STUDIA UBB PHYSICA, Vol. 66 (LXVI), 1-2, 2021, pp. 47-53
(RECOMMENDED CITATION)
doi:10.24193/subbphys.2021.05

LORENTZ NUMBER WITH PHENOMENOLOGICAL TRANSMISSION

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ABSTRACT. We analyzed the Lorentz number for thermoelectric phenomena in the case of electronic systems, using the Landauer-Büttiker method. For the transmission coefficient we will adopt two simple phenomenological forms, constant and linear. The case of graphene with a quadratic transmission is also analyzed.

Keywords: *Thermoelectric properties, Wiedemann-Franz law, Lorentz number, Transmission, Electrons, Graphene.*

Since their discovery thermoelectric effects [1, 2, 3] have attracted attention through their theoretical explanation and many applications. At a given temperature T, in common conductors, the ratio between the heat conductance and the product temperature-electrical conductance is constant and equal to the Lorentz number $\mathcal{L}$. This result is a consequence of the fact that both charge and heat are carried by the same particles [4, 5], and this ratio is called the Wiedemann-Franz law [6]. Deviations from the Wiedemann-Franz law indicate departures from the Fermi liquid behavior [7]. In mesoscopic systems, Coulomb interaction and charge quantization can also lead to departures from the Wiedemann-Franz law [8, 9]. The importance of the Wiedemann-Franz ratio lies in the fact that the figure of merit for thermoelectric conversion ZT is directly proportional to the inverse of this ratio. In this respect it is desirable to maximize the charge flow and to minimize that of heat. The thermoelectric response of nanostructures has increased the interest in this research area [10, 11]. Recently, the thermoelectric transport properties in graphene connected molecular junctions and in interacting quantum dots in graphene were studied in Refs. [12, 13]. The effect of magnetic field on thermoelectric properties of monolayer graphene was analyzed in [14].

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In this paper we will calculate the Lorentz number taking into account the electronic system and for two simple phenomenological forms of the transmission factor (constant and linear). Then we will discuss the Lorentz number for the case of graphene with a quadratic transmission. The obtained results can be useful in order to find out the efficiency of thermoelectric conversion.

The Wiedemann-Franz law states that the ratio between electronic thermal conductivity (K_{el}) and electrical conductivity (σ) is proportional to temperature:

$$\frac{K_{el}}{\sigma} = \mathcal{L}\,\mathrm{T} \tag{1}$$

where $\mathcal{L}$ is the Lorentz number. In the case of an ideal Fermi gas, $\beta\mu \gg 1$ ($\beta = 1/k_B T$, k_B - the Boltzmann constant, and μ is the chemical potential), the Lorentz number is:

$$\mathcal{L}_0 = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 \tag{2}$$

e – is the electron charge. For mesoscopic systems, in the presence of leads, using the Landauer-Büttiker formalism, one can express the Lorentz number through the energy dependent transmission $T(\varepsilon)$ by the following formula:

$$\mathcal{L} = \frac{K_{el}}{\sigma T} = \frac{L_0 L_2 - L_1^2}{e^2 T L_0^2} \tag{3}$$

where:

$$L_n = \frac{g}{h}\int d\varepsilon\ T(\varepsilon)\left(-\frac{\partial f}{\partial \varepsilon}\right)(\varepsilon - \mu)^n \tag{4}$$

with n= 0, 1, 2. Here g is the degeneracy (for classical Fermi gas $g=g_s=2$, and for graphene $g=g_s g_v=2\mathrm{x}2=4$, where g_s and g_v are the spin and valley degeneracies), and $f(\varepsilon)$ is the Fermi-Dirac distribution function. Using:

$$f(\varepsilon) = \frac{1}{2}\left[1 - \tanh\frac{\beta(\varepsilon - \mu)}{2}\right] \tag{5}$$

we obtain:

$$L_n = \frac{g\beta}{4h}\int d\varepsilon\, T(\varepsilon)\ \frac{(\varepsilon-\mu)^n}{\left(\cosh\left[\frac{\beta(\varepsilon-\mu)}{2}\right]\right)^2} \tag{6}$$

where h is the Planck constant. In the following we will analyze the Lorentz number, using several simple forms for the transmission.

Case 1: Electronic system with $T(\varepsilon)=T_0$=const.

