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Information theory and heat transport in relativistic gases

D Jou† and M Zakari

Universitat Autònoma de Barcelona, Departament de Física, 08193 Bellaterra, Catalonia, Spain

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Abstract. We study the behaviour of the thermal conductivity for an ideal ultra-relativistic gas far from equilibrium by using information theory and the fluctuation–dissipation theorem in non-equilibrium steady states. We compare two different proposals for the nonlinear generalization of the fluctuation–dissipation theorem to the far-from-equilibrium regime. Both proposals lead to a saturation of the heat flux for high temperature gradients, but one of them is in better agreement with the expressions most often used in radiation hydrodynamics.

1. Introduction

Information theory provides a useful tool for the analysis of the distribution function of macroscopic systems subjected to a given set of restrictions [1, 2]. The best known applications of this method refer to systems in thermodynamic equilibrium, i.e. subjected to restrictions on such quantities as the mean energy and the mean number of particles. However, there is an increasing interest in using this method in the analysis of non-equilibrium steady states [3–8]; for instance, systems under constraints on the mean internal energy u and mean heat flux Q. To obtain information on the transport coefficients one should relate Q and ∇T. However, ∇T does not appear in a natural way in the non-equilibrium distribution function when one requires u and Q, rather than u and ∇T, to have definite values. Nevertheless, one can obtain the transport coefficient, i.e. the thermal conductivity, by using the second moments of the fluctuations of the heat flux and the fluctuation–dissipation theorem (FDT).

In full generality, one needs to know not only the second moments of the fluctuations of the flux but also their time correlation, i.e. one needs the evolution of the fluctuations. Here, we will deal with a simple illustration where it is assumed that the decay of the fluctuations is a simple exponential with a relaxation time that does not depend on the flux. Of course, this is an oversimplification but, even in this case, we will show that one may obtain non-trivial results. In this work, we shall focus our attention on the thermal conductivity of an ideal ultra-relativistic gas [8] and, by means of the FDT in non-equilibrium steady states, we shall obtain a flux-dependent thermal conductivity which leads to a saturation of the heat flux when the temperature gradient is large enough, by using two different extensions of the FDT.

The FDT is a classical topic in modern non-equilibrium statistical mechanics [9, 10]. The best grounded formulation of the theorem corresponds to an analysis of transport coefficients near equilibrium, in the so-called linear response theory. The corresponding extension far from equilibrium, or, in other words, the nonlinear response theory, is a topic of current

† Fellow of the Institut d'Estudis Catalans, Carme 47, 08001 Barcelona, Spain.

development [11–14], with many open problems. For instance, several ambiguities may appear in nonlinear situations. Since the ratio of the flux to the force is not a constant, but depends on the force itself, such a ratio will differ in principle from the differential transport coefficient defined as the derivative of the flux with respect to the force. Therefore, it has to be clarified which of them (the usual transport coefficient $Q/\nabla T$ or the differential transport coefficient $\partial Q/\partial \nabla T$) is related to the fluctuations of the flux.

The plan of this article is as follows. In the second section we explore two posssible generalizations of the FDT to non-equilibrium states, and in the third section we use the results of information theory to obtain the corresponding values for the nonlinear thermal conductivity and we compare them with some of the expressions which are currently used in radiation hydrodynamics.

2. Fluctuation–dissipation theorem

The FDT [9–12] relates the transport coefficients with the time-correlation function of the fluctuations of dissipative fluxes. One of the best known formulations of the theorem is the so-called Green–Kubo relations for the transport coefficients, which, in the particular case of the thermal conductivity, reads [10–12]

$$\lambda(T) = \frac{1}{kT^2} \int_0^\infty \langle \delta\tilde{Q}(t)\delta\tilde{Q}(0)\rangle_{\mathrm{eq}}\,\mathrm{d}t. \tag{1}$$

