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Behavior of entropy in hyperbolic heat conduction

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It is shown that the classical entropy of an isolated system does not increase monotonically when the approach to equilibrium is described by hyperbolic equations for the temperature evolution. In contrast, the generalized entropy of extended irreversible thermodynamics does increase monotonically, and is therefore better suited than the classical theory for the description of hyperbolic heat transport.

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I. INTRODUCTION

The classical theory of heat conduction, based on Fourier's law, leads to parabolic equations for the evolution of temperature. This approach is very useful in many practical circumstances, but it fails when the frequency of the perturbations is comparable to the relaxation time of the heat flux (of the order of the collision time) as, for instance, in light scattering in fluids and neutron scattering in gases, or during the first stages of very sudden perturbations, as in the irradiation of a sample with a pulse of laser light, or in the propagation of heat pulses in solids at low temperatures, where the parabolic theory would predict an infinite speed in contrast with the finite speed observed experimentally [1–9].

These practical motivations, and other theoretical considerations based, for instance, on the kinetic theory of gases or on the infinite speed of heat in Fourier's theory, have led to generalize Fourier's law [1,2] by including relaxational effects, either in the form of some memory kernel or by adding to the equation relaxational terms such as the time derivative of the heat flux, which convert the usual constitutive equation for the heat flux into an evolution equation for this quantity.

Relaxational equations for the heat flux $\mathbf{q}$, of which the simplest one would be the Maxwell-Cattaneo equation [1–9]

$$\tau\dot{\mathbf{q}}+\mathbf{q}=-\lambda\nabla T \ , \tag{1}$$

lead to hyperbolic equations for the temperature T as, for instance, in the case of constant λ and τ

$$\tau\frac{\partial^2 T}{\partial t^2}+\frac{\partial T}{\partial t}=\chi\nabla^2 T \ , \tag{2}$$

with $\chi=\lambda/(\rho c)$ the thermal diffusivity, ρ being the mass density and c the heat capacity per unit mass. Much work has been devoted to solving this equation (of the form of the so-called telegraphist equation) analytically or numerically in many different circumstances [5–7]. In spite of the very wide effort on this equation, the thermodynamic implications of an equation such as (1) have been almost ignored, though, in fact, Eq. (1) asks for a deep reformulation of nonequilibrium thermodynamics [1,9–14]. It is our purpose here to call attention to these thermodynamic implications by analyzing explicitly the behavior of the entropy according to Eq. (1). This will make completely clear the need for a more complete thermodynamic theory.

II. OSCILLATORY APPROACH TO EQUILIBRIUM

We will consider an isolated rigid system of length L. We assume an initial temperature profile of the form

$$T(x,0)=T_0+\delta T_0\cos\frac{2\pi n x}{L} \ , \tag{3}$$

where T_0 is a homogeneous constant-temperature reference and n is a natural number. We assume that the internal energy of the system is simply given by $\rho u=\rho c T$, with u the internal energy per unit mass, ρ the mass density and c the heat capacity per unit mass. We want to study the evolution of the system towards the equilibrium. We assume that the perturbation δT is of the form

$$\delta T=\delta T_0 f(t)\cos kx \ , \tag{4}$$

with $f(t)$ a function of time to be determined from the evolution equations and k the wave number $k=2\pi n/L$. By introducing (4) into (2) one finds

$$f(t)=a'\exp(a_+ t)+b'\exp(a_-,t) \ , \tag{5}$$

with

$$a_\pm=\frac{1}{2\tau}[-1\pm(1-4\chi k^2\tau)^{1/2}] \ . \tag{6}$$

For $4\chi k^2\tau<1$ the decay of the system to the final homogeneous equilibrium state is exponential, and given by

$$\delta T=\delta T_0\exp\left[-\frac{1+[1-4\chi k^2\tau]^{1/2}}{2\tau}t\right]\cos kx \ . \tag{7}$$

