Temperature dependence of the kinetic coefficients of interference ballistic structures

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(Submitted 25 November 1997)
Zh. Éksp. Teor. Fiz. **114**, 1827–1835 (November 1998)

The effect of the temperature on the kinetic coefficients of a mesoscopic sample in contact with two electron reservoirs is considered for the case in which the electron transmission coefficient of the sample undergoes oscillations near the Fermi energy. © *1998 American Institute of Physics.* [S1063-7761(98)02011-3]

1. INTRODUCTION

One of the important properties of mesoscopic systems[1] at low temperatures is the preservation of phase coherence during propagation of electrons. Therefore, in such systems it is possible to observe effects that are sensitive to the phase of the electron wave function. As an example, we consider the Aharonov–Bohm effect,[2] which leads to oscillations with period $\Phi_0=h/e$ of the physical characteristics of nonsuperconducting doubly-connected samples immersed in a magnetic flux Φ (Refs. 3 and 4). This effect is observed in both the kinetic[5] and thermodynamic[6] properties of the samples.

The creation of structures in which electrons propagate ballistically has made it possible to imagine a number of devices based on the phenomenon of interference.[7–12] A peculiarity of such interference ballistic structures is the fact that the electron transmission coefficient $g(\varepsilon)$ of these structures varies substantially, $\Delta g \simeq g$, in response to an insignificant change in the energy $\Delta\varepsilon/\varepsilon \simeq \lambda/L$ (λ is the electron wavelength, L is the characteristic length of the device).

This fact is important in any consideration of electron and heat transport in an interference ballistic structure in contact with electron reservoirs. On the one hand, in the given case the range of temperature T and voltage V over which the linear-response approximation is valid is substantially narrowed: $\Delta T,\ V \ll \varepsilon_F \lambda_F/L$, where ε_F is the Fermi energy and λ_F is the wavelength of a Fermi electron. On the other hand, in such a system the electron thermal voltage coefficient should be significant.[13] This leads, in particular, to a violation of the Wiedemann–Franz law despite the fact that an interference ballistic structure is a purely elastic scatterer.

Transport phenomena in mesoscopic samples in contact with electron reservoirs at $T \neq 0$ are examined in Refs. 13 and 14, which consider both particle transport between electron reservoirs and electron transport only through a mesoscopic structure. In the first case, the calculation of the current (heat flux) takes into account both the resistance of the mesoscopic sample itself and the additional contact resistance (spreading resistance) between the leads and the electron reservoirs.[13,15] In the present paper, we consider only the first case (transport between electron reservoirs) as it more closely corresponds to the standard experimental situation (two-probe measurements). The feasibility of measuring the transport coefficients associated with the mesoscopic sample itself is discussed in Refs. 13 and 14.

We apply the results of Refs. 13 and 14 to the case in which the electron transmission coefficient $g(\varepsilon)$ of the mesoscopic sample oscillates as ε varies near the Fermi energy. In Sec. 2 we obtain an expression for the current I and heat flux Q at nonzero reservoir temperatures, with allowance for the oscillating nature of the dependence $g(\varepsilon)$. Section 3 considers the linear response regime. Section 4 derives expressions for I and Q for a large temperature difference between the reservoirs. Section 5 considers a one-dimensional ring enclosing magnetic flux Φ in terms of an interference ballistic structure, and shows that the presence of this flux can substantially alter the temperature dependence of the transport coefficients.

2. STATEMENT OF THE PROBLEM AND BASIC RELATIONS

Let a ballistic mesoscopic sample be connected by ballistic leads to two electron reservoirs, ''L'' and ''R'', The size of the sample is assumed to be small in comparison with the phase coherence length $L_\varphi(T)$. We denote the temperatures and chemical potentials of the reservoirs respectively by T_L, μ_L and T_R, μ_R. In the present paper, we consider a one-dimensional sample and one-dimensional leads. Generalization to the case of several conducting subzones in the absence of channel mixing is trivial. With channel mixing taken into account such a generalization can be made according to the results of Refs. 13 and 15.

