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Ballistic heat transport in semiconductors within the extended irreversible thermodynamics theory

A.Bourhaleb[1,2], A.Salhoumi[1], Y.Boughaleb[1,*] and M.Fliyou[2]
[1] *Laboratoire de Physique de la Matière Condensée, Faculté des sciences Ben M'Sik, BP 7955 Ben M'Sik Casablanca, Morocco.*
[2]*Equipe de l'énergie solaire E.N.S Marrakech, Morocco.*

The transport in miniaturised electronic devices requires to go beyond simple hydrodynamic descriptions. So, carrier transports in nano-length devices is no longer dominated by collisions among the particles but the ballistic transport governs at this level. This type of transport occurs when the perturbation characteristic time is of the order of the relaxation time and the mean free path is of the order of the device's dimension .

The aim of the present work is to calculate the ballistic velocity of heat transport by using a continued-fraction technique in the framework of extended irreversible thermodynamics. This ballistic speed must be less or equal to the maximum value c_0 corresponding to phonon speed. Note that the classical Fourier equation is only able to describe the diffusion regime and the Maxwell-Cattaneo equation predicts a second sound propagation at speed $c_0/\sqrt{3}$ but it is silent about the ballistic behaviour .

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I. INTRODUCTION

The classical theory of irreversible processes, based on the local equilibrium hypothesis, is valid at low frequencies and long wave-lengths. It's, of course, highly desirable to extend the domain of validity of the classical theory to high frequency and short wave-length phenomena. The classical formalism, i.e. Fourier 's law for heat flux, Newton-Stokes's law for diffusion and Ohm's law for electric current is valid at low frequencies and weak fluxes. However, when thermodynamic forces are important and at the regime of high frequency new fast phenomena appear. The EIT theory seems to deal with good tools in this application domain [1-3]. Indeed, this theory, motivated by some relaxational transport equations, includes in its general version memory, non-linear and non-local effects and considers the dissipative fluxes as independent supplementary variables. Then, one should generalise the hydrodynamic transport equations by including such effects. The latter should take into account the higher-order moments of the velocity distribution function. However, this procedure leads to a hierarchy of evolution equations, which should be closed [3,4]. Thus, the problem consists of finding an expression for the $(n+1)^{th}$ moment and the production terms in the corresponding evolution equation as suitable function of the first n^{th} moments.

The paradox of infinite propagation velocity of thermal pulses obtained in the classical formalism is among the problems which, have received great interest. In the framework of the EIT theory, the propagation speed of dissipative signals is finite. This implies that the corresponding flux can not reach arbitrarily high values. But one obtains a flux saturation phenomena. In fact, this saturation behaviour, which is well known, for instance, in radiation hydrodynamics [6], in plasma physics [7,8] and in electronics [9] is an important non-linear feature which should be taken into account in the formulation of transport laws valid at high values of thermodynamic forces. For instance, from information theory and fluctuation-dissipatif one, the identification of the physical meaning of the Lagrange multipliers corresponding to the heat flux yields an effective thermal conductivity [10,11], which leads itself to a heat flux limiter. It is close to other flux limiters found in the literature [6,12]. An important domain of application of these results is found in microelectronic devices.

In precedent work [13], we have treated this problem by truncating the development of the continued fraction (12) at the second row. The results were slightly superior to c_0 (limit velocity), and in order to improve the value of the ballistic velocity we were led to consider higher order in the development.

The plan of this paper is as follows: In the first part, we treat the hierarchy of higher moments taking into account memory, and non-local effects. By using a continued-fraction technique, we derive the expression of effective transport coefficients yielding flux limiters. In the third part, we evidence the transition from classical to ballistic transport and try to improve the calculation of the ballistic velocity for thermal pulses. Finally, we end with some concluding remarks.

