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Nine-moment phonon hydrodynamics based on the maximum-entropy closure: one-dimensional flow

Zbigniew Banach¹ and Wiesław Larecki²

¹ Department of Fluid Mechanics, Centre of Mechanics, Institute of Fundamental Technological Research, Polish Academy of Sciences, Swietokrzyska 21, 00-049 Warsaw, Poland

² Department of Theory of Continuous Media, Institute of Fundamental Technological Research, Polish Academy of Sciences, Swietokrzyska 21, 00-049 Warsaw, Poland

E-mail: zbanach@ippt.gov.pl and wlarecki@ippt.gov.pl

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Abstract

The maximum-entropy distribution functions applied to Callaway's model for phonon gas dynamics lead to a hierarchy of closed systems of moment equations. The system of equations for the energy density and the heat flux is the first member of this hierarchy of closures. Here emphasis is placed on analysing the next member, the 9-moment maximum-entropy system that involves the flux of the heat flux as an extra gas-state variable. After presenting a study of the one-dimensional, rotationally symmetric reduction of this system, we explicitly calculate a single generating function of three Lagrange multipliers in terms of which the reduced system of three evolution equations for these multipliers can be cast into a symmetric hyperbolic form. In the context of determining the Lagrange multipliers as explicit functions of the moment densities, we discuss new aspects of the expansion of various non-equilibrium quantities about quasi-equilibrium states. This expansion is fundamentally a non-equilibrium expansion that includes the heat flux in a non-perturbative manner, i.e., there are no unphysical limitations on the magnitude of the nonvanishing component of the heat flux to maintain a theory. Results are presented both at the first order in the expansion and at the second order. This enables us to verify the internal consistency of our approach and to justify the non-equilibrium generalization of the method of Grad.

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1. Introduction

As is well known, the Boltzmann–Peierls (BP) equation [1–3] provides a satisfactory description of phonon transport in dielectric materials and semiconductors. This equation

is valid in all transport regimes. However, even under the assumption of Callaway's model with nondispersion and isotropy for phonon frequency spectrum [4], it is very difficult to obtain closed-form analytic solutions of the BP equation except in the simplest situations. For more general problems, it is thus necessary to apply either advanced numerical schemes or approximate moment methods.

The method of moments replaces the problem of directly solving the BP equation with that of solving a system of generalized transport equations for various hydrodynamic quantities. Clearly, any finite set of these equations is not a determined system. Therefore, the moment closure prescription must be devised while remaining mindful that the resulting system should be well posed. In [5], a considerable effort has been put into demonstrating that the closure by entropy maximization leads to a well-defined hierarchy of closed systems of evolution equations for the Lagrange multipliers, in the sense that every member of this hierarchy of closures is symmetric hyperbolic and has an entropy.

The first member of the hierarchy is the 4-moment system [6], which is based on the quasi-equilibrium Planck distribution [2–4]. Since this distribution depends explicitly on the energy density and the heat flux, it yields a set of four evolution equations with the independent variables being the energy density and the three components of the heat flux. Inspection shows that the 4-moment closure properly captures phonon hydrodynamic phenomena in the case when the effective relaxation time τ_n for normal processes is much smaller than the effective relaxation time τ_r for resistive processes [3]. Then there is a physical reason to employ the quasi-equilibrium Planck distribution in place of the full distribution. The second member of the hierarchy is the 9-moment maximum-entropy system [7], which is obtained by including the deviatoric part of the flux of the heat flux in the set of independent gas-state variables. A main advantage of using the 9-moment model is that, unlike the 4-moment model, it is capable of representing the most important effects associated with both resistive and normal processes. More precisely, the 9-moment model is the simplest hydrodynamic model where the effective relaxation times τ_r and τ_n occur explicitly, thereby allowing the qualitative description of the aforementioned effects.

In this paper, emphasis is placed on discussing the 9-moment system. Precisely speaking, we first present a study of the one-dimensional, rotationally symmetric reduction of this system and then explicitly calculate a single generating function K of three Lagrange multipliers in terms of which the reduced system of three evolution equations for these multipliers can be cast into a symmetric hyperbolic form. As shown in [5], for more general systems of phonon hydrodynamic equations of divergence type, a single generating potential K can also be derived by employing an integral expression for it (which depends on the Lagrange multipliers through the maximum-entropy distribution function), but the biggest obstacle to any practical implementation of this expression is that the required integral proves to be impossible to determine. One important and explicit example of K is the construction of Larecki [6] who, using the 4-moment model with nondispersion and isotropy for phonon frequency spectrum, demonstrated how K is related to four Lagrange multipliers. A second example is new and is, in essence, that described in this paper.

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 9-moment 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 [8]. Most conventional methods consider only perturbative expansions of the Lagrange multipliers about

equilibrium states. In our two recent papers [9, 10], a new type of expansion about quasi-equilibrium states was introduced and the first-order approximation to the moment flux was discussed. Here we note that the above expansion is based on the modified Grad-type approach. It is fundamentally a non-equilibrium expansion that includes the heat flux in a non-perturbative manner, i.e., there are no unphysical limitations on the magnitude of the nonvanishing component of the heat flux to maintain a theory. Such a perturbative expansion technique seems particularly suited for describing phonon flows in the regime where $\tau_n \ll \tau_r$. The physical consequence of this condition 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.

Beginning from the maximum-entropy method, it is the aim of this paper to examine further aspects of the expansion of various non-equilibrium quantities about quasi-equilibrium states. Specifically, restricting our attention to the one-dimensional, rotationally symmetric geometry, we calculate the Lagrange multipliers and the moment flux (as well as the entropy density and the entropy flux) to second order in \tilde{N} , where \tilde{N} is the convenient gas-state variable defined by (4.26). No doubt, our perturbative expansion technique can be extended to a three-dimensional setting. However, the resulting formulae are not simple and a full treatment is too lengthy for the present work. We also mention the following. It is, of course, possible to perform the first-order calculations by means of the modified Grad-type approach³, but this approach does not enable one to expand the Lagrange multipliers and the moment flux in powers of \tilde{N} . The maximum-entropy method shows that corrections of second order in \tilde{N} can be systematically computed. Discussion of these corrections is important because they provide a nontrivial verification of the consistency of our postulates about the phonon gas close to quasi-equilibrium. In fact, we must prove that the second-order corrections are non-singular for all admissible values of the heat flux and that they can indeed be neglected if $\tilde{N} \ll 1$. Moreover, we encounter the problem of appropriately defining the small quantity \tilde{N} in which to expand the Lagrange multipliers and the moment flux.

For the sake of simplicity, we consider the BP equation with Callaway's collisional terms. The relaxation times τ_r and τ_n are assumed to depend only on the energy density. 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 $+\infty$. Throughout our work, we employ units which are defined by setting $k_B = \hbar = 1$.

Concerning the organization of this paper, section 2 first introduces the BP equation under the relaxation time approximation and then defines the 9-moment system. Section 3 is devoted to the study of the one-dimensional, rotationally symmetric reduction of 9-moment phonon hydrodynamics as well as to the construction of a single generating potential K . Section 4 discusses perturbative expansions of the Lagrange multipliers about quasi-equilibrium states. Section 5 is for discussion and final remarks. Some intermediate calculations are put into the appendix.

2. Preliminaries

2.1. Callaway's model

In kinetic theory, the state of a phonon gas is described by the distribution function f which represents the number density of phonons at position (x^i) and time t having wave vector \mathbf{k} .

³ Such calculations have been presented in [9, 10].

This distribution function obeys the BP equation of the form [1–3]

$$\partial_t f + c g^i \partial_i f = J_r(f) + J_n(f), \quad (2.1)$$

where

$$\partial_t := \frac{\partial}{\partial t}, \quad \partial_i := \frac{\partial}{\partial x^i}. \quad (2.2)$$

Here (g^i) are the components of a unit vector \mathbf{g} in the direction of \mathbf{k} and $(J_r(f), J_n(f))$ are the collision terms for resistive and normal processes, respectively.

We shall treat the left-hand side of the BP equation with great care, but shall handle the collision terms on the right-hand side schematically, as in [9, 10], by substituting for $(J_r(f), J_n(f))$ the Callaway model [4] with \mathbf{k} -independent relaxation times τ_r and τ_n . Precisely speaking, we assume that the true collision terms $J_r(f)$ and $J_n(f)$ may be adequately represented by

$$J_r(f) = \frac{1}{\tau_r}(F_o - f), \quad J_n(f) = \frac{1}{\tau_n}(F_* - f), \quad (2.3)$$

where $\tau_r = \tau_r(\epsilon)$ and $\tau_n = \tau_n(\epsilon)$ are given functions of the energy density ϵ , F_o is the equilibrium distribution function and F_* is the quasi-equilibrium distribution function. As regards the explicit form of (F_o, F_*) , we obtain the following well-known formulae:

$$F_o := \frac{1}{e^{\zeta_o} - 1}, \quad F_* := \frac{1}{e^{\zeta_*} - 1}, \quad (2.4)$$

where

$$\zeta_o := c|\mathbf{k}|\Delta_o, \quad \zeta_* := c|\mathbf{k}|\Delta(1 - \mathbf{v} \cdot \mathbf{g}). \quad (2.5)$$