For $4\chi k^2\tau>1$ the decay has an oscillatory behavior given by

$$\delta T=\delta T_0[A\sin\omega t+\cos\omega t]\exp\left[-\frac{t}{2\tau}\right]\cos kx \ , \tag{8}$$

where A is a constant and ω is given by

$$\omega=\frac{1}{2\tau}[4\chi k^2\tau-1]^{1/2} \ . \tag{9}$$

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The expression for the heat flux is, according to (2),

$$q(x,t)=-\lambda k\,\delta T_0[A'\sin\omega t+B'\cos\omega t]\exp\left[-\frac{t}{2\tau}\right]\sin kx\,, \tag{10}$$

where the new parameters A' and B' are defined as

$$A'=\frac{2A+4\omega\tau}{1+4\omega^2\tau^2}\,,\quad B'=\frac{2A-4\omega\tau}{1+4\omega^2\tau^2}\,. \tag{11}$$

Note that $q(0,t)=q(L,t)=0$, i.e., no heat flows into or out of the system, and the total internal energy of the system is constant because

$$U=\int_0^L \rho u\,dx=\int_0^L \rho c T(x,t)dx=\rho c T_0 L\,. \tag{12}$$

Thus our system is an isolated system. Now, we want to compute the evolution of the entropy along the approach of the system to equilibrium. The entropy of the rigid system is

$$\rho s=\rho c\ln\frac{T}{T_0}\,. \tag{13}$$

with s the entropy per unit mass.

If a McLaurin expansion is introduced in (13), we may write

$$\rho s=\rho c\sum_{j=1}^{\infty}\frac{(-1)^{j+1}}{j}\delta_0^j f(t)^j\cos^j(kx)\,, \tag{14}$$

where δ_0 is defined as $\delta T_0/T_0$. Integration over the whole system (i.e., from $x=0$ to $x=L$) yields

$$\tilde{S}(\tilde{t})=-\sum_{j=1}^{\infty}\delta_0^j F(j)\phi(\tilde{t})^{2j}\exp(-j\tilde{t})\,, \tag{15}$$

where the tilde is used for the set of dimensionless variables

$$\tilde{S}=S/(\rho c L),\quad \tilde{t}=t/\tau,\quad \tilde{\omega}=\tau\omega\,, \tag{16}$$

with S the total entropy of the system, and we also introduced the new functions

$$\phi(\tilde{t})=A\sin\tilde{\omega}t+\cos\tilde{\omega}t\,, \tag{17}$$

$$F(j)=\frac{(2j-1)!}{2^{2j}(j!)^2}\,. \tag{18}$$

Dealing with the extremal values of $\tilde{S}$, we can determine them in two trivial cases: when $A=1/(2\tilde{\omega})$ the entropy reaches a relative extremal for $\tilde{t}=n\pi/\tilde{\omega}$, while $A=-2\tilde{\omega}$ implies the existence of an extremal if $\tilde{t}=(1+2n)\pi/2\tilde{\omega}$, with $n=1,2,\ldots$ in both cases. When $A=1/(2\tilde{\omega})$, the initial value of $\partial T/\partial t$ is zero and $q(x,0)=0$, as it may be seen from the general expression (10).

From (15) we know the temporal dependence of the entropy of the isolated system. In Figs. 1 and 2, we plot the difference between the entropy at a given time and its value at $t=0$. Figure 1 corresponds to the case $A=1/(2\omega)$ and there is a transition from a reversible behavior to an irreversible behavior near the initial time. When other particular values of A are considered, as shown in Fig. 2, the behavior is irreversible already at the initial time.

