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Nine-moment phonon hydrodynamics based on the modified Grad-type approach: formulation

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Abstract
In this paper, we present the derivation of a new set of heat transport equations, called the equations of nine-moment phonon hydrodynamics, which are expected to describe transient processes under high thermal loads. The nine-moment model introduces the energy density, the heat flux and the flux of the heat flux as basic gas-state variables. The evolution equations for these variables are derived from the Grad-type expansion method applied to the Boltzmann–Peierls equation with Callaway's collisional terms. The basic idea is to expand the phase density about an anisotropic Planck distribution. The advantage of using this distribution is that the heat flux is incorporated into the model in a non-perturbative manner, thereby allowing virtually arbitrarily large values for the components of the heat flux. Special emphasis is placed on finding explicit closed-form expressions for the moment flux and collisional quantities in terms of independent gas-state variables. Our model involves two relaxation times and it seems particularly suited for describing phonon flows in the regime where the relaxation time for normal processes is much smaller than the relaxation time for resistive processes.

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1. Introduction

Heat transport by phonons is important in a variety of technological applications. Many of these applications involve transient processes under high thermal loads. A full description of thermal processes requires the study of phonon flows in the ballistic, hyperbolic and diffusive regimes. Here, the hyperbolic regime is studied with a view to a deeper understanding of the effect of short time scales of the order of the phonon relaxation times on heat transport. Moreover, our aim is to describe the nonlinear effects associated with the heat flux. At the end of the introduction, we mention how to incorporate the diffusive and ballistic flow into our model.

In the case when the particle description of phonons is valid [1–3], the Boltzmann–Peierls (BP) equation is often used [4] in conjunction with the relaxation-time approximation. Even under the assumption of Callaway's model [5, 6], the BP equation is a complicated nonlinear equation for the distribution function f (i.e., the phase density or the number density of phonons) and closed-form analytic solutions are virtually unobtainable. The method of moments provides a means of constructing approximate solutions as it replaces the problem of directly solving the BP equation with that of solving a system of generalized transport equations for various hydrodynamic and quasi-hydrodynamic variables.

In the work by Larecki [7], the four-moment system was presented as a possible model for heat transport in the hyperbolic regime. This model is based on the quasi-equilibrium Planck distribution[3] which incorporates the heat flux in a non-perturbative function; i.e., there are no unphysical limitations on the magnitudes of the individual components of the heat flux to maintain a positive distribution function. It yields a set of four quasi-linear differential equations with the independent variables being the energy density and the three components of the heat flux. In this context, a word should be said about the normal and resistive processes. As is well known, normal processes (scattering processes which conserve both energy and momentum) tend to return the phonon gas to a quasi-equilibrium Planck distribution F, whereas resistive processes (scattering processes which conserve only energy) try to force it towards an equilibrium Planck distribution F_E. We define τ_n to be the relaxation time for normal processes and τ_r to be the relaxation time for resistive processes. With these definitions, we conclude that the four-moment system can be used in the case when $\tau_n \ll \tau_r$ (then there is a physical reason to employ the quasi-equilibrium Planck distribution F in place of the full distribution f) and that it is a good model for time scales of the order of τ_r. Moreover, by what has been said above, this model is capable of representing the nonlinear effects associated with the heat flux.

Here, we want to propose a theory which describes phenomena at frequencies comparable to the inverse of τ_n. This can be achieved by enlarging the set of independent gas-state variables, through the introduction of higher-order moments of the distribution function f. A natural way to derive the evolution equations for these extra variables is to generalize the classical method of Grad [9, 10]. Thus, we begin by expanding the number density of phonons about a quasi-equilibrium Planck distribution F. We proceed in a systematic manner, i.e., we first set up a Hilbert space for the expansion and subsequently define an orthogonal basis in this Hilbert space. The use of the quasi-equilibrium Planck distribution F for the expansion differs significantly from the Banach–Piekarski approach [11] which uses the equilibrium Planck distribution F_E for it. In fact, the basic advantage of using the quasi-equilibrium Planck distribution F is that the heat flux is incorporated into the model in a non-perturbative manner, thereby allowing virtually arbitrarily large values for the individual components of the heat flux. Developing the theory along these lines, one can obtain a whole hierarchy of closed systems of moment equations corresponding to the hierarchy of truncated expansions of the distribution function f. Unlike the four-moment system which involves only the relaxation time τ_r, each member of this hierarchy of closures contains the relaxation times τ_n and τ_r. These closure models are linear in the excessive variables and nonlinear in the energy density and the heat flux. Such an approach seems particularly useful if we assume that $\tau_n \ll \tau_r$.

[3] In the main text and [8], we also call this distribution the anisotropic Planck function.

The physical consequence of this assumption is clear. During the first time period τ_n, normal processes make the phonon gas approach F, and then during the longer time period τ_r, resistive processes return it to F_E. Also, because of $\tau_n \ll \tau_r$, the excessive variables are fast variables that dacay to their quasi-equilibrium values after a short relaxation time τ_n. For time scale of the order of τ_n, we are thus justified in assuming that f is close to F. Moreover, having a separation of two time scales, we can expand f about F.

Denoting by $\mathcal{M}^{ij}$ the flux of the heat flux, the simplest model which may be expected to offer a description of the aforementioned effects is obtained by including the deviatoric part of $\mathcal{M}^{ij}$ in the set of independent gas-state variables. We interpret this model as the nine-moment closure model or, in a phenomenological setting, the quasi-hydrodynamic description in which the state of the phonon gas is assumed to be defined completely by the usual four variables (here the energy density and the heat flux) supplemented by the five components of the deviatoric part of $\mathcal{M}^{ij}$ as extra gas-state variables. Using the BP equation under the relaxation-time approximation, our purpose in this paper is to derive and display the equations of phonon hydrodynamics in the nine-moment closure model; in particular, to obtain explicit closed-form expressions for the moment flux and collisional terms. In a sense, the idea to use the deviatoric part of $\mathcal{M}^{ij}$ as an extra dynamical variable is not entirely new. The equations of nine-moment phonon hydrodynamics were first derived by Banach and Piekarski [12]. They assumed that the phonon gas is close to local equilibrium and thus required that the components of the heat flux are small. For a linear model, further simplifications are possible and this has been exploited by Dreyer and Struchtrup [13]. In their work, numerical calculations based on the linearized nine-moment closure were successfully fitted to the experimental data on heat pulses in crystals. Applications of this closure to the gradient expansions of q^i and $\mathcal{M}^{ij}$ have been discussed by Karlin *et al* [14] and Karlin and Gorban [15]. In the present nonlinear model, one can handle problems with large components of the heat flux. This is a definite improvement over previous approaches which restrict attention to small deviations in the heat flux from zero.

In the context of classical kinetic theories, a similar strategy for deriving a hierarchy of moment closure systems was developed by Groth *et al* [16, 17] based on an expansion about an ellipsoidal distribution function[4] (EDF). This strategy permits the inclusion of fluid stresses in a non-perturbative fashion. It also results in quasi-linear moment equations that are hyperbolic for significant ranges of physical conditions, thereby preventing the breakdown of the transport equations. However, these authors did not set up a Hilbert space for the expansion. They also did not define an orthogonal basis in this Hilbert space because emphasis was placed on describing the 35-moment closure. Another observation is that collision processes do not attempt to make the classical Boltzmann gas approach an EDF.

Now, we take the opportunity to offer some comments on the so-called diffusive and ballistic regimes. As is well known, diffusive and ballistic phonon transport under small time and spatial scales play a crucial role in fast-switching electronic devices and pulsed-laser processing of materials. The Fourier law represents only diffusive transport and predicts an infinite speed for the propagation of heat. Given the results of [8], we expect that the equations of nine-moment phonon hydrodynamics are hyperbolic in a convex set of states containing all quasi-equilibrium states and thus that they lead to a finite heat wave speed. However, although these equations may be a good model for short time scales and high thermal loads, they cannot describe ballistic phonon transport in short spatial scales. Instead of suggesting the hydrodynamic model, Joshi and Majumdar [20] used an equation of phonon radiative transfer to analyse heat transport under both short time and spatial scales. Salhoumi *et al* [21],

[4] In [18, 19], this distribution is also called the anisotropic Gaussian distribution.

in turn, considered including higher-order moments of the distribution function in the set of basic independent variables.

From the viewpoint of this paper, an interesting approach to transient heat transport was developed by Chen [22, 23]. His approach is called the ballistic-diffusive approximation. It begins by dividing the distribution function at any point into two components: $f = f_b + f_m$. The first component represents carriers originating from the boundaries and experiencing out-scattering only, whereas the second one represents those originating from inside the medium due to the excitation and the boundary contributions converted into scattered or emitted phonons after absorption. An equation for f_b can be extracted from the formalism of Pomraning [24]. For f_m, Chen used the hydrodynamic description that is familiar in thermal radiation. This description differs from the standard hyperbolic heat conduction, derived on the basis of the Cattaneo constitutive relation, mainly in the incorporation of an additional ballistic term. An advantage of using the Chen hybrid method to represent transient heat conduction from nano to macroscale is that the Cattaneo equation can always be replaced by a more accurate hydrodynamic model. For example, one can employ the four-moment system [7] or the equations of nine-moment hydrodynamics in place of the Cattaneo constitutive relation. Of course, further investigation of these issues may well represent our best opportunity to gain further insight into the nature of hybrid approaches, and such investigations are presently being pursued.

We finally mention the following. For the sake of simplicity, we ignore most of the intricacies of the phonon model. No distinction is made between longitudinal and transverse phonons. The dispersion relation for all three types of phonons has the form $\omega = c|\mathbf{k}|$, where c is the constant Debey speed. We let the components of the wave vector $\mathbf{k}$ range from $-\infty$ to $+\infty$.

Our paper is organized as follows. Section 2 is devoted to a brief treatment of the more relevant aspects of phonon kinetics. Section 3 first sets up a Hilbert space for the expansion and then defines an orthogonal basis in this Hilbert space. Section 4 shows how to relate the obtained expansion coefficients to the energy density, the heat flux and the deviatoric part of $\mathcal{M}^{ij}$. Section 5 centres around nine-moment phonon hydrodynamics. Section 6 is for final remarks. The auxiliary technical material is included as appendices A and B.

2. Phonon kinetics

The fundamental equation of phonon kinetic theory is the BP equation [4]. This equation governs the time evolution of the distribution function f describing the number density of phonons at position (x^i) having wave vector $\mathbf{k}$ and is given by

$$\partial_t f + c g^i \partial_i f = J(f), \tag{2.1}$$

where

$$\partial_t := \frac{\partial}{\partial t}, \qquad \partial_i := \frac{\partial}{\partial x^i}. \tag{2.2}$$

Here $J(f)$ is the collision term and (g^i) are the components of a unit vector $\mathbf{g}$ in the direction of $\mathbf{k}$. One knows fully well that $J(f)$ can be decomposed as

$$J(f) = J_r(f) + J_n(f), \tag{2.3}$$

where $J_r(f)$ and $J_n(f)$ are the collision terms representing the rates of change of f produced by resistive and normal processes, respectively. These collision terms must satisfy the conditions [1–3]

$$\int |\mathbf{k}| J_r(f)\, \mathrm{d}^3\mathbf{k} = 0, \tag{2.4a}$$

$$\int |\mathbf{k}| J_n(f)\, \mathrm{d}^3\mathbf{k} = 0, \qquad \int k^i J_n(f)\, \mathrm{d}^3\mathbf{k} = 0. \tag{2.4b}$$

Equations (2.4*b*) tell us that normal processes conserve both energy and momentum, while equation (2.4*a*) states that resistive processes conserve only energy.