The objects (Δ_o, Δ) and \mathbf{v} are a set of scalar and vector quantities that may depend on (t, x^i) . Here, defining the energy density ϵ and the heat flux q^i by the integral equations⁴

$$\epsilon := cy \int |\mathbf{k}| f \, d^3\mathbf{k}, \quad q^i := c^2 y \int k^i f \, d^3\mathbf{k}, \quad (2.6)$$

in which⁵

$$y := 3(2\pi)^{-3}, \quad (2.7)$$

we fix (Δ_o, Δ) and \mathbf{v} so as to satisfy the conditions [11]

$$\epsilon = cy \int |\mathbf{k}| F_o \, d^3\mathbf{k}, \quad \epsilon = cy \int |\mathbf{k}| F_* \, d^3\mathbf{k}, \quad q^i = c^2 y \int k^i F_* \, d^3\mathbf{k}. \quad (2.8)$$

Using these conditions, it is possible to relate Δ_o to ϵ and to express (Δ, \mathbf{v}) in terms of (ϵ, \mathbf{q}) . Explicitly, we have for $(\Delta_o, \Delta, \mathbf{v})$

$$\Delta_o = \chi \left(\frac{3}{\epsilon} \right)^{1/4}, \quad \Delta = \frac{\chi}{\epsilon^{1/4}} \frac{(3+u)^{1/4}}{(1-u)^{3/4}}, \quad \mathbf{v} = \frac{3}{2c\epsilon + \sqrt{4c^2\epsilon^2 - 3|\mathbf{q}|^2}} \mathbf{q}, \quad (2.9)$$

where

$$\chi := \left(\frac{4\pi^5 y}{45c^3} \right)^{1/4}, \quad u := |\mathbf{v}|^2 = \frac{3(2c\epsilon - \sqrt{4c^2\epsilon^2 - 3|\mathbf{q}|^2})}{2c\epsilon + \sqrt{4c^2\epsilon^2 - 3|\mathbf{q}|^2}}. \quad (2.10)$$

⁴ For any two wave vectors \mathbf{k} and \mathbf{k}' , we easily show that $\mathbf{k} \cdot \mathbf{k}' \leq |\mathbf{k}||\mathbf{k}'|$. Multiplying this inequality by $(c^2 y)^2 f(t, x^i, \mathbf{k}) f(t, x^i, \mathbf{k}')$ and integrating over $(\mathbf{k}, \mathbf{k}')$ yields $|\mathbf{q}|^2 \leq c^2 \epsilon^2$. This inequality is a strict inequality unless f is a delta function.

⁵ In (2.7), we need to multiply $(2\pi)^{-3}$ by 3; this is because there are three types of phonons corresponding to one longitudinal and two transversal sound waves.

Since Δ diverges for $|\mathbf{q}| = c\epsilon$, we postulate that $|\mathbf{q}| < c\epsilon$. Given (2.9) and (2.10), this postulate yields the inequalities $|\mathbf{v}| < 1$ and $0 \leq u < 1$. Clearly, $u = |\mathbf{v}|^2 = 0$ if and only if $|\mathbf{q}| = 0$.

To sum up, the approximation involved in Callaway’s model, especially if (τ_r, τ_n) are regarded as independent of \mathbf{k} , is that of disregarding the detailed statistics and dynamics of the phonon collisions. The original basis for this approximation was presumably its physically appealing form, corresponding to a relaxation phenomenon, together with the fact that equations (2.3) and (2.8) allow the model to represent the conservation laws inherent in the true collision terms $J_r(f)$ and $J_n(f)$. Specifically, using these equations, we obtain

$$\int |\mathbf{k}| J_r(f) d^3\mathbf{k} = 0, \tag{2.11a}$$

$$\int |\mathbf{k}| J_n(f) d^3\mathbf{k} = 0, \quad \int k^i J_n(f) d^3\mathbf{k} = 0. \tag{2.11b}$$

Equations (2.11b) tell us that normal processes conserve both energy and momentum, while equation (2.11a) states that resistive processes conserve only energy. For further details, including the proof that Callaway’s model leads to a non-negative entropy production, the reader is referred to [7, 9].

2.2. Nine-moment equations and maximum-entropy closure

At this stage, we need to introduce the so-called flux of the heat flux:

$$\mathcal{M}^{ij} := c^3 y \int k^i g^j f d^3\mathbf{k}. \tag{2.12}$$

Since $g^i = k^i/|\mathbf{k}|$, it is obvious that $\mathcal{M}^{ij} = M^{ij}$. The deviatoric part of \mathcal{M}^{ij} is defined by

$$M^{ij} := c^3 y \int k^{(i} g^{j)} f d^3\mathbf{k}. \tag{2.13}$$

As usual, angle brackets denote the symmetric traceless part, e.g.,

$$k^{(i} g^{j)} := k^i g^j - \frac{1}{3} |\mathbf{k}| \delta^{ij}, \quad k^{(i} g^j g^{k)} := k^i g^j g^k - \frac{2}{5} k^{(i} \delta^{jk)}. \tag{2.14}$$

Round brackets indicate symmetrization and δ^{ij} stands for the Kronecker delta. Now, using the BP equation with Callaway’s collisional terms and the kinetic-theory definitions of (ϵ, q^i, M^{ij}) , the evolution equations for (ϵ, q^i, M^{ij}) are of the form

$$\partial_t \epsilon + \partial_i q^i = 0, \tag{2.15a}$$

$$\partial_t q^i + \frac{c^2}{3} \delta^{ij} \partial_j \epsilon + \partial_j M^{ij} = -\frac{1}{\tau_r} q^i, \tag{2.15b}$$

$$\partial_t M^{ij} + \frac{2c^2}{5} \delta^{k(i} \partial_k q^{j)} + \partial_k M^{ijk} = -\frac{1}{\tau_r} M^{ij} - \frac{1}{\tau_n} N^{ij}, \tag{2.15c}$$

where

$$M^{ijk} := c^4 y \int k^{(i} g^j g^{k)} f d^3\mathbf{k}, \quad N^{ij} := c^3 y \int k^{(i} g^{j)} (f - F_*) d^3\mathbf{k}. \tag{2.16}$$

Note that the resistive (i.e., Umklapp and other momentum-destroying) processes are the only processes which give rise to the occurrence of a collisional relaxation term on the right-hand side of (2.15b). Because of this, even if the normal processes dominate the phonon

distribution ($\tau_n \ll \tau_r$), we also take into account the resistive processes when deriving the evolution equations for (ϵ, q^i, M^{ij}) . Setting

$$M_*^{ij} := c^3 y \int k^{(i} g^{j)} F_* d^3 \mathbf{k} \quad (2.17)$$

and observing that

$$M_*^{ij} = \frac{4c^2 \epsilon}{3+u} v^{(i} v^{j)} = \frac{3c}{2c\epsilon + \sqrt{4c^2 \epsilon^2 - 3|\mathbf{q}|^2}} q^{(i} q^{j)},$$

the quantity N^{ij} (see (2.16)) can also be written as

$$N^{ij} = M^{ij} - M_*^{ij} = M^{ij} - \frac{4c^2 \epsilon}{3+u} v^{(i} v^{j)} = M^{ij} - \frac{3c}{2c\epsilon + \sqrt{4c^2 \epsilon^2 - 3|\mathbf{q}|^2}} q^{(i} q^{j)}. \quad (2.18)$$

The number of independent components in (ϵ, q^i, M^{ij}) is nine. Consequently, it is natural to refer to equations (2.15a)–(2.15c) as the 9-moment system.

Of course, the 9-moment system is not a determined system since there appears the additional quantity M^{ijk} . Before showing that the closure by entropy maximization [5] applied to equations (2.15a)–(2.15c) leads to a determined system of partial differential equations for the Lagrange multipliers, we first introduce the following formulae for the entropy density s and the entropy flux Φ^i :

$$s = s(f) := -y \int H(f) d^3 \mathbf{k}, \quad \Phi^i = \Phi^i(f) := -cy \int g^i H(f) d^3 \mathbf{k}, \quad (2.19)$$

where

$$H(f) := f \ln f - (1+f) \ln(1+f). \quad (2.20)$$

Maximization of $s(f)$ subject to the constraints of fixed values of (ϵ, q^i, M^{ij}) implies maximizing the functional

$$\begin{aligned} Y(f) := & s(f) + \Lambda \left(\epsilon - cy \int |\mathbf{k}| f d^3 \mathbf{k} \right) + \Lambda_i \left(q^i - c^2 y \int k^i f d^3 \mathbf{k} \right) \\ & + \Lambda_{ij} \left(M^{ij} - c^3 y \int k^{(i} g^{j)} f d^3 \mathbf{k} \right), \end{aligned} \quad (2.21)$$

where

$$\Lambda_L := (\Lambda, \Lambda_i, \Lambda_{ij}) \quad (2.22)$$

are the Lagrange multipliers corresponding to the aforementioned constraints. Without any loss of generality, we can assume that Λ_{ij} is symmetric and traceless:

$$\Lambda_{ij} = \Lambda_{ji}, \quad \delta^{ij} \Lambda_{ij} = 0. \quad (2.23)$$

Variation of $Y(f)$ yields the formula

$$\delta Y(f) = -y \int \left[\ln \left(\frac{f}{1+f} \right) + \zeta \right] \delta f d^3 \mathbf{k}, \quad (2.24)$$

in which

$$\zeta := c|\mathbf{k}|(\Lambda + c\Lambda_i g^i + c^2 \Lambda_{ij} g^{(i} g^{j)}). \quad (2.25)$$

Then the maximum-entropy distribution function is easily seen from $\delta Y(f) = 0$ to be

$$f = F := \frac{1}{e^\zeta - 1}. \quad (2.26)$$

Because of the dependence of ζ on Λ_L and \mathbf{k} , the natural variables of F are Λ_L and \mathbf{k} . Thus we obtain

$$F = F(\Lambda_L, \mathbf{k}), \tag{2.27}$$

which means that F depends on (t, x^i) through Λ_L .

