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ORIGINAL ARTICLE

Nanrong Zhao · Masaru Sugiyama

Analysis of heat conduction in a rarefied gas at rest with a temperature jump at the boundary by consistent-order extended thermodynamics

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Abstract In the context of the first- and second-order theories of consistent-order extended thermodynamics, a systematic approach is established for analyzing the temperature jump at the boundary through studying one-dimensional stationary heat conduction in a rarefied gas at rest. Thereby an approach to the free boundary-value problem in general is explored. Boundary values of temperature are assumed to be in the form of power expansion with respect to the Knudsen number, based on which analytical expressions of the temperature jump as well as entropy production at the boundary are derived explicitly. Dependencies of these two boundary quantities on both the Knudsen number and accommodation factor are also extensively discussed. The present analysis is expected to be the basis for the study of higher-order theories of consistent-order extended thermodynamics.

Keywords Consistent-order extended thermodynamics · Rarefied gas · Temperature jump · Entropy production at the boundary

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1 Introduction

Extended thermodynamics (ET) [1,2] is a theory of nonequilibrium phenomena in macroscopic physical systems that is valid even beyond the assumption of local equilibrium—the assumption that thermodynamic properties of a subsystem that is sufficiently large microscopically but sufficiently small macroscopically can be described well by the same relationships as those of a globally equilibrium system. Therefore ET may be required when there are steep gradients and rapid changes taking place in nonequilibrium phenomena, which are constantly observed nowadays in modern technology such as nanotechnologies and space technologies. ET is a natural generalization of thermodynamics of irreversible processes based on the local equilibrium assumption [3] by introducing many field variables in addition to the ordinary thermodynamic fields such as mass density, momentum density and energy density into its well-posed basic field equations. In order to

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N. Zhao (✉)
Department of Physics, Sichuan University, Chengdu 610064, China
E-mail: zhaonanr@yahoo.com

Present address:
N. Zhao
Graduate School of Engineering, Nagoya Institute of Technology, Nagoya 466-8555, Japan

M. Sugiyama
Graduate School of Engineering, Nagoya Institute of Technology, Nagoya 466-8555, Japan

deeply understand its mathematical structure and physical implications and to find clues to its further improvement, extended thermodynamic study of rarefied gases is crucially important because here we already have a well-established basic equation, that is the Boltzmann equation [4–6]. We also have the advantage of referring to ingenious methods developed so far: Chapman–Enskog method [4,5,7], Grad's moment method [8,9], and some newly proposed methods [10,11].

In extended thermodynamics of rarefied gases, there generally still remains the problem concerning boundary values imposed on the basic field equations, which actually takes on two aspects. One is the so-called uncontrollable boundary-value problem, that is, how to pose the appropriate boundary condition for most of the fields which are uncontrollable experimentally and are difficult to be understood intuitively. Another is related to possible jumps of physical quantities at the boundary between the system under consideration and its environment. These jumps indicate a free boundary-value problem in the sense that the related boundary values are, in general, not given at the beginning of our analysis. Both aspects are entangled with each other. In order to formulate and solve such a boundary-value problem, it is important to develop a systematic method by which the solution for the field equations and the jumps can be simultaneously derived and calculated in a consistent manner. It is worth emphasizing that there is essentially the same problem in the Chapman–Enskog method, Grad's moment method, and some newly proposed methods mentioned above.

Many studies have been made on determining the jumps of physical quantities at the boundary, or more generally boundary properties. For general references see, for example, monographs written by Chapman and Cowling [4], by Cercignani [5], and by Sone [6]. Beskok and Karniadakis [12] presented a second-order model for jumps; Lockerby and Reese [13] used the Burnett equations to compute second-order boundary conditions. Studies based on Grad's moment methods and extended thermodynamics were also made [14–17]. The results obtained so far mostly rely on numerical computation. For example, one typical procedure uses the method [14,15], based on which a set of basic relations can be established to provide the jumps. Nevertheless, due to the nonlinearity of these relations only numerical solutions have been available, which obviously cannot help us solve, in a systematic manner, the boundary-value problem, which always involves both jumps and uncontrollable values. There are also analytical studies [16,17] where the difficulty of the derivation of the jumps has been greatly reduced by using the assumption of an ideal wall. That is, it is assumed that there is no entropy production at the interface between the wall and the gas. This assumption, however, has its limitations. Indeed, according to the present analysis, one can safely adopt the concept of an ideal wall only when thermodynamic states are very near equilibrium (see Sect. 4.2).

In the present paper we study analytically the jump of temperature at the boundary on the basis of consistent-order extended thermodynamics (COET) [18]. By studying one-dimensional stationary heat conduction in a rarefied gas at rest (see Fig. 1), we try to gain a deep insight into the systematic approach to the free boundary-value problem in general. Moreover, as a measure of irreversibility in the process occurring at the boundary with the temperature jump, the entropy production there is also of physical importance. We will provide a specific confirmation to the positivity of this quantity in the context of COET by using our analytical derivation of the temperature jump. As we will see, COET has a good theoretical structure to carry out the systematic analysis of these boundary processes owing to its key concept called order. In our recent work [19], taking into account the concept carefully, we constructed a consistent solution of the field equations for the same heat conduction problem in a power-series form with respect to the space coordinate.