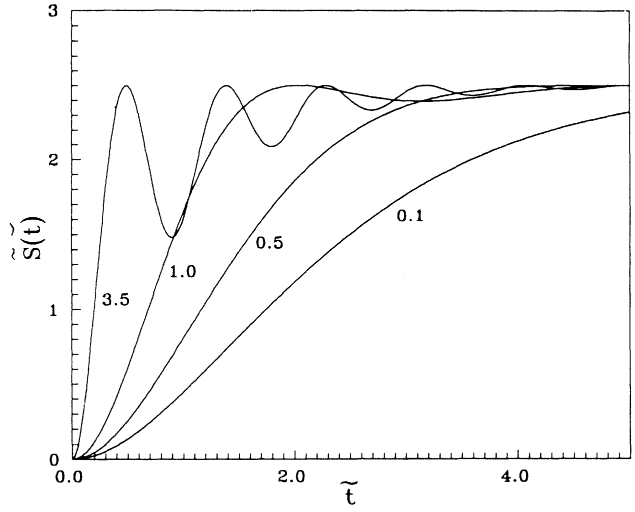

FIG. 1. Reduced entropy as a function of $\tilde{t}$ calculated from local-equilibrium hypothesis for different values of $\tilde{\omega}$ when $A=1/(2\tilde{\omega})$. The represented values of $\tilde{S}$ are multiplied by a factor 10^{-7} and the origin is fixed at $\tilde{S}(0)$.

The behavior shown in Figs. 1 and 2 is rather surprising. In fact, it is not incompatible with the requirements of the second law of thermodynamics, because the initial entropy is less than the final entropy. However, the nonmonotonic behavior of the entropy raises interesting questions about the local-equilibrium formulation of the second law. This law requires that the entropy production must be everywhere positive, but the results shown in Figs. 1 and 2 do not exhibit such monotonic increase of the entropy. Then we have seen that a physically well-motivated transport equation [1–4] does not satisfy the local-equilibrium formulation of the second law of thermodynamics. As a consequence, such a local-equilibrium formulation must be generalized.

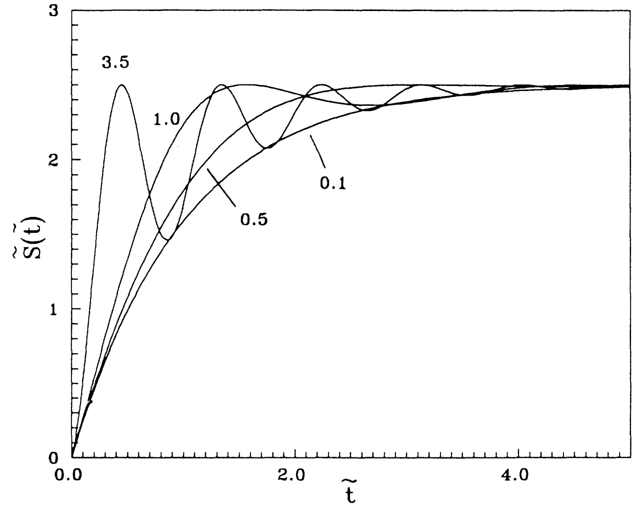

FIG. 2. Reduced entropy as a function of $\tilde{t}$ calculated from local-equilibrium hypothesis for different values of $\tilde{\omega}$ when $A=0$. The represented values of $\tilde{S}$ are multiplied by a factor 10^{-7} and the origin is fixed at $\tilde{S}(0)$.

III. EXTENDED IRREVERSIBLE THERMODYNAMICS

Extended irreversible thermodynamics (EIT) provides such a reformulation of the second law [1,9–14]. This theory assumes that the thermodynamic fluxes are independent variables of the system in addition to the classical slow variables (internal energy in this case). In the present situation, the generalized entropy would depend not only on u (or T) but also on $\mathbf{q}$. According to EIT the generalized entropy has the form [1]

$$\rho s^*(u,\mathbf{q})=\rho s_{\text{eq}}(u)-\frac{\tau}{2\lambda T^2}\mathbf{q}\cdot\mathbf{q} \ . \tag{19}$$