Since the exact kinetic-theory expressions for $J_r(f)$ and $J_n(f)$ are quite formidable, a more phenomenological approach was proposed by Callaway [5], based on the use of a relaxation-time approximation of the form

$$J_r(f) = \frac{1}{\tau_r}(F_o - f), \qquad J_n(f) = \frac{1}{\tau_n}(F_* - f), \tag{2.5}$$

where all the physics is supposed to be included in **k**-dependent quantities τ_r and τ_n that should be evaluated elsewhere with a specific model. We refer to τ_r as the relaxation time for resistive processes and to τ_n as the relaxation time for normal processes. In order to list the explicit form of the functions F_o and F_*, we require some preliminary definitions:

$$\zeta_o := c\hbar|\mathbf{k}|\Delta_o, \qquad \zeta_* := c\hbar|\mathbf{k}|\Delta_*(1 - \mathbf{v}_* \cdot \mathbf{g}). \tag{2.6}$$

The objects (Δ_o, Δ_*) and $\mathbf{v}_*$ are a set of scalar and vector quantities that may depend on (t, x^i) and $\hbar$ is the Planck constant divided by 2π. With this notation, we obtain for F_o and F_*

$$F_o := \frac{1}{\mathrm{e}^{\zeta_0} - 1}, \qquad F_* := \frac{1}{\mathrm{e}^{\zeta_*} - 1}. \tag{2.7}$$

Combining (2.4) and (2.5), the values of $(\Delta_o, \Delta_*, \mathbf{v}_*)$ are then determined by the conditions

$$\int |\mathbf{k}| \frac{1}{\tau_r}(F_o - f)\, \mathrm{d}^3\mathbf{k} = 0, \tag{2.8a}$$

$$\int |\mathbf{k}| \frac{1}{\tau_n}(F_* - f)\, \mathrm{d}^3\mathbf{k} = 0, \tag{2.8b}$$

$$\int k^i \frac{1}{\tau_n}(F_* - f)\, \mathrm{d}^3\mathbf{k} = 0. \tag{2.8c}$$

Clearly, there are two tendencies: the normal processes will attempt to make the phonon gas approach F_* and the resistive processes will try to force it towards F_o. The original basis for approximation (2.5) was presumably its physically appealing form, corresponding to a relaxation phenomenon, together with the fact that a suitable choice of $(\Delta_o, \Delta_*, \mathbf{v}_*)$ allows the model to represent the conservation laws inherent in the true collision terms $J_r(f)$ and $J_n(f)$. In this context, we mention that the connection between the exact collision operator and the Callaway model for it was clarified by Simons [6].

Using the above definitions, the BP equation under the relaxation-time approximation is given by

$$\partial_t f + c g^i \partial_i f = \frac{1}{\tau_r}(F_o - f) + \frac{1}{\tau_n}(F_* - f). \tag{2.9}$$

Before showing that this equation leads to a non-negative entropy production, we first introduce the following formulae for the entropy density s and the entropy flux Φ^i:

$$s := -k_B y \hbar^3 \int H(f)\, \mathrm{d}^3\mathbf{k}, \qquad \Phi^i := -c k_B y \hbar^3 \int g^i H(f)\, \mathrm{d}^3\mathbf{k}, \tag{2.10}$$

where k_B is the Boltzmann constant and

$$y := 3(2\pi\hbar)^{-3}, \tag{2.11a}$$

$$H(f) := f \ln f - (1+f)\ln(1+f). \tag{2.11b}$$

In (2.11a), we need to multiply $(2\pi\hbar)^{-3}$ by 3; this is because there are three types of phonons corresponding to one longitudinal and two transversal sound waves. Now, we come to the entropy law. Multiplying (2.9) by $-k_B y\hbar^3[\mathrm{d}H(f)/\mathrm{d}f]$ and integrating over wave-vector space yields

$$\partial_t s + \partial_i \Phi^i = \sigma := \sigma_r + \sigma_n, \tag{2.12}$$

where

$$\sigma_r := -k_B y\hbar^3 \int \frac{\mathrm{d}H(f)}{\mathrm{d}f}\frac{1}{\tau_r}(F_o - f)\,\mathrm{d}^3\mathbf{k}, \tag{2.13a}$$

$$\sigma_n := -k_B y\hbar^3 \int \frac{\mathrm{d}H(f)}{\mathrm{d}f}\frac{1}{\tau_n}(F_* - f)\,\mathrm{d}^3\mathbf{k}. \tag{2.13b}$$

For essentially obvious reasons, we call σ the entropy production. With the aid of

$$\frac{\mathrm{d}H(f)}{\mathrm{d}f} = -\ln\left(\frac{1+f}{f}\right) \tag{2.14}$$

and

$$F_* - f = F_*(1+f) - f(1+F_*), \tag{2.15}$$

the quantity σ_n may be expressed in the form

$$\sigma_n = k_B y\hbar^3 \int \frac{1}{\tau_n}\,[F_*(1+f) - f(1+F_*)]\ln\left(\frac{1+f}{f}\right)\mathrm{d}^3\mathbf{k}. \tag{2.16}$$

Since

$$\ln\left(\frac{F_*}{1+F_*}\right) = -\zeta_* = -c\hbar|\mathbf{k}|\Delta_*(1 - \mathbf{v}_*\cdot\mathbf{g}), \tag{2.17}$$

it follows from (2.8b) and (2.8c) that

$$\int \frac{1}{\tau_n}(F_* - f)\ln\left(\frac{F_*}{1+F_*}\right)\mathrm{d}^3\mathbf{k} = 0. \tag{2.18}$$

As a consequence of (2.15) and (2.18), we may replace (2.16) by

$$\sigma_n = k_B y\hbar^3 \int \frac{1}{\tau_n}\,[F_*(1+f) - f(1+F_*)]\ln\left[\frac{F_*(1+f)}{f(1+F_*)}\right]\mathrm{d}^3\mathbf{k}. \tag{2.19}$$

This expression for σ_n is non-negative because elementary inspection shows that the integrand is non-negative; it vanishes for $f = F_*$. Precisely in the same way, we can prove that $\sigma_r \geqslant 0$, the equality holds if and only if $f = F_o$.

In phonon kinetic theory, one defines the energy density ϵ, the heat flux q^i and the flux of the heat flux $\mathcal{M}^{ij}$ by the integral formulae

$$\epsilon := cy\hbar^4 \int |\mathbf{k}| f\,\mathrm{d}^3\mathbf{k}, \tag{2.20a}$$

$$q^i := c^2 y\hbar^4 \int k^i f\,\mathrm{d}^3\mathbf{k}, \tag{2.20b}$$

$$\mathcal{M}^{ij} := c^3 y\hbar^4 \int k^i g^j f\,\mathrm{d}^3\mathbf{k}. \tag{2.20c}$$

Since $g^i = k^i/|\mathbf{k}|$, it is obvious that $\mathcal{M}^{ij} = \mathcal{M}^{ji}$. Moreover, from the above definitions of $(\epsilon, \mathbf{q})$ and the reasoning of [25] it follows that[5] $|\mathbf{q}| \leqslant c\epsilon$. This condition is a strict inequality unless f is a delta function. The deviatoric part of $\mathcal{M}^{ij}$ is given by

$$M^{ij} := c^3 y\hbar^4 \int k^{\langle i} g^{j\rangle} f \,\mathrm{d}^3\mathbf{k}. \tag{2.21}$$

As usual, angle brackets denote the symmetric trace-free part, e.g.,

$$k^{\langle i} g^{j\rangle} := k^i g^j - \tfrac{1}{3}|\mathbf{k}|\delta^{ij}, \qquad k^{\langle i} g^j g^{k\rangle} := k^i g^j g^k - \tfrac{3}{5} k^{(i}\delta^{jk)}. \tag{2.22}$$

Round brackets indicate symmetrization and δ^{ij} stands for the Kronecker delta.

By means of (2.9), we obtain at once

$$\partial_t \epsilon + \partial_i q^i = 0, \tag{2.23a}$$

$$\partial_t q^i + \frac{c^2}{3}\delta^{ij}\partial_j \epsilon + \partial_j M^{ij} = P_r^i, \tag{2.23b}$$

$$\partial_t M^{ij} + \frac{2c^2}{5}\delta^{k\langle i}\partial_k q^{j\rangle} + \partial_k M^{ijk} = P_r^{ij} + P_n^{ij}, \tag{2.23c}$$

where

$$M^{ijk} := c^4 y\hbar^4 \int k^{\langle i} g^j g^{k\rangle} f \,\mathrm{d}^3\mathbf{k}, \tag{2.24a}$$

$$P_r^i := c^2 y\hbar^4 \int k^i \frac{1}{\tau_r}(F_o - f)\,\mathrm{d}^3\mathbf{k}, \tag{2.24b}$$

$$P_r^{ij} := c^3 y\hbar^4 \int k^{\langle i} g^{j\rangle} \frac{1}{\tau_r}(F_o - f)\,\mathrm{d}^3\mathbf{k}, \tag{2.24c}$$

$$P_n^{ij} := c^3 y\hbar^4 \int k^{\langle i} g^{j\rangle} \frac{1}{\tau_n}(F_* - f)\,\mathrm{d}^3\mathbf{k}. \tag{2.24d}$$

In a similar fashion, it is also possible to derive the equations for M^{ijk} and higher-order moments of the distribution function. Of course, any finite set consisting of the moment equations is not a determined system since there appear more variables than equations. It can be made so, however, by choosing a specific functional form for $f = f(\mathbf{k})$ that depends on parameters which are taken to be functions of (t, x^i), where there are as many parameters as there are moment equations. For example, in the case of equations (2.23*a*)–(2.23*c*), the closure problem reduces to the problem of finding the distribution function that depends on (t, x^i) through (ϵ, q^i, M^{ij}). This observation will be of interest to us subsequently.

3. Expansion about an anisotropic Planck function

3.1. Local quasi-equilibrium

We regard as being appropriate to quasi-equilibrium any phase density f such as to be left unaltered by normal processes:

$$J_n(f) = 0. \tag{3.1}$$

[5] For any two wave vectors $\mathbf{k}$ and $\mathbf{k}'$, we easily show that $\mathbf{k}\cdot\mathbf{k}' \leqslant |\mathbf{k}|\,|\mathbf{k}'|$. Multiplying this inequality by $(c^2 y\hbar^4)^2 f(t, x^i, \mathbf{k}) f(t, x^i, \mathbf{k}')$ and integrating over $(\mathbf{k}, \mathbf{k}')$ yields $|\mathbf{q}|^2 \leqslant c^2\epsilon^2$.