The present analysis is based on the first- and second-order COET, from which we take the advantage that there is no uncontrollable boundary-value problem entangled. In contast to the first impression we may have that the results from the first- and second-order COET seem to be trivially simple, we can grasp several important points for the purpose mentioned above, which can be summarized as follows:

1) An analytical expression of the temperature jump in a power expansion form with respect to Knudsen number is derived explicitly. This expression will afford us a sound basis for further study of the third-order theory, or higher-order theories where we will encounter the uncontrollable boundary-value problem as well. A preliminary study in the case of the third-order COET has been reported recently [20].
2) An analytical expression for the entropy production at the boundary is also explicitly derived. On the basis of this expression, we make clear that the positivity of such a quantity is guaranteed within the validity range of our analysis, and is closely related to the proper sign of temperature jump at the boundary (see Sect. 4.2). The validity of the concept of an ideal wall is also studied explicitly.
3) The analytical results obtained here are compared with the results derived from Ohwada's numerical simulations [21]. Quantitatively good agreement between them strongly indicates the validity and usefulness of COET.

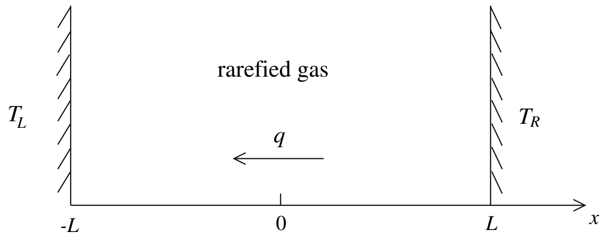

Fig. 1 One-dimensional heat conduction experiment (heat flux q) between rigid walls with temperatures T_L and T_R ($T_L < T_R$)

2 The first- and second-order COET for the heat conduction problem

COET [18] was proposed as a revised version of ET [1]. COET makes use of combinations of ordinary moments in ET as its field variables, and each of these combinations, called a G-moment, may be assigned an order of magnitude that is a measure of the importance of the moment in a physical process of nonequilibrium phenomena under consideration. As a result, closure of the hierarchical moment equations is automatically achieved. Similar ideas were also adopted in recent developments for transport equations of rarefied gases [10,11].

In the context of COET, a simplified form of the kinetic equation known as the Bhatnagar–Gross–Krook (BGK) equation [22] may be adopted, where a relaxation time τ is introduced into the collision term. For a problem of stationary one-dimensional heat conduction in a rarefied gas at rest, every G-moment can be expressed by the terms containing expressions of the type $[\tau(\mathrm{d}\theta/\mathrm{d}x)]^n$ and/or $\tau^n(\mathrm{d}^n\theta/\mathrm{d}x^n)$, which are regarded as of order n [18]. Here θ is the temperature field that depends only on the x-coordinate ($\theta \equiv kT/m$, where T is the kinetic temperature of the gas, k is the Boltzmann constant and m is the mass of an atom). If an irreversible process is deemed to be steep of order n, the necessary number of the G-moments is known and the field equations are closed by omitting all terms of order higher than n. In such a manner, COET gives us a sequence of field equations of increasing order that starts from the zero-order theory for equilibrium.

The nonequilibrium begins at the first-order theory, which is composed of the following three equations [18]:

$$\begin{aligned} &\text{1st order} \\ &0 = \frac{\mathrm{d}P}{\mathrm{d}x}, \\ &0 = \frac{\mathrm{d}G_{1,1}}{\mathrm{d}x}, \\ &G_{1,1} = \sqrt{\tfrac{5}{2}}P\tau\frac{\mathrm{d}\theta}{\mathrm{d}x} \end{aligned} \tag{1}$$

with three independent variables: pressure P , temperature θ and the first-order moment $G_{1,1}$, which is proportional to the heat flux q such that $G_{1,1} = -\sqrt{\frac{2}{5}}q$.

The system for the second-order theory is enlarged by introducing the second-order moments $G_{2,0}$, $G_{1,2}$, $G_{3,0}$ and $G_{2,2}$ such that [18]

$$\begin{aligned} &\text{2nd order} \\ &\left.\begin{aligned} 0 &= \frac{\mathrm{d}P}{\mathrm{d}x}, \\ 0 &= \frac{\mathrm{d}G_{1,1}}{\mathrm{d}x}, \\ G_{1,1} &= \sqrt{\tfrac{5}{2}}P\tau\frac{\mathrm{d}\theta}{\mathrm{d}x}, \end{aligned}\right\}(A) \\ &\left.\begin{aligned} G_{2,0} &= \frac{7}{\sqrt{3}}G_{1,1}\tau\frac{\mathrm{d}\theta}{\mathrm{d}x}, \\ G_{1,2} &= -4\sqrt{\tfrac{7}{15}}G_{1,1}\tau\frac{\mathrm{d}\theta}{\mathrm{d}x}, \\ G_{3,0} &= -\sqrt{14}\theta G_{1,1}\tau\frac{\mathrm{d}\theta}{\mathrm{d}x}, \\ G_{2,2} &= 2\sqrt{\tfrac{21}{5}}\theta G_{1,1}\tau\frac{\mathrm{d}\theta}{\mathrm{d}x}. \end{aligned}\right\}(B) \end{aligned}, \tag{2}$$

Obviously, this system of equations can be split into two parts (A) and (B) as indicated above, where part (A), the same as Eq. (1), is closed for the variables P, θ and $G_{1,1}$. Once part (A) is solved, part (B) provides us with the other quantities.

