Note on the relation between thermophoresis and slow uniform flow problems for a rarefied gas

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A relation between the problem of thermophoresis of a sphere and that of a uniform flow past a sphere is discussed on the basis of the linearized Boltzmann equation. First pointed out is the disagreement between the relation predicted by the representation theorem recently developed by the author and that of the existing theory by Sharipov. The two contradicting predictions are assessed by the asymptotic theory for small Knudsen numbers, which results in showing the failure of the latter. The reason of this failure is also explained. Finally, new data of a slip coefficient, which is predominantly responsible for the thermal polarization in a slightly rarefied gas, are obtained for the hard-sphere Boltzmann equation by the use of the correct relation. © 2009 American Institute of Physics. [doi:10.1063/1.3263707]

I. INTRODUCTION

A body in an infinite expanse of a resting rarefied gas with a uniform temperature gradient, or a very small particle in a gas of ordinary pressure in the corresponding situation, is forced by the gas to be set into motion. This interesting phenomenon is called the thermophoresis.¹ The problem of thermophoresis of a sphere, especially the force acting on the sphere sustained at a fixed position, is one of the fundamental problems in rarefied gas dynamics and in aerosol science and has been attracting many researchers, together with the problem of slow uniform flow past a sphere (e.g., Refs. 2-10 for the thermophoresis, Refs. 11-18 for the uniform flow problem, and references therein). For the latter problem, it has been pointed out that a nonuniform temperature field is induced by the gas flow even when the temperature of the sphere is uniform and the same as the upstream one.¹⁴ This interesting phenomenon is called the thermal polarization¹⁹ of the gas. In the present paper, we will discuss a cross relation that holds between the above fundamental problems, to be a little more specific between the force acting on (or the momentum flux onto) the sphere in the former and the temperature field (or the heat flux) established in the bulk gas in the latter.

The cross relation mentioned above was discussed earlier²⁰ in the connection to the Onsager–Casimir reciprocity in nonequilibrium thermodynamics. There are, however, contradicting assertions in the literature about the concrete form of the relation.^{20–23} The cross relation itself comes from a fascinating symmetry of the systems described by the linearized Boltzmann equation. We recently established a representation theorem²⁴ based on the symmetry that explains such relations in a general context without a connection to the entropy production argument. In the present paper, we will start with presenting a consequence of the representation theorem and point out the disagreement with the existing relation²¹ reported by Sharipov (Sec. II B). The disagreement motivated us to provide a numerical evidence of the validity of our representation, leading to the use of the well established results of the asymptotic theory for small Knudsen numbers^{25–27} (Sec. III). The numerical data of a couple of slip coefficients obtained for the Bhatnagar-Gross-Krook model^{28,29} (BGK model, for short³⁰) will be used for the assessment. It will be shown that the results of the asymptotic theory are consistent with our representation, not with the relation by Sharipov^{21,31} (Sec. IV). The source of the inconsistency will be explained. By the use of our representation, we will further report the value of one of the slip coefficients, which is predominantly responsible for the thermal polarization of the gas in a slightly rarefied gas, for the original Boltzmann equation for hard-sphere molecules. The other slip coefficient reported in Ref. 8 will be used to this end.

II. PROBLEM

A. Basic problems and their formulation

We begin with the statement of the problem of thermophoresis of a sphere (problem I) and that of uniform flow past a sphere (problem II).

Problem I. Consider a sphere with a uniform temperature (radius L and temperature T_0) placed in an infinite expanse of a rarefied gas at rest with uniform pressure p_0 and temperature $T_0(1+c_TX_1/L)$, where c_T is a dimensionless constant and X_i is the rectangular coordinate system with its origin at the center of the sphere [see Fig. 1(a)].

Problem II. Consider the same sphere as in problem I placed in a uniform rarefied gas flow with pressure p_0 , temperature T_0 , and flow velocity $(U_0, 0, 0)$ [see Fig. 1(b)].