From the properties of $J_n(f)$ we conclude that any such f is of the form

$$f = F := \frac{1}{\mathrm{e}^{\zeta} - 1}, \tag{3.2}$$

where

$$\zeta := c\hbar|\mathbf{k}|\Delta(1 - \mathbf{v}\cdot\mathbf{g}). \tag{3.3}$$

If $f = F$, equations (2.8b) and (2.8c) have the simple solution for $(\Delta_*, \mathbf{v}_*)$: $\Delta_* = \Delta$, $\mathbf{v}_* = \mathbf{v}$. In what follows, we call F the quasi-equilibrium Planck distribution or the anisotropic Planck function. This distribution contains the scalar function $\Delta = \Delta(t, x^i)$ and the vector function $\mathbf{v} = \mathbf{v}(t, x^i)$ which are largely at our disposal. Here we fix Δ and $\mathbf{v}$ so as to reproduce the actual energy density ϵ and the actual heat flux q^i:

$$\epsilon = cy\hbar^4 \int |\mathbf{k}| F \, \mathrm{d}^3\mathbf{k}, \qquad q^i = c^2 y\hbar^4 \int k^i F \, \mathrm{d}^3\mathbf{k}. \tag{3.4}$$

Hence we have for Δ and $\mathbf{v}$

$$\Delta = \frac{\chi}{\epsilon^{1/4}} \frac{(3+u)^{1/4}}{(1-u)^{3/4}}, \qquad \mathbf{v} = \frac{3}{2+W} \frac{\mathbf{q}}{c\epsilon}, \tag{3.5}$$

where

$$\chi := \left(\frac{4\pi^5 y}{45c^3}\right)^{1/4}, \qquad W := \sqrt{4 - 3\left(\frac{|\mathbf{q}|}{c\epsilon}\right)^2}, \qquad u := |\mathbf{v}|^2 = \frac{3(2-W)}{2+W}. \tag{3.6}$$

Assuming that we know ϵ and q^i, we express Δ and v^i as functions of ϵ and q^i. These functions were first derived by Larecki [7]. Since Δ diverges for $|\mathbf{q}| = c\epsilon$, we postulate that $|\mathbf{q}| < c\epsilon$. Given (3.5) and (3.6), this postulate yields the inequalities $|\mathbf{v}| < 1$ and $0 \leqslant u < 1$. Clearly, $u = |\mathbf{v}|^2 = 0$ if and only if $|\mathbf{q}| = 0$.

The closure procedure for the four-moment system is based on F. With the definitions

$$M_F^{ij} := c^3 y\hbar^4 \int k^{\langle i} g^{j\rangle} F \, \mathrm{d}^3\mathbf{k}, \qquad P_{rF}^i := c^2 y\hbar^4 \int k^i \frac{1}{\tau_r}(F_o - F) \, \mathrm{d}^3\mathbf{k}, \tag{3.7}$$

this closure procedure may be stated simply. Let M^{ij} and P_r^i in (2.23b) have the form

$$M^{ij} = M_F^{ij}, \qquad P_r^i = P_{rF}^i. \tag{3.8}$$

Having also (2.23a), this results in the system of equations from which the evolution of (ϵ, q^i) can in principle be determined:

$$\partial_t \epsilon + \partial_i q^i = 0, \tag{3.9a}$$

$$\partial_t q^i + \partial_j\left(\frac{c^2}{3}\delta^{ij}\epsilon + M_F^{ij}\right) = P_{rF}^i. \tag{3.9b}$$

Such is indeed the case because equations (3.7) provide the motivation for expressing M_F^{ij} and P_{rF}^i in terms of ϵ and q^i. Explicitly, given (3.2) and (3.3) as well as (3.5) and (3.6), we obtain for M_F^{ij},

$$M_F^{ij} = \frac{4c^2\epsilon}{3+u} v^{\langle i} v^{j\rangle} = \frac{3c}{2c\epsilon + \sqrt{4c^2\epsilon^2 - 3|\mathbf{q}|^2}} q^{\langle i} q^{j\rangle}. \tag{3.10}$$

Moreover, when τ_r does not depend on $\mathbf{k}$ and $\tau_r = \tau_r(\epsilon)$, (3.4) and (3.7) yield P_{rF}^i in the form

$$P_{rF}^i = -\frac{1}{\tau_r} q^i. \tag{3.11}$$

More details on the four-moment system (3.9) can be found in [7]. There, it was shown how the closure by entropy maximization leads naturally to both the anisotropic Planck function and the formulae equivalent to (3.5), (3.6) and (3.10).

If f satisfies the condition $J_r(f) = 0$, then f is an equilibrium Planck distribution given by

$$f = F_E := \frac{1}{e^{\zeta_E} - 1}, \tag{3.12}$$

where

$$\zeta_E := c\hbar|\mathbf{k}|\Delta_E. \tag{3.13}$$

Considering the case in which

$$cy\hbar^4 \int |\mathbf{k}| F_E \, d^3\mathbf{k} = \epsilon, \tag{3.14}$$

we find that

$$\Delta_E = \frac{\chi}{\epsilon^{1/4}}. \tag{3.15}$$

A limitation of the distribution function F_E is that it admits no heat flux. Consequently, the use of this function for the expansion leads to the theory which treats the heat flux as a small perturbative quantity.

3.2. Perturbations and the weighted Hilbert space

If $\tau_n \ll \tau_r$, we can assume that f is close to F. Then it is natural to define the perturbation with respect to F and thus to look for a distribution function in the form

$$f = F\left[1 - c\hbar|\mathbf{k}|\Delta(1+F)\varphi\right], \tag{3.16}$$

where

$$\varphi = \varphi(t, x^i, \mathbf{k}) = \varphi(t, x^i, |\mathbf{k}|, \mathbf{g}) = \varphi(t, x^i, \zeta, \mathbf{g}). \tag{3.17}$$

In (3.17), we have proposed the passage from $\mathbf{k}$ to $(\zeta, \mathbf{g})$. Because of (3.3), this passage is a diffeomorphic change of variables if $|\mathbf{k}| \neq 0$:

$$\mathbf{k} = |\mathbf{k}|\,\mathbf{g} = \frac{\zeta}{c\hbar\Delta(1 - \mathbf{v}\cdot\mathbf{g})}\,\mathbf{g}. \tag{3.18}$$

Setting $R_+ := (0, \infty)$ and denoting by S^2 the unit sphere, we observe that $\zeta \in R_+$ and $\mathbf{g} \in S^2$. Therefore, for each (t, x^i), the perturbation φ is a function of the three independent variables $(\zeta, \mathbf{g}) \in R_+ \times S^2$.

In order to construct the appropriate Hilbert space for φ, we introduce the following objects:

$$V_1 := V_1(\mathbf{v}\cdot\mathbf{g}) := \frac{1}{2\pi(1 - \mathbf{v}\cdot\mathbf{g})^5}, \tag{3.19a}$$

$$V_2 := V_2(\zeta) := \frac{15}{4\pi^4}\zeta^4 F(1+F) = \frac{15}{4\pi^4}\frac{\zeta^4 e^{\zeta}}{(e^{\zeta} - 1)^2}. \tag{3.19b}$$

Using these objects, the scalar product between two perturbations is defined by

$$\langle\varphi_1|\varphi_2\rangle := \int_{S^2}\int_{R_+} V_1 V_2 \varphi_1\varphi_2 \, d\zeta \, d^2\mathbf{g}, \tag{3.20}$$

where $d^2\mathbf{g}$ is the incremental solid angle. If $\theta \in [0, \pi]$ denotes the polar angle ($\cos\theta = \mathbf{v}\cdot\mathbf{g}/|\mathbf{v}|$) and $\phi \in [0, 2\pi)$ denotes the azimuthal angle, then $d^2\mathbf{g}$ can be identified with $\sin\theta\, d\theta\, d\phi$. Let $\mathcal{H}$ be the set of all the perturbations which are square-integrable on $R_+ \times S^2$ with weight $V_1 V_2$. We find it convenient to refer to $\mathcal{H}$ as the weighted Hilbert space. Since $\langle\cdot\,|\,\cdot\rangle$ is the scalar product in $\mathcal{H}$, the norm of $\varphi \in \mathcal{H}$ is the square root of $\langle\varphi\,|\,\varphi\rangle$; thus $\|\varphi\| := \sqrt{\langle\varphi\,|\,\varphi\rangle}$.

We now show that the norm $\|\cdot\|$ can be used to evaluate the entropy density s in the neighbourhood of quasi-equilibrium. Substitution of (3.16) into (2.11*b*) leads to an expression for the quantity $H(f)$ which is a function of the perturbation φ. Because of the complicated nature of this expression, the entropy density s as defined by (2.10) is very difficult to analyse. In the neighbourhood of quasi-equilibrium, however, a simple approximation can be obtained by using the first three terms of the expansion of $H(f)$:

$$H(f) = H(F) + c\hbar|\mathbf{k}|\zeta\Delta F(1+F)\varphi + \tfrac{1}{2}c^2\hbar^2|\mathbf{k}|^2\Delta^2 F(1+F)\varphi^2 + O(\varphi^3). \tag{3.21}$$

In view of this approximation to $H(f)$, the structure of (2.10) may be further exposed by a change to quasi-equilibrium coordinates in the integral. If we employ the quasi-radial variable ζ and the unit vector $\mathbf{g}$, so that $\mathbf{k}$ is given by (3.18) and

$$d^3\mathbf{k} = |\mathbf{k}|^2\, d|\mathbf{k}| d^2\mathbf{g} = \frac{\zeta^2}{c^3\hbar^3\Delta^3(1-\mathbf{v}\cdot\mathbf{g})^3}\, d\zeta\, d^2\mathbf{g}, \tag{3.22}$$

then (2.10) takes the form

$$s = s_F\big[1 - \tfrac{3}{2}(1-u)^2\big(\langle 1-\mathbf{v}\cdot\mathbf{g}\,|\,\varphi\rangle + \tfrac{1}{2}\|\varphi\|^2\big)\big], \tag{3.23}$$

where

$$s_F := -k_B y\hbar^3 \int H(F)\, d^3\mathbf{k} = 4k_B\epsilon\Delta\frac{1-u}{3+u}. \tag{3.24}$$

In the process of deriving the above approximate formula for s, we have used (3.5), (3.6), (3.19), (3.20) and (A.1). Introducing φ instead of f, we easily verify that (2.20*a*), (2.20*b*) and (3.4) imply the following conditions on φ:

$$\langle 1\,|\,\varphi\rangle = 0, \qquad \langle g^i\,|\,\varphi\rangle = 0; \tag{3.25}$$

thus

$$\langle 1-\mathbf{v}\cdot\mathbf{g}\,|\,\varphi\rangle = 0. \tag{3.26}$$

With the aid of these results, (3.23) gives

$$s = s_F\big[1 - \tfrac{3}{4}(1-u)^2\|\varphi\|^2\big], \tag{3.27}$$

showing the small deviations of s from s_F to be proportional to the square root of $\langle\varphi\,|\,\varphi\rangle$.