Expressions for the current I and dissipative heat loss Q between electron reservoirs in the single-channel approximation have the form

$$I=\frac{2e}{h}\int d\varepsilon\, g(\varepsilon)\left[f_0\left(\frac{\varepsilon-\mu_L+e\varphi}{T_L}\right)-f_0\left(\frac{\varepsilon-\mu_R+e\varphi}{T_R}\right)\right], \quad (1)$$

$$Q=\frac{2}{h}\int d\varepsilon\, g(\varepsilon)\left[(\varepsilon-\mu_L+e\varphi)f_0\left(\frac{\varepsilon-\mu_L+e\varphi}{T_L}\right)\right.$$
$$\left.-(\varepsilon-\mu_R+e\varphi)f_0\left(\frac{\varepsilon-\mu_R+e\varphi}{T_R}\right)\right]. \quad (2)$$

Here $g(\varepsilon)$ is the electron transmission coefficient of the mesoscopic sample as a function of electron energy ε, $f_0(x)=(1+e^x)^{-1}$ is the Fermi distribution function, φ is the potential of the sample relative to the electron reservoirs. The quantity φ should be determined self-consistently from the Poisson equation.[16–18]

Below we assume that the energy dependence of the transmission coefficient, $g(\varepsilon)$, derives from interference processes. Therefore, the transmission coefficient is an oscillating function of electron wavelength $\lambda = 2\pi/k$. We write

$$g(\varepsilon) = \overline{g} + \sum_n g_n, \tag{3}$$

$$g_n = A_n \cos(nkL) + B_n \sin(nkL).$$

Here $\overline{g}$ is the mean transmission coefficient, $\varepsilon = (\hbar k)^2/2m^*$, and m^* is the effective mass of the electron. If

$$L \gg \lambda_F, \tag{4}$$

then near the Fermi energy the quantity $g(\varepsilon)$ can accurately be assumed to be an oscillating function of the electron energy. Substituting the expansion (3) into expressions (1) and (2) in this case and assuming that

$$T_L \ll \mu_L,\ T_R \ll \mu_R, \quad \Delta\mu = \mu_R - \mu_L \ll \mu_L, \mu_R, \tag{5}$$

we obtain

$$I = -\frac{2e}{h}\left\{ \overline{g}\Delta\mu + \pi^2 T^{*2} \sum_n \frac{1}{n} (\psi_n(T_L)\partial_\varepsilon g_n|_{\mu_L - e\varphi} - \psi_n(T_R)\partial_\varepsilon g_n|_{\mu_R - e\varphi}) \right\}, \tag{6}$$

$$Q = \frac{2\pi^2}{h}\left\{ \overline{g}\frac{T_L^2 - T_R^2}{6} + T^{*2}\sum_n \frac{\Delta\mu}{n}(\psi_n(T_L)\partial_\varepsilon g_n|_{\mu_L - e\varphi} + \psi_n(T_R)\partial_\varepsilon g_n|_{\mu_R - e\varphi}) + T^{*2}\sum_n \left(\cosh\frac{nT_L}{T^*}\psi_n^2(T_L) g_n(\mu_L - e\varphi) - \cosh\frac{nT_R}{T^*}\psi_n^2(T_R) g_n(\mu_R - e\varphi) \right) \right\}. \tag{7}$$

Here $\psi_n(T) = (T/T^*)[\sinh(nT/T^*)]^{-1}$, $T^* = \Delta_F/2\pi^2$, $\Delta_F = 2\varepsilon_F\lambda_F/L$, and we use the notation $\partial_\varepsilon \equiv \partial/\partial\varepsilon$. The Fermi energy $\varepsilon_F = \mu - e\varphi_0$ is defined in equilibrium: $\mu = \mu_L = \mu_R, T = T_L = T_R$. The quantity $\Delta\mu$ is determined both by the difference of electrostatic potentials V applied to the electron reservoirs and the difference of chemical potentials of the electron reservoirs due to their temperature dependence. Note that the dependence $\mu(T)$ is absent for a two-dimensional reservoir.

Expressions (6) and (7) are central to the present work and will be used below to determine the temperature dependence of the kinetic coefficients. We assume that inelastic processes are absent in the sample, $L \ll L_\varphi(T)$, and that the effect of the temperature reduces merely to energy averaging of the transmission coefficients $g(\varepsilon)$ (3).