This expression for the entropy may be obtained from kinetic theory by using the Boltzmann definition $s=-k\int f \ln f\, dc$, with c the molecular velocity and f the nonequilibrium steady-state distribution function: following this procedure, Grad's thirteen-moments method [15] yields precisely (19). A further possible way to understand the nonclassical term in (19) is to use the following operational method to define the nonequilibrium entropy [1]: A small element of the nonequilibrium system is suddenly isolated and it is allowed to decay to equilibrium. The final entropy of the system s_{fin} is the equilibrium entropy corresponding to the local energy and volume of the subsystem $s_{\text{eq}}(u)$ and its initial entropy s_{in} is the nonequilibrium entropy to be defined and denoted by $s^*(u,\mathbf{q})$. Both values of the entropy are related through $s_{\text{fin}}=s_{\text{in}}+\int \sigma\, dv\, dt$, with σ the entropy production during the decay of the flux to its zero equilibrium value. If one takes into account that

$$\sigma=\frac{1}{\lambda T^2}\mathbf{q}\cdot\mathbf{q} \tag{19$'$}$$

and that $\mathbf{q}$ decays exponentially according to the Maxwell-Cattaneo law, one gets again (19) after performing the integration of σ from $t=0$ to $t=\infty$. In more general situations, the simple form (19) could be generalized to a more complicated expression for $s(u,\mathbf{q})$ [16] but this is not necessary to stress the fundamental physical features.

The differential of (19) is

$$ds^*=T^{-1}du-\frac{\tau}{\rho\lambda T^2}\mathbf{q}\cdot d\mathbf{q} \ , \tag{20}$$

where we have neglected nonlinear terms of second order in q in T^{-1}.

Taking into account the energy-balance equation

$$\rho\dot{u}=-\nabla\cdot\mathbf{q} \tag{21}$$

and introducing it into (20), we find for the entropy production

$$\sigma=-\frac{1}{T^2}\mathbf{q}\cdot\left[\nabla T+\frac{\tau}{\lambda}\dot{\mathbf{q}}\right] \ . \tag{22}$$

If the Maxwell-Cattaneo equation (2) is introduced in (22) one finds

$$\sigma=\frac{1}{\lambda T^2}\mathbf{q}\cdot\mathbf{q} \ . \tag{23}$$

In contrast, the classical entropy production has the form

$$\sigma_{\text{eq}}=-\frac{1}{T^2}\mathbf{q}\cdot\nabla T \ , \tag{24}$$

which in combination with the Maxwell-Cattaneo equation leads to

$$\rho\dot{s}_{\text{eq}}=\frac{1}{\lambda T^2}\mathbf{q}\cdot\mathbf{q}+\frac{\tau}{\lambda T^2}\dot{\mathbf{q}}\cdot\mathbf{q} \ . \tag{25}$$

From (19) we conclude that ρs^* can only increase during the approach to equilibrium. After integration from $x=0$ to $x=L$, we can write the following generalization of (15):

$$\tilde{S}^*(\tilde{t})=\tilde{S}(\tilde{t})-\tilde{S}'(\tilde{t}) \ , \tag{26}$$

where the explicit expression for $\tilde{S}'$ is obtained using the same arguments previously employed in the derivation of (15). The result is

$$\tilde{S}'(\tilde{t})=\frac{\delta_0^2}{8}\frac{h(\tilde{t})e^{-\tilde{t}}}{1+4\omega^2}\left[\frac{1}{2}+\sum_{j=1}^{\infty}\delta_0^{2j}(2j+1)[G(j)-G(j+1)]\times\phi(\tilde{t})^{2j}\exp(-j\tilde{t})\right] \ , \tag{27}$$

where we have introduced the new functions

$$h(\tilde{t})=(2A+4\tilde{\omega})\sin\tilde{\omega}\tilde{t}+(2-4A\tilde{\omega})\cos\tilde{\omega}\tilde{t} \ , \tag{28}$$

$$G(j)=\frac{(2j)!}{2^{2j}(j!)^2} \ . \tag{29}$$

In Figs. 3 and 4 we represent the behavior of the generalized entropy as compared with the local-equilibrium entropy. In contrast with the latter, the generalized entropy of extended irreversible thermodynamics shows a