We investigate the steady behavior of the gas under the following assumptions:

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FIG. 1. Sketch of the problems: (a) thermophoresis and (b) uniform flow past a sphere.

- (1) The behavior of the gas can be described by the Boltzmann equation for monatomic gases.
- (2) On the surface of the sphere, the gas molecules are reflected according to the reflection rule to be prescribed later.
- (3) $|c_{\rm T}| \ll 1$ and $|U_0/(2kT_0/m)^{1/2}| \ll 1$, so that the problems can be linearized around the reference equilibrium state at rest with pressure p_0 and temperature T_0 . Here *m* is the mass of a molecule and *k* is the Boltzmann constant.

We denote the space coordinates X_i by Lx_i , the molecular velocity by $(2kT_0/m)^{1/2}\zeta_i$, the velocity distribution function for problem I by $\rho_0(2kT_0/m)^{-3/2}(1+c_T\phi^I)E(\zeta)$, and that for problem II by $\rho_0(2kT_0/m)^{-3/2}(1+u_0\phi^{II})E(\zeta)$, where $\rho_0 = p_0/(kT_0/m)$, $u_0 = U_0/(2kT_0/m)^{1/2}$, and $E(\zeta) = \pi^{-3/2} \exp(-|\zeta|^2)$. Then, the problems are formulated as follows:

(i) Problem I (thermophoresis):

$$\zeta_i \frac{\partial \phi^{\rm I}}{\partial x_i} = \frac{2}{\sqrt{\pi}} \frac{1}{\rm Kn} \mathcal{L}(\phi^{\rm I}), \tag{1a}$$

$$\phi^{\mathrm{I}} = \int_{\zeta_n^* < 0} \frac{|\zeta_n^*| E^*}{|\zeta_n| E} R(\boldsymbol{\zeta}^*, \boldsymbol{\zeta}; \boldsymbol{x}) \phi^{\mathrm{I}*} \mathrm{d} \boldsymbol{\zeta}^*$$

for $\zeta_n > 0$, $|\boldsymbol{x}| = 1$, (1b)

$$\phi^{\mathrm{I}} \to \left(|\boldsymbol{\zeta}|^2 - \frac{5}{2} \right) x_1 - \frac{\sqrt{\pi}}{2} \mathrm{Kn} \, \boldsymbol{\zeta}_1 A(|\boldsymbol{\zeta}|) \quad \text{as} \quad |\boldsymbol{x}| \to \infty.$$
(1c)

(ii) Problem II (uniform flow):

$$\zeta_i \frac{\partial \phi^{\rm II}}{\partial x_i} = \frac{2}{\sqrt{\pi}} \frac{1}{\rm Kn} \mathcal{L}(\phi^{\rm II}), \qquad (2a)$$

$$\phi^{\mathrm{II}} = \int_{\zeta_n^* < 0} \frac{|\zeta_n^*| E^*}{|\zeta_n| E} R(\boldsymbol{\zeta}^*, \boldsymbol{\zeta}; \boldsymbol{x}) \phi^{\mathrm{II}*} \mathrm{d} \boldsymbol{\zeta}^*$$

for $\zeta_n > 0$, $|\boldsymbol{x}| = 1$, (2b)

$$\phi^{\mathrm{II}} \to 2\zeta_1 \quad \mathrm{as} \quad |\mathbf{x}| \to \infty.$$
 (2c)