3. KINETIC COEFFICIENTS IN THE LINEAR REGIME

For small differences of the reservoir chemical potentials $\Delta\mu$ and temperatures $\Delta T = T_R - T_L$

$$\Delta\mu \ll \Delta_F, \quad \Delta T \ll \min(T, T^*), \tag{8}$$

where Δ_F is the distance between electron energy levels near the Fermi level, the expressions for the current I and heat flux Q can be represented in matrix form:[13]

$$\begin{pmatrix} I \\ Q \end{pmatrix} = -\begin{pmatrix} L_0 & L_1/T \\ L_1 & L_2/T \end{pmatrix}\begin{pmatrix} \Delta\mu/e \\ \Delta T \end{pmatrix}. \tag{9}$$

In the present paper, we consider kinetic coefficients describing charge and energy transport between the electron reservoirs. For this case, as emphasized in Ref. 13, the Onsager relations are satisfied, as reflected in Eq. (9).

Expressions for the kinetic coefficients L_i can be obtained from expressions (6) and (7). The temperature T^* divides the low-temperature from the high-temperature range; in the former, the effect of the temperature can be neglected, while in the latter, averaging over energy leads to compensation of the interference contributions to the transmission coefficient, as a result of which $g(\varepsilon) \simeq \overline{g}$.

We now write out asymptotic expressions for the coefficients L_i.

1) Low temperatures: $T \ll T^*$,

$$L_0 = \frac{2e^2}{h} g(\varepsilon_F), \tag{10a}$$

$$L_1 = \frac{2e\pi^2}{3h} T^2 \partial_\varepsilon g|_{\varepsilon_F}, \tag{10b}$$

$$L_2 = \frac{2\pi^2}{3h} T^2 g(\varepsilon_F). \tag{10c}$$

2) High temperatures: $T \gg T^*$,

$$L_0 = \frac{2e^2}{h}\left[\overline{g} + \frac{2T}{T^*}\exp\left(-\frac{T}{T^*}\right) g_1(\varepsilon_F) \right], \tag{11a}$$

$$L_1 = \frac{4e\pi^2}{h} T^2 \exp\left(-\frac{T}{T^*}\right)\partial_\varepsilon g_1|_{\varepsilon_F}, \tag{11b}$$

$$L_2 = \frac{2e^2}{3h} T^2 \left[\overline{g} - \frac{6T}{T^*}\exp\left(-\frac{T}{T^*}\right) g_1(\varepsilon_F) \right]. \tag{11c}$$

We also write out expressions for the electron thermal voltage coefficient $\alpha = -\Delta\mu/e\Delta T$ and the thermal conductivity $\kappa = -Q/\Delta T$, which are measured at $I = 0$:

1) $T \ll T^*$,

$$\alpha = \frac{\pi^2}{3e} T \partial_\varepsilon \ln(g)|_{\varepsilon_F}, \tag{12a}$$

$$\kappa = \frac{2\pi^2}{3h} T g(\varepsilon_F)\left[1 - \frac{3(e\alpha)^2}{\pi^2} \right]. \tag{12b}$$

2) $T \gg T^*$,

$$\alpha = \frac{\pi^2}{e} T^* (\overline{g})^{-1} \partial_\varepsilon g_1|_{\varepsilon_F}, \tag{13a}$$

$$\kappa = \frac{2\pi^2}{3h} T \left[\overline{g} - \frac{6T}{T^*}\exp\left(-\frac{T}{T^*}\right) g_1(\varepsilon_F) \right]. \tag{13b}$$

Expressions (10), obtained in Ref. 13, and expressions (12) have the usual form for the theory of metals (see, e.g., Ref. 19). However, in contrast to normal metals, for which $e\alpha_0 \simeq T/\varepsilon_F$ (without allowance for phonon entrainment), in the case under consideration the electron thermal voltage is not small: $\alpha/\alpha_0 \simeq \varepsilon_F/T^* \gg 1$. This leads, in particular, to a breakdown of the Wiedemann–Franz law:

$$\frac{3e^3}{\pi^2}\frac{\kappa}{GT}=\begin{cases}1-3(e\alpha)^2/\pi^2, & T\ll T^*,\\ 1-\dfrac{8T}{T^*}\exp\left(-\dfrac{T}{T^*}\right)\dfrac{g_1(\varepsilon_F)}{\overline{g}}, & T\gg T^*.\end{cases} \tag{14}$$

Here $G=L_0$ is the conductance of the system. The greatest deviation should be observed for $T\simeq T^*$; it decreases at both lower and higher temperatures. We emphasize that in the present work we derive the deviation from the Aharonov–Bohm law for the transport coefficients between the electron reservoirs, whereas in Refs. 13 and 14 such a deviation was derived for the coefficients associated with the mesoscopic sample itself.