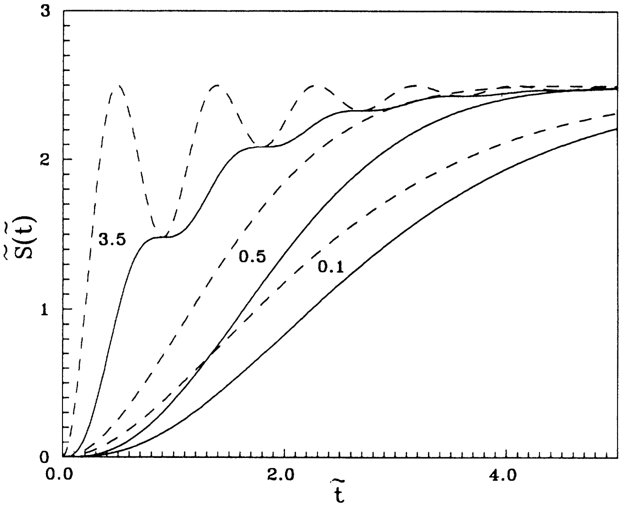

FIG. 3. Reduced entropies as a function of $\tilde{t}$ calculated from the local-equilibrium hypothesis (dashed curves) and from the EIT model (solid curves) for different values of $\tilde{\omega}$ when $A=1/(2\tilde{\omega})$. The represented values of $\tilde{S}$ are multiplied by a factor 10^{-7} and the origin is fixed at $\tilde{S}(0)$.

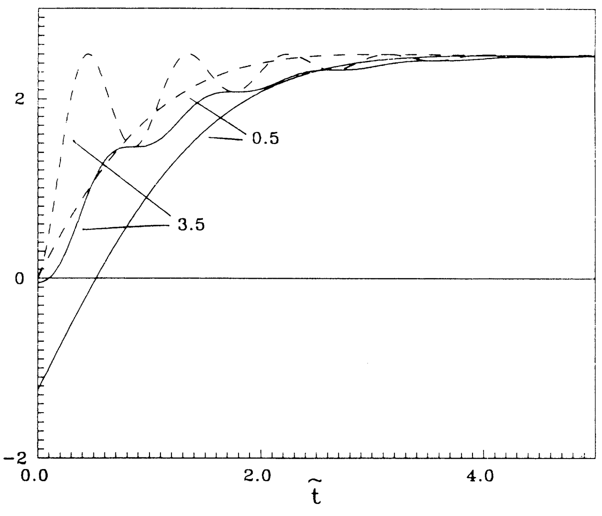

FIG. 4. Reduced entropies as a function of $\tilde{t}$ calculated from the local-equilibrium hypothesis (dashed curves) and from the EIT model (solid curves) for different values of $\tilde{\omega}$ when $A = 0$. The represented values of $\tilde{S}$ are multiplied by a factor 10^{-7} and the origin is fixed at $\tilde{S}(0)$.

monotonic increase with some stationary points, corresponding to the minima of the local-equilibrium entropy.

IV. CONCLUSIONS

We have tried in this paper to show with a very simple example that the usual formulation of the second law in terms of the monotonic increase of the local-equilibrium entropy is not always a safe criterion for restricting the constitutive equations, as it may forbid equations, as the Maxwell-Cattaneo equation, which are well founded either from experimental or theoretical points of view. However, the entropy of extended irreversible thermodynamics, which takes into account the independent character of the heat flux at short times, is suitable as an expression for the second law in hyperbolic heat transport as it makes compatible the monotonical increase of the entropy with the use of the Maxwell-Cattaneo equation.

A situation similar to that analyzed in this paper could be found if relaxational equations are taken for other fluxes, as for instance the viscous-pressure tensor. Numerical simulations in the context of molecular hydrodynamics have shown that for sufficiently short wavelengths, shear waves can propagate in fluids, i.e., the usual diffusive behavior of tangential velocity perturbations is changed to a propagative behavior [17]. The tangential velocity perturbation would play in that case a role analogous to that of the temperature perturbations in the problem dealt with in this paper.

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