With these preparations, the closure procedure for the 9-moment system may now be stated simply. Let $(\epsilon, q^i, M^{ij}, M^{ijk})$ in equations (2.15a)–(2.15c) have the form

$$\epsilon = \epsilon(\Lambda_L), \quad q^i = q^i(\Lambda_L), \quad M^{ij} = M^{ij}(\Lambda_L), \quad M^{ijk} = M^{ijk}(\Lambda_L), \tag{2.28}$$

where

$$\epsilon(\Lambda_L) := cy \int |\mathbf{k}| F(\Lambda_L, \mathbf{k}) d^3\mathbf{k}, \quad q^i(\Lambda_L) := c^2 y \int k^i F(\Lambda_L, \mathbf{k}) d^3\mathbf{k}, \tag{2.29a}$$

$$M^{ij}(\Lambda_L) := c^3 y \int k^{(i} g^{j)} F(\Lambda_L, \mathbf{k}) d^3\mathbf{k}, \quad M^{ijk}(\Lambda_L) := c^4 y \int k^{(i} g^j g^{k)} F(\Lambda_L, \mathbf{k}) d^3\mathbf{k}. \tag{2.29b}$$

Since we have used F to express $(\epsilon, q^i, M^{ij}, M^{ijk})$ in terms of Λ_L , this procedure gives us a closed set of equations from which the evolution of Λ_L can, in principle, be determined.

In order to proceed further, we employ the unit vector \mathbf{g} and the quasi-radial variable ζ defined by (2.25). It is easy to confirm that

$$|\mathbf{k}| = \frac{1}{cz} \zeta, \quad d^3\mathbf{k} = \frac{1}{c^3 z^3} \zeta^2 d\zeta d^2\mathbf{g}, \tag{2.30}$$

where

$$z := \Lambda + c\Lambda_i g^i + c^2 \Lambda_{ij} g^{(i} g^{j)} \tag{2.31}$$

and $d^2\mathbf{g}$ is the incremental solid angle. If $\theta \in [0, \pi]$ denotes the polar angle and $\phi \in [0, 2\pi]$ denotes the azimuthal angle, then $d^2\mathbf{g}$ can be identified with $\sin\theta d\theta d\phi$. With the help of

$$\int_0^\infty \frac{\zeta^3}{e^\zeta - 1} d\zeta = \frac{1}{4} \int_0^\infty \frac{\zeta^4 e^\zeta}{(e^\zeta - 1)^2} d\zeta = \frac{\pi^4}{15}, \tag{2.32}$$

the quantities in equations (2.29a) and (2.29b) reduce to integrals over the unit sphere S^2 . The resulting formulae for $(\epsilon, q^i, M^{ij}, M^{ijk})$ are then given by

$$\epsilon = \frac{3}{4\pi} \chi^4 \int_{S^2} \frac{1}{z^4} d^2\mathbf{g}, \quad q^i = \frac{3c}{4\pi} \chi^4 \int_{S^2} g^i \frac{1}{z^4} d^2\mathbf{g}, \tag{2.33a}$$

$$M^{ij} = \frac{3c^2}{4\pi} \chi^4 \int_{S^2} g^{(i} g^{j)} \frac{1}{z^4} d^2\mathbf{g}, \quad M^{ijk} = \frac{3c^3}{4\pi} \chi^4 \int_{S^2} g^{(i} g^j g^{k)} \frac{1}{z^4} d^2\mathbf{g}. \tag{2.33b}$$

Also, inserting $f = F$ into (2.19) and knowing that

$$\int_0^\infty H(F) \zeta^2 d\zeta = -\frac{4\pi^4}{45}, \tag{2.34}$$

we obtain for (s, Φ^i)

$$s = \frac{1}{\pi} \chi^4 \int_{S^2} \frac{1}{z^3} d^2\mathbf{g}, \quad \Phi^i = \frac{c}{\pi} \chi^4 \int_{S^2} g^i \frac{1}{z^3} d^2\mathbf{g}. \tag{2.35}$$

Equations (2.33a), (2.33b) and (2.35) will be of interest to us subsequently.

3. One-dimensional flow

3.1. Reduction to three Lagrange multipliers

In the one-dimensional, rotationally symmetric geometry, all variables are functions of time and a single spatial coordinate $x := x^1$. The components $(q^1, v^1, \Phi^1, \Lambda_1)$ may vary, whereas the remaining components in $(q^i, v^i, \Phi^i, \Lambda_i)$ are set equal to zero. The symmetric traceless tensors M^{ij} and Λ_{ij} specialize to

$$M^{11} = -2M^{22} = -2M^{33}, \quad \Lambda_{11} = -2\Lambda_{22} = -2\Lambda_{33}. \quad (3.1)$$

Since the flow is assumed to be one-dimensional, there are no off-diagonal components of M^{ij} and Λ_{ij} . As regards the moment flux M^{ijk} , which is a rank-three symmetric traceless tensor, we can use the component M^{111} as a basis for the representation of this moment flux. In fact, the relevant components of M^{ijk} are characterized by

$$M^{111} = -2M^{221} = -2M^{331}, \quad M^{ij1} = 0 \quad (i \neq j). \quad (3.2)$$

Now, it is convenient to introduce the following notation:

$$q := q^1, \quad v := v^1, \quad \Phi := \Phi^1, \quad (3.3a)$$

$$m := \frac{3}{2}M^{11}, \quad M := \frac{3}{2}M^{111}, \quad (3.3b)$$

$$N := \frac{m}{c^2\epsilon} - \frac{4u}{3+u}, \quad u := |v|^2, \quad (3.3c)$$

$$a_1 := \Lambda, \quad a_2 := \Lambda_1, \quad a_3 := \Lambda_{11}. \quad (3.3d)$$

Equations (2.9), (2.10) and (3.3c) enable us to show that

$$v = \frac{3}{2c\epsilon + \sqrt{4c^2\epsilon^2 - 3|q|^2}}q, \quad u = \frac{3(2c\epsilon - \sqrt{4c^2\epsilon^2 - 3|q|^2})}{2c\epsilon + \sqrt{4c^2\epsilon^2 - 3|q|^2}} \quad (3.4)$$

and

$$N = \frac{m}{c^2\epsilon} - \frac{2c\epsilon - \sqrt{4c^2\epsilon^2 - 3|q|^2}}{c\epsilon}. \quad (3.5)$$

In view of these relations, we can think of (v, u) as being the functions of (ϵ, q) and of N as being the function of (ϵ, q) and m .

Given the above definitions, equations (2.15a)–(2.15c) reduce to a system of three equations for (ϵ, q, m) :

$$\partial_t \epsilon + \partial_x q = 0, \quad (3.6a)$$

$$\partial_t q + \partial_x \left(\frac{c^2}{3}\epsilon + \frac{2}{3}m \right) = -\frac{1}{\tau_r}q, \quad (3.6b)$$

$$\partial_t m + \partial_x \left(\frac{2c^2}{5}q + M \right) = -\frac{1}{\tau_r}m - \frac{c^2\epsilon}{\tau_n}N, \quad (3.6c)$$

where

$$\partial_x := \frac{\partial}{\partial x}. \quad (3.7)$$

Additional simplification is realized when the quantities (ϵ, q, m, M) and (s, Φ) are expressed in terms of the Lagrange multipliers (a_1, a_2, a_3) . We first introduce the polar and azimuthal angles (θ, ϕ) that define the unit vector \mathbf{g} with respect to the x -axis:

$$g^1 = \sigma := \cos \theta, \quad g^2 = \sin \theta \cos \phi, \quad g^3 = \sin \theta \sin \phi. \quad (3.8)$$

Substitution into (2.31) yields the result

$$z = a_1 + ca_2\sigma + \frac{1}{2}c^2a_3(3\sigma^2 - 1). \quad (3.9)$$

Then the integral formulae (2.33a), (2.33b) and (2.35) simplify to

$$\epsilon = \frac{3}{2}\chi^4 \int_{-1}^1 \frac{1}{z^4} d\sigma, \quad q = \frac{3c}{2}\chi^4 \int_{-1}^1 \frac{\sigma}{z^4} d\sigma, \quad (3.10a)$$

$$m = \frac{3c^2}{4}\chi^4 \int_{-1}^1 \frac{3\sigma^2 - 1}{z^4} d\sigma, \quad M = \frac{9c^3}{20}\chi^4 \int_{-1}^1 \frac{\sigma(5\sigma^2 - 3)}{z^4} d\sigma, \quad (3.10b)$$

$$s = 2\chi^4 \int_{-1}^1 \frac{1}{z^3} d\sigma, \quad \Phi = 2c\chi^4 \int_{-1}^1 \frac{\sigma}{z^3} d\sigma. \quad (3.10c)$$

For the convergence of the above integrals, we assume that

$$a_1 > c|a_2| + c^2|a_3| \quad (\Rightarrow z \geq a_1 - c|a_2| - c^2|a_3| > 0). \quad (3.11)$$

Then the integrations over σ are elementary if we take into account the reasoning presented in section 3.2. Condition (3.11) is not optimal, but it suffices to calculate the generating potential K by means of equations (3.24a)–(3.24e). In the case of quasi-equilibrium states $(a_1, a_2, 0)$, equations (3.10a) and (3.10b) enable us to express analytically (a_1, a_2) and (m, M) in terms of the principal moment variables (ϵ, q) (see, e.g., equations (4.7) and (4.9)). Moreover, the solvability close to equilibrium and quasi-equilibrium states of the above one-dimensional model can easily be shown by using the inverse function theorem. Finally, if the non-equilibrium Lagrange multipliers a_2 and a_3 are arbitrary, the existence of the inverse relations (3.36) may be deduced from the standard theorems of convex analysis [12].