Comparing expressions (12a) and (13a), we see that $\alpha(T)$ has a maximum (in absolute value) at $T\simeq T^*$. To order of magnitude, the maximum is $|e\alpha(T^*)|\simeq 1$. Note also that the sign of α can be different for $T\ll T^*$ and $T\gg T^*$.

The conductance G of the system and the thermal conductivity κ for $T\ll T^*$ depend on the Fermi energy ε_F, which in turn depends on the chemical potentials of the electron reservoirs. For $T\gg T^*$ the small interference terms in the conductance and the thermal conductivity exhibit such a dependence (see (11a) and (13b)).

4. CURRENT AND HEAT FLUX FOR A LARGE TEMPERATURE DIFFERENCE BETWEEN THE ELECTRON RESERVOIRS

We fix the temperature of one of the reservoirs, e.g., T_L, and consider the dependence of the current and heat flux in the system on the temperature of the second reservoir (T_R). As follows from Eq. (6), in the limit

$$T_R \gg T^* \tag{15}$$

the current I is independent of T_R. Moreover, if we write

$$Q=Q_0+\delta Q, \quad Q_0=\frac{\pi^2}{6e^2}\overline{g}(T_L^2-T_R^2), \tag{16}$$

then it follows from Eq. (7) that the interference term δQ in the heat flux under condition (15) is also independent of T_R.

Inasmuch as inelastic processes take place only in the reservoirs and not in the sample, temperature averaging of the contributions to the current (and heat flux Q) due to electrons propagating from the left reservoir to the right reservoir (with temperature T_L) and in the reverse direction (with temperature T_R) takes place independently, as is immediately clear from (6) and (7).

In what follows we set $\mu_L=\mu_R$. If condition (15) is met, the dependence on T_L of the thermoelectric current I_T and the interference term δQ in the heat flux have the following form:

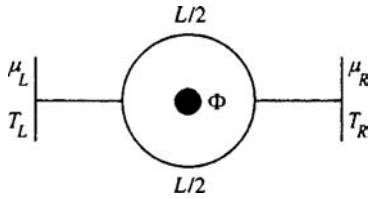

FIG. 1. Model of a one-dimensional ballistic ring of length L enclosing a magnetic flux Φ. The ring is connected by one-dimensional wires to two electron reservoirs at temperatures T_L and T_R and chemical potentials μ_L and μ_R.

1) $T_L \ll T^*$,

$$I_T=\frac{2e}{h}\int_{\varepsilon_0}^{\varepsilon_F} d\varepsilon[g(\varepsilon)-\overline{g}], \tag{17a}$$

$$\delta Q=\frac{2}{h}\int_{\varepsilon_0}^{\varepsilon_F} d\varepsilon(\varepsilon-\varepsilon_F)[g(\varepsilon)-\overline{g}]. \tag{17b}$$

Here $\varepsilon_0=\Delta_F[\varepsilon_F/\Delta_F]$ ($[x]$ is the integer part of x). In this regime, the thermoelectric current and the interference term in the heat flux are independent of the temperatures of the electron reservoirs T_L and T_R.

2) $T_L \gg T^*$, $T_R > T_L$,

$$I_T=-\frac{4e\pi^2}{h}T_L T^*\exp\left(-\frac{T_L}{T^*}\right)\partial_\varepsilon g_1|_{\varepsilon_F}, \tag{18a}$$

$$\delta Q=\frac{4\pi^2}{h}T_L^2\exp\left(-\frac{T_L}{T^*}\right)g_1(\varepsilon_F). \tag{18b}$$

Thus, the difference between the regime with a large temperature difference and the linear response regime ($\Delta T \ll T$) is that the thermoelectric current and the interference term in the heat flux are independent of the temperature of the hotter reservoir (T_R), and fail to vanisih in the limit $T_L \to 0$.