In this case:

$$L_0 = \frac{g\beta T_0}{4h}\int_0^\infty d\varepsilon\ \frac{1}{\left(\cosh\left[\frac{\beta(\varepsilon-\mu)}{2}\right]\right)^2} = \frac{gT_0}{2h}\left[1 + \tanh\left(\frac{\beta\mu}{2}\right)\right] \tag{7}$$

When βμ≫ 1 (low temperatures):

$$L_0 \cong \frac{gT_0}{h} \tag{8}$$

Then:

$$L_1 = \frac{g\beta T_0}{4h}\int_0^\infty d\varepsilon\ \frac{\varepsilon - \mu}{\left(\cosh\left[\frac{\beta(\varepsilon-\mu)}{2}\right]\right)^2} \tag{9}$$

or:

$$L_1 = \frac{gT_0}{\beta h}\left\{ln\left[2\cosh\left(\frac{\beta\mu}{2}\right)\right] - \frac{\beta\mu}{2}\tanh\left(\frac{\beta\mu}{2}\right)\right\} \tag{10}$$

which, for βμ≫ 1, reduces to:

$$L_1 \cong \frac{gT_0\mu}{h}\ e^{-\beta\mu} \to 0 \tag{11}$$

Finally, L_2 is:

$$L_2 = \frac{g\beta T_0}{4h}\int_0^\infty d\varepsilon\ \frac{(\varepsilon - \mu)^2}{\left(\cosh\left[\frac{\beta(\varepsilon-\mu)}{2}\right]\right)^2} \tag{12}$$

After integration we obtain:

$$L_2 = \frac{2gT_0}{h\beta^2}\left\{\frac{\pi^2}{6} + polylog\left(2, -e^{-\beta\mu}\right) - \beta\mu\ ln\left[2\cosh\left(\frac{\beta\mu}{2}\right)\right] + \left(\frac{\beta\mu}{2}\right)^2\left[1 + \tanh\left(\frac{\beta\mu}{2}\right)\right]\right\} \tag{13}$$

where *polylog(n,y)* is the polylogarithmic function. In the low temperatures limit, βμ≫ 1, L_2 becomes:

$$L_2 \cong \frac{2\pi^2 gT_0}{6h\beta^2} \tag{14}$$

Having these results, and in the low temperatures limit, we obtain for the Lorentz number:

$$\mathcal{L} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 \equiv \mathcal{L}_0 \tag{15}$$

Now we will consider the opposite limit when βμ≪ 1. This case correspond to high temperatures or to low electron concentration. In this case we have the following approximations:

$$L_0 \cong \frac{gT_0}{2h}\left[1+\frac{\beta\mu}{2}\right] \tag{16}$$

$$L_1 \cong \frac{gT_0 \ln 2}{\beta h}\left[1-\frac{(\beta\mu)^2}{8\ln 2}\right] \tag{17}$$

and:

$$L_2 \cong \frac{gT_0\pi^2}{6h\beta^2}\left[1+\frac{(\beta\mu)^3}{2\pi^2}\right] \tag{18}$$

The Lorentz number becomes:

$$\mathcal{L} \cong \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2\left\{1-\frac{12(\ln 2)^2}{\pi^2}+\beta\mu\left[\frac{12(\ln 2)^2}{\pi^2}-\frac{1}{2}\right]\right\} \tag{19}$$

After evaluating the numerical factors we get:

$$\mathcal{L} \cong 0.416\,(1+0.2019\,\beta\mu)\mathcal{L}_0 \cong 0.416\,\mathcal{L}_0 \tag{20}$$

Case 2: Electronic system with linear transmission $T(\varepsilon)=a\varepsilon$.
In this case, using eq. (4), the L_n terms will be:

$$L_0 = \frac{ga}{h\beta}\left\{\frac{\beta\mu}{2}+\ln\left[2\cosh\left(\frac{\beta\mu}{2}\right)\right]\right\} \tag{21}$$

with the approximations:

$$L_0 \cong \frac{ga\mu}{h} \tag{22}$$

for $\beta\mu \gg 1$, and:

$$L_0 \cong \frac{ga}{h\beta}\left(\ln 2+\frac{\beta\mu}{2}\right) \tag{23}$$

for $\beta\mu \ll 1$.