3.3. Expansion in terms of orthogonal functions

Before constructing an orthogonal basis in $\mathcal{H}$, we first define $\mathcal{H}_1$ ($\mathcal{H}_2$) to be the Hilbert space of real functions which are square-integrable on S^2 (R_+) with weight V_1 (V_2). The scalar products in $\mathcal{H}_1$ and $\mathcal{H}_2$ are given by

$$(\beta_1\,|\,\beta_2) := \int_{S^2} V_1\beta_1\beta_2\, d^2\mathbf{g} \qquad (\beta_1 \in \mathcal{H}_1, \beta_2 \in \mathcal{H}_1) \tag{3.28a}$$

and

$$[\rho_1\,|\,\rho_2] := \int_{R_+} V_2\rho_1\rho_2\, d\zeta \qquad (\rho_1 \in \mathcal{H}_2, \rho_2 \in \mathcal{H}_2), \tag{3.28b}$$

respectively. Let $\boldsymbol{\beta}_1$ and $\boldsymbol{\beta}_2$ be the tensor functions on S^2. Then we set

$$(\boldsymbol{\beta}_1 \,|\, \boldsymbol{\beta}_2) := \int_{S^2} V_1(\boldsymbol{\beta}_1 \otimes \boldsymbol{\beta}_2)\, \mathrm{d}^2\mathbf{g}. \tag{3.29}$$

For real functions, (3.29) reduces to (3.28*a*).

If we orthogonalize the set of non-negative powers of ζ,

$$\{\zeta^n\} := \{\, \zeta^n \mid n = 0, 1, 2, \ldots, \infty\}, \tag{3.30}$$

in the sense explained in [26, p 23], we obtain a set of polynomials,

$$\{\Omega_n\} := \{\Omega_n(\zeta) \mid n = 0, 1, 2, \ldots, \infty\}, \tag{3.31}$$

uniquely determined by the following two conditions: (i) $\Omega_n(\zeta)$ is a polynomial of precise degree n in which the coefficient of ζ^n is positive; (ii) $\{\Omega_n\}$ is the orthonormal system, i.e., $[\Omega_n \,|\, \Omega_n] = \delta_{nm}$. Because of (A.1), we obtain for $\Omega_0(\zeta)$

$$\Omega_0(\zeta) = 1. \tag{3.32}$$

Using the lemma of Dijkstra and van Leeuwen as formulated in [27, p 468], it is possible to prove that the system $\{\Omega_n\}$ forms an orthonormal basis in $\mathcal{H}_2$.

As a next step, we define $\mathbf{g}_\perp$ and γ by

$$\mathbf{g}_\perp := \mathbf{g} - \frac{1}{u}(\mathbf{v}\cdot\mathbf{g})\mathbf{v}, \qquad \gamma := \boldsymbol{\delta} - \frac{1}{u}(\mathbf{v}\otimes\mathbf{v}), \tag{3.33}$$

where $\boldsymbol{\delta}$ is the unit tensor. We may interpret $\mathbf{g}_\perp$ as the part of $\mathbf{g}$ orthogonal to $\mathbf{v}$ and γ as the projection tensor. The components of $\mathbf{g}_\perp$ and γ are

$$g_\perp^i = g^i - \frac{1}{u}(\mathbf{v}\cdot\mathbf{g})v^i, \qquad \gamma^{ij} = \delta^{ij} - \frac{1}{u}v^i v^j. \tag{3.34}$$

Now, if we orthogonalize the set of tensorial powers of $\mathbf{g}$,

$$\{\otimes^n\mathbf{g}\} := \{\, \otimes^n\mathbf{g} \mid n = 0, 1, 2, \ldots, \infty\}, \tag{3.35}$$

we obtain a set of tensor functions,

$$\{\boldsymbol{\Pi}_n\} := \{\, \boldsymbol{\Pi}_n(\mathbf{g}, \mathbf{v}) \mid n = 0, 1, 2, \ldots, \infty\}, \tag{3.36}$$

such that $(\boldsymbol{\Pi}_n \,|\, \boldsymbol{\Pi}_m) = \mathbf{0}$ for $n \neq m$. The first few functions $\boldsymbol{\Pi}_n$ can be expressed as

$$\boldsymbol{\Pi}_0 := \Pi_0 := 1 - u, \tag{3.37a}$$

$$\boldsymbol{\Pi}_1 := \Pi_1 := \mathbf{v}\cdot\mathbf{g} - \frac{u(5+u)}{3(1+u)}, \tag{3.37b}$$

$$\boldsymbol{\Pi}_2 := \sqrt{1-u}\;\mathbf{g}_\perp, \tag{3.37c}$$

$$\boldsymbol{\Pi}_3 := \Pi_3 := \frac{1}{3-u}\,[1 + u - 2(\mathbf{v}\cdot\mathbf{g})] - \frac{1}{2}\,|\mathbf{g}_\perp|^2, \tag{3.37d}$$

$$\boldsymbol{\Pi}_4 := (\mathbf{v}\cdot\mathbf{g} - u)\mathbf{g}_\perp, \tag{3.37e}$$

$$\boldsymbol{\Pi}_5 := \mathbf{g}_\perp \otimes \mathbf{g}_\perp - \frac{1}{2}|\mathbf{g}_\perp|^2\gamma. \tag{3.37f}$$

The components of $\boldsymbol{\Pi}_2$, $\boldsymbol{\Pi}_4$ and $\boldsymbol{\Pi}_5$ are

$$\Pi_2^i = \sqrt{1-u}\; g_\perp^i, \tag{3.38a}$$

$$\Pi_4^i = (\mathbf{v}\cdot\mathbf{g} - u)g_\perp^i, \tag{3.38b}$$

$$\Pi_5^{ij} = g_\perp^i g_\perp^j - \tfrac{1}{2}|\mathbf{g}_\perp|^2\gamma^{ij}. \tag{3.38c}$$

Note that

$$\Pi_2^i v_i = \Pi_4^i v_i = 0, \tag{3.39a}$$

$$\Pi_5^{ij} = \Pi_5^{ji}, \qquad \Pi_5^{ij} v_j = 0, \qquad \Pi_5^{ij} \gamma_{ij} = 0. \tag{3.39b}$$

Here and throughout this paper, we adopt the useful convention whereby the component indices are lowered and raised with δ_{ij} and δ^{ij}, respectively. The system $\{\mathbf{\Pi}_n\}$ forms a basis in $\mathcal{H}_1$, in the sense that $\beta \in \mathcal{H}_1$ can be expanded as

$$\beta = \sum_{n=0}^{\infty} \beta^n \cdot \mathbf{\Pi}_n, \tag{3.40}$$

where the tensor quantities β^n are the expansion coefficients and the dot stands for the inner product of the tensors involved.

For the perturbation $\varphi \in \mathcal{H}$, since $\{\mathbf{\Pi}_m \, \Omega_n\}$ is a complete set of orthogonal functions, we have

$$\varphi = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} (\varphi^{n|m} \cdot \mathbf{\Pi}_m) \Omega_n, \tag{3.41a}$$

or using a component notation,

$$\varphi = \sum_{n=0}^{\infty} \left(\varphi^{n|0} \, \Pi_0 + \varphi^{n|1} \, \Pi_1 + \varphi_i^{n|2} \, \Pi_2^i + \varphi^{n|3} \, \Pi_3 + \varphi_i^{n|4} \, \Pi_4^i + \varphi_{ij}^{n|5} \, \Pi_5^{ij} + \cdots \right) \Omega_n. \tag{3.41b}$$

The expansion coefficients $\varphi^{n|m}$ are functions of (t, x^i) and the dependence of φ on (t, x^i) is contained in

$$\varphi^{n|m} = \varphi^{n|m}(t, x^i) \tag{3.42}$$

and

$$\mathbf{\Pi}_m = \mathbf{\Pi}_m(\mathbf{g}, \mathbf{v}(t, x^i)). \tag{3.43}$$

As a consequence of (3.39*a*) and (3.39*b*), it is possible to assume without any loss of generality that

$$\varphi_i^{n|2} v^i = \varphi_i^{n|4} v^i = 0, \tag{3.44a}$$

$$\varphi_{ij}^{n|5} = \varphi_{ji}^{n|5}, \qquad \varphi_{ij}^{n|5} v^j = 0, \qquad \varphi_{ij}^{n|5} \gamma^{ij} = 0. \tag{3.44b}$$

According to (3.37*a*)–(3.37*c*) and (3.41), equations (3.25) are equivalent to the conditions

$$\varphi^{0|0} = 0, \qquad \varphi^{0|1} = 0, \qquad \varphi_i^{0|2} = 0. \tag{3.45}$$

With the exception of these conditions, the expansion coefficients $\varphi^{n|m}$ are arbitrary except for certain inequalities that express the fact that $(1-u)\,\|\varphi\|$ is small[6] (see (3.27) and (3.51)). The first significant coefficients are the coefficients $\left(\varphi^{0|3}, \varphi_i^{0|4}, \varphi_{ij}^{0|5}\right)$ which can be used to evaluate the deviation of M^{ij} from M_F^{ij} (see section 4).

[6] For example, abbreviating $(\varphi^{n|m} \cdot \varphi^{n|m})^{1/2}$ as $|\varphi^{n|m}|$, it follows from $(1-u)\,\|\varphi\| \ll 1$ that $|\varphi^{n|m}| \ll 1$.

3.4. Expansion coefficients and the entropy density

Expansion (3.41) enables us to relate an approximate expression for the entropy density s, namely (3.27), to the expansion coefficients $\varphi^{n|m}$. As a first step in the explicit evaluation of this expression in terms of $\varphi^{n|m}$, it is convenient to introduce the following quantities:

$$R := \frac{1}{2\sqrt{u}} \ln\left(\frac{1+\sqrt{u}}{1-\sqrt{u}}\right), \tag{3.46a}$$

$$A := \frac{1}{u^2}\left[(1-u)^2 R + \frac{1}{3}(5u-3)\right], \tag{3.46b}$$

$$D := \frac{2}{3} - A, \qquad E := 3(3-u)A - 4. \tag{3.46c}$$

In view of (3.6), we may think of these quantities as being the functions of ϵ and $\mathbf{q}$. Definitions (3.46a) and (3.46b) are readily understood in the case when $u > 0$ (i.e., when $|\mathbf{q}| \neq 0$). To get precise values for R and A (and hence for D and E) as u approaches 0 ($0 \leqslant u < 1$), it need only be observed that

$$R = \sum_{n=0}^{\infty} \frac{1}{2n+1} u^n, \tag{3.47a}$$

$$A = \sum_{n=0}^{\infty} \frac{8}{(2n+1)(2n+3)(2n+5)} u^n. \tag{3.47b}$$

Thus, if $u = 0$, the values of (R, A, D, E) are

$$R = 1, \qquad A = \tfrac{8}{15}, \qquad D = \tfrac{2}{15}, \qquad E = \tfrac{4}{5}. \tag{3.48}$$

Because of this, there is no true singularity in (3.46) and the quantities R, A, D and E are regular, continuously differentiable functions of ϵ and $\mathbf{q}$.