Here $d\zeta^* = d\zeta_1^* d\zeta_2^* d\zeta_3^*$, Kn is the Knudsen number defined by $\text{Kn} = \ell_0 / L$ with ℓ_0 being the mean free path of a gas molecule at the reference equilibrium state, and \mathcal{L} is the linearized collision operator. $\zeta_n = \zeta_i n_i$ and $\zeta_n^* = \zeta_i^* n_i$ with *n* being the unit vector normal to the surface of the sphere at position *x* pointing to the gas side, ϕ^{I*} , ϕ^{II*} , and E^* represent $\phi^I(x, \zeta^*)$, $\phi^{II}(x, \zeta^*)$, and $E(\zeta^*)$ respectively, *R* is the so-called reflection kernel of the boundary at the reference equilibrium state, and $A(|\zeta|)$ is the solution of

$$\mathcal{L}(\zeta_i A) = -\zeta_i \Big(|\boldsymbol{\zeta}|^2 - \frac{5}{2} \Big),$$

such that $\int_0^{\infty} z^4 A(z) \exp(-z^2) dz = 0$. The specific form of \mathcal{L} and R is suppressed here because we require them only to have the properties listed in Appendix A. In the following discussion, \mathcal{L} , R, and Kn are assumed to be common to problems I and II.

B. Cross relation between problems I and II

According to the representation theorem developed by the author,²⁴ the force acting on the sphere $p_0L^2c_T(F_1^I, 0, 0)$ in problem I can be written in terms of the quantities in problem II, irrespective of the Knudsen number, in the form (see example 3 in Ref. 24):

$$F_{1}^{\mathrm{I}} = -\lim_{r \to \infty} \int_{|\mathbf{x}|=r} \left(x_{1} Q_{n}^{\mathrm{II}}(\mathbf{x}) + \frac{\sqrt{\pi}}{2} \mathrm{Kn} \langle \zeta_{n} \zeta_{1} A(|\boldsymbol{\zeta}|) \phi^{\mathrm{II}}(\mathbf{x}, \boldsymbol{\zeta}) \rangle \right) \mathrm{dS},$$
(3)

or equivalently

$$F_{1}^{\mathrm{I}} = \int_{|\mathbf{x}|=1} \left(x_{1} Q_{n}^{\mathrm{II}}(\mathbf{x}) + \frac{\sqrt{\pi}}{2} \mathrm{Kn} \langle \zeta_{n} \zeta_{1} A(|\boldsymbol{\zeta}|) \phi^{\mathrm{II}}(\mathbf{x}, \boldsymbol{\zeta}) \rangle \right) \mathrm{dS},$$
(4)

where dS is the surface element at position x, $\langle \cdots \rangle$ represents the moment of the quantity inside:

$$\langle f \rangle = \int f E(\boldsymbol{\zeta}) \mathrm{d}\boldsymbol{\zeta},$$
 (5)

 $p_0(2kT_0/m)^{3/2}u_0Q_i^{\text{II}}(\mathbf{x})$ is the heat flow in problem II:

$$Q_i^{\rm II} = \left\langle \zeta_i \left(|\boldsymbol{\zeta}|^2 - \frac{5}{2} \right) \boldsymbol{\phi}^{\rm II} \right\rangle$$

and $Q_n^{II}(\mathbf{x}) = Q_i^{II}(\mathbf{x})n_i(\mathbf{x})$. In what follows, we call Eqs. (3) and (4) the first and the second representations of the cross relation between problems I and II, respectively.

On the other hand, Sharipov presented the formula²¹

$$F_1^{\mathrm{I}} = \int_{|\mathbf{x}|=1} x_1 Q_n^{\mathrm{II}} \mathrm{dS} + \int_{|\mathbf{x}|\ge 1} Q_1^{\mathrm{II}} \mathrm{dx}$$

which can be transformed into

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$$F_1^{\mathrm{I}} = -\lim_{r \to \infty} \int_{|\mathbf{x}|=r} x_1 Q_n^{\mathrm{II}}(\mathbf{x}) \mathrm{dS}, \qquad (6)$$

by applying the Gauss divergence theorem to the first term. Obviously his formula contradicts ours: the term containing $A(|\zeta|)$ in Eq. (3) is absent in Eq. (6). We shall show below the failure of his formula (6) by presenting a numerical evidence. To this end, we will make use of the well established results of the asymptotic theory for small Knudsen numbers. We also explain the source of the failure and provide new data of a slip coefficient which is predominantly responsible for the thermal polarization of a slightly rarefied gas.