II. HIERARCHY OF HIGHER-ORDER FLUXES.

The starting point of the present paper is the evolution equations of E.I.T compatible with the second law of thermodynamics, namely generalised Maxwell-Cattaneo equation for the particle diffusion flux J (the heat flux Q or the electric current J,...etc). In this equation, it should

* E-mail: yboughaleb@yahoo.fr

appear the divergence of the second order flux $J^{(2)}$ [12,14] as

$$\text{ô}_{1}\frac{\partial J}{\partial t}+J=-D_{1}\nabla n-\nabla .J^{(2)} \tag{1}$$

where τ_1 is the relaxation time, D_1 the diffusion coefficient and n the concentration of the particles (electrons e^-, holes e^+ or other carriers). $J^{(2)}$ represents the flux of J or, in microscopic terms, the higher order moment immediate to J, when $J^{(2)} = 0$. Equation (1) reduces to the well-known Maxwell-Cattaneo equation [1-3]. Equation (1) is not compatible with local-equilibrium hypothesis, as it leads to negative values for the classical entropy production. Instead, it is compatible with the generalised entropy production of EIT, which depends itself on J. This transport equation, as the similar ones for the higher-order fluxes, is satisfactory to describe high-frequency phenomena as the second sound, light scattering in gases, neutron scattering in solids or liquids,...etc.

The general form of the evolution equations for the fluxes of n^{th} order and the balance equation of internal energy have the forms

$$\frac{\partial \mathrm{J}^{(n)}}{\partial t}=-\nabla .\mathrm{J}^{(n+1)}+\sigma^{(n)} \tag{2}$$

where $n=1, 2, 3, \ldots$

$$\rho\frac{\partial u}{\partial t}=-\nabla .J+J.E \tag{3}$$

where $\sigma^{(n)}$ is the production term corresponding to the flux $J^{(n)}$, ρ density and E the external electric field.

In the framework of EIT, the generalized expression of entropy S, which takes into account not only the classical variables (internal energy u, volume v and particles density n) but also the dissipative ones, is sufficient to give a most detailed description of the system far from equilibrium.

For these systems, the dissipative fluxes are considered as independent variables, then the entropy is given by $S = S(u, n, J, J^{(n)},\ldots)$ and the generalised Gibbs equation takes the form [1,3]

$$ds=\theta^{-1}du-\theta^{-1}\mu\, dn-\sum_{n=1}^{\infty}\alpha_{n}J^{(n)}\otimes dJ^{(n)} \tag{4}$$

where θ is the non-equilibrium temperature, μ the non-equilibrium chemical potential of electrons and parameters α_n will be identified below.

The entropy flux J^S takes the form

$$J^{s}=\theta^{-1}Q-\theta^{-1}\mu\, J-\sum_{n=1}^{\infty}\beta_{n}J^{(n+1)}\otimes J^{(n)} \tag{5}$$

where β_n are coefficients which depend only on u and n (i.e. $\beta_n = \beta_n(u, n)$).

The entropy production σ^s per unit time and volume is written as

$$\sigma^{s}=\rho\frac{\partial s}{\partial t}+\nabla .J^{s} \tag{6}$$

By considering equations (4), (5) and (6), we can derive the following form of entropy production σ^s

$$\sigma^{s}=J\otimes\left[-\alpha_{1}\frac{\partial J}{\partial t}-\nabla\theta^{-1}\mu+\beta_{1}\nabla .J^{(2)}\right]+\ldots.$$
$$+\sum_{n=2}^{\infty}J^{(n)}\otimes\left[-\alpha_{n}\frac{\partial J^{(n)}}{\partial t}-\beta_{(n-1)}\nabla .J^{(n-1)}+\beta_{n}\nabla .J^{(n+1)}\right] \tag{7}$$

The simplest form of the evolution equation compatible with the second law of thermodynamics (i.e. with the positive character of the entropy production), assumes that thermodynamic forces are proportional to the corresponding flux. This leads to a set of equations of the form

$$\tau_{1}\frac{\partial J}{\partial t}+J=\text{ë}_{1}\nabla\text{è}^{-1}+\text{ã}_{1}\nabla .J^{(2)} \tag{8}$$

$$\tau_{n}\frac{\partial J^{(n)}}{\partial t}+J^{(n)}=\text{ë}_{n}\nabla .J^{(n-1)}+\text{ã}_{n}\nabla .J^{(n+1)} \tag{9}$$

$n=1, 2, 3, \ldots$

where $J^{(n+1)}$ is a tensor of order n, which is identified as the flux of $J^{(n)}$, τ_n is the relaxation time of the flux $J^{(n)}$, λ_n transport coefficient corresponding to $\nabla .J^{(n-1)}$ and γ_n positive definite coefficients. For the sake of simplicity, we have neglected here the coupling between Q and J.

