# Thermal Conductivity and Lorenz Number for One-Dimensional Ballistic Transport

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We study the thermal conductivity and Lorenz number of charge carriers for one-dimensional ballistic transport within the correlation function formalism. The carrier transit time between two ideal contacts is found to substitute for the collision time in the definition of a ballistic thermal conductivity. A universal thermal conductance $K = 2\pi^2 k_B^2 T/3h$ is naturally obtained for the degenerate case. Dispersion curves for the thermal conductivity and the Lorenz number associated with different time scales belonging to the microscopic system are given for the first time. [S0031-9007(97)02335-1]

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One-dimensional structures offer a fascinating scenario to look for fundamental physics as well as to develop innovative devices. As important achievements in this field we recall the fundamental unity of electrical conductance, the quantum and fractional Hall effect, the universal conductance fluctuations, etc. [1]. In this respect, thermal conductivity of charge carriers has been recently studied for a variety of systems in an attempt to investigate its properties and analogies with the electrical conductivity [2–5]. In particular, in a seminal experiment of the Philips group [6], the thermoelectrical properties of a quantum point contact have been interpreted as experimental evidence for the Wiedemann-Franz law to hold.

The aim of this Letter is to present a first principle calculation of thermal conductivity and Lorenz number for one-dimensional ballistic transport thus providing the fundamental properties of this physical quantity. The generality of the theoretical approach enables us to investigate continuously the transition from nondegenerate to completely degenerate conditions and recover well known results under the diffusive regime, when transport is controlled by scattering of carriers with lattice imperfections.

In the linear response regime, the fluxes are connected to the externally applied fields by the kinetic (or Kelvin-Onsager) coefficients $L_{\mu\nu}$ according to

$$\mathbf{j}_\mu = \sum_\nu L_{\mu\nu}\mathbf{X}_\nu\,, \tag{1}$$

where $\mu, \nu = 1, 2$, while $\mathbf{j}_1$ and $\mathbf{j}_2$ denote the electrical current and the heat-flux densities, respectively, and $\mathbf{X}_1$ and $\mathbf{X}_2$ the electric field and temperature gradient, respectively. As a consequence of the fluctuation-dissipation theorem [7] the linear responses to a weak external disturbance can be derived from the spectral properties of fluctuations. Those are given in the following by the symmetrized correlation function in thermal equilibrium

$$C_{\mu\nu}(t) = \tfrac{1}{2}\langle J_\mu(0)J_\nu(t) + J_\nu(0)J_\mu(t)\rangle\,, \tag{2}$$

where $J_\nu$ and $J_\mu$ denote the operators of the respective observed quantities, and $\langle\cdots\rangle$ indicate their expectation (or quantum mechanically averaged) value. In the ballistic regime the theory may be extended to the nonequilibrium case according to [8], while with collisions it depends on the details of the scattering processes as shown for the nondegenerate regime in [5].

We apply the above relations to a one-dimensional conductor of active length $L$ limited in the $z$ direction by ideal contacts (i.e., completely absorbing and thermalizing). Following a Wigner function formalism [9] the general correlation functions (2) are found to be

$$C_{\mu\nu}(t) = \frac{1}{\pi}\left(\frac{e\hbar}{mL}\right)^2\left(\frac{\hbar^2}{2me}\right)^{(\mu+\nu-2)} e^{-t/\tau_c} \times \int_{-L/2}^{L/2} dz \int_{k^-}^{k^+} k^{2(\mu+\nu-1)} f_0(1 - f_0)\, dk\,, \tag{3}$$

where $e$ is the electron charge, $\hbar$ the reduced Planck constant, $m$ the carrier effective mass, $\tau_c$ the average scattering time describing the diffusive regime, $k$ the wave vector, and $f_0$ the Fermi distribution. The integration limits for the $k$ integration are

$$k^\pm = \frac{m}{\hbar t}\left(\pm\frac{L}{2} - z\right). \tag{4}$$

Equation (3) describes the continuous transition from a ballistic [i.e., $\exp(-t/\tau_c) = 1$] to a diffusive regime [i.e., $C_{\mu\nu}(t) \sim \exp(-t/\tau_c)$]. The normalized correlation functions for the ballistic case calculated numerically according to Eq. (3) are reported in Fig. 1. In the degenerate case, the decay of the correlations is found to