Equations (3.10a)–(3.10c), in conjunction with relation (3.9), imply that (ϵ, q, m, M) and (s, Φ) are functions of (a_1, a_2, a_3) . Differentiating (s, Φ) with respect to (a_1, a_2, a_3) , we obtain

$$\epsilon = -\frac{1}{4} \frac{\partial s}{\partial a_1}, \quad q = -\frac{1}{4} \frac{\partial s}{\partial a_2}, \quad m = -\frac{1}{4} \frac{\partial s}{\partial a_3}, \quad (3.12a)$$

$$q = -\frac{1}{4} \frac{\partial \Phi}{\partial a_1}, \quad \frac{c^2}{3}\epsilon + \frac{2}{3}m = -\frac{1}{4} \frac{\partial \Phi}{\partial a_2}, \quad \frac{2c^2}{5}q + M = -\frac{1}{4} \frac{\partial \Phi}{\partial a_3}. \quad (3.12b)$$

We further define s^{ij} , Φ^{ij} and (Q^i) by

$$s^{ij} := -\frac{1}{4} \frac{\partial^2 s}{\partial a_i \partial a_j}, \quad \Phi^{ij} := -\frac{1}{4} \frac{\partial^2 \Phi}{\partial a_i \partial a_j}, \quad (3.13a)$$

$$(Q^i) := \left(0, -\frac{1}{\tau_r} q, -\frac{1}{\tau_r} m - \frac{c^2 \epsilon}{\tau_n} N \right). \quad (3.13b)$$

The introduction of this notation enables equations (3.6a)–(3.6c) to be written as

$$s^{ij} \partial_i a_j + \Phi^{ij} \partial_x a_j = Q^i \quad (i = 1, 2, 3). \quad (3.14)$$

Here, we adopt the summation convention whereby a repeated index implies summation over all values of that index.

Clearly, the above system of partial differential equations for (a_1, a_2, a_3) is symmetric because the matrices (s^{ij}) and (Φ^{ij}) are symmetric. Then it remains to show that the symmetric system (3.14) is hyperbolic in an open set D_M of ‘states’ (a_1, a_2, a_3) containing all equilibrium and quasi-equilibrium states, i.e., has a well-posed initial-value formulation there [13–15]. Observe that, for each $(r_1, r_2, r_3) \in \mathbb{R}^3$, equations (3.10c) and (3.13a) lead directly to the result

$$s^{ij}r_i r_j = -6\chi^4 \int_{-1}^1 \frac{\mathcal{B}^2}{z^5} d\sigma, \quad (3.15)$$

in which \mathcal{B} is defined by

$$\mathcal{B} := r_1 + cr_2\sigma + \frac{1}{2}c^2r_3(3\sigma^2 - 1). \quad (3.16)$$

Since $s^{ij}r_i r_j < 0$ if $\delta^{ij}r_i r_j \neq 0$, the matrix (s^{ij}) is negative definite and system (3.14) is verified to be symmetric hyperbolic and hence hyperbolic for all ‘states’ $(a_1, a_2, a_3) \in D_M$. In this context, it is perhaps important to stress the following. For the moment systems corresponding to the relativistic Boltzmann equation, cases are known [16] where the equilibrium states are located on the boundary of the domain of definition of the connected maximum-entropy problems. These complications do not arise in the present approach as the equilibrium states $(a_1, 0, 0) \in D_M$ and the quasi-equilibrium states $(a_1, a_2, 0) \in D_M$, which satisfy the obvious conditions $a_1 > 0$ and $a_1 > c|a_2|$, are inner points of $\overline{D_M}$.

3.2. The generating potential

Introduce the potential K , a function of (a_1, a_2, a_3) , defined by

$$K := -\chi^4 \int_{-1}^1 \frac{1}{z^2} d\sigma. \quad (3.17)$$

Differentiation of K with respect to (a_1, a_2) gives

$$s = \frac{\partial K}{\partial a_1}, \quad \Phi = \frac{\partial K}{\partial a_2}. \quad (3.18)$$

The integral in equation (3.17) may be explicitly evaluated. We first observe that expression (3.9) for z is conveniently rewritten as

$$z = a + b\sigma + d\sigma^2, \quad (3.19)$$

where

$$a := a_1 - \frac{1}{2}c^2a_3, \quad b := ca_2, \quad d := \frac{3}{2}c^2a_3. \quad (3.20)$$

Condition (3.11) is then equivalent to the inequality

$$a > \frac{1}{3}(2|d| - d) + |b|. \quad (3.21)$$

Let

$$X := 4ad - b^2. \quad (3.22)$$

Note that

$$(X < 0) \implies (a - d > \sqrt{-X}), \quad (3.23a)$$

$$(X = 0) \implies (a > d \geq 0), \quad (3.23b)$$

$$(X > 0) \implies (d > 0). \quad (3.23c)$$

For $X < 0$, the potential X appears in the form

$$K = -\frac{2\chi^4}{X} \left[\frac{2d(d-a)+X}{(a-d)^2+X} + \frac{2d}{\sqrt{-X}} \operatorname{arctanh} \left(\frac{\sqrt{-X}}{a-d} \right) \right]. \tag{3.24a}$$

For $X = 0$, equation (3.17) yields at once

$$K = -\frac{2}{3}\chi^4 \frac{3a+d}{(a-d)^3}. \tag{3.24b}$$

If $X > 0$ and $a > d$, the potential K is given by

$$K = -\frac{2\chi^4}{X} \left[\frac{2d(d-a)+X}{(a-d)^2+X} + \frac{2d}{\sqrt{X}} \operatorname{arctan} \left(\frac{\sqrt{X}}{a-d} \right) \right]. \tag{3.24c}$$

If $X > 0$ and $d > a$, one finds

$$K = -\frac{2\chi^4}{X} \left\{ \frac{2d(d-a)+X}{(a-d)^2+X} + \frac{2d}{\sqrt{X}} \left[\pi + \operatorname{arctan} \left(\frac{\sqrt{X}}{a-d} \right) \right] \right\}. \tag{3.24d}$$

In the case when $X > 0$ and $a = d$, it follows that

$$K = -\frac{2\chi^4}{X} \left(1 + \frac{\pi a}{\sqrt{X}} \right). \tag{3.24e}$$

With the help of these formulae for K , the corresponding formulae for $(s, \Phi, \epsilon, q, m, M)$ are determined directly from (3.18), (3.12a) and (3.12b). Here, it is also important to stress that, since the potential K was originally defined by (3.17), this potential is a continuous and differentiable function of (a_1, a_2, a_3) .

Setting

$$\varpi := \begin{cases} \sqrt{-X}/(a-d) & \text{for } X \leq 0, \\ \sqrt{X}/(a-d) & \text{for } X > 0, \end{cases} \tag{3.25}$$

the functions $\operatorname{arctanh} \varpi$ and $\operatorname{arctan} \varpi$ may be expanded in absolutely convergent power series in ϖ valid for $\varpi^2 < 1$ [17]:

$$\operatorname{arctanh} \varpi = \sum_{n=0}^{\infty} \frac{1}{2n+1} \varpi^{2n+1}, \quad \operatorname{arctan} \varpi = \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} \varpi^{2n+1}. \tag{3.26}$$

The inequality $\varpi^2 < 1$ is automatically satisfied if $X \leq 0$. However, in the case $X > 0$, this inequality is not automatically satisfied because it imposes an additional condition on the possible values of (a_1, a_2, a_3) . When $\varpi^2 < 1$, equations (3.24a)–(3.24c) can alternatively be written as

$$K = -\frac{2\chi^4}{a-d} \left[\frac{a+d}{(a-d)^2+X} - \frac{2d}{(a-d)^2} \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+3} \frac{X^n}{(a-d)^{2n}} \right]. \tag{3.27}$$

Substitution of

$$\frac{1}{(a-d)^2+X} = \frac{1}{(a-d)^2} \sum_{n=0}^{\infty} (-1)^n \frac{X^n}{(a-d)^{2n}} \tag{3.28}$$

into (3.27) then gives

$$K = -\frac{2\chi^4}{(a-d)^3} \sum_{n=0}^{\infty} (-1)^n \left(a + \frac{2n+1}{2n+3} d \right) \frac{X^n}{(a-d)^{2n}}, \tag{3.29}$$

where

$$a + \frac{2n+1}{2n+3}d > 0. \quad (3.30)$$

Clearly, this form of K is only valid if $a > d$ and

$$\varpi^2 = \frac{|X|}{(a-d)^2} < 1. \quad (3.31)$$

For a phonon gas that departs slightly from local equilibrium, we easily verify that

$$\frac{c|a_2|}{a_1} \ll 1, \quad \frac{c^2|a_3|}{a_1} \ll 1, \quad \frac{|b|}{a} \ll 1, \quad \frac{|d|}{a} \ll 1, \quad \varpi^2 \ll 1. \quad (3.32)$$

Thus, with these conditions, expansion (3.29) is expected to play a key role in the description of a phonon gas close to local equilibrium. If the non-equilibrium Lagrange multiplier a_3 is small, one way of further transforming the potential K is to expand $(a-d)^{-3}$ and $(a-d)^{-2n}$ in powers of a_3 . Formally, such an approach enables us to expand K into the Taylor series with respect to (a_2, a_3) and to replace K by the truncated series K_T . Whether the latter, if appropriately chosen, can generate the hyperbolic system

$$s_T^{ij} \partial_t a_j + \Phi_T^{ij} \partial_x a_j = Q_T^i \quad (i = 1, 2, 3) \quad (3.33)$$

remains an open question. In order to answer it, one must show that the symmetric matrix⁶

$$(s_T^{ij}) := -\frac{1}{4} \left(\frac{\partial^3 K_T}{\partial a_1 \partial a_i \partial a_j} \right) \quad (3.34)$$

is negative definite.