Here $\langle\ldots\rangle_{\mathrm{eq}}$ stands for the equilibrium average, k is the Boltzmann constant and $\tilde{Q}$ is the so-called reduced heat flux, which will be explicated below. A natural question to ask is how this relationship can be extended to situations far from equilibrium, and how can it yield a thermal conductivity dependent not only on temperature T but also on the temperature gradient ∇T or, alternatively, on the heat flux Q. In particular, for an ultra-relativistic gas it is expected that λ will depend on ∇T in such a way that in the high ∇T limit the heat flux remains finite and tends to the asymptotic value $Q_{\max} = uc$, with u the internal energy density and c the speed of light. This limit to the heat flux, with its physical origin in the finite character of the speed of light, is known in radiation hydrodynamics as the flux limit problem [15–18]. Of course, nonlinear response theory has received much attention, but usually these analyses have been either abstract and formal or applied to more complicated systems [11, 12].

Here, we will deal with this problem under simple assumptions which are, however, useful in understanding some problems arising in the nonlinear context. In this way, we assume an exponential decay for the fluctuations of $\tilde{Q}$, i.e. $\delta\tilde{Q}(t) = \delta\tilde{Q}(0)\exp(-t/\tau)$ with the relaxation time τ independent of $\tilde{Q}$. This simple hypothesis has often been made in recent thermodynamic formalisms [19–23], which have paid attention to the thermodynamic implications of relaxational extensions of hydrodynamical transport equations. In the simplifying hypothesis of exponential relaxation, (1) reduces to

$$\lambda = \frac{\tau}{kT^2}\langle \delta\tilde{Q}(0)\delta\tilde{Q}(0)\rangle_{\mathrm{eq}} \tag{2}$$

with $\delta\tilde{Q}$ the fluctuation of the subtracted heat flux, $\tilde{Q} \equiv Q - cu$. In non-equilibrium situations, relation (2) could be naively generalized as

$$\begin{aligned} -\frac{Q}{\nabla T} &= \frac{\tau}{kT^2}\langle \delta\tilde{Q}\delta\tilde{Q}\rangle_{\mathrm{neq}} \\ &= \frac{\tau}{kT^2}[c^2\langle\delta u\delta u\rangle - 2c\langle\delta u\delta Q\rangle + \langle\delta Q\delta Q\rangle]_{\mathrm{neq}} \end{aligned} \tag{3}$$

with $\langle\ldots\rangle_{\text{neq}}$ being an average over a non-equilibrium steady-state distribution function characterizing the physical situation under study. In our case, we will use the non-equilibrium distribution function (6) which will be discussed in the next section.

A different version of the FDT [13, 14], instead of (1), relates the second moments of the fluxes to the differential transport coefficient $\partial Q/\partial\nabla T$ rather than to the usual conductivity $\lambda = -Q/\nabla T$, i.e.

$$-\frac{\partial Q}{\partial \nabla T} = \frac{1}{kT^2}\int_0^\infty \langle \delta\tilde{Q}(t)\delta\tilde{Q}(0)\rangle_{\text{neq}}\,\mathrm{d}t. \tag{4}$$

An expression analogous to this one (though more general and abstract and written for the quantum case and valid only for Hamiltonian perturbations) was obtained in [14] by solving the von Neumann equation for a system exposed to external perturbations and using the invariant part of the time-dependent density matrix to generalize the linear reponse theory to non-equilibrium states. We will comment further on this expression in the concluding section. In the hypothesis of an exponential decay of fluctuations, (4) reduces to

$$-\frac{\partial Q}{\partial \nabla T} = \frac{\tau}{kT^2}\langle \delta\tilde{Q}\delta\tilde{Q}\rangle_{\text{neq}}. \tag{5}$$

Of course, since in the neighbourhood of equilibrium one has $Q = -\lambda\nabla T$, it follows that (3) and (5) are completely equivalent near equilibrium.

For an ultra-relativistic gas under a heat flux, the distribution function very far from equilibrium is explicitly known [8] and it allows us to obtain the second moment of the fluctuations of u and Q around their mean values. We will resort to them to obtain the coefficient of thermal conductivity by using the above generalizations, (3) and (5), of the FDT to non-equilibrium steady states.