From Eqs. (1) and (2), we may conclude that both theories predict a constant pressure P that may be fixed by a boundary value, a constant heat flux $G_{1,1}$ due to the energy balance and a Fourier-type temperature field θ. The boundary values for θ, i.e. θ_L and θ_R at the left and right sides respectively, determine the specific forms of both $G_{1,1}$ and $\theta(x)$ as follows:

$$G_{1,1} = \sqrt{\frac{5}{2}} P\tau \frac{\theta_R - \theta_L}{2L} \tag{3}$$

and

$$\theta(x) = \frac{\theta_R - \theta_L}{2L} x + \frac{\theta_R + \theta_L}{2}, \tag{4}$$

where $2L$ is the length of the domain. Note that in Eq. (3), τ introduced in the BGK model generally depends on temperature [23], and so does the heat conductivity. However we assumed τ is a constant in the derivation of the above equations, which should be only valid for a small temperature difference. In such a case, Eq. (3) indicates a constant heat conductivity and then we obtain straight lines for the temperature field in Fig. 2. On the other hand, generally, the study of the third- and even higher-order theories which is constructed by introducing higher-order modification terms into the Fourier's law above becomes more complicated—not only is the general solution for the basic equations difficult to properly obtain [19], but also the uncontrollable boundary-value problem occurs, which is still unclear at present. We therefore restrict ourselves to studying Eqs. (3) and (4) as the first step.

The remaining problem is to determine explicitly the boundary values for θ, which is far from trivial. And we now clearly recognize the essential difference of temperature fields derived from first- and second-order theories. In fact, as we will see in Sect. 3.1, the boundary values θ_L and θ_R of the first-order theory are different from those of the second-order theory because of the difference between their distribution functions f. They are, respectively, given by

$$f^{1\mathrm{st}} = \left(1 + \frac{G_{1,1}}{P\sqrt{\theta}} \varphi_{1,1}\right) f_E \tag{5}$$

and

$$f^{2\mathrm{nd}} = \left(1 + \frac{G_{1,1}}{P\sqrt{\theta}} \varphi_{1,1} + \frac{G_{2,0}}{P\theta} \varphi_{2,0} + \frac{G_{1,2}}{P\theta} \varphi_{1,2} + \frac{G_{3,0}}{P\theta^2} \varphi_{3,0} + \frac{G_{2,2}}{P\theta^2} \varphi_{2,2}\right) f_E, \tag{6}$$

where $\varphi_{r,l}$ denotes the orthonormal irreducible Hermite polynomials in C_i of the atomic velocity, with r the number of traces and l the number of free indices [18]. $G_{r,l}$ is the corresponding moment defined by $G_{r,l} = m\sqrt{\theta}^{2r+l} \int \varphi_{r,l} f \mathrm{d}\mathbf{C}$. $f_E = \frac{P/\theta}{m\sqrt{2\pi\theta}^3} \mathrm{e}^{-\frac{C^2}{2\theta}}$ is the phase density at equilibrium. The distribution function $f^{2\mathrm{nd}}$ for the second-order theory obviously involves additional second-order terms.

3 Formulations for the temperature jump and entropy production at the boundary

In this section we analyze the temperature jump and the entropy production at the boundary on the assumption of a Maxwellian boundary condition, i.e. atoms are reflected at the wall either specularly or diffusively with velocities obeying the Maxwellian distribution (thermalization). By introducing an accommodation factor λ, whose meaning is self-evident from Eq. (7), the phase density at the wall $\hat{f}$ is expressed as [14,15]

$$\hat{f} = \begin{cases} \lambda f^w + (1-\lambda) f(-n_1 C_1) & : n_1 C_1 > 0 \\ f(n_1 C_1) & : n_1 C_1 \leq 0, \end{cases} \tag{7}$$

where C_1 is the x-component of the velocity of an atom, and n_1 denotes the x-component of the unit normal vector to the wall pointing inside the gas, so that we have the condition $n_1 C_1 > 0$ for the reflected atoms from the wall and $n_1 C_1 \le 0$ for the incident atoms on the wall. In Eq. (7), for simplicity, the other velocity components are not shown explicitly. The phase density f refers to that of the gas in front of the wall, which reads Eqs. (5) and (6) for the first- and second-order theories, respectively. While the phase density f^w represents the Maxwellian of the thermalized particles:

$$f^w = \frac{\rho^w}{m\sqrt{2\pi\theta^w}^3} \mathrm{e}^{-\frac{C^2}{2\theta^w}} \tag{8}$$

with mass density ρ^w and a given wall temperature θ^w ($\theta^w \equiv kT^w/m$, where T^w is the thermodynamic temperature of the wall, i.e. T_L at the left side and T_R at the right side, as shown in Fig. 1).