In the general case of phonon gas hydrodynamics based on the maximum-entropy principle, the analysis leading to a single generating function K of a set of Lagrange multipliers has been previously published by Larecki and Piekarski [5]. This analysis is possible whenever the moments of the distribution function happen to be symmetric tensors. Their work may provide the motivation for further developments, but the difficulty is that a closed-form analytic expression for K in terms of the Lagrange multipliers proves to be impossible to obtain except in the two situations. One of these situations has been examined in [6]. There, the 4-moment model with nondispersion and isotropy for phonon frequency spectrum was presented and the potential K was calculated. The second situation is, in essence, that described in this paper. Clearly, the disadvantage of using the potential K is that equations (3.12a) and (3.18) define only the relations

$$\epsilon = \epsilon(a_1, a_2, a_3), \quad q = q(a_1, a_2, a_3), \quad m = m(a_1, a_2, a_3) \quad (3.35)$$

and the inverse relations

$$a_1 = a_1(\epsilon, q, m), \quad a_2 = a_2(\epsilon, q, m), \quad a_3 = a_3(\epsilon, q, m) \quad (3.36)$$

are not easily determined. Although one can try to solve equations (3.14) for (a_1, a_2, a_3) and subsequently evaluate the hydrodynamic quantities (ϵ, q, m) , transport equations for (ϵ, q, m) cannot be formulated explicitly. This is a drawback because transport equations for the hydrodynamic quantities are highly desirable. The perturbative expansion technique, which is presented in section 4, provides a means of overcoming this difficulty.

We finally mention the following. As discussed in detail by Pennisi [18] and Geroch and Lindblom [19], for dissipative relativistic theories of divergence type it is also true that there exists a single generating function K , since the conservation of energy–momentum–stress is one of the evolution equations. A characteristic feature of [18] is that the route from

⁶ The symmetric matrix (Φ_T^{ij}) is defined by $(\Phi_T^{ij}) := -\frac{1}{4} \left(\frac{\partial^3 K_T}{\partial a_2 \partial a_i \partial a_j} \right)$.

a rather simple starting point (the precise definition of K) to an interesting final result (an explicit expression for K in terms of the Lagrange multipliers) required an introduction of the expansion of K about equilibrium states. Here, since the number of independent Lagrange multipliers is small and the dispersion relation is given by $\Omega = c|\mathbf{k}|$, we were able to calculate K in another way.

4. Expansion about quasi-equilibrium states

4.1. Derivation of the linearized formulae

In the one-dimensional geometry, using the results of section 4, we can express

$$\mathcal{M} := (\epsilon, q, m) \tag{4.1}$$

and M as explicit functions of

$$\mathcal{A} := (a_1, a_2, a_3). \tag{4.2}$$

The inverse problem to that just mentioned is that of recovering the relations

$$\mathcal{A} = \mathcal{A}(\mathcal{M}) \tag{4.3}$$

and

$$M = M(\mathcal{M}) \tag{4.4}$$

if the relations

$$\mathcal{M} = \mathcal{M}(\mathcal{A}) \tag{4.5}$$

and

$$M = M(\mathcal{A}) \tag{4.6}$$

are given. However, for the case $a_3 \neq 0$, it is impossible to invert equation (4.5) analytically so as to obtain equations (4.3) and (4.4). This can only be done for the case $a_3 = 0$, in the sense that a knowledge of (ϵ, q) enables one to determine m and (a_1, a_2) :

$$\begin{aligned} m = m_* &:= \frac{4c^2\epsilon u}{3+u}, & a_1 = \Delta &= \frac{\chi}{\epsilon^{1/4}} \frac{(3+u)^{1/4}}{(1-u)^{3/4}}, \\ a_2 &= -\frac{1}{c} \Delta v = -\frac{\chi v}{c\epsilon^{1/4}} \frac{(3+u)^{1/4}}{(1-u)^{3/4}}. \end{aligned} \tag{4.7}$$

Here, we recall that the quantities v and u are related to the energy density ϵ and the heat flux q through equations (3.4). From the assumption $a_3 = 0$, and from the definition

$$A := \frac{1}{u^2} \left[\frac{(1-u)^2}{2\sqrt{u}} \ln \left(\frac{1+\sqrt{u}}{1-\sqrt{u}} \right) + \frac{1}{3}(5u-3) \right], \tag{4.8}$$

a direct analysis of (3.10b), (3.9) and (4.7) then yields the following expression for M in terms of (ϵ, q) :

$$M = M_* := \frac{9c^3\epsilon u}{5(3+u)} Gv = \frac{27c^2(2c\epsilon - \sqrt{4c^2\epsilon^2 - 3|q|^2})}{20(2c\epsilon + \sqrt{4c^2\epsilon^2 - 3|q|^2})} Gq, \tag{4.9}$$

where

$$G := \frac{1}{2u} \left[\frac{8}{3} - 5(1-u)A \right]. \tag{4.10}$$

The coefficient G is well-behaved as a function of (ϵ, q) near $q = 0$. Indeed, a simple calculation employing the series

$$A = \sum_{n=0}^{\infty} \frac{8u^n}{(2n+1)(2n+3)(2n+5)} \quad (0 \leq u < 1) \quad (4.11)$$

shows that, in the limit $q \rightarrow 0$, this coefficient becomes

$$G = \frac{8}{7} \quad (4.12)$$

since $u \rightarrow 0_+$ as $q \rightarrow 0$.

In the case $a_3 \neq 0$, we shall find it advantageous to write \mathcal{A} in the form

$$a_1 = \Delta(1 + \lambda_1), \quad a_2 = -\frac{1}{c}\Delta(1 + \lambda_2)v, \quad a_3 = \frac{1}{c^2}\Delta\lambda_3. \quad (4.13)$$

Although the analytic (i.e., exact and tractable) solution for \mathcal{A} of equation (4.5) is not possible to get, we now see that, at least in principle, the problem of determining relations (4.3) and (4.4) reduces to the problem of expressing the quantities $(\lambda_1, \lambda_2, \lambda_3)$ in terms of \mathcal{M} . Combining (3.9) and (4.13) gives

$$z = \Delta\omega, \quad \omega := \omega_* + \delta\omega_*, \quad (4.14)$$

where

$$\omega_* := 1 - v\sigma, \quad \delta\omega_* := \lambda_1 - \lambda_2v\sigma + \frac{1}{2}\lambda_3(3\sigma^2 - 1). \quad (4.15)$$

Let

$$\delta\left(\frac{1}{\omega_*^4}\right) := \frac{1}{\omega^4} - \frac{1}{\omega_*^4}. \quad (4.16)$$

With the additional notation

$$\delta M_* := M - M_*, \quad (4.17)$$

equations (3.10a)–(3.10c) can then be rewritten as follows:

$$\int_{-1}^1 \delta\left(\frac{1}{\omega_*^4}\right) d\sigma = 0, \quad \int_{-1}^1 \sigma \delta\left(\frac{1}{\omega_*^4}\right) d\sigma = 0, \quad (4.18a)$$

$$\frac{3}{4}\left(\frac{\chi}{\Delta}\right)^4 \int_{-1}^1 (3\sigma^2 - 1) \delta\left(\frac{1}{\omega_*^4}\right) d\sigma = \epsilon N, \quad (4.18b)$$

$$\frac{9c^3}{20}\left(\frac{\chi}{\Delta}\right)^4 \int_{-1}^1 \sigma(5\sigma^2 - 3) \delta\left(\frac{1}{\omega_*^4}\right) d\sigma = \delta M_*, \quad (4.18c)$$

where the quantities $(\chi/\Delta)^4$ and N (see (2.9), (3.3c), (3.5) and (4.7)) are characterized by

$$\left(\frac{\chi}{\Delta}\right)^4 = \frac{\epsilon(1-u)^3}{3+u}, \quad N = \frac{m-m_*}{c^2\epsilon}. \quad (4.19)$$

In obtaining these formulae, we have made use of the fact that

$$\epsilon = \frac{3}{2}\left(\frac{\chi}{\Delta}\right)^4 \int_{-1}^1 \frac{1}{\omega_*^4} d\sigma, \quad q = \frac{3c}{2}\left(\frac{\chi}{\Delta}\right)^4 \int_{-1}^1 \frac{\sigma}{\omega_*^4} d\sigma, \quad (4.20a)$$

$$m_* = \frac{3c^2}{4}\left(\frac{\chi}{\Delta}\right)^4 \int_{-1}^1 \frac{3\sigma^2 - 1}{\omega_*^4} d\sigma, \quad M_* = \frac{9c^3}{20}\left(\frac{\chi}{\Delta}\right)^4 \int_{-1}^1 \frac{\sigma(5\sigma^2 - 3)}{\omega_*^4} d\sigma. \quad (4.20b)$$

When (4.16) is substituted into (4.18a)–(4.18c) and the integration is performed, the resulting system yields a set of equations from which the relation between $(\lambda_1, \lambda_2, \lambda_3, M)$ and \mathcal{M} can, in principle, be determined. More precisely, the solution of equations (4.18a) and (4.18b) gives expressions for $(\lambda_1, \lambda_2, \lambda_3)$,

$$\lambda_i = \lambda_i(\mathcal{M}) \quad (i = 1, 2, 3), \tag{4.21}$$

and these are fed back into (4.18c), which in turn is solved for M to give $M = M(\mathcal{M})$.