5. TEMPERATURE DEPENDENCE OF THE KINETIC COEFFICIENTS OF A ONE-DIMENSIONAL BALLISTIC RING WITH MAGNETIC FLUX

Consider a one-dimensional ballistic ring connected by one-dimensional leads to two electron reservoirs (Fig. 1). The ring encloses a magnetic flux Φ. The length of the ring L is assumed to be small in comparison with the phase coherence length: $L \ll L_\varphi$. Within the framework of quantum waveguide theory[20] in the approximation of noninteracting electrons, the transmission coefficient g for such a system for symmetrically located contacts is[20,21]

$$g=\frac{(1-\cos(kL))(1+\cos(2\pi\Phi/\Phi_0))}{(\cos(2\pi\Phi/\Phi_0)-1.25\cos(kL)+0.25)^2+\sin^2(kL)}. \tag{19}$$

The first two terms in expansion (3) have the form

$$\overline{g}=\frac{2(1+\cos(2\pi\Phi/\Phi_0))}{3+2\cos(2\pi\Phi/\Phi_0)}, \tag{20}$$

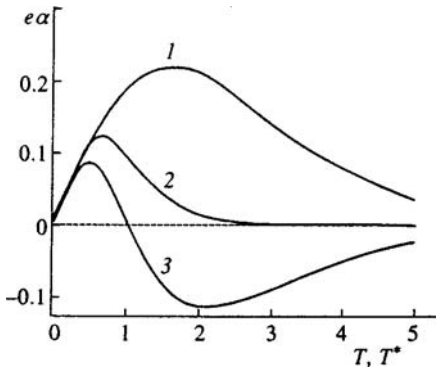

FIG. 2. Dependence of the thermoelectric coefficient α of a one-dimensional ring on the temperature T in the linear response regime ($\Delta T \ll T$) for $\Phi=0$ (*1*), Φ^* (*2*), and $0.15\Phi_0$ (*3*). $\{L/\lambda_F\}=0.75$.

$$g_1=\frac{2}{9}g\left(4\cos\left(\frac{2\pi\Phi}{\Phi_0}\right)-3\right)\cos(kL). \tag{21}$$

The kinetic coefficients of the system depend on the magnetic flux Φ, and this dependence can be manifested in a nontrivial way. We show this in the case of the thermoelectric coefficient α.

Figure 2 plots the dependence $\alpha(T)$ for three values of Φ and $\{L/\lambda_F\}=0.75$, where $\{x\}$ is the fractional part of x. The quantity α is governed by the transmission coefficient g for $T<T^*$ (see Eq. (12a)), and by its first harmonic g_1 for $T>T^*$ (see Eq. (13a)). The signs of the derivatives $\partial_\varepsilon g$ and $\partial_\varepsilon g_1$ depend on the magnetic flux Φ (and on the product k_FL). For some values of Φ these quantities have the same sign (Fig. 2, curve *1*) while for others their signs are different (Fig. 2, curve *3*). Therefore, by varying the magnetic flux Φ it is possible to go from a fixed-sign dependence of $\alpha(T)$ to a dependence that changes sign with increasing or decreasing temperature.

Furthermore, for $\Phi=\pm\Phi^*$ (where $\Phi^*/\Phi_0=(2\pi)^{-1}\arccos(3/4)\simeq 0.115$) the quantity g_1 (see Eq. (21)) governing the high-temperature ($T>T^*$) asymptotic limit of the thermoelectric coefficient α vanishes. Therefore, in expansion (6) it is necessary to retain the $n=2$ term. As a result, for $\Phi=\pm\Phi^*$ and $T>T^*$ we obtain

$$e\alpha\simeq\exp\left(-\frac{2T}{T^*}\right)\frac{2T}{T^*}\sin(2k_FL). \tag{22}$$

In the given case α falls off more rapidly with temperature (than for $\Phi\neq\pm\Phi^*$) (Fig. 2, curve *2*). Moreover, the temperature separating the low-temperature and high-temperature regions is reduced by a factor of two.