III. ASYMPTOTIC THEORY FOR SMALL KNUDSEN NUMBERS

A. Brief summary of general framework

Before starting the discussions of individual problems, we shall give a brief summary of the asymptotic theory for small Knudsen numbers for steady gas flows described by the linearized Boltzmann equation.²⁵ The reader is also referred to Refs. 26 and 27 for detailed descriptions.

According to the asymptotic theory, the perturbed velocity distribution function and macroscopic quantities defined as its moment in molecular velocity space, which we generically denote by f, can be split into two parts:

$$f = f_{\rm H} + f_{\rm K}$$

where $f_{\rm H}$ is the part which changes in (dimensionless) space with the length scale of O(1), while $f_{\rm K}$ is the correction to $f_{\rm H}$ which is appreciable only in the thin layer (the so-called Knudsen layer) with the thickness of $O(\varepsilon)$ adjacent to the boundary, where $\varepsilon = (\sqrt{\pi}/2)$ Kn is a small parameter.³² We call $f_{\rm H}$ and $f_{\rm K}$ the Hilbert part and the Knudsen-layer part of the solution (or the quantity f), respectively. They can be expanded as a power series of ε :

$$f_{\rm H} = f_{\rm H0} + f_{\rm H1}\varepsilon + f_{\rm H2}\varepsilon^2 + \cdots,$$

$$f_{\rm K} = f_{\rm K1}\varepsilon + f_{\rm K2}\varepsilon^2 + \cdots.$$

Note that the Knudsen-layer part does not appear at the leading order, i.e., the order of $O(\varepsilon^0)$, of the expansion. The Hilbert part of the velocity distribution function takes a special form as a function of ζ and the study of its behavior is reduced to solving the following Stokes set of equations for macroscopic quantities:

$$\partial_i P_{\rm H0} = 0, \tag{7a}$$

$$\partial_i u_{i\mathrm{H}\ell} = 0, \tag{7b}$$

$$\partial_i P_{\mathrm{H}\ell+1} = \gamma_1 \Delta u_{i\mathrm{H}\ell},\tag{7c}$$

$$\Delta \tau_{\mathrm{H}\ell} = 0, \tag{7d}$$

with the so-called slip boundary conditions. Here $p_0(1+P)$ is the pressure, $T_0(1+\tau)$ is the temperature, $(2kT_0/m)^{1/2}u_i$ is the flow velocity, γ_1 is a constant defined later in Eq. (10), $\partial_i = \partial/\partial x_i$, Δ is the Laplacian, and $\ell = 0, 1, 2, \cdots$. The slip boundary condition for Eq. (7) up to $O(\varepsilon^2)$ is summarized in Appendix B. The Hilbert part describes the overall behavior of the gas outside the Knudsen-layer with the thickness of $O(\varepsilon)$. We shall use Eqs. (3) and (6) for the assessment of two contradicting statements, so that the information about the Knudsen-layer part is not necessary and is omitted here.

In summary, we can obtain the overall behavior of the gas outside of the Knudsen layer up to $O(\varepsilon^2)$ by solving the Stokes system (7) with the slip boundary condition (B1) in Appendix B. As to the Hilbert part of the stress and heat flow, fortunately we can get them with higher accuracy of $O(\varepsilon^3)$ from the information above. We show below the general form of the Hilbert part of the perturbed velocity distribution function $\phi_{\rm H}$ and heat flow $Q_{i\rm H}$ up to $O(\varepsilon^2)$ and $O(\varepsilon^3)$ respectively, which will be necessary in the subsequent discussions:

$$\phi_{\rm H0} = P_{\rm H0} + 2\zeta_i u_{i\rm H0} + \left(|\boldsymbol{\zeta}|^2 - \frac{5}{2} \right) \tau_{\rm H0}, \tag{8a}$$