Comparatively simple results are obtained only when we use a linearized theory of small departures from local quasi-equilibrium. This theory is accomplished by observing that local quasi-equilibrium states are defined by

$$(a_1^{(0)}, a_2^{(0)}, a_3^{(0)}) := (\Delta, -\Delta v/c, 0), \tag{4.22}$$

by verifying that these states comprise a two-dimensional subspace parametrized by (ϵ, q) , by assuming that $|\lambda_i| \ll 1$ ($i = 1, 2, 3$), by showing that

$$\delta \left(\frac{1}{\omega_*^4} \right) = -\frac{4}{\omega_*^4} \left(\frac{\delta\omega_*}{\omega_*} \right) + \frac{10}{\omega_*^4} \left(\frac{\delta\omega_*}{\omega_*} \right)^2 - \left[20 + 45 \left(\frac{\delta\omega_*}{\omega_*} \right) + 36 \left(\frac{\delta\omega_*}{\omega_*} \right)^2 + 10 \left(\frac{\delta\omega_*}{\omega_*} \right)^3 \right] \frac{1}{\omega_*^4} \left(\frac{\delta\omega_*}{\omega_*} \right)^3, \tag{4.23}$$

and by postulating (as in fact happens in the case of typical values of $|v|$) that the above exact expression for $\delta(1/\omega_*^4)$ can be approximated by

$$\delta \left(\frac{1}{\omega_*^4} \right) = -\frac{4}{\omega_*^4} \left(\frac{\delta\omega_*}{\omega_*} \right). \tag{4.24}$$

With the integral formulae presented in the appendix, we then derive from (4.18a)–(4.18c) and (4.24) the following manageable system of linear relations:

$$3(1 + u)\lambda_1 - u(5 + u)\lambda_2 + 6u\lambda_3 = 0, \tag{4.25a}$$

$$(5 + u)\lambda_1 - (1 + 5u)\lambda_2 + 2(1 + 2u)\lambda_3 = 0, \tag{4.25b}$$

$$24u\lambda_1 - 8u(1 + 2u)\lambda_2 - 3[4(1 - 3u) - 9(1 - u)^2 A]\lambda_3 = -(1 - u)(3 + u)N, \tag{4.25c}$$

$$72u^2 v\lambda_1 - 6uv[15(1 - u)^2 A - 4(2 - 5u)]\lambda_2 - 9v[4(2 - u)(5 - 7u) - 75(1 - u)^2 A]\lambda_3 = -\frac{5u}{c^3 \epsilon}(1 - u)(3 + u)\delta M_*. \tag{4.25d}$$

Before exploiting these relations, we set

$$E := 3(3 - u)A - 4, \quad I := \frac{3}{u} [3(3u - 5)A + 4(2 - u)], \quad \tilde{N} := -\frac{(9 - u^2)N}{3(1 - u)E}. \tag{4.26}$$

Given the integral identity

$$E = \frac{3(1 - u)^2}{2(3 - u)} \int_{-1}^1 \frac{[(3 - u)\sigma^2 - 4v\sigma + 3u - 1]^2}{(1 - v\sigma)^5} d\sigma \tag{4.27}$$

and series (4.11), elementary inspection shows that $E > 0$ if $|v| = \sqrt{u} < 1$ and that

$$E \rightarrow \frac{4}{5}, \quad I \rightarrow -\frac{36}{35} \tag{4.28}$$

as q (and hence u) approaches 0. Evidently, equations (4.25a)–(4.25d) imply the formulae

$$\lambda_1 = \frac{4u}{3(3 - u)}\tilde{N}, \quad \lambda_2 = \frac{2}{3 - u}\tilde{N}, \quad \lambda_3 = \frac{1}{3}\tilde{N} \tag{4.29}$$

and

$$M = \frac{9c^3\epsilon}{3+u} \left[\frac{1}{5}Gu + \frac{1-u}{3(3-u)}I\tilde{N} \right] v, \quad (4.30)$$

in which

$$\tilde{N} = -\frac{9-u^2}{3(1-u)E} \left(\frac{m}{c^2\epsilon} - \frac{4u}{3+u} \right). \quad (4.31)$$

Within the framework of a linearized theory of small departures from local quasi-equilibrium, using (4.10), (4.26), (4.8) and (3.4), it thus appears that the quantities $\lambda_1, \lambda_2, \lambda_3$ and M can all be expressed as linear functions of \tilde{N} and nonlinear functions of (ϵ, q) . Also, the conditions $|\lambda_i| \ll 1$ ($i = 1, 2, 3$) are readily seen to be equivalent to the condition $|\tilde{N}| \ll 1$. Next, since the solution for m of equation (4.31) has the form

$$m = \frac{c^2\epsilon}{3+u} \left[4u - \frac{3(1-u)}{3-u}E\tilde{N} \right], \quad (4.32)$$

the passage from (ϵ, q, m) to (ϵ, q, \tilde{N}) is a diffeomorphic change of independent gas-state variables. Insertion of relations (4.30) and (4.32) into equations (3.6a)–(3.6c) and use of the formula

$$N = -\frac{3(1-u)}{9-u^2}E\tilde{N}, \quad (4.33)$$

where E is defined by (4.26), leads to the differential equations for (ϵ, q, \tilde{N}) . Finally, the transport equations for (ϵ, q, m) can be derived from this starting point by taking into account relation (4.31).

Now, a word should be said about the physical interpretation of our results. As a matter of fact, the perturbative treatment of equations (4.18a)–(4.18c) given here relies implicitly on the postulate that the relaxation time τ_n for normal processes is much smaller than the relaxation time τ_r for resistive processes. If $\tau_n \ll \tau_r$, during the first time period τ_n , normal processes make the phonon gas approach a quasi-equilibrium Planck distribution F_* , and then during the longer time period τ_r , resistive processes return it to an equilibrium Planck distribution F_o . Consequently, for time scales of the order of τ_n , we are justified in assuming that (a_1, a_2, a_3) is close to $(a_1^{(0)}, a_2^{(0)}, a_3^{(0)})$. Moreover, having a separation of two time scales, we can expand (m, M) about (m_*, M_*) and linearize in \tilde{N} .

An alternative strategy for obtaining the equations of 9-moment phonon hydrodynamics is offered by the modified Grad-type approach [9]. This approach proposes to expand the phase density (i.e., the number density of phonons) about a quasi-equilibrium Planck distribution F_* and to include the flux of the heat flux in the expansion. In the one-dimensional case [10], the phase density to the 9-moment order of approximation takes the form [9, 10]:

$$f = F_*[1 - c|\mathbf{k}|\Delta(1 + F_*)\varphi^{0|3}\Pi_3], \quad (4.34)$$

where (F_*, Δ) are defined by (2.4) and (2.9), $\varphi^{0|3}$ is the expansion coefficient and Π_3 is the ‘special’ function given by

$$\Pi_3 := \frac{1}{3-u} (1+u-2v\sigma) - \frac{1}{2}(1-\sigma^2). \quad (4.35)$$

Note that Π_3 is independent of $|\mathbf{k}|$ and depends on $\sigma := g^1 = \cos\theta$ and on (ϵ, q) through (v, u) (see (3.4)). Because of (4.34) and (4.35), we can show that f has the same principal moments as F_* :

$$\epsilon = cy \int |\mathbf{k}|f \, d^3\mathbf{k} = cy \int |\mathbf{k}|F_* \, d^3\mathbf{k}, \quad q = c^2y \int |\mathbf{k}|\sigma f \, d^3\mathbf{k} = c^2y \int |\mathbf{k}|\sigma F_* \, d^3\mathbf{k}. \quad (4.36)$$

In view of (3.3b), equations (2.13) and (2.16) for (M^{ij}, M^{ijk}) reduce to

$$m = \frac{1}{2}c^3 y \int |\mathbf{k}|(3\sigma^2 - 1)f \, d^3\mathbf{k}, \quad M = \frac{3}{10}c^4 y \int |\mathbf{k}|\sigma(5\sigma^2 - 3)f \, d^3\mathbf{k}. \quad (4.37)$$

Substituting (4.34) into (4.37) and recalling the definitions of (G, E, I, \tilde{N}) (see (4.10) and (4.26)), we obtain $\varphi^{0|3} = \tilde{N}$ and relations (4.30)–(4.33). Consequently, since the resulting closing relation for M is linear in \tilde{N} and nonlinear in (ϵ, q) , the modified Grad-type approach [9, 10] delivers essentially the same transport equations for (ϵ, q, \tilde{N}) or (ϵ, q, m) as those originating from the present method. Such an approach seems particularly useful if we assume that $\tau_n \ll \tau_r$. Then it is natural to expand f about F_* . Moreover, with the exception of the obvious condition $|q| < c\epsilon$, there are effectively no unphysical limitations on the value of $|q|$, i.e., one can handle problems with a large nonvanishing component of the heat flux. We believe that this is an improvement over traditional approaches which only make allowances for small deviations in the heat flux from zero.

