the distribution of dT/dE was computed recently from random-matrix theory [8]. The energy derivative of the transmission probability has the parametrization

$$\frac{dT}{dE} = \frac{c}{\hbar}(\tau_1 - \tau_2)\sqrt{T(1-T)}, \tag{15}$$

with independent distributions

$$P(c) \propto (1-c^2)^{-1+\beta/2}, \qquad |c| < 1, \tag{16}$$

$$P(\tau_1, \tau_2) \propto |\tau_1 - \tau_2|^{\beta}(\tau_1\tau_2)^{-2(\beta+1)} e^{-(1/\tau_1 + 1/\tau_2)\pi\beta\hbar/\Delta}, \qquad \tau_1, \tau_2 > 0, \tag{17}$$

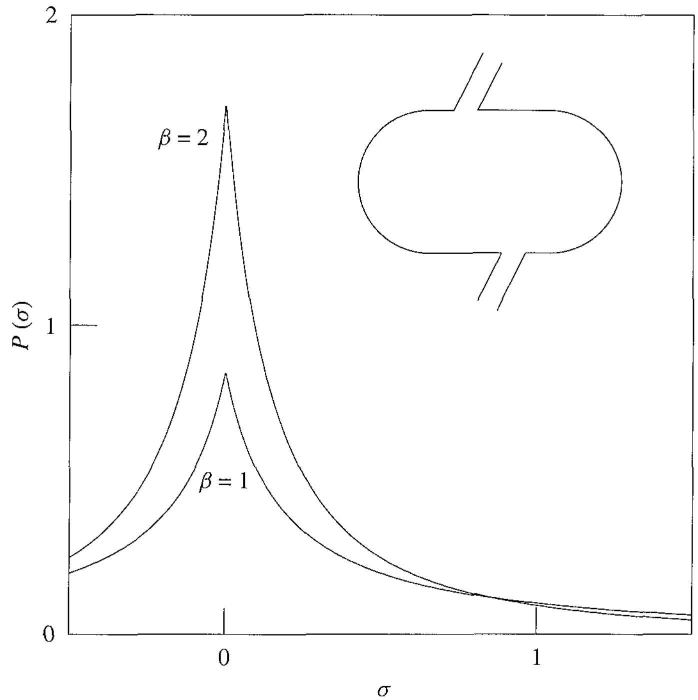

Fig. 3. Distribution of the dimensionless thermopower of a chaotic cavity with two single-channel ballistic point contacts (inset), computed from eqn (19) for the case of broken ($\beta = 2$) and unbroken ($\beta = 1$) time-reversal symmetry

$$P(T) \propto T^{-1+\beta/2}, \qquad 0 < T < 1. \tag{18}$$

The integer β equals 1 or 2, depending on whether time-reversal symmetry is present or not. The times τ_1, τ_2 are the eigenvalues of the Wigner–Smith time-delay matrix (see [8, 14]). Their sum $\tau_1 + \tau_2$ is the density of states (multiplied by $2\pi\hbar$). The thermopower distribution follows from

$$P(\sigma) \propto \int_{-1}^{1} dc\, P(c) \int_0^\infty d\tau_1 \int_0^\infty d\tau_2\, P(\tau_1, \tau_2) \int_0^1 dT\, P(T)$$
$$\times (\tau_1 + \tau_2)\delta\left(\sigma - (\Delta/2\pi\hbar)c(\tau_1 - \tau_2)\sqrt{1/T - 1}\right). \tag{19}$$

As in [8, 15], the density of states appears as a weight factor $\tau_1 + \tau_2$ in the ensemble average (19), because the ensemble is generated by uniformly varying the charge on the quantum dot rather than its Fermi energy. This is the correct thing to do in the Hartree (self-consistent potential) approximation. A more sophisticated treatment of the electron–electron interactions (as advocated in [16]) does not yet exist for this problem. The resulting distributions are plotted in Fig. 3. The curves have a cusp at $\sigma = 0$, and asymptotes $P(\sigma) \propto |\sigma|^{-1-\beta} \ln|\sigma|$ for $|\sigma| \gg 1$.

4. Conclusion

The results we have reported hold for single-channel conductors. The generalization to multi-channel conductors is of interest. Multi-channel diffusive conductors were studied in [3]. For a chaotic cavity with ballistic point contacts having a large number of modes (N modes per point contact), the distribution of the thermopower is Gaussian The mean is zero and the variance is

$$\operatorname{Var} S = \frac{k_B^4 T^2 \pi^6}{9e^2 N^4 \Delta^2 \beta} \tag{20}$$

(We have used the results of [17]) Analogously to universal conductance fluctuations, the variance of the thermopower is reduced by a factor of 2 upon breaking time-reversal symmetry ($\beta = 1 \rightarrow \beta = 2$)

For an N-mode wire in the localized regime, our derivation of the exponential distribution of the thermopower remains valid This is not true for the Lorentzian distribution The reason is that the Herbert–Jones–Thouless formula for $N > 1$ relates the density of states to the sum of the inverse localization lengths, [18] and there is no simple relation between this sum and the thermopower We expect that the tail of the distribution remains quadratic, $P(S) \propto S^{-2}$—because of the argument of Section 2 3, which is still valid for $N > 1$ It remains a challenge to determine analytically the entire thermopower distribution of a multi channel disordered wire

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