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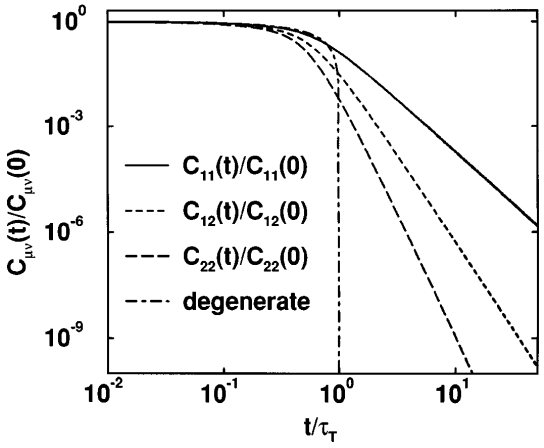


FIG. 1. Correlation functions for the nondegenerate and degenerate ballistic cases.

be linear for all $\mu$ and $\nu$. This is because, due to the Pauli principle, only carriers at the Fermi energy and thus with the same transit time contribute to (3). On the contrary, in the nondegenerate case the correlation functions exhibit different time decays because of the different weighting with the exponents $\mu$ and $\nu$. As can be easily verified, in the long time limit the correlation functions decay as $t^{-2(\mu+\nu)+1}$, which is in accordance with the results given in [10].

The dynamic coefficients $L_{\mu\nu}(\omega)$ are now calculated by means of the Fourier-Laplace transforms $S_{\mu\nu}(\omega)$ of the respective correlation functions $C_{\mu\nu}(t)$ from [11]:

$$L_{\mu\nu}(\omega) = \frac{LS_{\mu\nu}(\omega)}{k_B T}, \tag{5}$$

where $k_B$ is the Boltzmann constant and $T$ the absolute temperature. Performing first the integrations over space and time analytically, and then transforming the remaining integration in $k$ to an integration over the energy variable $E$, we get $S_{\mu\nu}(\omega)$ in the compact form:

$$S_{\mu\nu}(\omega) = \frac{2^{3/2} e^{4-\mu-\nu}}{\pi L \hbar m^{1/2}} \int_0^\infty dE\, E^{\mu+\nu-3/2} f_0(1 - f_0) \times \Gamma(\omega)\left[1 - \frac{\Gamma(\omega)}{\tau(E)}(1 - e^{-\tau(E)/\Gamma(\omega)})\right]. \tag{6}$$

Here $\tau(E) = L\sqrt{m/2E}$ is the microscopic ballistic transit time of a carrier with kinetic energy $E$, and $\Gamma(\omega) = \tau_c/(1 + i\omega\tau_c)$ is the Lorentzian line-shape function. Equation (6) describes the continuous transition from a diffusive to a ballistic regime, the former and latter corresponding to the limits $\tau/\tau_c \to \infty$ and $\tau/\tau_c \to 0$, respectively, in the range of energies determined by the factor $f_0(1 - f_0)$. In the static (i.e., $\omega = 0$) and ballistic limit inserting the microscopic $\tau(E)$ Eq. (6) reads

$$S_{\mu\nu}(0) = \frac{2e^2}{h} \int_0^\infty dE \left(\frac{E}{e}\right)^{\mu+\nu-2} f_0(1 - f_0). \tag{7}$$