3.1 Temperature jump at the boundary

In order to obtain the jump of temperature, we first establish the jump conditions, which can be derived by applying the conservation laws of mass and energy at the boundary as follows:

$$m \int C_1 \hat{f} \mathrm{d}\mathbf{C} = 0, \tag{9}$$

$$\frac{1}{2} m \int C^2 C_1 \hat{f} \mathrm{d}\mathbf{C} = \frac{1}{2} m \int C^2 C_1 f \mathrm{d}\mathbf{C}, \tag{10}$$

where $\hat{f}$ takes the form of Eq. (7). By inserting f in Eq. (6) for the second-order theory as well as f^w in Eq. (8) into Eqs. (9) and (10), the jump conditions are reduced, after some calculations, to be

$$\sqrt{\frac{1}{2\pi}} \rho^w \sqrt{\theta^w} = \left(\sqrt{\frac{1}{2\pi}} P - \frac{G_{2,0}}{4\sqrt{15\pi}\theta} + \frac{G_{1,2}}{2\sqrt{21\pi}\theta} - \frac{G_{3,0}}{4\sqrt{70\pi}\theta^2} + \frac{G_{2,2}}{4\sqrt{21\pi}\theta^2} \right) \sqrt{\frac{1}{\theta}}, \tag{11}$$

$$\begin{aligned} \sqrt{\frac{2}{\pi}} \lambda \rho^w \sqrt{\theta^w}^3 = & \sqrt{\frac{2}{\pi}} \lambda P \sqrt{\theta} - \frac{1}{2} \sqrt{\frac{5}{2}} G_{1,1} n_1 (2 - \lambda) \\ & + \lambda \left(\sqrt{\frac{3}{5\pi}} \frac{G_{2,0}}{2} - \sqrt{\frac{3}{7\pi}} \frac{G_{1,2}}{2} + \frac{G_{3,0}}{2\sqrt{70\pi}\theta} - \frac{G_{2,2}}{4\sqrt{21\pi}\theta} \right) \sqrt{\frac{1}{\theta}}, \end{aligned} \tag{12}$$

where both θ and $G_{r,l}$ should be evaluated at the boundary.

Elimination of the density ρ^w from Eqs. (11) and (12), and utilizing the relations in Eq. (2) for reduction, we obtain

$$\begin{aligned} \theta_L - \theta_L^w = & \ \tfrac{\sqrt{5\pi}}{4} \tfrac{(2-\lambda)}{\lambda} \tfrac{G_{1,1}\sqrt{\theta_L}}{P} - \left(\tfrac{\theta_L^w}{5\theta_L} + \tfrac{9}{10} \right) \tfrac{G_{1,1}^2}{P^2} \ , \\ \theta_R - \theta_R^w = & -\tfrac{\sqrt{5\pi}}{4} \tfrac{(2-\lambda)}{\lambda} \tfrac{G_{1,1}\sqrt{\theta_R}}{P} - \left(\tfrac{\theta_R^w}{5\theta_R} + \tfrac{9}{10} \right) \tfrac{G_{1,1}^2}{P^2} \ . \end{aligned} \tag{13}$$

Introducing Eq. (3) for $G_{1,1}$ as well as the dimensionless quantities according to

$$K_n = \tfrac{\tau}{L/\sqrt{kT_0/m}}, \quad \hat{\theta} = \tfrac{\theta}{kT_0/m}, \tag{14}$$

where K_n is the Knudsen number and $T_0 \equiv \frac{T_L+T_R}{2}$, we may slightly rewrite Eq. (13) in a dimensionless form as

$$\begin{aligned} (\hat{\theta}_L - \hat{\theta}_L^w) = & \ \tfrac{5}{8} \sqrt{\tfrac{\pi}{2}} \tfrac{(2-\lambda_L)}{\lambda_L} K_n (\hat{\theta}_R - \hat{\theta}_L) \sqrt{\hat{\theta}_L} - \tfrac{5}{8} \left(\tfrac{\hat{\theta}_L^w}{5\hat{\theta}_L} + \tfrac{9}{10} \right) K_n^2 (\hat{\theta}_R - \hat{\theta}_L)^2 \ , \\ (\hat{\theta}_R - \hat{\theta}_R^w) = & -\tfrac{5}{8} \sqrt{\tfrac{\pi}{2}} \tfrac{(2-\lambda_R)}{\lambda_R} K_n (\hat{\theta}_R - \hat{\theta}_L) \sqrt{\hat{\theta}_R} - \tfrac{5}{8} \left(\tfrac{\hat{\theta}_R^w}{5\hat{\theta}_R} + \tfrac{9}{10} \right) K_n^2 (\hat{\theta}_R - \hat{\theta}_L)^2. \end{aligned} \tag{15}$$