The continued fraction techniques have been used to take into account non-equilibrium thermodynamic implications of the hierarchy (8) and (9) for non-local and memory effects for transport coefficients [13,15]. Here, we enlarge the previous developments to show how nonlinear effects yielding flux limiters may be incorporated in this formalism.

To do that, we generalize (8) and (9) incorporating the electric field E, in the compact form for the hierarchy of hydrodynamic moments as [5]

$$\tau_{m}\frac{\partial J^{(m)}}{\partial t}+J^{(m)}=\lambda_{m}\nabla J^{(m-1)}+\gamma_{m}\nabla .J^{(m+1)}+$$
$$\lambda_{m}'E.J^{(m+1)}+\gamma_{m}'E.J^{(m+1)} \tag{10}$$

where λ_m, γ_m, λ'_m and γ'_m, are transport coefficients corresponding to the terms
$\nabla.J^{(m+1)}, \nabla.J^{(m+1)}, E.J^{(m-1)}$ and $E.J^{(m+1)}$
Equation (10) can be written in the Fourier-Laplace space (ω, k) as

$$A_m = B_m J^{(m-1)} + C_m J^{(m+1)} \tag{11}$$

and the parameters A_m, B_m and C_m take the following expressions respectively.

$$A_m = (1 + i\text{ù}\,\tau_m),\ B_m = (i\text{ë}_m k + \text{ë}'_m E)$$
$$\text{and} \qquad C_m = (\text{ã}'_m E + i\text{ã}_m k)$$

where ω is the frequency and k is the wave-vector. It has been shown [5] that for $\omega=0$ and $k=0$, (11) yields a continued fraction which give a flux saturation for high value of the electric field
In the following we consider :

$$A_m = (1 + i\text{ù}\,\tau_m),\ B_m = i\text{ë}_m k$$
$$\text{and} \qquad C_m = i\text{ã}_m k$$

and we focus our attention on ballistic heat pulse propagation.

III. CLASSICAL AND BALLISTIC TRANSPORT

Now, we investigate the transition from the classical transport to ballistic one in the Maxwell-Cattaneo context. This formalism is qualitatively satisfactory to describe the behaviour of thermal pulses travelling across the crystals and reduced devices. However, it presents some problems in the fast transport phenomena. Indeed, the experiments describing this kind of behaviour at very low temperature exhibit the presence of wave propagation with a speed ranging from $c_0/\sqrt{3}$ to c_0 in the sample, where c_0 is the limit velocity (Debye speed for phonons or light speed for photons). It is of course well-known that transport of heat in dielectric crystals is well treated by means of the phonon model [16]. Generally, there are three mechanisms of particle transport: ballistic, second sound and diffusion. These mechanisms depend on temperature, purity of the crystals and on the frequency of the pertubation. At low frequency, one should observe diffusion transport (i.e. classical transport). At intermediate frequencies, we obtain second sound transport and at high frequencies the ballistic transport dominates.

Our goal is to derive the ballistic velocity by using the continued fraction techniques (i.e. for ballistic phonons in dielectric crystals and for ballistic electrons in micro-electronic devices). This phase velocity should be lower or equal to c_0 , where c_0 represents the speed of sound for thermal problems and the speed of light for electrical ones.

If we truncate the hierarchy at order $(n+1)^{th}$, i.e. $J^{(m)} = 0$ for m great than $n+1$, we obtain from (11) a continued-fraction expansion of $(n+1)^{th}$ order[1,2] as:

$$i\omega = \cfrac{-\xi_0 k^2}{1 + i\omega\tau_1 + \cfrac{\lambda_1^2 k^2}{1 + i\omega\tau_2 + \cfrac{\lambda_2^2 k^2}{\begin{array}{c} \cdot \\ \cdot \\ \cdot \\ 1 + i\omega\tau_n + \cfrac{\lambda_n^2 k^2}{1 + i\omega\tau_{n+1}} \end{array}}}} \tag{12}$$

where, for phonons and photons, according to Dreyer and Struchtrup[16], λ_n and τ_n are related as follows:

$$\frac{\lambda_n^2}{\tau_n^2} = \frac{(n+1)^2}{4(n+1)^2 - 1} c_0^2 \tag{13}$$

At the first row, we fall on the Maxwell-Cattaneo approximation, in this case the velocity propagation tends to $c_0/\sqrt{3}$, which correspond to second sound velocity (Fig. 2)
Our aim is to explore the influence of the ratios τ_1/τ_2 and τ_2/τ_3 on several truncations of the continued fraction (12).