$$\phi_{\mathrm{H1}} = P_{\mathrm{H1}} + 2\zeta_{i}u_{i\mathrm{H1}} + \left(|\boldsymbol{\zeta}|^{2} - \frac{5}{2}\right)\tau_{\mathrm{H1}} - \zeta_{i}\zeta_{j}B(|\boldsymbol{\zeta}|)\partial_{j}u_{i\mathrm{H0}} - \zeta_{i}A(|\boldsymbol{\zeta}|)\partial_{j}\tau_{\mathrm{H0}},$$
(8b)

$$\phi_{\mathrm{H2}} = P_{\mathrm{H2}} + 2\zeta_{i}u_{i\mathrm{H2}} + \left(|\boldsymbol{\zeta}|^{2} - \frac{5}{2}\right)\tau_{\mathrm{H2}} - \zeta_{i}\zeta_{j}B(|\boldsymbol{\zeta}|)\partial_{j}u_{i\mathrm{H1}}$$
$$- \zeta_{i}A(|\boldsymbol{\zeta}|)\partial_{i}\tau_{\mathrm{H1}} + \frac{1}{\gamma_{1}}\zeta_{i}D_{1}(|\boldsymbol{\zeta}|)\partial_{i}P_{\mathrm{H1}}$$
$$+ \zeta_{i}\zeta_{j}\zeta_{k}D_{2}(|\boldsymbol{\zeta}|)\partial_{j}\partial_{k}u_{i\mathrm{H0}} - \zeta_{i}\zeta_{j}F(|\boldsymbol{\zeta}|)\partial_{i}\partial_{j}\tau_{\mathrm{H0}}, \qquad (8c)$$

and

$$Q_{i\mathrm{H0}} = 0, \tag{9a}$$

$$Q_{i\mathrm{H}1} = -\frac{5}{4} \gamma_2 \partial_i \tau_{\mathrm{H}0}, \tag{9b}$$

$$Q_{iH2} = -\frac{5}{4} \gamma_2 \partial_i \tau_{H1} + \frac{\gamma_3}{2} \Delta u_{iH0},$$
 (9c)

$$Q_{i\rm H3} = -\frac{5}{4}\gamma_2\partial_i\tau_{\rm H2} + \frac{\gamma_3}{2}\Delta u_{i\rm H1}.$$
 (9d)

Here B, D_1 , D_2 , and F are the solutions of the following equations:

$$\mathcal{L}[\zeta_{ij}B(|\boldsymbol{\zeta}|)] = -2\zeta_{ij}, \quad \mathcal{L}[\zeta_{ij}F(|\boldsymbol{\zeta}|)] = \zeta_{ij}A(|\boldsymbol{\zeta}|),$$
$$\mathcal{L}[\zeta_{ijk}D_1(|\boldsymbol{\zeta}|) + \zeta_i\zeta_j\zeta_kD_2(|\boldsymbol{\zeta}|)] = \gamma_1\zeta_{ijk} - \zeta_i\zeta_j\zeta_kB(|\boldsymbol{\zeta}|),$$

such that $\int_0^\infty [5D_1(z) + z^2D_2(z)]z^4e^{-z^2}dz = 0$, where $\zeta_{ij} = \zeta_i\zeta_j - (1/3)|\zeta|^2\delta_{ij}$, $\zeta_{ijk} = \zeta_i\delta_{jk} + \zeta_j\delta_{ik} + \zeta_k\delta_{ij}$, and δ_{ij} is Kronecker's delta. The γ_1 , γ_2 , and γ_3 occurring in Eqs. (7)–(9) are constants defined by

$$\gamma_1 = I_6(B), \quad \gamma_2 = 2I_6(A),$$
 (10a)

$$\gamma_3 = I_6(AB) = 5I_6(D_1) + I_8(D_2) = -2I_6(F),$$
 (10b)

where $I_n(Z) = (8/15\sqrt{\pi}) \int_0^{\infty} z^n Z(z) \exp(-z^2) dz$. They are dependent on the molecular model. For instance, $\gamma_1 = \gamma_2 = \gamma_3 = 1$ for

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the BGK model, while $\gamma_1 = 1.270\ 042$, $\gamma_2 = 1.922\ 284$, and $\gamma_3 = 1.947\ 906$ for a hard-sphere gas.