Equation (15) provides us with the relations for the boundary values of temperature $\hat{\theta}$ (or temperature jump) based on the second-order theory. It is noticeable that: (1) in the case of the first-order theory, the second-order terms on the right-hand side of these relations play no role; (2) under the special conditions that only the first-order term is remained and that $\lambda_L = \lambda_R = 1$, the above set of relations recovers that derived in [14,15] based on Grad's 13-moment phase density; (3) as indicated by this equation, besides $\hat{\theta}_L^w$ and $\hat{\theta}_R^w$, two parameters influence the temperature jump, that is, the accommodation factor $\lambda_{L(R)}$ and Knudsen number K_n. Specifically, for $K_n \to 0$, the difference between the gas temperatures at the wall $\theta_{L(R)}$ and the wall temperatures $\theta^w_{L(R)}$, that is, the temperature jump vanishes. While for $\lambda_{L(R)} \to 0$, gas temperatures at both sides $\hat{\theta}_L$ and $\hat{\theta}_R$ become equal as $\frac{\theta^w_R+\theta^w_L}{2}$, being independent of the Knudsen number, which just indicates an adiabatic wall. Same limiting behaviors were also demonstrated by the numerical solutions derived in [15].

As Eq. (15) is nonlinear with respect to $\hat{\theta}_L$ and $\hat{\theta}_R$ it is, in general, difficult to obtain explicit expressions for the temperature jump as a function of the wall temperatures, even in the first-order case. Although the implicit result Eq. (15) can easily be solved numerically, we emphasize the importance of its analytical solution which is consistent with the order of the theory adopted. We believe that an explicit analytical result will play an essential role in the construction of a systematic formalism of boundary-value problems that may contain two types of boundary values, as we mentioned at the beginning of this paper; we can then understand more deeply the mathematical structure of ET itself. Therefore, although the first- and second-order theories that we are considering here only require the determination of jumps, we expect that the present study will be a sound basis for the study of higher-order theories with uncontrollable boundary-value problems [20].

In order to solve Eq. (15) analytically we may assume the temperature jump to be analytic with respect to Knudsen number. This point seems to be also supported by numerical results [14,15,21]. In such a case we propose the following expansions in Knudsen number

$$\begin{aligned} \hat{\theta}_L^{1\text{st}} &= \hat{\theta}_L^w + \alpha_1 K_n, \\ \hat{\theta}_R^{1\text{st}} &= \hat{\theta}_R^w + \beta_1 K_n \end{aligned} \tag{16}$$

and

$$\begin{aligned} \hat{\theta}_L^{2\text{nd}} &= \hat{\theta}_L^w + \alpha_1 K_n + \alpha_2 K_n^2, \\ \hat{\theta}_R^{2\text{nd}} &= \hat{\theta}_R^w + \beta_1 K_n + \beta_2 K_n^2, \end{aligned} \tag{17}$$

respectively for first- and second-order theories with coefficients α_i and β_i $(i = 1, 2)$. Naturally, the temperature jump should be identical to each other on the level of the first order. Notice that the above expansions are performed for boundary quantities—in the present case, temperature jump. Such expansions do not conflict with the order concept used in the derivation of the field equations in COET. Inserting these expansions into Eq. (15), we obtain

$$\begin{aligned} \alpha_1 &= \frac{5\sqrt{\pi/2}\sqrt{\hat{\theta}_L^w}(\hat{\theta}_R^w-\hat{\theta}_L^w)(2-\lambda_L)}{8\lambda_L}, \\ \beta_1 &= -\frac{5\sqrt{\pi/2}\sqrt{\hat{\theta}_R^w}(\hat{\theta}_R^w-\hat{\theta}_L^w)(2-\lambda_R)}{8\lambda_R} \end{aligned} \tag{18}$$

and

$$\begin{aligned} \alpha_2 = {} & \frac{1}{256\lambda_L^2\lambda_R}(\hat{\theta}_L^w - \hat{\theta}_R^w)\Big[176(\hat{\theta}_R^w - \hat{\theta}_L^w)\lambda_L^2\lambda_R + 25\pi(2-\lambda_L) \\ & \times\left(2\sqrt{\hat{\theta}_L^w\hat{\theta}_R^w}(2-\lambda_R)\lambda_L + (3\hat{\theta}_L^w - \hat{\theta}_R^w)(2-\lambda_L)\lambda_R\right)\Big], \\ \beta_2 = {} & \frac{1}{256\lambda_R^2\lambda_L}(\hat{\theta}_L^w - \hat{\theta}_R^w)\Big[176(\hat{\theta}_R^w - \hat{\theta}_L^w)\lambda_R^2\lambda_L - 25\pi(2-\lambda_R) \\ & \times\left(2\sqrt{\hat{\theta}_L^w\hat{\theta}_R^w}(2-\lambda_L)\lambda_R + (3\hat{\theta}_R^w - \hat{\theta}_L^w)(2-\lambda_R)\lambda_L\right)\Big]. \end{aligned} \tag{19}$$

Now, the boundary values $\hat{\theta}_{L(R)}$ have been explicitly expressed in terms of the wall temperatures $\hat{\theta}^w_{L(R)}$ as well as the parameters of Knudsen number K_n and the accommodation factors λ_L and λ_R. By using these analytical expressions above, we may conveniently discuss the general dependence of the temperature jump on these parameters.