For L_1 we will obtain:

$$L_1 = \frac{2ag}{h\beta^2}\left\{\frac{\pi^2}{6}+\left(\frac{\beta\mu}{2}\right)^2+polylog\left(2,-e^{-\beta\mu}\right)-\frac{\beta\mu}{2}\ln\left[2\cosh\left(\frac{\beta\mu}{2}\right)\right]\right\} \tag{24}$$

In the case $\beta\mu \gg 1$:

$$L_1 \cong \frac{\pi^2 ga}{3\,h\beta^2} \tag{25}$$

and for $\beta\mu \ll 1$:

$$L_1 \cong \frac{\pi^2 ga}{6\,h\beta^2}\left(1+\frac{6\ln 2}{\pi^2}\,\beta\mu\right) \tag{26}$$

The last factor is:

$$L_2 = \frac{2ag\mu}{h\beta^2}\left\{\frac{\pi^2}{6} - \left(\frac{\beta\mu}{2}\right)^2 + \frac{\beta\mu}{2}\ln\left[2\cosh\left(\frac{\beta\mu}{2}\right)\right] - 2\,polylog\left(2, -e^{-\beta\mu}\right) - \frac{3}{\beta\mu}\,polylog\left(3, -e^{-\beta\mu}\right)\right\} \quad (27)$$

In the low temperatures βμ≫ 1, and:

$$L_2 \cong \frac{\pi^2 ga\mu}{3\,h\beta^2} \quad (28)$$

and in the opposite limit βμ≪ 1 :

$$L_2 \cong \frac{ag}{2\,h\beta^3}\left[9\zeta(3) + \frac{\pi^2\beta\mu}{3}\right] \quad (29)$$

where ζ(x) is the Riemann's zeta function. Using the results above the Lorentz number in the low temperatures limit βμ≫ 1 becomes:

$$\mathcal{L} \cong \mathcal{L}_0\left[1 - \frac{\pi^2}{3\,(\beta\mu)^2}\right] \quad (30)$$

In the opposite limit βμ≪ 1, and the Lorentz number is:

$$\mathcal{L} \cong \mathcal{L}_0\,\frac{3\,q}{\pi^2}\,(1 + r\,\beta\mu) \quad (31)$$

Where *q* and *r* are complicated numerical factors given by *q*=2.1721…, and *r*=0.05638… . The Lorentz number will be:

$$\mathcal{L} \cong 0.66\,\mathcal{L}_0(1 + 0.05638\,\beta\mu) \cong 0.66\,\mathcal{L}_0 \quad (32)$$

Case 3: Graphene systems (electrons and holes) with quadratic transmission $T(\varepsilon)=a\varepsilon^2$.

In the case of graphene the integral over energies in (4) is taken over the entire interval $(-\infty, +\infty)$ taking into account the holes contribution (from $-\infty$ to μ), and the electrons contribution (from μ to $+\infty$). In this way, the first factor L_0 will be:

$$L_0 = \frac{\pi^2 g_s g_v a}{3\,h\beta^2}\left[1 + \frac{3(\beta\mu)^2}{\pi^2}\right] \quad (33)$$

the second factor L_1:

$$L_1 = \frac{\pi^2 g_s g_v \beta a\mu}{24\,h}\left(\frac{2}{\beta}\right)^3 \quad (34)$$

and the third factor L_2:

$$L_2 = \frac{7\pi^4 g_s g_v a}{15\, h\beta^4}\left[1 + \frac{5(\beta\mu)^2}{7\pi^2}\right] \tag{35}$$

The calculated Lorentz number will be:

$$\mathcal{L} = \frac{21}{5}\, f\, \mathcal{L}_0 \tag{36}$$

where:

$$f = \frac{1 + 3\left(\frac{\beta\mu}{2}\right)^2\left[1 + \frac{5}{7}\left(\frac{\beta\mu}{\pi}\right)^2\right]}{\left[1 + 3\left(\frac{\beta\mu}{\pi}\right)^2\right]^2} \tag{37}$$

At the Dirac point (μ=0) the Lorentz ratio becomes:

$$\mathcal{L} = \frac{21}{5}\, \mathcal{L}_0 \equiv 4.2\, \mathcal{L}_0 \tag{38}$$

and decreases as one departs from the Dirac point. When $\beta\mu \gg 1$, the Lorentz ratio is:

$$\mathcal{L} = \mathcal{L}_0 \tag{39}$$

For highly doped graphene, with this form of transmission, the Lorentz number is similar to the classical result for the Fermi systems. Close to the neutrality point the result changes appreciably. It remains to analyze the consequence of changing of the Lorentz number on the efficiency of thermoelectric conversion, by determining the figure of merit *ZT*.

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