Now, using (A.5), we obtain

$$(\mathbf{\Pi}_0\,|\,\mathbf{\Pi}_0) = \frac{2(1+u)}{(1-u)^2}, \tag{3.49a}$$

$$(\mathbf{\Pi}_1\,|\,\mathbf{\Pi}_1) = \frac{2u(3-u)}{9(1+u)(1-u)^2}, \tag{3.49b}$$

$$\left(\mathbf{\Pi}_2^i\middle|\mathbf{\Pi}_2^j\right) = \frac{2}{3(1-u)^2}\,\gamma^{ij}, \tag{3.49c}$$

$$(\mathbf{\Pi}_3\,|\,\mathbf{\Pi}_3) = \frac{E}{6(3-u)(1-u)^2}, \tag{3.49d}$$

$$\left(\mathbf{\Pi}_4^i\middle|\mathbf{\Pi}_4^j\right) = \frac{uD}{(1-u)^2}\,\gamma^{ij}, \tag{3.49e}$$

$$\left(\mathbf{\Pi}_5^{ij}\middle|\mathbf{\Pi}_5^{kl}\right) = \frac{A}{4(1-u)^2}(\gamma^{ik}\gamma^{jl} + \gamma^{il}\gamma^{jk} - \gamma^{ij}\gamma^{kl}), \text{ etc.} \tag{3.49f}$$

It follows from these formulae that

$$A > 0, \quad D > 0, \quad E > 0 \tag{3.50}$$

as long as $0 \leqslant u < 1$. With the aid of (3.41) and (3.49), the approximate formula (3.27) can be written in the form

$$s = s_F \left\{ 1 - \sum_{n=0}^{\infty} \left[\frac{3}{2}(1+u)\,|\varphi^{n|0}|^2 + \frac{u(3-u)}{6(1+u)}\,|\varphi^{n|1}|^2 + \frac{1}{2}\,|\varphi^{n|2}|^2 + \frac{E}{8(3-u)}\,|\varphi^{n|3}|^2 \right.\right.$$
$$\left.\left. + \frac{3}{4}\,u D\,|\varphi^{n|4}|^2 + \frac{3}{8}\,A\,|\varphi^{n|5}|^2 + \cdots \right]\right\}, \tag{3.51}$$

where

$$|\varphi^{n|m}| := \sqrt{\varphi^{n|m} \cdot \varphi^{n|m}}. \tag{3.52}$$

Consequently, expansion (3.41) diagonalizes the (linearized) entropy. Neglecting in (3.51) the terms that involve the expansion coefficients $\varphi^{n|m}$ other than $(\varphi^{0|3}, \varphi^{0|4}, \varphi^{0|5})$, we shall use the resulting expression for s in [8] to specify the region of hyperbolicity for the nine-moment system (5.22) in the one-dimensional case. Then the solutions to (5.22) have rotational symmetry about the x-axis ($x := x^1$) and the reduced system contains only three independent gas-state variables.

4. Connection between moments and expansion coefficients

In this section, we are concerned solely with the problem of relating M^{ij} or $M^{ij} - M_F^{ij}$ to $\left(\varphi^{0|3}, \varphi_i^{0|4}, \varphi_{ij}^{0|5}\right)$. It is out of place here to discuss similar problems for M^{ijk} and higher-order moments of the distribution function.

Remembering that M_F^{ij} is characterized by (3.7) and (3.10), it follows from (2.21), (3.16)–(3.20), (3.22), (3.5) and (3.6) that

$$N^{ij} := M^{ij} - M_F^{ij} = M^{ij} - \frac{4c^2\epsilon}{3+u} v^{\langle i} v^{j\rangle} = M^{ij} - \frac{3c}{2c\epsilon + \sqrt{4c^2\epsilon^2 - 3|\mathbf{q}|^2}} q^{\langle i} q^{j\rangle} \tag{4.1}$$

can be written as

$$N^{ij} = -6c^2\epsilon\,\frac{(1-u)^3}{3+u}\,\langle g^i g^j\,|\,\varphi\rangle. \tag{4.2}$$

Then equations (3.41) and (3.49), in conjunction with the conditions (3.45) and the relations

$$g^i g^j = \Omega_0\,\Pi_5^{ij} + 2\left[\frac{1}{\sqrt{1-u}}\,\Omega_0\,\Pi_2^{(i} + \frac{1}{u}\,\Omega_0\,\Pi_4^{(i}\right] v^{j)}$$
$$+ \frac{1}{u}\left[\frac{1+5u}{3(1-u^2)}\,\Omega_0\,\Pi_0 + \frac{4}{3-u}\,\Omega_0\,\Pi_1 + 2\,\Omega_0\,\Pi_3\right] v^i v^j$$
$$+ \frac{1}{2}\left[\frac{2}{3(1+u)}\,\Omega_0\,\Pi_0 - \frac{4}{3-u}\,\Omega_0\,\Pi_1 - 2\,\Omega_0\,\Pi_3\right]\gamma^{ij} \tag{4.3}$$

and $[\Omega_0\,|\,\Omega_n] = \delta_{0n}$, enable us to express

$$\tilde{N}^{ij} := \frac{1}{3c^2\epsilon}\left(\frac{3+u}{1-u}\right) N^{ij} \tag{4.4}$$

in the form

$$\tilde{N}^{ij} = -A\,\gamma^{ik}\gamma^{jl}\,\varphi_{kl}^{0|5} - 4D\,v^{(i}\gamma^{j)k}\,\varphi_k^{0|4} + \frac{E}{3(3-u)}\left(\gamma^{ij} - \frac{2}{u}\,v^i v^j\right)\varphi^{0|3}. \tag{4.5}$$

Using this formula for $\tilde{N}^{ij}$, we easily obtain

$$\varphi^{0|3} = -\frac{3(3-u)}{2uE}\,\tilde{N}^{kl}\,v_k v_l, \tag{4.6a}$$

$$\varphi_i^{0|4} = -\frac{1}{2uD}\left(\tilde{N}_{ij}\,v^j - \frac{1}{u}\,\tilde{N}^{kl}\,v_k v_l v_i\right), \tag{4.6b}$$

$$\varphi_{ij}^{0|5} = -\frac{1}{A}\left[\tilde{N}^{kl}\,v_k v_l\left(\frac{1}{2}\,\gamma_{ij} + \frac{1}{u}\,v_i v_j\right) - \frac{2}{u}\,v^k\tilde{N}_{k(i}v_{j)} + \tilde{N}_{ij}\right], \tag{4.6c}$$

where now $u \neq 0$.

Since equations (4.5) and (4.6) are ill-defined if $u = 0$, our purpose here is to construct the equivalent relations which have limits as the quantity $u = |\mathbf{v}|^2$ approaches 0. Defining the new tensor variable λ_{ij} by

$$\lambda_{ij} := -\frac{1}{6}\,\varphi^{0|3}\left(\gamma_{ij} - \frac{2}{u}\,v_i v_j\right) + \varphi_{(i}^{0|4}v_{j)} + \varphi_{ij}^{0|5}, \tag{4.7}$$

we first observe that the properties of this variable are very much analogous to those of M^{ij}:

$$\lambda_{ij} = \lambda_{ji}, \qquad \delta^{ij}\lambda_{ij} = 0. \tag{4.8}$$

In view of (3.6) and (3.34), we also observe that the expansion coefficients $\left(\varphi^{0|3}, \varphi_i^{0|4}, \varphi_{ij}^{0|5}\right)$ can be expressed in terms of λ_{ij}:

$$\varphi^{0|3} = -3\lambda_{kl}\,\gamma^{kl}, \tag{4.9a}$$

$$\varphi_i^{0|4} = \frac{2}{u}(\lambda_{ij}v^j + \lambda_{kl}\,\gamma^{kl}v_i), \tag{4.9b}$$

$$\varphi_{ij}^{0|5} = \lambda_{ij} - \frac{2}{u}\,v^k\lambda_{k(i}v_{j)} - \lambda_{kl}\,\gamma^{kl}\left(\frac{1}{u}\,v_i v_j + \frac{1}{2}\,\gamma_{ij}\right). \tag{4.9c}$$

Substituting the above formulae into (4.5) yields

$$\tilde{N}^{ij} = -A\,\lambda^{ij} - \frac{8}{3+u}\,B\,v^k\lambda_k^{\ \langle i}v^{j\rangle} - C\,\lambda_{kl}\,v^k v^l\,v^{\langle i}v^{j\rangle}, \tag{4.10}$$

where

$$B := \frac{3+u}{4u}\left(\frac{8}{3} - 5A\right), \tag{4.11a}$$

$$C := \frac{8(4u-21) + 105(3-u)A}{6u^2(3-u)}. \tag{4.11b}$$

Recalling (3.46) and (3.6), the coefficients B and C are well-behaved as functions of (ϵ, q) near $u = 0$. Indeed, a direct calculation using (3.47b) shows that B and $(3-u)C/3$ may be expanded in absolutely convergent power series in u valid for $u < 1$. In the limit $u \to 0$, these series expansions lead to

$$B = -\tfrac{2}{7}, \qquad C = 0. \tag{4.12}$$

Given the useful identities (B.3) and (B.4), we are able to transform relation (4.10) for $\tilde{N}^{ij}$ into the following relation for λ_{ij}:

$$\lambda^{ij} = -\frac{1}{A}\left[\tilde{N}^{ij} - \frac{1}{2D}\left(\frac{4}{3+u}\,B\,v^k\tilde{N}_k^{\ \langle i}v^{j\rangle} + \frac{K}{6E}\,\tilde{N}_{kl}\,v^k v^l\,v^{\langle i}v^{j\rangle}\right)\right], \tag{4.13}$$

where

$$K := \frac{1}{u^2}[45\,(3-u)A^2 + 6\,(3u-17)A + 16]. \tag{4.14}$$

In the limit $u \to 0$, (4.14) becomes

$$K = -\tfrac{64}{147}. \tag{4.15}$$

The net upshot of these calculations may be stated very neatly. Instead of defining the variable λ_{ij} by (4.7) valid for $u \neq 0$, it is also possible to define λ_{ij} as a regular function of $(\epsilon, \mathbf{q})$ and M^{ij}; see (4.13), (4.4) and (4.1) together with (B.5), (4.14) and (5.10)–(5.13). This function reduces to $\lambda^{ij} = -15M^{ij}/8c^2\epsilon$ as u approaches 0.