3. Information theory

The distribution function f for a system under the constraints of a given mean energy u and non-vanishing heat flux Q is, according to standard maximum entropy arguments [3–8],

$$f = Z^{-1}\exp(-\beta\hat{H} - I\hat{Q}) \tag{6}$$

where $\hat{H}$ is the Hamiltonian, $\hat{Q}$ the microscopic operator for the heat flux, and β and I the Lagrange multipliers related respectively to the mean energy $u = \langle\hat{H}\rangle$ and the mean heat flux $Q = \langle\hat{Q}\rangle$. Z is a generalized partition function ensuring the normalization of f. For an ideal ultra-relativistic gas, $\hat{H} = \sum_\alpha P_\alpha c$, $\hat{Q} = \sum_\alpha P_\alpha c\vec{c}_\alpha$, with P_α the modulus of the momentum of the α particle ($\alpha = 1, 2, \ldots, N$) and one obtains for $Z(\beta, I)$ the expression

$$Z(\beta, I) = \frac{1}{N!}\left[\frac{8\pi V}{\beta^3 c^3 h^3}\left(1 - \frac{c^2 I^2}{\beta^2}\right)^{-2}\right]^N \tag{7}$$

with N the number of particles, h the Planck constant and V the volume of the system. From the definition of entropy

$$S(u, Q) = -k\int f\ln(f)\,\mathrm{d}\Gamma \tag{8}$$

the Gibbs equation takes the generalized form

$$\mathrm{d}s = k\beta\,\mathrm{d}u + kI\,\mathrm{d}Q \tag{9}$$

where $d\Gamma$ is the element of volume in the phase space. The Lagrange multipliers have the explicit form [8]

$$\theta = T\left[\sqrt{4-3x^2} - 1\right] \tag{10}$$

$$cI = -\frac{3x}{T}\left[2 - 3x^2 + \sqrt{4-3x^2}\right]^{-1} \tag{11}$$

with $x \equiv Q/Q_0$ and $Q_0 = cu$ the saturation heat flux. Note that in the limit of a vanishing heat flux, i.e. when $x = 0$, θ reduces to T, the local-equilibrium temperature, and I tends to zero, so that one recovers, from (8), the classical Gibbs equations $ds = T^{-1}\,du$ and the distribution function (6) takes the standard form of the canonical equilibrium distribution function.

The second moments of the fluctuations of u and Q are given from a standard procedure as

$$\begin{aligned} \langle \delta u \delta u \rangle &= \frac{\partial^2 \ln Z}{\partial \beta^2} \\ \langle \delta Q \delta Q \rangle &= \frac{\partial^2 \ln Z}{\partial I^2} \\ \langle \delta u \delta Q \rangle &= \frac{\partial^2 \ln Z}{\partial I \partial \beta}. \end{aligned} \tag{12}$$

From expression (7) of the partition function, the latter set of fluctuations can be expressed as

$$\begin{aligned} \langle \delta u \delta u \rangle &= \frac{3N}{\beta^2} + \frac{4N}{\beta^2}\frac{c^2I^2(3\beta^2 - c^2I^2)}{(\beta^2 - c^2I^2)^2} \\ \langle \delta Q \delta Q \rangle &= \frac{4Nc^2}{(\beta^2 - c^2I^2)^2}(\beta^2 + c^2I^2) \\ \langle \delta u \delta Q \rangle &= -\frac{8Nc^2I\beta}{(\beta^2 - c^2I^2)^2} \end{aligned} \tag{13}$$

respectively.

Introducing equations (13) into equation (3), the nonlinear thermal conductivity may be written as

$$-\frac{Q}{\nabla T} = \frac{\tau}{kT^2}\frac{3Nc^2}{\beta^2}\left[1 - \frac{4}{3}\frac{4cI\beta^2 - (\beta + cI)(\beta^2 + c^2I^2)}{(\beta - cI)(\beta + cI)^2}\right] \tag{14}$$

whereas in the approach of (5) we have

$$-\frac{\partial Q}{\partial \nabla T} = \frac{\tau}{kT^2}\frac{3Nc^2}{\beta^2}\left[1 - \frac{4}{3}\frac{4cI\beta^2 - (\beta + cI)(\beta^2 + c^2I^2)}{(\beta - cI)(\beta + cI)^2}\right]. \tag{15}$$

Since β and I are complicated functions of T and Q, it is not easy to write Q explicitly in terms of ∇T. Instead of that, in figure 1 we plot Q/Q_0 against the temperature gradients obtained from (14) and (15). In either case Q/Q_0 does increase linearly with ∇T for small values of ∇T but it asymptotically tends to $Q/Q_0 = 1$ in the limit of high ∇T.