Another remark is also in order. Originally, the modified Grad-type approach was used in [9] to derive a closed system of equations for (ϵ, q^i, M^{ij}) . These equations are more general than those presented here, since they are based on the 9-moment closure that, in addition to the energy density ϵ and the heat flux \mathbf{q} , involves all components of the flux of the heat flux as extra gas-state variables. Although this closure permits the inclusion of the heat flux \mathbf{q} in a non-perturbative fashion, the presence of nine independent gas-state variables complicates the discussion of the properties of the resulting differential equations. For example, whether the 9-moment closure leads to a system of equations which are hyperbolic in a convex set of states containing all equilibrium and quasi-equilibrium states is an open problem that remains to be seen. It should be emphasized, however, that equations (3.6a)–(3.6c), in conjunction with the closing relations of this section, yield a nontrivial system of three evolution equations⁷ which, for a well-defined region of parameter space, is a symmetrizable quasi-linear hyperbolic system. The region of symmetric hyperbolicity in parameter space (the space defined by either ϵ, q, \tilde{N} or ϵ, q, m) is described in detail in [10]. Hyperbolicity is an important property for it ensures finite propagation speeds⁸, well-posedness and prevents the breakdown of the closure model. In this context, we mention that the notation in [10] slightly differs from ours as follows: the non-equilibrium quantity \tilde{N} is identified with the expansion coefficient $\varphi^{0|3}$ (i.e., $\tilde{N} := \varphi^{0|3}$) and the quasi-equilibrium Planck distribution F_* (also called the anisotropic Planck function) is denoted by F .

4.2. Approximation up to terms of second order

Equation (4.30) is, as has already been mentioned, also derivable from the modified Grad-type approach [10]. To go beyond this result, we must calculate M to second order in \tilde{N} . If $|\tilde{N}| \ll 1$, is it possible to neglect the second-order correction, i.e., is the postulate of section 4.1 about the replacement of $\delta(1/\omega_*^4)$ by (4.24) consistent even though we do not assume that q is small? Since this problem is directly related to the justification of the first-order approximation and the modified Grad-type approach, we now discuss it in detail. First of all, from equations (4.23), (4.15) and (4.29) we obtain, correct to second order,

$$\delta \left(\frac{1}{\omega_*^4} \right) = -\frac{4}{\omega_*^4} \left(\frac{\delta\omega_*}{\omega_*} \right) + \frac{10}{\omega_*^4} \left(\frac{\tilde{\delta}\omega_*}{\omega_*} \right)^2, \quad (4.38)$$

⁷ These equations are of course consistent with the full 9-moment system, because they correspond to the one-dimensional, rotationally symmetric reduction of this system [10].

⁸ In [10], restricting our attention to the one-dimensional geometry, we consider the eigenvalue problem and calculate approximately the characteristic speeds.

where (see (4.15)) $\delta\omega_* := \lambda_1 - \lambda_2 v\sigma + \frac{1}{2}\lambda_3(3\sigma^2 - 1)$ and

$$\tilde{\delta}\omega_* := \left[\frac{4u}{3(3-u)} - \frac{2v\sigma}{3-u} + \frac{1}{6}(3\sigma^2 - 1) \right] \tilde{N}. \quad (4.39)$$

Substitution of (4.38) into (4.18a)–(4.18c) and use of the integral formulae listed in the appendix yields a complete system of linear algebraic equations for the quantities $(\lambda_1, \lambda_2, \lambda_3, \delta M_*)$:

$$\delta M_* := M - \frac{9c^3\epsilon u}{5(3+u)} Gv. \quad (4.40)$$

Without entering into the details, by a direct analysis of this system, which in view of equations (4.38) and (4.39) contains the terms quadratic in \tilde{N} , it is possible to show that

$$\lambda_1 = \frac{4u}{3(3-u)} \tilde{N} + \frac{\alpha}{8(3-u)^2 E} \tilde{N}^2, \quad (4.41a)$$

$$\lambda_2 = \frac{2}{3-u} \tilde{N} + \frac{3\beta}{8(3-u)^2 E} \tilde{N}^2, \quad (4.41b)$$

$$\lambda_3 = \frac{1}{3} \tilde{N} + \frac{(1-u)\kappa}{2(3-u)^2 E} \tilde{N}^2, \quad (4.41c)$$

$$M = \frac{9c^3\epsilon u}{5(3+u)} Gv + \frac{3c^3\epsilon(1-u)I}{9-u^2} \left[1 + \frac{3\zeta}{4(3-u)EI} \tilde{N} \right] \tilde{N}v, \quad (4.41d)$$

where

$$\alpha := 45(5+u)(3-u)^2 A^2 - 24(171 - 142u + 31u^2)A + 16(101 - 87u + 16u^2), \quad (4.42a)$$

$$\beta := \frac{1}{u} [45(1+u)(3-u)^2 A^2 - 12(123 - 105u + 21u^2 + u^3)A + 16(42 - 39u + 7u^2)], \quad (4.42b)$$

$$\kappa := \frac{1}{u} [8(27 - 14u + 2u^2) - 45(3-u)^2 A], \quad (4.42c)$$

$$\begin{aligned} \zeta := & \frac{1}{u^2} [135u(1+u)(3-u)^2 A^3 + 9(405 - 1092u + 470u^2 - 4u^3 - 19u^4)A^2 \\ & - 36(129 - 309u + 171u^2 - 31u^3)A + 32(45 - 102u + 59u^2 - 12u^3)]. \end{aligned} \quad (4.42d)$$

The coefficients $(\alpha, \beta, \kappa, \zeta)$ tend to the limits

$$\alpha = \frac{16}{5}, \quad \beta = \frac{48}{7}, \quad \kappa = \frac{8}{7}, \quad \zeta = -\frac{192}{245} \quad (4.43)$$

as $u \rightarrow 0_+$. Also, in the limit $u \rightarrow 1_-$, we have

$$G = \frac{4}{3}, \quad I = \frac{\alpha}{E} = \frac{\beta}{E} = \frac{(1-u)\kappa}{E} = \frac{\zeta}{EI} = 0. \quad (4.44)$$

Owing to these explicit formulae, equations (4.41a)–(4.41d) are non-singular for all admissible values of q ($|q| < c\epsilon$). Moreover, except for the case of equation (4.41a), which reduces to

$$\lambda_1 = \frac{1}{18} \tilde{N}^2 \quad (4.45)$$

as $u \rightarrow 0_+$, it turns out that the second-order terms can be neglected when $|\tilde{N}| \ll 1$.

We are now ready to evaluate the entropy density s and the entropy flux Φ up to terms of second order in \tilde{N} . To this end, we first observe that (3.10c) can be cast into the form

$$s = 2\Delta \left(\frac{\chi}{\Delta}\right)^4 \int_{-1}^1 \frac{1}{\omega^3} d\sigma, \quad \Phi = 2c\Delta \left(\frac{\chi}{\Delta}\right)^4 \int_{-1}^1 \frac{\sigma}{\omega^3} d\sigma. \tag{4.46}$$

Here, in analogy with equation (4.23), the quantity $1/\omega^3$ is written as

$$\frac{1}{\omega^3} = \frac{1}{\omega_*^3} - \frac{3}{\omega_*^3} \left(\frac{\delta\omega_*}{\omega_*}\right) + \frac{6}{\omega_*^3} \left(\frac{\delta\omega_*}{\omega_*}\right)^2 - \left[10 + 15 \left(\frac{\delta\omega_*}{\omega_*}\right) + 6 \left(\frac{\delta\omega_*}{\omega_*}\right)^2\right] \frac{1}{\omega_*^3} \left(\frac{\delta\omega_*}{\omega_*}\right)^3. \tag{4.47}$$

Next, we replace the above exact expression for $1/\omega^3$ by the following approximate formula:

$$\frac{1}{\omega^3} = \frac{1}{\omega_*^3} - \frac{3}{\omega_*^3} \left(\frac{\delta\omega_*}{\omega_*}\right) + \frac{6}{\omega_*^3} \left(\frac{\tilde{\delta}\omega_*}{\omega_*}\right)^2. \tag{4.48}$$

Since $\delta\omega_*$ is defined by (4.15) and $(\lambda_1, \lambda_2, \lambda_3)$ are given by (4.41a)–(4.41c), it is then straightforward to conclude (after a bit of algebra and using (4.39) and the integrals presented in the appendix) that

$$s = s_* \left[1 - \frac{1}{8(3-u)} E \tilde{N}^2\right], \tag{4.49a}$$

$$\Phi = cs_* \left\{1 + \frac{1}{2(3-u)} \left[1 + \frac{\rho}{2(3-u)E} \tilde{N}\right] E \tilde{N}\right\} v, \tag{4.49b}$$

where

$$s_* := 4\epsilon\Delta \left(\frac{1-u}{3+u}\right), \quad \rho := \frac{1}{2u} [3(3-u)(13u-15)A + 4(3u^2-19u+18)]. \tag{4.50}$$

As shown in [9, 10], equations (4.29), (4.30) and (4.49a) can also be obtained by means of the modified Grad-type approach (see especially [10, equations (2.15), (3.21)–(3.25) and (3.50)]). However, equations (4.41a)–(4.41d) and (4.49b) are new: the modified Grad-type approach does not lead to them. The first-order expression for Φ is given by

$$\Phi = cs_* \left[1 + \frac{1}{2(3-u)} E \tilde{N}\right] v. \tag{4.51}$$

We easily deduce from $E > 0$ and $s - s_* = -s_* E \tilde{N}^2 / (8(3-u)) \leq 0$ that among all states (ϵ, q, \tilde{N}) having the same values of the energy density and the heat flux, the quasi-equilibrium state $(\epsilon, q, 0)$ gives s its greatest value. In the limit $u \rightarrow 1_-$, we find

$$E = 0, \quad \frac{\rho}{E} = -1. \tag{4.52}$$

Moreover, the coefficient ρ becomes

$$\rho = \frac{2}{35} \tag{4.53}$$

as $u \rightarrow 0_+$. Consequently, if the magnitude of \tilde{N} is much smaller than 1, then equations (4.49a) and (4.49b) represent an acceptable approximation. A simpler approximation to apply, and one expected to be satisfactory also for the quantities $(\lambda_2, \lambda_3, M)$, is to neglect all terms quadratic in \tilde{N} .