3.2 Entropy production at the boundary

We now analyze entropy production at the boundary with the results of temperature jump obtained in the preceding subsection.

By taking into account the continuity condition of the normal component of heat flux q at the boundary and assuming the entropy flux in the solid wall to be heat flux divided by the thermodynamic temperature of the wall, i.e., $q/T_{L(R)}$, the entropy production rate σ per unit area at the boundary can be obtained according to the following relations:

$$\begin{aligned}\sigma_L &= h_L - \tfrac{q}{T_L},\\ \sigma_R &= \tfrac{q}{T_R} - h_R,\end{aligned} \tag{20}$$

respectively, for the left and right sides, where the entropy flux h is determined by the kinetic theory of gases [8], i.e.,

$$h = -k\int C_1 \ln\left(\frac{f}{y}\right) f\,\mathrm{d}\mathbf{C}, \tag{21}$$

with $\frac{1}{y}$ the smallest element in the one-body phase space. Keeping terms up to and including O(3), h can be specified as

$$h = \frac{k}{m}\left(-\sqrt{\frac{5}{2}}\frac{G_{1,1}}{\theta} - \frac{37}{5\sqrt{10}}\frac{G_{1,1}^3}{P^2\theta^2} - 2\sqrt{\frac{7}{15}}\frac{G_{1,1}G_{1,2}}{P\theta^2} + \frac{2}{\sqrt{3}}\frac{G_{1,1}G_{2,0}}{P\theta^2}\right). \tag{22}$$

Then by using the relations in Eq. (2) and introducing a dimensionless entropy production defined by $\hat{\sigma} = \sigma\left(P\sqrt{\frac{k}{mT_0}}\right)^{-1}$, we finally obtain

$$\begin{aligned}\hat{\sigma}_L &= \sqrt{\tfrac{5}{2}}\tfrac{\hat{G}_{1,1}}{\hat{\theta}_L(\hat{\theta}_L^w)}(\hat{\theta}_L - \hat{\theta}_L^w) + \tfrac{47}{10}\sqrt{\tfrac{2}{5}}\tfrac{\hat{G}_{1,1}^3}{\hat{\theta}_L^2}\ ,\\ \hat{\sigma}_R &= -\sqrt{\tfrac{5}{2}}\tfrac{\hat{G}_{1,1}}{\hat{\theta}_R(\hat{\theta}_R^w)}(\hat{\theta}_R - \hat{\theta}_R^w) - \tfrac{47}{10}\sqrt{\tfrac{2}{5}}\tfrac{\hat{G}_{1,1}^3}{\hat{\theta}_R^2},\end{aligned} \tag{23}$$

where $G_{1,1}$ follows from Eq. (3), and $\hat{\theta}_{L(R)}$ from Eqs. (17)–(19). The omission of the second terms in the right-hand side of above expressions gives us the entropy production compatible to the first-order theory. As shown in the next section, positivity of entropy production is surely satisfied.

Clearly, entropy production at the boundary is also affected by both the Knudsen number and the accommodation factor through θ_L and θ_R. Specifically, for $\lambda \to 0$, vanishing entropy production independent of Knudsen number should be expected, since $G_{1,1}$ vanishes due to the identical θ_L and θ_R in such a limiting case [see the discussion (3) after Eq. (15)].

Here let us discuss the ideal wall briefly. Inserting Eqs. (3), (17)–(19) into Eq. (23), and with the condition of vanishing entropy production at the boundary, we easily derive the temperature jumps $\Delta\hat{\theta}_L(=\hat{\theta}_L - \hat{\theta}_L^w)$ and $\Delta\hat{\theta}_R(=\hat{\theta}_R - \hat{\theta}_R^w)$ to be

$$\triangle\hat{\theta}_L = \triangle\hat{\theta}_R = -\frac{47}{40}(\hat{\theta}_R^w - \hat{\theta}_L^w)^2 K_n^2. \tag{24}$$

It is remarkable that both jumps are equal to each other.

4 Typical results and discussions

4.1 Results for specific parameters

With the aid of the analytical expressions in the preceding section, we may conveniently calculate the temperature jump and entropy production for specific wall temperatures $\hat{\theta}_L^w$, $\hat{\theta}_R^w$ and parameters K_n, λ_L and λ_R. For simplicity, a simpler case with $\lambda_L = \lambda_R \equiv \lambda$ is studied here.

Figure 2 shows the temperature profiles for three Knudsen numbers derived from the second-order theory with the boundary values given by Eqs. (17)–(19), where $\hat{x} = \frac{x}{L}$. The classical Fourier's law

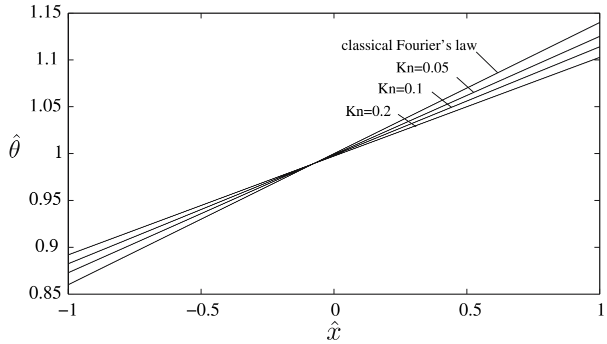

Fig. 2 Temperature profiles in the second-order theory of COET and the classical Fourier's law ($\hat{\theta}_L^w = 0.86$, $\hat{\theta}_R^w = 1.14$ and $\lambda = 0.826$)

$\hat{\theta} = \frac{\hat{\theta}_R^w + \hat{\theta}_L^w}{2} + \frac{\hat{\theta}_R^w - \hat{\theta}_L^w}{2}\hat{x}$ is also depicted for comparison. Due to the limit of the applicability range of second-order theory, only small Knudsen numbers are considered here and hereafter in the present paper.