To decide which of the two relationships between Q and ∇T is the more satisfactory, we compare our results with some well known expressions for the nonlinear λ used in radiation hydrodynamics. In fact, several different forms of flux limiters are used in radiation hydrodynamics [15]; some of them are based on specific physical arguments (kinetic theory, for instance), whereas some others are purely *ad hoc* expressions. Here, we will take

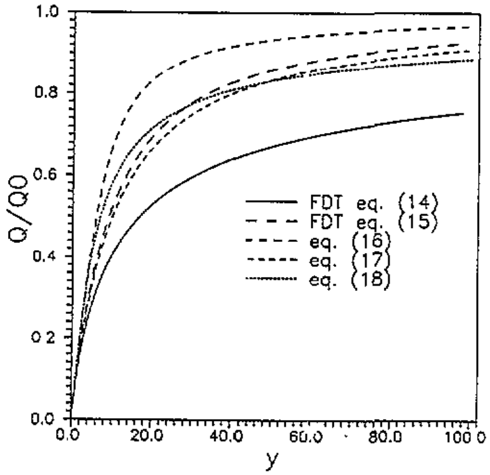

Figure 1. Plot of Q/Q_0 against $y = l\nabla T/T$. For large temperature gradients all the curves tend to saturation ($Q = Q_0$), whereas in the limit of low ∇T, Fourier's law is recovered.

two different expressions for the flux limiter. One of them proposed by Levermore and Pomraning [16] is based on the kinetic theory of radiation:

$$\lambda = \frac{3\lambda_0}{y}\left[\coth(y) - \frac{1}{y}\right]. \tag{16}$$

Here $y \equiv l'|\nabla T|/T$, l' is a coefficient with units of length and has the meaning of a mean-free path of order $c\tau$, and λ_0 is the thermal conductivity in the limit of low heat flux. Expression (16) has been obtained by a Chapman–Enskog approach from a flux-limited diffusion theory which starts from a transport equation for the specific intensity of radiation [16]. Other versions of flux limiters do not have a sound physical basis, but they are often in the analysis of astrophysical problems, used because of their simplicity.

For instance, the nonlinear thermal conductivity is often written as a ratio of two simple polynomials [16–18]:

$$\lambda = \lambda_0\left(\frac{6+3y}{6+3y+y^2}\right). \tag{17}$$

Another expression for the nonlinear thermal conductivity has been obtained [17] from the assumption that the density of the integrated frequency is isotropic in some inertial frame. This yields a relation between the thermal conductivity λ and the dimensionless temperature gradient y given by the expressions

$$\lambda(y) = 9\lambda_0\frac{(1-\beta^2)^2}{(3+\beta^2)^2} \qquad y = 4\beta\frac{(3+\beta^2)}{(1-\beta^2)^2} \tag{18}$$

where β is a parameter that changes between 0 and 1, yielding $y = 0$ for $\beta = 0$ and $y = \infty$ for $\beta = 1$. Thermodynamic arguments [24] yield the conclusion that this is the form of $\lambda(y)$ implied by thermodynamic arguments based on the existence of an entropy dependent on the first two moments of radiative distribution function.

The three flux limiters (16)–(18) behave as $\lambda \to \lambda_0$ when $y \to 0$ and as $Q = Q_0$ when $y \to \infty$. In figure 1 we also plot Q/Q_0 as a function of y corresponding to equations (14)–(18).

Inspection of figure 1 shows that the behaviour described by equation (15) is much closer to the flux limiters (16) than that of equation (14). In fact, (15) yields a behaviour intermediate between the one described by kinetic theory in the Chapman–Enskog approximation and the practical expression (17), and it provides a better approximation to (16) than the *ad hoc* version (17). Note also that the curve based on (15) is very close to the curve obtained from the nonlinear thermal conductivity (18), whereas the curve obtained from (14) is too low to be acceptable. From this we conclude that Ichiyanagi's generalization of the FDT is more reliable than the naive extentions (3) of Kubo's equation, under the assumption of an exponential decay for the fluctuations.