First of all, we truncate the continued-fraction at the third row, and the dispersion relation becomes $(1 << \omega\tau_3 \leq \omega\tau_2 \leq \omega\tau_1)$:

$$i\omega = \cfrac{\xi k^2}{i\omega\tau_1 + \cfrac{\lambda_1^2 k^2}{i\omega\tau_2 + \cfrac{2\lambda_2^2 k^2}{i\omega\tau_3 + \sqrt{4\lambda_3^2 k^2 - \omega^2\tau_3^2}}}} \tag{14}$$

we explore the effects of the ratios τ_1/τ_2 and τ_2/τ_3 on the ballistic speeds derived from (14) in the high-frequency limit, we take for λ_1, λ_2 and λ_3 the values given by expression (13).Our results are given in numerical form in table 1 and are plotted with more detail on Fig. 1.

Table 1: ballistic velocity of thermal pulses for several values of the ratios τ_1/τ_2 and τ_2/τ_3

τ_1/τ_2	τ_2/τ_3	v_p/c_0
1,16	1,18	0,9999
1,17	1,16	0,99984

1,35	1,17	0,99899
1,5	1,12	0,99944

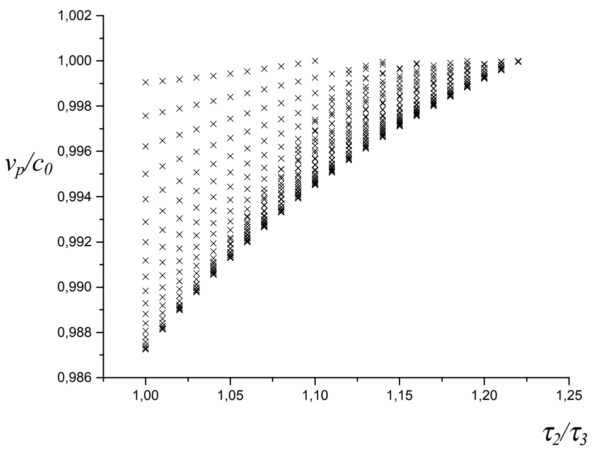

FIG. 1: variation of the ballistic velocity as a function of relaxation times ratio τ_2/τ_3 for τ_1/τ_2 ranging from 1 to 1.5. the lowest curve corresponds to $\tau_1/\tau_2=1.5$ and the highest one to $\tau_1/\tau_2=1$

Contrary to the truncation at the first and the second rows (Maxwell-Cattaneo Approximation, [18]), we can see clearly from this curve, that all values of ballistic velocity converge to the maximal speed (the speed of sound or of light), so we conclude that this truncation is sufficient to describe the ballistic transport. It is interesting to note that for higher values of τ_1/τ_2, higher value of τ_2/τ_3 are required to approach the maximal speed.

We notice that for a high value of τ_2/τ_3 $(\tau_2/\tau_3>>1)$, we find again the equation of Maxwell-Cattaneo and consequently the regime of the second sound $c_0/\sqrt{3}$ (Fig 2). In contrast with the Fig.1, where τ_2/τ_3 was of order *1*, here the ratio τ_2/τ_3 is of order *10* .i.e. τ_3 is rather lower than τ_2. In this case, instead of approaching the ballistic regime, the speed of the pulses approaches the speed of the second sound, i.e. $c_0/\sqrt{3}$.

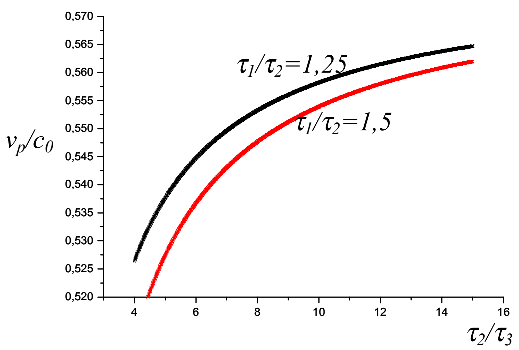

FIG. 2 : Variation of ballistic velocity as a function of relaxation times ratio τ_2/τ_3 for different value of τ_1/τ_2 for high value of τ_2/τ_3.