Equation (7), referring to the *ballistic* limit, is independent of the energy wave-vector dispersion and thus valid also for nonparabolic bands. By introducing $\tau_T$ as an average transit time, defined later, the static kinetic coefficients in the ballistic regime are given by the following equations. In the nondegenerate case

$$L_{11}^{\mathrm{ndg}} = \frac{e^2 n}{m} \tau_T^{\mathrm{ndg}}, \tag{8}$$

$$L_{22}^{\mathrm{ndg}} = \frac{2n(k_B T)^2}{m} \tau_T^{\mathrm{ndg}}, \tag{9}$$

$$L_{12}^{\mathrm{ndg}} = L_{21}^{\mathrm{ndg}} = \frac{enk_B T}{m} \tau_T^{\mathrm{ndg}}, \tag{10}$$

and, neglecting exponentially small terms of the order of $\exp(-E_F/k_B T)$, in the degenerate case

$$L_{11}^{\mathrm{deg}} = \frac{e^2 n}{2m} \tau_T^{\mathrm{deg}} = L\frac{2e^2}{h}, \tag{11}$$

$$L_{22}^{\mathrm{deg}} = \frac{n}{2m} \tau_T^{\mathrm{deg}} E_F^2 \left(1 + \frac{\pi^2}{3} \frac{(k_B T)^2}{E_F^2}\right), = L\frac{2}{h} E_F^2 \left(1 + \frac{\pi^2}{3} \frac{(k_B T)^2}{E_F^2}\right), \tag{12}$$

$$L_{12}^{\mathrm{deg}} = L_{21}^{\mathrm{deg}} = \frac{en}{2m} \tau_T^{\mathrm{deg}} E_F = L\frac{2e}{h} E_F. \tag{13}$$

In the above equations $n$ is the one-dimensional carrier concentration, $E_F = (\pi\hbar n)^2/8m$ the Fermi energy, and the average transit time $\tau_T$ is given by

$$\tau_T^{\mathrm{ndg}} = L\left(\frac{m}{2\pi k_B T}\right)^{1/2} = \frac{L}{v_{\mathrm{ndg}}}, \tag{14}$$

$$\tau_T^{\mathrm{deg}} = L\left(\frac{m}{2E_F}\right)^{1/2} = \frac{L}{v_{\mathrm{deg}}}, \tag{15}$$

where $v_{\mathrm{ndg}}$ and $v_{\mathrm{deg}}$ are the average velocity of carriers injected from the contacts pertaining to the nondegenerate and degenerate cases, respectively. The two cases are specified by $\delta = E_F/k_B T \ll -1$ for the nondegenerate case and $\delta \gg 1$ for the degenerate case.

The dynamic thermal conductivity $\kappa(\omega)$ calculated from the standard relation

$$\kappa(\omega) = \frac{L_{11}(\omega)L_{22}(\omega) - L_{12}(\omega)L_{21}(\omega)}{L_{11}(\omega)T} \tag{16}$$

exhibits in general a frequency dispersion, and for the static case is given by the following relations:

$$\kappa^{\mathrm{ball,ndg}} = \frac{nk_B^2 T}{m} \tau_T^{\mathrm{ndg}} = \frac{nLk_B^{3/2} T^{1/2}}{(2\pi m)^{1/2}}, \tag{17}$$

$$\kappa^{\mathrm{ball,deg}} = \frac{\pi^2}{6} \frac{nk_B^2 T}{m} \tau_T^{\mathrm{deg}} = \frac{2\pi^2}{3} \frac{Lk_B^2 T}{h} \tag{18}$$

for the nondegenerate and degenerate cases, respectively, where the right-hand side of (18) has accounted for the relation $4Lm/n\tau_T^{\mathrm{deg}} = h$. For completeness we report also the values of the diffusive regime which are given by

$$\kappa^{\mathrm{diff,ndg}} = \frac{3}{2} \frac{nk_B^2 T}{m} \tau_c, \tag{19}$$

$$\kappa^{\mathrm{diff,deg}} = \frac{\pi^2}{3}\frac{nk_B^2T}{m}\tau_c\,, \tag{20}$$

for the nondegenerate and degenerate cases, respectively.