In (3.41), the part of φ which contains only a contribution from the expansion coefficients $\left(\varphi^{0|3}, \varphi_i^{0|4}, \varphi_{ij}^{0|5}\right)$ is given by

$$\psi := \varphi^{0|3}\,\Pi_3 + \varphi_i^{0|4}\,\Pi_4^i + \varphi_{ij}^{0|5}\,\Pi_5^{ij}. \tag{4.16}$$

Remarkably, employing (3.37*d*)–(3.37*f*) and (4.9), we can write ψ in the form

$$\psi = \lambda_{ij}\left[g^i\,(g^j - 2v^j) + \frac{2}{3-u}\,(2 - \mathbf{v}\cdot\mathbf{g})\,v^i v^j\right]. \tag{4.17}$$

Upon relating λ_{ij} to (ϵ, q^i, M^{ij}) and using (5.13) and (B.5), $\psi \in \mathcal{H}_1$ is to be expressed in terms of the unit vector $\mathbf{g} := \mathbf{k}/|\mathbf{k}|$ and the physical variables $(\epsilon, \mathbf{q}, M^{ij})$.

5. Nine-moment closure

5.1. Specification of the relaxation times

Given (2.5)–(2.8) and (3.12)–(3.15), we shall treat the collision term $J_n(f) = (F_* - f)/\tau_n$ with great care, but shall handle the collision term $J_r(f) = (F_o - f)/\tau_r$ schematically, as in [12], by assuming an effective relaxation tima τ_r which depends on ϵ and is independent of $\mathbf{k}$:

$$\tau_r = \tau_r(\epsilon). \tag{5.1}$$

In that case, the quantity Δ_o can be identified with $\Delta_E = \chi/\epsilon^{1/4}$ (see (3.6) and (3.15)) and this ensures that the rate of change of the energy density due to resistive processes is zero.

For our purposes, we postulate that τ_n is independent of M^{ij} and depends on $(|\mathbf{k}|, \mathbf{g})$ and $(\epsilon, \Delta_*, \mathbf{v}_*)$ as

$$\tau_n = \tau_n(\epsilon, \zeta_*), \tag{5.2}$$

where ζ_* is defined by (2.6)–(2.8). Given (3.15), as a useful example of the above dependence of τ_n on $(|\mathbf{k}|, \mathbf{g})$ and $(\epsilon, \Delta_*, \mathbf{v}_*)$, we consider the relation

$$\tau_n = \alpha\,\Delta_E^5\,\zeta_*^{m-5} = \alpha\left(\frac{\chi}{\epsilon^{1/4}}\right)^5 \zeta_*^{m-5} \tag{5.3}$$

in which $\alpha > 0$ and $2 < m \leqslant 4$. Here α is a constant and m is an exponent determined by the interaction mechanism (see, e.g., [28]). If $|\mathbf{v}_*| \ll 1$, then $\zeta_* \cong c\hbar\,|\mathbf{k}|\,\Delta_*$ and (5.3) reduces to

$$\tau_n = \alpha\,\Delta_E^5\,(c\hbar|\mathbf{k}|\Delta_*)^{m-5}. \tag{5.4}$$

It is natural to interpret $T_* := 1/k_B\Delta_*$ as the relaxation temperature [6]. In the case when this temperature does not differ significantly from the local equilibrium temperature $T_E := 1/k_B\Delta_E$, we see that (5.4) is just the equivalent of Herring's formula [29].

The typical relaxation time τ_n tends to ∞ as $|\mathbf{k}| \to 0$, and long-wavelength phonons (i.e., phonons with $|\mathbf{k}| \cong 0$) have a very long lifetime. As was already pointed out by

Jäckle [30] and Buot [31], an important consequence of this behaviour of τ_n is the non-existence of a gap in the eigenvalue spectrum of the linearized collision operator $\mathcal{L}_n$ and the breakdown of the usual justification of the hydrodynamic equations by means of perturbation theory. In order to derive phonon hydrodynamics from the linearized BP equation, the distribution of the low-lying eigenvalues of $\mathcal{L}_n$ must be taken into account.

However, there are physical arguments for the validity of the hydrodynamic description. First, the hydrodynamic equations for local temperature and drift velocity, which were proposed by many authors in spite of the mathematical problems originating in the gapless spectrum of $\mathcal{L}_n$, were able to describe observations associated with second sound and Poiseuille flow in a satisfactory way, at least qualitatively (see, e.g., [1–3]). Second, considering the smallness of the phase space of the long-wavelength phonons, Beck [32] arrived at the following result in connection with the low-lying eigenvalues of $\mathcal{L}_n$. As long as the relation (5.4) holds true and $2 < m \leqslant 4$, the fact that τ_n^{-1} reaches values arbitrarily close to zero will not have a strong influence on the hydrodynamic equations. Physically, the inequality $m > 2$ means that the lifetime τ_n of long-wavelength phonons diverges with a power that is smaller than the power with which their phase space goes to zero. Herring [29] and Holland [33] suggested that the values $m = 4$ for transverse and $m = 3$ for longitudinal phonons seem most probable in crystals of high symmetry.

If $2 < m \leqslant 4$, the major contribution to the integrals in (2.20) stems from wave vectors of thermal phonons, i.e., from wave vectors such that $|\mathbf{k}| \cong k_{th} := k_B T_E / c\hbar$. Because of this, one can try to restrict the Brillouin zone to thermal phonons making the main contribution to quantities like energy density, etc and treat $\mathcal{L}_n$ as if it had a spectral gap [34]. Relation (5.4) is then replaced by

$$\bar{\tau}_n := \alpha\,(k_B T_E)^{-m}\,(c\hbar\,k_{th})^{m-5} \tag{5.5}$$

and, in the case when normal processes dominate the phonon distribution, we may assume that

$$\bar{\tau}_n \ll \tau_r. \tag{5.6}$$

The physical meaning of this inequality is clear: during the first time period, the normal time, the distribution relaxes to a quasi-equilibrium Planck distribution, and then during the longer, resistive time, the distribution settles into an equilibrium Planck distribution.

5.2. The moment flux and collision terms

An arbitrary local state of the phonon gas is specified by primary variables $(\epsilon, \mathbf{q})$ and by additional variables $(\varphi^{n|m})$. For complete specification of a non-equilibrium state the set of additional variables needed is, in general, infinite. In order to arrive at a manageable system of evolution equations for $(\epsilon, \mathbf{q}, \varphi^{n|m})$, the infinite set $(\varphi^{n|m})$ has to be truncated. Following Grad [9,10], we assume that the phonon gas is sufficiently close to local quasi-equilibrium for the function φ to be approximated by three terms of its expansion:

$$\varphi = \psi := \varphi^{0|3}\,\Pi_3 + \varphi_i^{0|4}\,\Pi_4^i + \varphi_{ij}^{0|5}\,\Pi_5^{ij}. \tag{5.7}$$

Adopting this approximation, we obtain for f,

$$f = F\,[1 - c\hbar|\mathbf{k}|\Delta(1+F)\psi]\,, \tag{5.8}$$

where Δ is given by (3.5). Thus, the variables defining the state of the phonon gas are $\left(\epsilon, q^i, \varphi^{0|3}, \varphi_i^{0|4}, \varphi_{ij}^{0|5}\right)$ or (ϵ, q^i, M^{ij}) which are nine in number. This leads to a description involving only quantities that appear in the fundamental balance equations (2.23*a*) and (2.23*b*). If $\bar{\tau}_n \ll \tau_r$, the classical formulation of phonon hydrodynamics starts from the evolution equations for the energy density ϵ and the heat flux $\mathbf{q}$. These quantities are slowly varying, since they are not altered by the normal processes. The higher moment M^{ij}, however, tends to its local quasi-equilibrium value M_F^{ij} on the fast time scale determined by $\bar{\tau}_n$. Whereas many authors (see, e.g., [14, 15]) have studied the elimination of a fast variable M^{ij} in order to obtain a description of the phonon gas in terms of slow variables $(\epsilon, \mathbf{q})$, our aim is the opposite one: we want to derive the evolution equation for M^{ij}.

The moment flux M^{ijk} is calculated by inserting (5.8) into (2.24*a*), using identity (4.17) and relations (4.13), (4.4), (4.1), (3.5) and (3.6). These manipulations, when combined with the auxiliary formulae (A.1)–(A.6) and (B.1)–(B.4), lead after some algebra to

$$M^{ijk} = -\frac{S}{4\epsilon^2 E}\, q^{\langle i} q^j q^{k\rangle} - \frac{1}{A}\left[\frac{3B}{\epsilon}\, q^{\langle i} M^{jk\rangle} - \frac{1}{c^2\epsilon^3 D} \times \left(2L\, q^l M_l{}^{\langle i} q^j q^{k\rangle} - \frac{Q}{c^2\epsilon^2 E}\, M_{lm} q^l q^m\, q^{\langle i} q^j q^{k\rangle}\right)\right], \tag{5.9}$$

where

$$B := \frac{3+u}{4u}\left(\frac{8}{3} - 5A\right), \tag{5.10a}$$

$$D := \frac{2}{3} - A, \qquad E := 3(3-u)A - 4, \tag{5.10b}$$

$$L := \left(\frac{3+u}{4}\right)^3 \frac{1}{u^2}\left[\frac{15}{8}(3+u)A^2 - 13A + \frac{16}{3}\right], \tag{5.10c}$$

$$Q := \left(\frac{3+u}{4}\right)^5 \frac{1}{u^3}\left[\frac{45}{4}(1-u^2)A^3 + 3(19u-27)A^2 - 4(7u-15)A - \frac{32}{3}\right], \tag{5.10d}$$

$$S := \left(\frac{3+u}{4}\right)^2 \frac{1}{u}\left[\frac{45}{2}(1-u)(3-u)A^2 + 6(39-23u)A - 16(9-5u)\right]. \tag{5.10e}$$

Because of (3.46*a*) and (3.46*b*), we find

$$A = \frac{1}{u^2}\left[\frac{(1-u)^2}{2\sqrt{u}} \ln\left(\frac{1+\sqrt{u}}{1-\sqrt{u}}\right) + \frac{1}{3}(5u-3)\right]. \tag{5.11}$$

Inspection shows that the new coefficients (L, Q, S) tend to the limits

$$L = \frac{3}{980}, \qquad Q = -\frac{27}{377300}, \qquad S = \frac{81}{35} \tag{5.12}$$

as the quantity u approaches 0. The limits for (A, B, D, E) are given by (3.48) and (4.12). Using (3.6) yields

$$u = \frac{3\left(2c\epsilon - \sqrt{4c^2\epsilon^2 - 3|\mathbf{q}|^2}\right)}{2c\epsilon + \sqrt{4c^2\epsilon^2 - 3|\mathbf{q}|^2}}. \tag{5.13}$$

With equations (5.11) and (5.13), we clearly see the following: substitution of (5.10) into (5.9) enables us to represent M^{ijk} as a function of $(\epsilon, \mathbf{q})$ and M^{ij}.