For more precision, we have computed the ballistic velocity by truncating the continued fraction at the 10^{th} order .As in table 1 and Fig. 1, the value of τ_1/τ_2 and τ_2/τ_3 are of order *1*. The difference is that we have gone up to the 10^{th} order approximation in the continued fraction (12)

Table 2: Influence of the residue on the velocity of thermal pulses for several values of the ratio τ_1/τ_2 and τ_2/τ_3

τ_1/τ_2	τ_2/τ_3	v_p/c_0 *(1)*	v_p/c_0 *(2)*
1,12	1,25	0,83405	0,99558
1,15	1,27	0,84027	0,99943
1,2	1,22	0,83401	0,99252
1,25	1,24	0,84148	0,99607
1,3	1,25	0,8466	0,99922
1,4	1,24	0,84874	0,99988

v_p/c_0 *(1)* is calculated from (12) at the 10^{th} order.
v_p/c_0 *(2)* is calculated from (12) also at the 10^{th} order by introducing a residue R_n which, incorporate the rest of development of the continued fraction in order to insure its convergence.
A simple calculation will lead to the following expression of R_n:

$$R_n=-\frac{1}{2}\left(i\omega\tau_n-\sqrt{4\lambda_n^2 k^2-\omega^2\tau_n^2}\right) \qquad (15)$$

The introduction of the residue R_n allows better results of the ballistic velocity in a good agreement with the one obtained from equation (14), in the sense that they are close to the maximum value $v_p/c_0=1$ which is expected in the high frequency limit.

IV. CONCLUDING REMARKS

The speed of sound (Debye speed) in semiconductors for thermal waves or the speed of light for the electric one are the highest admissible velocities of signal propagation. This property is lost in the classical transport theory which predicts an unphysical divergence of the speed in the high-frequency limit. Extended irreversible thermodynamic goes beyond the classical formulation, and consequently resolves this problem. By introducing this theory we have computed the ballistic velocity, which is in agreement with the physical one. In particular, and for the first time, we have examined the influence of the ratios τ_1/τ_2 and τ_2/τ_3, which are the relaxation times corresponding to the fluxes of first, second and third order respectively. Up to now, in previous literature the ratio τ_1/τ_2 was taken from a microscopic Boltzman equation for phonon [1] and it was assumed that $\tau_1/\tau_2=\tau_2/\tau_3$. Our results give more information, which is indeed useful because the microscopic determination of τ_3 is in general very difficult. It is seen that the ratios τ_1/τ_2 and τ_2/τ_3 play a

role on the speed of the ballistic pulses, which in general is lower than the theoretical upper bound provided by the speed of sound or of light. This is physically interesting, because in the literature it is often assumed that that the ballistic speed coincides with the mentioned upper bound; in fact, the previous calculation in [1] gave a value which was very close to the upper bound. Our study opens a new view on the saturation. This is interesting, because of the important role of the ballistic speed in microscopic devices. The second remarkable point in our analysis in that we have worked both in a third-order truncation (14) as well as in a tenth-order approach to the continued fraction (12). It turns out from our calculation that the difference between both results is not very relevant. Thus, as it may be seen in Fig.1, the ballistic speed for τ_2/τ_3 higher than *1.20* are very close to the maximum allowable speed, independently of the value of the ratio τ_1/τ_2. This is, too, an interesting result.
Indeed, in previous analysis [1,15], it was assumed $\tau_2/\tau_3=1$, for simplicity, but it was asked what could be the influence of the actual value of τ_2/τ_3 on the ballistic speed. Here we have shown that it is sufficient that τ_2/τ_3 is of the order of *1.25* to obtain a ballistic speed very close to the upper bound, independently of τ_1/τ_2 .

Note, however, that if $\tau_3 << \tau_2$, as in Fig.2, the ballistic situation is no longer recovered, but the speed of propagation is the one corresponding to the second sound, namely $c_0 / \sqrt{3}$.

Therefore, the role of τ_2/τ_3 is more important than it was previously thought. An interesting problem would be to evaluate it from microscopic models in actual devices. Another topic of interest would be to analyze the influence of τ_2/τ_3 on the saturation value of the fluxes in the flux-limiter proposed in equation (10). The existing illustrations [5] have been obtained under the simplifying assumption $\tau_2/\tau_3 = \tau_1/\tau_2$, but the situation could be richer in practical cases.

In this article ballistic heat transport have received special attention, but this study can also be applied to the ballistic electric transport by using appropriate value of ξ_0 in development (12).

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