Equations (17)–(20) evidence the similarity and differences of the thermal conductivity formulas for different transport regimes and degeneracy conditions. Accordingly, we notice that transit time takes the place of collision time in passing from diffusive to ballistic regimes while different numerical factors, of the order of unit, characterize different cases. Furthermore, one should note that the thermal conductance of the ballistic regime $K^{\mathrm{ball}} = \kappa^{\mathrm{ball}}/L$ is independent of the sample geometry and has the following interesting properties. In the nondegenerate case, for a given carrier concentration and effective mass, it is proportional to the square root of the absolute temperature. In the degenerate case, it takes the universal form

$$K^{\mathrm{ball,deg}} = \frac{2\pi^2}{3}\frac{k_B^2T}{h}\,, \tag{21}$$

the presence of the Planck constant being associated with full quantum conditions. In analogy with the quantized electrical conductance $G = 2e^2/h$, we expect that Eq. (20) represents a fundamental unit of thermal conductance at temperature $T$, associated with a single subband. This latter case confirms experimental findings on the observation of universal thermopower fluctuations [3] and thermoelectric power of point contacts [12], as well as recent studies in thermal transport properties of a Luttinger liquid [4]. We further point out that in the nondegenerate diffusive regime the numerical coefficient $3/2$ is the result of a scaling behavior as $(1 + D/2)$ with $D = 1, 2, 3$ the dimensionality of the system. In the degenerate case we find the standard $\pi^2/3$ numerical coefficient independently from the dimensionality. Note that this result is obtained for the single relaxation time approach used for the diffusive regime. In general we expect that, when the energy relaxation time scale is comparable with momentum relaxation, significant deviations should occur. The frequency dispersion of the thermal conductivity in the ballistic regime exhibits interesting spectra which deviate considerably from the Lorentzian line shape of the corresponding diffusive regime. These are reported in Figs. 2 and 3 for the nondegenerate and degenerate cases, respectively. In the nondegenerate case the structure at $\omega\tau_T \simeq 10$ in the real part of the thermal conductivity $\mathrm{Re}[\kappa(\omega)]$ originates from the long time tails of the associated correlation functions (see Fig. 1). A corresponding structure, even if strongly smoothed out, is also detectable in the imaginary part $\mathrm{Im}[\kappa(\omega)]$. In the degenerate case we recover the oscillatory behavior of $\mathrm{Re}[\kappa(\omega)]$ already found for the case of current noise spectral density in [13] and associated with the geometrical resonances coming from the triangular shape of the current correlation function. Again, a corresponding structure is detectable in the imaginary part $\mathrm{Im}[\kappa(\omega)]$.

By recalling that the electrical conductivity $\sigma(\omega)$ is given by $\sigma(\omega) = L_{11}(\omega)$, for the Lorenz number $L_0(\omega)$, here generalized to account for frequency dispersion as

$$L_0(\omega) = \frac{\kappa(\omega)}{\sigma(\omega)T}\,, \tag{22}$$

we get, in the static case

$$L_0^{\mathrm{ball,ndg}} = \frac{2}{3}L_0^{\mathrm{diff,ndg}} = \frac{k_B^2}{e^2}\,, \tag{23}$$

$$L_0^{\mathrm{ball,deg}} = L_0^{\mathrm{diff,deg}} = \frac{\pi^2}{3}\frac{k_B^2}{e^2}\,. \tag{24}$$

Equation (24) is rigorous at all frequencies for the ballistic regime, deriving from a unique decay of the degenerate correlation functions (see Fig. 1). Conversely, for the diffusive regime (24) is an approximation due to the assumption of an average scattering time. Thus, the robust property of the universal Lorenz number, pointed out in [2], actually does not seem to be fulfilled in general. Note that in the ballistic nondegenerate case the