Although the temperature profiles according to the second-order theory of COET are straight lines as that of classical Fourier's law, they have jumps at the boundaries as listed in Table 1. Here, in order to investigate the validity of the expansion (17), numerical values obtained directly from Eq. (15) are also presented for comparison. The difference is, as naturally expected, small for relatively small Knudsen numbers. Moreover, we may also compare the column with $K_n = 0.1546$ in Table 1 with Ohwada's data obtained by numerical simulations [21]. For proper comparison, Knudsen numbers in both data should be properly converted to each other: For Ohwada's system of hard sphere molecules, Knudsen number is related to the heat conductivity γ by $K_n^{\text{Ohwada}} = \frac{32}{75}\sqrt{\frac{2}{\pi}}\frac{\gamma}{2PL}\sqrt{\frac{mT_0}{k}}$ [4]. While our Knudsen number, being compatible with BGK equation, is proportional to the relaxation time τ [see Eq. $(14)_1$ where τ can be properly adjusted to the heat conductivity by Fourier's law expressed as Eq. (3)] such that $K_n = \frac{2\gamma}{5LP}\sqrt{\frac{mT_0}{k}}$. As a result, ratio $\frac{K_n^{\text{Ohwada}}}{K_n} \approx 0.4255$ may be followed. For $K_n = 0.1546$, Ohwada obtained $\hat{\theta}_L^{\text{numerical}} = 0.886$ and $\hat{\theta}_R^{\text{numerical}} = 1.109$, with which, obviously, our data coincide well.

Inserting the data of $\hat{\theta}_L$ and $\hat{\theta}_R$ in Table 1 into Eq. (23), we can further estimate the values of entropy production at the boundary as shown in Table 2 for four Knudsen numbers, where the data for $K_n = 0.1546$ are listed in order to compare them with our recent data based on the third-order theory: $\hat{\sigma}_L = 0.00161$ and $\hat{\sigma}_R = 0.00103$ [19]. Both sets of values also agree with each other well.

4.2 K_n and λ dependencies of the temperature jump and entropy production at the boundary

Owing to the analytical expressions obtained in Sect. 3 for both the temperature jump and entropy production at the boundary we can make clear explicit dependencies of the quantities on Knudsen number and the accommodation factor. In this subsection their typical results are shown.

Table 1 The boundary values of temperature $\hat{\theta}$ in the second-order theory of COET ($\hat{\theta}_L^w = 0.86$, $\hat{\theta}_R^w = 1.14$ and $\lambda = 0.826$)

K_n	0.05	0.1	0.1546	0.2
$\hat{\theta}_L$	0.873	0.882	0.889	0.892
$\hat{\theta}_R$	1.125	1.114	1.106	1.103
$\hat{\theta}_L^{\text{direct}}$	0.873	0.884	0.893	0.900
$\hat{\theta}_R^{\text{direct}}$	1.125	1.113	1.102	1.094

Table 2 Entropy production rate at the boundary in the second-order theory of COET ($\hat{\theta}_L^w = 0.86$, $\hat{\theta}_R^w = 1.14$ and $\lambda = 0.826$)

K_n	0.05	0.1	0.1546	0.2
$\hat{\sigma}_L$	0.000274	0.000879	0.00167	0.00233
$\hat{\sigma}_R$	0.000180	0.000577	0.00108	0.00147

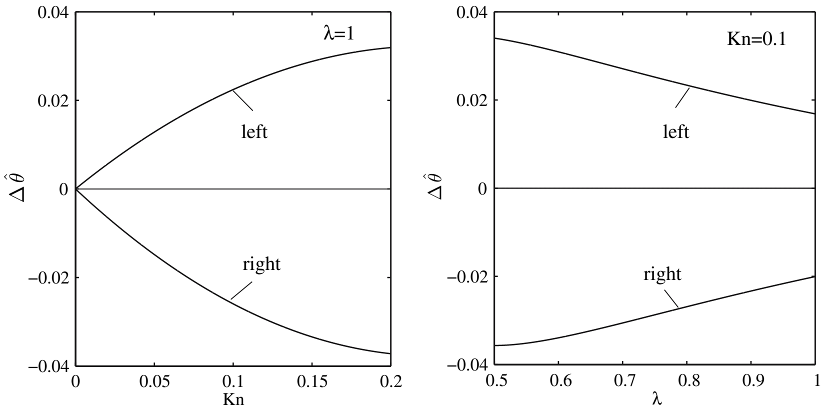

Fig. 3 Knudsen number K_n and accommodation factor λ dependencies of the temperature jumps at the boundary ($\hat{\theta}_L^w = 0.86$ and $\hat{\theta}_R^w = 1.14$)