Let us finally point out that it is not surprising that our result does not coincide with the one obtained in kinetic theory. Indeed, neither our result nor the result (16) is an exact first-principles expression, but they are approximated expressions based on very different physical approaches. In fact, it is rather satisfactory that such different starting points lead to final results which are significantly similar.

4. Conclusions

It is seen that the results obtained from two possible versions of the FDT, namely the direct extension of the Kubo formula for thermal conductivity (3) and the Ichiyanagi expression (5) for the differential transport coefficient lead to a saturation for the heat flux in non-equilibrium steady state (equations (14) and (15) respectively) and that their general behaviour is rather similar. Comparison with the expressions for radiation hydrodynamics *indicate that extension (5) is preferable to extension (3) of the fluctuation–dissipation* expression to the nonlinear regime, because it yields a behaviour which is closer to the results given by the flux limiters used in radiation hydrodynamics.

Let us also comment on the hypothesis that τ does not depend on Q; although admittedly this is an oversimplification, it is not an internally inconsistent hypothesis. For instance, in the relaxation-time approximation of kinetic theory of gases, one often assumes kinetic equations of the form

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla f = -\frac{1}{\tau}(f - f_0) \tag{19}$$

with $\boldsymbol{v}$ the molecular velocity, f the distribution function and f_0 the local-equilibrium distribution. In this formalism, if one goes to the nonlinear order in the solution, one finds a nonlinear thermal conductivity $\lambda(T, \nabla T)$ in spite of the fact that τ only depends on T and does not depend on ∇T or Q. Note that in this paper we have used, instead of the *solution of (19), an expression for f based on maximum-entropy arguments. This is due* to the fact that we need a solution that remains valid even very far from equilibrium, in highly nonlinear regimes in which solutions of kinetic equations are not easily available.

The derivation of the fluctuation–dissipation expression for the differential transport coefficient, analogous to (4), was based [14] on a non-equilibrium Hamiltonian of the form

$$H(t) = H - \sum_j A_j E_j(t) \tag{20}$$

H being the Hamiltonian of the unperturbed system, E_j the external fields, for instance an electric field, and A_j the operators of the system conjugate to the external fields. In our case, no Hamiltonian is directly related to the perturbation. Instead, we have used an expression of the form (6), i.e.

$$f \sim \exp\left[-\beta\left(\hat{H}+\frac{1}{\beta}\boldsymbol{I}\cdot\hat{\boldsymbol{Q}}\right)\right]. \tag{21}$$

Therefore, if follows that the expression $(-\boldsymbol{I}/\beta)\cdot\hat{\boldsymbol{Q}}$ plays the role of the $\sum_j A_j E_j$ in (20). In fact, according to extended irreversible thermodynamics, the quantity $-\boldsymbol{I}/\beta$ may be identified [8] as $\tau\nabla\theta^{-1}$, where τ is the relaxation time and $\nabla\theta^{-1}$ is the force conjugate to the heat flux. Thus, the non-equilibrium distribution (6) may be interpreted as giving an effective perturbed Hamiltonian describing the thermal perturbation due to the temperature gradient.

It must also be pointed out that in [14] the evolution and probability of the fluctuations are not exactly described by the same non-equilibrium Hamiltonian. To a certain extent, the inclusion of the effects of the non-vanishing $\boldsymbol{Q}$ in the statistics but not in the dynamics of the fluctuations in the present problem may be seen as a particular and very simplified consequence of this fact.

Let us finally mention that, to the best of our knowledge, fluctuation–dissipation ideas have not been used in the context of the nonlinear thermal conduction in relativistic gases nor in the context of radiation hydrodynamics, so that this work may be regarded as a contribution to the study of flux limiters, the thermodynamic analysis of which has received fresh attention from the thermodynamic point of view in recent years [24, 25].

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