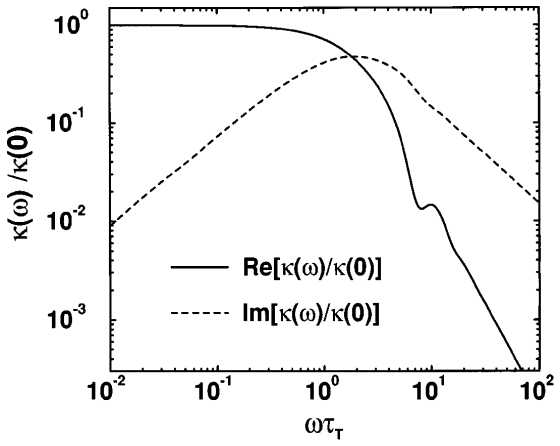


FIG. 2. Spectrally resolved thermal conductivity for the ballistic regime in the nondegenerate case. Continuous and dashed curves refer to the real and imaginary parts, respectively.

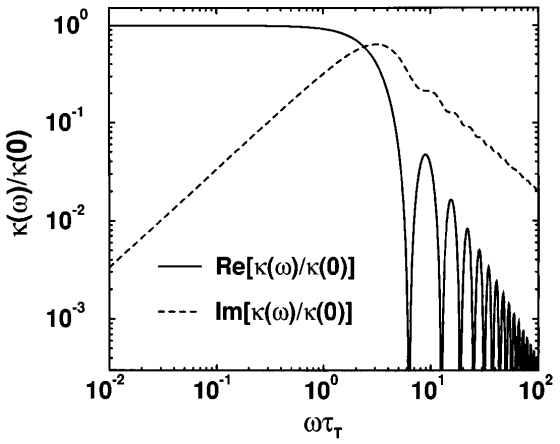


FIG. 3. Spectrally resolved thermal conductivity for the ballistic regime in the degenerate case. Continuous and dashed curves refer to the real and imaginary parts, respectively.

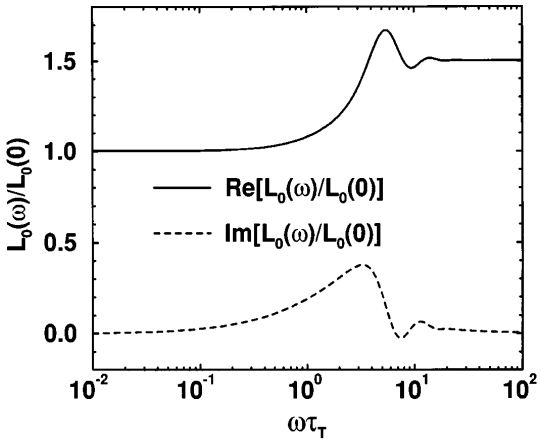


FIG. 4. Spectrally resolved Lorenz number for the ballistic regime in the nondegenerate case. Continuous and dashed curves refer to the real and imaginary parts, respectively.

Lorenz number exhibits a frequency dispersion because of the different long time tails exhibited by different correlation functions. This effect, whose behavior is shown in Fig. 4, is expected to be present whenever momentum and energy relaxation have comparable time scales.

In conclusion, a rigorous calculation of the thermal conductivity of charge carriers for one-dimensional ballistic transport has proven several fundamental properties of this quantity. Its formal definition looks similar to the diffusive regime provided the average transit time replaces the average collision time. For the degenerate ballistic regime, a single time scale for all correlation functions is found to be its universal property. This property leads to a fundamental unit of thermal conductance at the given temperature in agreement with experiments and to a Lorenz number without dispersion. For the nondegenerate ballistic regime long time tails of the correlation functions, decaying with increasing odd integer exponent, are found. As a consequence the Lorenz number exhibits a dispersion behavior which is recognized as a general property of this physical quantity.

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