Firstly, Fig. 3 shows the dependencies of the temperature jumps, i.e., $\Delta\hat{\theta}_L (= \hat{\theta}_L - \hat{\theta}_L^w)$ and $\Delta\hat{\theta}_R (= \hat{\theta}_R - \hat{\theta}_R^w)$ on Knudsen number K_n under $\lambda = 1$ and their dependencies on the accommodation factor λ under $K_n = 0.1$. It is evident from Fig. 3 that the temperature jump at the left side is positive while that at the opposite side is negative, under the premise of $\hat{\theta}_R^w > \hat{\theta}_L^w$. On the other hand, magnitudes of both jumps monotonously increase with the increase of Knudsen number, while decrease with the increase of the accommodation factor. The same tendency has been obtained in numerical work [15].

Secondly, Fig. 4 presents the dependencies of the entropy production at the boundary ($\hat{\sigma}_L$ and $\hat{\sigma}_R$) on K_n and λ. As a fundamental requisite of the second law of thermodynamics, the entropy production in any case is positive. Moreover, this quantity whether on the left or on the right, increases in magnitude with increasing Knudsen number, while decreasing with increasing accommodation factor. In addition, $\hat{\sigma}_L$ is always bigger than $\hat{\sigma}_R$, which may be accepted as another necessary consequence of the prescribed condition $\hat{\theta}_R^w > \hat{\theta}_L^w$.

The sign of the temperature jump and the positivity of entropy production in the case of small Knudsen number can be understood by taking a close look at the leading term [the first term of $O(1)$] in Eq. (13) (or Eq.(15)) for temperature jump and that in Eq. (23) for entropy production at the boundary. If $\hat{\theta}_R^w > \hat{\theta}_L^w$ (or $T_R > T_L$ as in Fig. 1), the heat flux should point from right to left, which is equivalent to $G_{1,1} > 0$. As a consequence, the temperature jumps appear to be positive at the left side while negative at the right side, as shown in Table. 1 and Fig. 3, and then entropy production arises positively at both sides, as shown in Fig. 4. It is therefore clear that this positivity is closely related to the proper sign of the temperature jump at the boundary.

Finally, it is noticeable from Figs. 3 and 4 that the magnitude of the entropy production tends to vanish more quickly than that of the temperature jump when $K_n \to 0$. In fact, the leading term of $\hat{\sigma}_{L(R)}$ in Eq. (23)

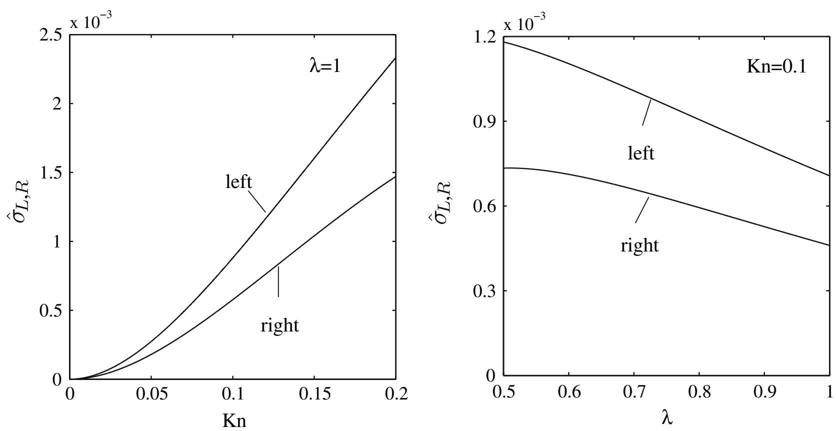

Fig. 4 Knudsen number and accommodation factor dependencies of the entropy production at the boundary ($\hat{\theta}_L^w = 0.86$, $\hat{\theta}_R^w = 1.14$)

should be of $O(K_n^2)$ while that of the temperature jump given by Eq. (15) is of $O(K_n)$. This result implies an interesting fact that if the system under consideration is very near equilibrium so that the first-order theory of COET is sufficient for the description of the process, then the entropy production is negligible even though there exists a nonzero temperature jump. Therefore the assumption of an ideal wall adopted, for example, in [16,17] is reasonable only when the system is very near equilibrium.

5 Summary

We have explored a systematic approach to the temperature jump by studying one-dimensional stationary heat conduction in a rarefied gas at rest. By assuming a power expansion with respect to the Knudsen number like Eqs. (16) and (17), we have obtained analytical expressions for the temperature jump for first- and second-order theories of COET, based on which we also calculated the entropy production at the boundary. The general dependencies of both boundary quantities on the Knudsen number and the accommodation factor have been extensively discussed. Owing to the systematic structure of this approach, it may be easily extrapolated to the higher-order theory of COET where we will encounter the uncontrollable boundary-value problem. We may expect that the present analysis provides us with a sound basis to study such a crucial problem in extended thermodynamics.

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