Now we are ready to proceed to individual problems.

B. Application to individual problems

1. Application to the thermophoresis: Problem I

The problem of thermophoresis of a sphere in a slightly rarefied gas has been intensively studied in Refs. 6–8 and 11 on the basis of the asymptotic theory. According to these references, the force $p_0L^2c_T(F_1^1,0,0)$ acting on the sphere with uniform temperature T_0 is induced by the reaction of the slip flow caused by the thermal stress (thermal stress slip flow⁶) and is given by

$$F_1^{\rm I} = 12\pi\gamma_1 a_4 \left(\frac{\sqrt{\pi}}{2} {\rm Kn}\right)^3 + o({\rm Kn}^3) \quad ({\rm Kn} \ll 1),$$
 (11)

where a_4 is a slip coefficient related to thermal stress [see Eq. (B1) in Appendix B]. This force acting on the sphere is sometimes called the thermal force in the literature.

2. Application to the uniform flow problem: Problem II

Because of the general form (8), $\langle \zeta_i \zeta_1 A \phi_{H\ell} \rangle$ ($\ell = 0, 1, 2$) is given by

$$\langle \zeta_i \zeta_1 A \phi_{\rm H0} \rangle = \frac{5}{4} \gamma_2 \tau_{\rm H0} \delta_{i1}, \qquad (12a)$$

$$\langle \zeta_i \zeta_1 A \phi_{\rm H1} \rangle = \frac{5}{4} \gamma_2 \tau_{\rm H1} \delta_{i1} - \frac{\gamma_3}{2} (\partial_1 u_{i\rm H0} + \partial_i u_{\rm 1H0}), \qquad (12b)$$

$$\langle \zeta_i \zeta_1 A \phi_{\text{H2}} \rangle = \frac{5}{4} \gamma_2 \tau_{\text{H2}} \delta_{i1} - \frac{\gamma_3}{2} (\partial_1 u_{i\text{H1}} + \partial_i u_{1\text{H1}}) + \frac{\gamma_3}{2} \partial_1 \partial_i \tau_{\text{H0}}.$$
(12c)

Hence, taking account of Eq. (9), we can obtain the righthand side of Eqs. (3) and (6) up to $O(\varepsilon^3)$, if we know u_{iH0}^{II} , u_{iH1}^{II} , τ_{H0}^{II} , τ_{H1}^{II} , and τ_{H2}^{II} , where superscripted II indicates that the individual quantities are those of problem II. Fortunately, they have already been obtained in Refs. 11 and 14,³³

$$u_{r\rm H0}^{\rm II} = \left(1 - \frac{3}{2}r^{-1} + \frac{1}{2}r^{-3}\right)\cos\,\theta,\tag{13a}$$

$$u_{r\mathrm{H1}}^{\mathrm{II}} = -\frac{3}{2}k_0(r^{-1} - r^{-3})\cos\,\theta,\tag{13b}$$

$$u_{\theta H0}^{\rm II} = -\left(1 - \frac{3}{4}r^{-1} - \frac{1}{4}r^{-3}\right)\sin\theta, \tag{13c}$$

$$u_{\theta H1}^{\rm II} = \frac{3}{4}k_0(r^{-1} + r^{-3})\sin \theta,$$
(13d)

$$u_{\varphi H0}^{\rm II} = 0, \quad u_{\varphi H1}^{\rm II} = 0,$$
 (13e)

$$\tau_{\rm H0}^{\rm II} = 0, \quad \tau_{\rm H1}^{\rm II} = 0, \quad \tau_{\rm H2}^{\rm II} = 6d_4 r^{-2} \cos \theta.$$
 (13f)

Here we introduced the spherical coordinates (r, θ, φ) , i.e., $r = |\mathbf{x}|$, θ is the polar angle from the x_1 -direction, and φ is the azimuthal angle; $(u_r, u_{\theta}, u_{\varphi})$ is the *r*-, θ -, and φ -components of the (dimensionless) flow velocity u_i . It should be noted

that the nonuniform temperature field is induced at the order of ε^2 [see Eq. (13f)] despite the fact that the temperature of the sphere is the same as the upstream uniform temperature. This is the phenomenon of thermal polarization.