We now turn to the collision terms $\left(P_r^i, P_r^{ij}, P_n^{ij}\right)$. The case when τ_r is a function of ϵ alone is particularly simple since then the collision terms P_r^i and P_r^{ij} are easily shown to be

$$P_r^i = -\frac{1}{\tau_r}\, q^i, \qquad P_r^{ij} = -\frac{1}{\tau_r}\, M^{ij}. \tag{5.14}$$

Note that the integrations in (2.24*b*) and (2.24*c*) can be performed explicitly. The more difficult problem with τ_n allowed to be a function of ϵ and ζ_* (see (5.2)) can also be solved, but only in the nine-moment approximation. However, before proceeding further, we must analyse conditions (2.8b) and (2.8c) in which f is assumed to have the form (5.8). The validity of these conditions is ensured by setting

$$\Delta_* = \Delta = \frac{\chi}{\epsilon^{1/4}} \frac{(3+u)^{1/4}}{(1-u)^{3/4}}, \qquad \mathbf{v}_* = \mathbf{v} = \left(\frac{3+u}{4}\right)\frac{\mathbf{q}}{c\epsilon}. \tag{5.15}$$

Then, since $\zeta_* = \zeta$ and $F_* = F$, (2.8b) and (2.8c) are equivalent to

$$\left\langle \frac{1}{\tau_n} \middle| \psi \right\rangle = 0, \qquad \left\langle \frac{1}{\tau_n}\, g^i \middle| \psi \right\rangle = 0. \tag{5.16}$$

The proof that equations (5.16) hold true is immediate and is based on the fact that

$$\left\langle \frac{1}{\tau_n} \middle| \psi \right\rangle = \frac{1}{\tilde{\tau}_n\,(1-u)}\,\mathcal{X}, \tag{5.17a}$$

$$\left\langle \frac{1}{\tau_n}\, g^i \middle| \psi \right\rangle = \frac{1}{\tilde{\tau}_n}\left[\left(\frac{5+u}{3(1-u^2)}\,\mathcal{X} + \frac{1}{u}\,\mathcal{Y}\right)v^i + \frac{1}{\sqrt{1-u}}\,\mathcal{Z}^i\right], \tag{5.17b}$$

where

$$\tilde{\tau}_n := \left[\frac{1}{\tau_n}\middle| 1\right]^{-1} = \frac{4\pi^4}{15}\left(\int_0^\infty \frac{\zeta^4}{\tau_n(\epsilon,\zeta)}\,\frac{\mathrm{e}^\zeta}{(\mathrm{e}^\zeta-1)^2}\,\mathrm{d}\zeta\right)^{-1}, \tag{5.18a}$$

$$\mathcal{X} := \varphi^{0|3}\,(\Pi_0\,|\,\Pi_3) + \varphi^{0|4}_j\,\left(\Pi_0\middle|\Pi^j_4\right) + \varphi^{0|5}_{kl}\,\left(\Pi_0\middle|\Pi^{kl}_5\right) = 0, \tag{5.18b}$$

$$\mathcal{Y} := \varphi^{0|3}\,(\Pi_1\,|\,\Pi_3) + \varphi^{0|4}_j\,\left(\Pi_1\middle|\Pi^j_4\right) + \varphi^{0|5}_{kl}\,\left(\Pi_1\middle|\Pi^{kl}_5\right) = 0, \tag{5.18c}$$

$$\mathcal{Z}^i := \varphi^{0|3}\,\left(\Pi^i_2\middle|\Pi_3\right) + \varphi^{0|4}_j\,\left(\Pi^i_2\middle|\Pi^j_4\right) + \varphi^{0|5}_{kl}\,\left(\Pi^i_2\middle|\Pi^{kl}_5\right) = 0. \tag{5.18d}$$

Here, it may be noted that the effective relaxation time $\tilde{\tau}_n$ for normal processes depends on ϵ through τ_n (see (5.18a)). At this stage, the combination of (2.24d), (5.8) and (5.15) yields an expression for P^{ij}_n in the form

$$P^{ij}_n = \frac{6c^2\epsilon\,(1-u)^3}{\tilde{\tau}_n(3+u)}\,(g^i g^j\,|\,\psi). \tag{5.19}$$

Let us now use (4.16) and (3.41b). With the aid of

$$(g^i g^j\,|\,\psi) = \langle g^i g^j\,|\,\varphi\rangle \tag{5.20}$$

which is a consequence of (3.32) and (4.3), we finally obtain from (4.1) and (4.2) that

$$P^{ij}_n = -\frac{1}{\tilde{\tau}_n}\left(M^{ij} - \frac{3c}{2c\epsilon + \sqrt{4c^2\epsilon^2 - 3|\mathbf{q}|^2}}\,q^{\langle i}q^{j\rangle}\right). \tag{5.21}$$

Given (5.18a), the collision term P^{ij}_n is thus represented as a linear function of M^{ij} and a nonlinear function of $(\epsilon, \mathbf{q})$.

Insertion of relations (5.9), (5.14) and (5.21) into system (2.23) leads to the differential equations for $(\epsilon, \mathbf{q})$ and M^{ij}:

$$\partial_t\epsilon + \partial_i q^i = 0, \tag{5.22a}$$

$$\partial_t q^i + \partial_j\left(\frac{c^2}{3}\delta^{ij}\epsilon + M^{ij}\right) = -\frac{1}{\tau_r}\,q^i, \qquad \tau_r = \tau_r(\epsilon), \tag{5.22b}$$

$$
\begin{aligned}
\partial_t M^{ij} + \partial_k \Bigg\{ & \frac{2c^2}{5}\delta^{k\langle i} q^{j\rangle} - \frac{S}{4\epsilon^2 E}\, q^{\langle i} q^j q^{k\rangle} - \frac{1}{A}\Bigg[\frac{3B}{\epsilon}\, q^{\langle i} M^{jk\rangle} \\
& - \frac{1}{c^2\epsilon^3 D}\left(2L\, q^l M_l{}^{\langle i} q^j q^{k\rangle} - \frac{Q}{c^2\epsilon^2 E}\, M_{lm} q^l q^m\, q^{\langle i} q^j q^{k\rangle}\right)\Bigg]\Bigg\} \\
= & -\frac{1}{\tau_r}\, M^{ij} - \frac{1}{\tilde{\tau}_n}\left(M^{ij} - \frac{3c}{2c\epsilon + \sqrt{4c^2\epsilon^2 - 3|\mathbf{q}|^2}} q^{\langle i} q^{j\rangle}\right),
\end{aligned} \tag{5.22c}
$$

where the coefficients (A, B, D, E, L, Q, S) depend on $(\epsilon, \mathbf{q})$ according to the relations (5.10)–(5.13) and the effective relaxation time $\tilde{\tau}_n = \tilde{\tau}_n(\epsilon)$ is defined by (5.18*a*). We call these differential equations, which originate from the modified Grad-type approach, the equations of nine-moment phonon hydrodynamics. System (5.22) is based on an expansion about an anisotropic Planck function and thus permits the inclusion of the heat flux in a non-perturbative fashion. Precisely speaking, with the exception of the natural condition $|\mathbf{q}| < c\epsilon$, there are effectively no unphysical limitations on the value of $|\mathbf{q}|$, i.e., one can handle problems with large components of the heat flux. This is a definite improvement over previous approaches [12–15] which only make allowances for small deviations in the heat flux from zero. Also, the explicit presence of two relaxation times $(\tau_r, \tilde{\tau}_n)$ in equation (5.22*c*) introduces important physical features not found in the four-moment system (3.9). First of all, unlike the latter, the nine-moment system is expected to be a useful tool in dealing with both normal and resistive processes. Moreover, assuming a separation of two time scales $(\tilde{\tau}_n \ll \tau_r)$, one can treat phenomena at frequencies comparable to the inverse of the normal time. However, since the infinite set $(\varphi^{n|m})$ was truncated and the flux M^{ijk} and the collision term P_n^{ij} were approximated by linear functions of M^{ij}, a limitation of the nine-moment system is that it is incapable of representing the effects of large departures from local quasi-equilibrium.

In the work of Banach and Piekarski [12], the nine-moment closure was based on the following relations for M^{ijk} and P_n^{ij}:

$$
M^{ijk} = \frac{45}{28\epsilon}\, q^{\langle i} M^{jk\rangle}, \qquad P_n^{ij} = -\frac{1}{\tilde{\tau}_n}\, M^{ij}. \tag{5.23}
$$

These relations are consistent with the present results, in the sense that they can be obtained by evaluating the right-hand sides of (5.9) and (5.21) to first order in the heat flux. Then the terms in (5.9) and (5.21) containing $M_{lm} q^l q^m\, q^{\langle i} q^j q^{k\rangle}$, $q^l M_l{}^{\langle i} q^j q^{k\rangle}$, $q^{\langle i} q^j q^{k\rangle}$ and $q^{\langle i} q^{j\rangle}$ are neglected and the coefficients (A, B) in (5.9) are given by (3.48) and (4.12). For a linear model in which $M^{ijk} = 0$, a further simplification of (5.22*c*) is possible and this has been exploited by Dreyer and Struchtrup [13], with a view to an interpretation of the experimental data on heat pulses in crystals. Finally, a word should be said about the limit $|\mathbf{q}| \to c\epsilon$. Equations (5.9) and (5.21) become[7]

$$
M^{ijk} = -\frac{4}{\epsilon^2}\, q^{\langle i} q^j q^{k\rangle} + \frac{3}{\epsilon}\, q^{\langle i} M^{jk\rangle} + \frac{3}{2c^2\epsilon^3}\left(q^l M_l{}^{\langle i} q^j q^{k\rangle} + \frac{1}{c^2\epsilon^2}\, M_{lm} q^l q^m\, q^{\langle i} q^j q^{k\rangle}\right), \tag{5.24a}
$$

$$
P_n^{ij} = -\frac{1}{\tilde{\tau}_n}\left(M^{ij} - \frac{1}{\epsilon}\, q^{\langle i} q^{j\rangle}\right) \tag{5.24b}
$$

as $|\mathbf{q}|$ approaches $c\epsilon$. This leads to the conclusion that, for all values of $|\mathbf{q}|$, the flux M^{ijk} and the production term P_n^{ij} are finite.

[7] Formally, in the limit $|\mathbf{q}| \to c\epsilon$, we obtain $S/E = 16$, $A = 2/3$, $B = -2/3$, $L/D = 1/2$ and $Q/DE = -1$.

6. Final remarks

Our modification of the Grad-type approach, which begins by expanding the phase density about an anisotropic Planck function, may be used to present a systematic derivation of a whole hierarchy of closed systems of moment equations. The system of equations for the energy density and the heat flux is the first, non-perturbative member of this hierarchy of closures. Here we have investigated in detail the next member, the nine-moment closure that involves the deviatoric part of the flux of the heat flux as an extra gas-state variable. In addition to this, our reasoning shows that the method of Grad can be generalized in the following sense: instead of using the equilibrium distribution for the expansion, one can use for it any non-equilibrium distribution that maximizes the Boltzmann entropy under the constraints of fixed values of appropriately chosen moments [35].