The interference terms in the conductance $G=L_0$ (see Eq. (11a)) and the thermal conductivity κ (see Eq. (13b)) have an analogous dependence on Φ and T for $T>T^*$. Specifically, they change sign with varying Φ; moreover, their magnitude falls off exponentially with increasing temperature, with a characteristic temperature of $T^*/2$ for $\Phi=\pm\Phi^*$ and T^* for other values of magnetic flux Φ.

For $\Phi\neq 0$ the conductance of the ring (19) vanishes near integer values of the ratio $k_FL/2\pi=L/\lambda_F$. Therefore, near these values the thermoelectric coefficient α has a significant value (at low temperatures). It can be seen from Fig. 3 that as the ratio L/λ_F approaches an integer, the peak in the dependence $\alpha(T)$ becomes sharper and shifts toward lower temperatures. Note that when we make the substitution $\{L/\lambda_F\}\to 1-\{L/\lambda_F\}$ the thermoelectric coefficient changes sign.

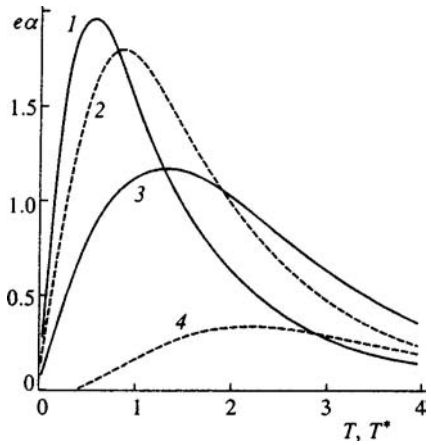

FIG. 3. Dependence of the thermoelectric coefficient α of a one-dimensional ring on the temperature T in the linear response regime ($\Delta T \ll T$) for $\{L/\lambda_F\}=0.05$ (*1*), 0.1 (*2*), 0.2 (*3*), and 0.4 (*4*). $\Phi=0.3\Phi_0$.

6. CONCLUSION

In the present paper we have considered the effect of the temperature on the kinetic coefficients of a mesoscopic sample in contact with two electron reservoirs. Charge and energy transport are described by the electron transmission coefficient $g(\varepsilon)$ of the sample. It is assumed that inelastic processes are absent in the sample and that the effect of temperature T reduces simply to energy averaging of the electron transmission coefficient g in a neighborhood $\Delta\varepsilon\simeq T$ about ε_F. Expressions have been obtained for the current I (6) and dissipative heat flux Q (7) which take account of oscillations in g near ε_F. Such oscillations are characteristic of ballistic mesoscopic systems in which interference has a substantial influence on the transmission of an electron wave.[7–12] Note that in contrast to the Sommerfeld expansion customarily used in the theory of normal metals, which takes account of variations of physical quantities of the system on a scale ε_F (or more precisely, on a scale $\Delta\varepsilon \gg T$), the expansion proposed here takes account of variation of physical characteristics of the system near ε_F in the energy range $\Delta\varepsilon\ll T,\varepsilon_F$.

We have shown that the thermoelectric coefficient α significantly exceeds the value α_0 characteristic of ordinary metals (without allowance for phonon entrainment and in the absence of magnetic impurities), $\alpha\simeq\alpha_0\varepsilon_F/T^*$, which is due to oscillations in the electron transmission coefficient near ε_F (Ref. 13). We have calculated the dependence $\alpha(T)$. In the linear regime ($\Delta T\ll T^*,T$) the dependence $\alpha(T)$ has a maximum (in absolute value) at $T\simeq T^*$. Note that the sign of α can be different for $T<T^*$ and for $T>T^*$. At high temperatures ($T>T^*$) the thermoelectric coefficient falls exponentially with temperature, $\alpha\propto\exp(-2\pi^2T/\Delta_F)$, and this dependence can be used to determine Δ_F. It should be noted

that the present work treats the one-channel approximation. For a multichannel sample without channel mixing, the high-temperature asymptotic limit of the dependence $\alpha(T)$ has a form analogous to that of the dependence $\Delta_F = \max(\Delta_F(n))$, where n is the channel number.

In the case of the Aharonov–Bohm effect for doubly-connected, one-dimensional samples, we predict a nontrivial dependence of the thermoelectric coefficient and the interference terms in the conductance and the thermal conductivity at high temperatures ($T > T^*$) on the temperature and magnetic flux.

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Translated by Paul F. Schippnick