To sum up, our perturbative expansion scheme is both consistent with the modified Grad-type approach and goes beyond it. Yet it is also clear that this scheme is not trivial in the following sense. In principle, there may be no small quantity in which to expand; or even if such a small quantity exists, it may be that the Lagrange multipliers and the moments we are studying are not described by formulae which can be expanded in that small quantity—such an expansion may contain the singular terms. Here, however, expressions (4.41a)–(4.41d) are well-behaved as functions of (ϵ, q, \tilde{N}) and these problems do not appear.

5. Discussion and final remarks

Concentrating on the 9-moment closure and assuming for simplicity the one-dimensional geometry, we have presented a systematic derivation of the closed systems of equations for (a_1, a_2, a_3) and (ϵ, q, \tilde{N}) . In contrast with our previous analysis in [9, 10] where the modified Grad-type approach was used, we have used here the maximum-entropy method [5] as the starting point. Given this method, it was advantageous to provide a new example of the single generating potential, i.e., calculate explicitly a function K of a set of three Lagrange multipliers (a_1, a_2, a_3) in terms of which the derived system of partial differential equations for (a_1, a_2, a_3) assumes a symmetric hyperbolic form. Moreover, in the case when the phonon gas is close to quasi-equilibrium ($f \cong F_*$) and the normal processes dominate the phonon distribution ($\tau_n \ll \tau_r$), it was possible to discuss new aspects (as compared with those already discussed [9, 10]) of the expansion of various non-equilibrium quantities about quasi-equilibrium states. For definiteness, and in order to show that the basic postulates of the theory can be verified self-consistently, explicit perturbative expressions for $(\lambda_1, \lambda_2, \lambda_3, M)$ and (s, Φ) were presented both at the first order in the expansion and at the second order. To first order in \tilde{N} , the results are consistent with, and appear complementary to, those obtained by means of the modified Grad-type approach [9, 10]. In essence, these results explain why one is justified in neglecting the second-order terms if $|\tilde{N}| \ll 1$.

Our strategy to describe small deviations from quasi-equilibrium was to close equations (3.6a)–(3.6c) by using relation (4.33) and by expanding $\delta M_* := M - M_*$ in powers of \tilde{N} . Most perturbative expansion techniques (e.g., those originating from the methods of Chapman and Enskog [20] and Grad [21, 22]) are based on an expansion about local equilibrium states and, as such, require that the components of \mathbf{q} are small. The main advantage of using the present technique is that the heat flux is incorporated into the model in a non-perturbative fashion, thereby allowing virtually arbitrarily large values for the nonvanishing component of \mathbf{q} . As noted already in section 4.1, such an approach suggests itself if the heat flux is finite and the relaxation time τ_n for normal processes is much smaller than the relaxation time τ_r for resistive processes. Then the quantities (ϵ, q) are slowly varying, since they are not altered by the normal processes. The higher moments (m, M) , however, tend to their local quasi-equilibrium values (m_*, M_*) on the fast time scale determined by τ_n . Developing the theory along these lines and considering only the lowest-order (in \tilde{N}) approximation to δM_* , one obtains the closing relations (4.30), (4.32) and (4.33) for equations (3.6a)–(3.6c) which are linear in the fast variable \tilde{N} and nonlinear in the slow variables (ϵ, q) . Moreover, it turns out that the resulting evolution system for (ϵ, q, \tilde{N}) is a symmetrizable quasi-linear hyperbolic system [10]. Because of this, the solutions to well-posed initial-value and/or boundary-value problems exist locally in a classical sense and the development of shocks can be expected.

If q is finite and \tilde{N} is the only small variable, the complexity of equations (4.41a)–(4.41d) is unavoidable and its presence reassures us as to the generality of our approach in the regime where $\tau_n \ll \tau_r$. For example, the fact that scattering processes tend to return the phonon gas first to a quasi-equilibrium Planck distribution F_* and then to an equilibrium Planck distribution F_o is included both in the description of the moment flux (see (4.41d)) and the collisional term (see the right-hand side of (3.6c)). The traditional approaches differ from ours in that they consider the phonon gas close to local equilibrium, i.e., they lead to the theory which treats the heat flux as a small perturbative quantity. Under these circumstances, it seems natural to expand (m, N, M) in powers of q and \tilde{N} . From this expansion we obtain [7], correct to leading order,

$$m = -\frac{4}{15}c^2\epsilon\tilde{N}, \quad N = -\frac{4}{15}\tilde{N}, \quad M = 0, \quad (5.1)$$

so that equation (3.6c) simplifies to

$$\partial_t m + \partial_x \left(\frac{2c^2}{5} q \right) = - \left(\frac{1}{\tau_r} + \frac{1}{\tau_n} \right) m. \tag{5.2}$$

The evolution system for $(\epsilon, q, m) \in \mathbb{R}^3$, derivable from (3.6a), (3.6b) and (5.2), is strictly hyperbolic in \mathbb{R}^3 . Here, unlike the case corresponding to the closing relations of section 4.1, it follows that the characteristic speeds do not depend on (ϵ, q, m) ; these speeds are 0 and $\pm\sqrt{15}c/5$. All the equations involved are linear if the relaxation times (τ_r, τ_n) are assumed to be the constant quantities. With this extra assumption, the principle of superposition of solutions applies and then one can employ the extensively developed theory of linear operators.

We believe that the above observations clearly demonstrate how the present nonlinear model is related to the linear one. In order to proceed further, we must carefully analyse the properties of solutions of our evolution equations for (ϵ, q, \tilde{N}) . The hyperbolic structure of these equations, evident in the lowest-order $O(\tilde{N})$ analysis of [10], lends itself to solution techniques that take advantage of the wave-like nature of the transport phenomena. Such techniques require the construction of good approximate Riemann solvers. There have been a number of approximate Riemann solvers proposed. One of the most popular currently in use in the computational fluid dynamics community is due to Roe [23, 24]. The basic idea is to approximate locally the original quasi-linear system of partial differential equations by a constant-coefficient linear system. We think that this idea may be useful, even though it is not yet developed for application to our system of evolution equations. Certainly, it must lead to separate numerical problems, the discussion of which is beyond the scope of this work.

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Appendix. Useful integrals

In this appendix, we present a set of integrals that are needed to derive the results of section 4.

Put $\omega_* := 1 - v\sigma$. With the abbreviation

$$\phi_m^n := (1 - u)^{m-1} \int_{-1}^1 \frac{\sigma^n}{\omega_*^m} d\sigma, \tag{A.1}$$

the following formulae can be obtained:

$$\phi_3^0 = 2, \quad \phi_3^1 = 2v, \quad \phi_4^0 = \frac{2}{3}(3 + u), \quad \phi_4^1 = \frac{8}{3}v, \quad \phi_4^2 = \frac{2}{3}(1 + 3u), \tag{A.2a}$$

$$\phi_4^3 = \frac{2}{3}[4 - 3(1 - u)A]v, \quad \phi_5^0 = 2(1 + u), \quad \phi_5^1 = \frac{2}{3}(5 + u)v, \quad \phi_5^2 = \frac{2}{3}(1 + 5u), \tag{A.2b}$$

$$\phi_5^3 = 2(1 + u)v, \quad \phi_5^4 = \frac{2}{3}[3(1 - u)^2 A - 1 + 7u], \tag{A.2c}$$

$$\phi_5^5 = \frac{2}{3u}[15(1 - u)^2 A - 8 + 17u - 3u^2]v, \quad \phi_6^0 = \frac{2}{5}(5 + 10u + u^2), \tag{A.2d}$$

$$\phi_6^1 = \frac{4}{5}(5 + 3u)v, \quad \phi_6^2 = \frac{2}{15}(5 + 38u + 5u^2), \quad \phi_6^3 = \frac{4}{5}(3 + 5u)v, \tag{A.2e}$$

$$\phi_6^4 = \frac{2}{5}(1 + 10u + 5u^2), \quad \phi_6^5 = \frac{2}{15u}[8 - 10u + 50u^2 - 15(1 - u)^3 A]v, \quad (\text{A.2f})$$

$$\phi_6^6 = \frac{2}{5u}[16 - 45u + 50u^2 - 5u^3 - 30(1 - u)^3 A], \quad (\text{A.2g})$$

$$\phi_6^7 = \frac{2}{5u^2}[56 - 160u + 150u^2 - 30u^3 - 105(1 - u)^3 A]v, \quad (\text{A.2h})$$

where the quantity A is defined by (4.8). These formulae are introduced in order to facilitate the understanding of equations (4.7), (4.9), (4.20a), (4.20b), (4.25a)–(4.25d), (4.27), (4.41a)–(4.41d) and (4.49a). In the limit $u \rightarrow 0_+$, we find

$$\frac{1}{v}\phi_6^5 \rightarrow \frac{10}{7}, \quad \frac{1}{v}\phi_6^6 \rightarrow \frac{12}{7}, \quad \phi_6^6 \rightarrow \frac{2}{7}, \quad \frac{1}{v}\phi_6^7 \rightarrow \frac{4}{3}. \quad (\text{A.3})$$

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