An alternative strategy for obtaining determined systems of moment equations is based on the closure by entropy maximization [35]. The main advantage of using this closure prescription is that if one expresses the moments and the collision operator moments as functions of the Lagrange multipliers, the evolution equations for these multipliers are then automatically symmetric hyperbolic at every order of truncation. Clearly, in order to derive transport equations for the hydrodynamic quantities, which are traditionally of interest, we need to relate the Lagrange multipliers to the moment densities. However, even in the simplest physically interesting situation of a one-dimensional, rotationally symmetric geometry applied to the nine-moment phonon system (then only three independent gas-state variables are involved), one cannot express analytically the Lagrange multipliers in terms of moment densities without first performing a perturbative expansion of various non-equilibrium quantities as is done, e.g., in rational extended thermodynamics [35]. Most conventional methods propose to introduce perturbative expansions of the Lagrange multipliers about equilibrium states. Because of this, in a linearized theory, they deliver essentially the same closing relations for the moment systems as those originating from the Grad-type expansion of f about an equilibrium Planck distribution [12]. In a separate paper, we will discuss similar but much more difficult problems for a new type of expansion about quasi-equilibrium states. In particular, we will show there that the present method and the maximum-entropy approach are consistent with, and appear complementary to, each other.

A key feature of the maximum-entropy closures is that they generate a hierarchy of moment closure systems, each of which possesses realizability of its predicted moments, has an entropy and is symmetric hyperbolic. (Recently, Dreyer *et al* [36] developed an approximative scheme that allows numerical solutions of the Callaway equation[8] to be compared with numerical solutions of the maximum-entropy system.) Whether the closure of system (2.23), based on using the closing relations of section 5.2, leads to a system of equations which are hyperbolic in a convex set of states containing all quasi-equilibrium states is an open problem and remains to be seen. However, the one-dimensional, rotationally symmetric reduction of this model appears to be an interesting one as it reveals a nontrivial system of three evolution equations which, for a well-defined region of parameter space, is a symmetrizable hyperbolic system. The region of symmetric hyperbolicity in parameter space (the space defined by either $\epsilon, q^1, \varphi^{0|3}$ or ϵ, q^1, M^{11}) is characterized by the following conditions [8]:

$$|q^1| < c\epsilon, \qquad \varphi^{0|3} < \Xi := \frac{4(3-\sqrt{3u})}{9(1-u)|Y|}, \tag{6.1}$$

[8] In [36], the Callaway model is defined in a three-dimensional spacetime coordinatized by (t, x^1, x^2). Moreover, the relaxation times (τ_r, τ_n) are assumed to be the constant quantities.

where

$$Y := \frac{9[9(u^2 - 2u + 5)A^2 - 24(1 + u)A + 16u]}{u[3(3 - u)A - 4]^2} < 0. \tag{6.2}$$

These conditions show that the reduced system is certainly hyperbolic in the neighbourhood of quasi-equilibrium, i.e., in the range where relation (B.6) is valid. Moreover, in the case $\varphi^{0|3} < 0$, there are effectively no mathematical limitations on the magnitude of $\varphi^{0|3}$ as the second condition in (6.1) is then satisfied automatically. For any fixed value of ϵ, as q^1 moves towards 0, one can prove that $\varphi^{0|3} < \Xi = 28/27$. In the limit $|q^1| \to c\epsilon$, one obtains $\varphi^{0|3} < \Xi = \infty$. Consequently, the differential equations for $(\epsilon, q^1, \varphi^{0|3})$ or (ϵ, q^1, M^{11}) form a symmetrizable hyperbolic system even beyond the limits of their original derivation ($|\varphi^{0|3}| \ll 1$), and indeed this type of observation is one of the most unexpected features of the one-dimensional reduction of equations (5.22*a*)–(5.22*c*). More details on these issues can be found in [8].

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Appendix A. Some useful integrals

This appendix contains a set of integrals that are needed to derive equations (3.5), (3.6), (3.10), (3.15), (3.24), (3.32), (3.49) and (5.9).

We first observe that

$$3\int_0^\infty \zeta^2[\zeta - \ln(\mathrm{e}^\zeta - 1)]\,\mathrm{d}\zeta = \int_0^\infty \frac{\zeta^3}{\mathrm{e}^\zeta - 1}\,\mathrm{d}\zeta = \frac{1}{4}\int_0^\infty \frac{\zeta^4\,\mathrm{e}^\zeta}{(\mathrm{e}^\zeta - 1)^2}\,\mathrm{d}\zeta = \frac{\pi^4}{15}. \tag{A.1}$$

With the abbreviation

$$\phi^{i_1 i_2 \ldots i_n} := \frac{1}{2\pi}\int_{S^2} \frac{g^{i_1} g^{i_2} \ldots g^{i_n}}{(1 - \mathbf{v}\cdot\mathbf{g})^4}\,\mathrm{d}^2\mathbf{g}, \tag{A.2}$$

the following formulae can be obtained:

$$\phi = \frac{2(3 + u)}{3(1 - u)^3}, \qquad \phi^i = \frac{8}{3(1 - u)^3}\,v^i, \tag{A.3a}$$

$$\phi^{ij} = \frac{2}{3(1 - u)^2}\,\delta^{ij} + \frac{8}{3(1 - u)^3}\,v^i v^j, \tag{A.3b}$$

$$\phi^{ijk} = \frac{3A}{(1 - u)^2}\,\delta^{(ij}v^{k)} + \frac{2G}{(1 - u)^3}\,v^i v^j v^k, \tag{A.3c}$$

where the coefficients A and G are characterized by (5.11) and (B.1*a*), respectively.

Setting

$$\psi^{i_1 i_2 \ldots i_n} := \frac{1}{2\pi}\int_{S^2} \frac{g^{i_1} g^{i_2} \ldots g^{i_n}}{(1 - \mathbf{v}\cdot\mathbf{g})^5}\,\mathrm{d}^2\mathbf{g}, \tag{A.4}$$

we find that further useful formulae are

$$\psi = \frac{2(1+u)}{(1-u)^4}, \qquad \psi^i = \frac{2(5+u)}{3(1-u)^4}\, v^i, \tag{A.5a}$$

$$\psi^{ij} = \frac{2}{3(1-u)^3}\,\delta^{ij} + \frac{4}{(1-u)^4}\, v^i v^j, \tag{A.5b}$$

$$\psi^{ijk} = \frac{2}{(1-u)^3}\,\delta^{(ij} v^{k)} + \frac{4}{(1-u)^4}\, v^i v^j v^k, \tag{A.5c}$$

$$\psi^{ijkl} = d_1\,\delta^{(ij}\delta^{kl)} + d_2\,\delta^{(ij} v^k v^{l)} + d_3\, v^i v^j v^k v^l, \tag{A.5d}$$

$$\psi^{ijklm} = d_4\,\delta^{(ij}\delta^{kl} v^{m)} + d_5\,\delta^{(ij} v^k v^l v^{m)} + d_6\, v^i v^j v^k v^l v^m, \tag{A.5e}$$

where

$$d_1 := \frac{3A}{4(1-u)^2}, \qquad d_2 := \frac{8-15(1-u)A}{2u(1-u)^3}, \tag{A.6a}$$

$$d_3 := \frac{105(1-u)^2 A + 8(13u-7)}{12u^2(1-u)^4}, \qquad d_4 := \frac{5(15A-8)}{4u(1-u)^2}, \tag{A.6b}$$

$$d_5 := \frac{5[8(7-6u) - 105(1-u)A]}{6u^2(1-u)^3}, \tag{A.6c}$$

$$d_6 := \frac{315(1-u)^2 A - 8(21-39u+16u^2)}{4u^3(1-u)^4}. \tag{A.6d}$$

The coefficients $(d_1, d_2, \ldots, d_6)$ tend to the limits

$$d_1 = \tfrac{2}{5}, \qquad d_2 = \tfrac{24}{7}, \qquad d_3 = \tfrac{32}{9}, \tag{A.7a}$$

$$d_4 = \tfrac{10}{7}, \qquad d_5 = \tfrac{40}{9}, \qquad d_6 = \tfrac{32}{11} \tag{A.7b}$$

as u approaches 0.

Appendix B. Some useful identities

We first introduce the following quantities:

$$G := \frac{1}{2u}\left[\frac{8}{3} - 5(1-u)A\right], \tag{B.1a}$$

$$I := \frac{3}{u}\,[3(3u-5)A + 4(2-u)]\,, \tag{B.1b}$$

$$P := \frac{1}{u}\,[15(3-u)A - 4(6-u)]\,. \tag{B.1c}$$

In the limit $u \to 0$, we have

$$G = \tfrac{8}{7}, \qquad I = -\tfrac{36}{35}, \qquad P = -\tfrac{4}{7}. \tag{B.2}$$

Using the above definitions, it is straightforward to verify that the coefficients in (4.10), (4.13) and (5.9) satisfy the identities

$$A+\frac{4u}{3+u}\,B=4D,\qquad 2uK+\frac{12}{3+u}\,BE=3AP, \tag{B.3a}$$

$$3E-uP=6(3-u)D,\qquad K+\frac{8}{3+u}\,BP-6(3-u)CD=0, \tag{B.3b}$$

$$2u^2C+\frac{16u}{3+u}\,B+3A=\frac{6E}{3-u}, \tag{B.3c}$$

$$u^2K+\frac{24u}{3+u}\,BE-18DE=-9(3-u)AD, \tag{B.3d}$$

$$\frac{4}{3+u}\,B+2uC=\frac{2}{3-u}\,P,\qquad 3\left(\frac{4}{3+u}\right)^2S+9EG=-20I, \tag{B.3e}$$

$$2u^2\left(\frac{4}{3+u}\right)^5Q-4uE\left(\frac{4}{3+u}\right)^3L+\frac{36}{3+u}\,BDE=5ADI. \tag{B.3f}$$

Given (4.10), these identities are presented in order to facilitate an understanding of equations (4.13) and (5.9).

The deduction of (4.13) is also based on the additional formulae of the form

$$\lambda_{kl}v^kv^l=-\frac{3-u}{2E}\,\tilde{N}_{kl}v^kv^l, \tag{B.4a}$$

$$\lambda_{ij}v^j=-\frac{1}{4D}\left(\tilde{N}_{ij}v^j-\frac{P}{3E}\,\tilde{N}_{kl}v^kv^lv_i\right). \tag{B.4b}$$

To derive (B.4), we have used (4.10) and (B.3). Finally, recalling (4.1) and knowing that

$$v^i=\frac{3+u}{4c\epsilon}\,q^i=\frac{3}{2c\epsilon+\sqrt{4c^2\epsilon^2-3|\mathbf{q}|^2}}\,q^i, \tag{B.5}$$

we obtain from (5.9), (B.3*e*) and (B.3*f*)

$$M_{ijk}v^iv^jv^k=cu\left[\frac{6c^2\epsilon}{5(3+u)}\,Gu^2-\frac{I}{E}\,N_{ij}v^iv^j\right]. \tag{B.6}$$

This formula gives us a mathematical basis for studying the issues of [8].

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