Substitution of Eq. (13) into Eq. (12) eventually yields the following expressions for $\langle \zeta_n \zeta_1 A \phi_{H\ell}^{II} \rangle$ ($\ell = 0, 1, 2$) on the spherical control surface of radius *r*:

$$\left\langle \zeta_n \zeta_1 A \phi_{\text{H0}}^{\text{II}} \right\rangle |_{|\mathbf{x}|=r} = 0, \tag{14a}$$

$$\langle \zeta_n \zeta_1 A \phi_{\text{H1}}^{\text{II}} \rangle |_{|\mathbf{x}|=r} = \frac{3}{2} \gamma_3 \frac{\cos^2 \theta}{r^2} + O(r^{-4}),$$
 (14b)

$$\langle \zeta_n \zeta_1 A \phi_{\text{H2}}^{\text{II}} \rangle |_{|\mathbf{x}|=r} = \frac{3}{2} \gamma_3 k_0 \left(1 - 5 \frac{\gamma_2}{\gamma_3} \frac{d_4}{k_0} \right) \frac{\cos^2 \theta}{r^2} + O(r^{-4}),$$
(14c)

where k_0 and d_4 are slip coefficients related to shear stress and its derivative [see Eq. (B1) in Appendix B]. Substitution of Eq. (13) into Eq. (9) eventually yields the following expressions for $Q_{nH\ell}^{II}$ ($\ell = 0, 1, 2, 3$) on the spherical control surface of radius *r*:

$$Q_{nH0}^{II}|_{|\mathbf{x}|=r} = 0, \quad Q_{nH1}^{II}|_{|\mathbf{x}|=r} = 0,$$
 (15a)

$$Q_{nH2}^{II}|_{|\mathbf{x}|=r} = -\frac{3}{2}\gamma_3 r^{-3}\cos\theta,$$
(15b)

$$Q_{n\mathrm{H3}}^{\mathrm{II}}|_{|\mathbf{x}|=r} = -\frac{3}{2}\gamma_3 \left(k_0 + 10\frac{\gamma_2}{\gamma_3}d_4\right)r^{-3}\cos\,\theta.$$
 (15c)

3. Reduction of the relations (3) and (6)

Now all the information that we need is prepared. Keeping in mind that the Knudsen-layer part has vanished in a far field, we can calculate the right-hand side of Eqs. (3) and (6) for small Kn as follows:

$$-\lim_{r \to \infty} \int_{|\mathbf{x}|=r} x_1 Q_n^{\mathrm{II}}(\mathbf{x}) \mathrm{dS}$$

$$= -\lim_{r \to \infty} \int_{|\mathbf{x}|=r} x_1 Q_{n\mathrm{H}}^{\mathrm{II}} \mathrm{dS}$$

$$= -\lim_{r \to \infty} \int_{|\mathbf{x}|=r} x_1 [Q_{n\mathrm{H}2}^{\mathrm{II}} + Q_{n\mathrm{H}3}^{\mathrm{II}} \varepsilon] \varepsilon^2 \mathrm{dS} + o(\varepsilon^3)$$

$$= 2\pi \gamma_3 \bigg[1 + \bigg(k_0 + 10 \frac{\gamma_2}{\gamma_3} d_4 \bigg) \varepsilon \bigg] \varepsilon^2 + o(\varepsilon^3),$$

and

$$-\lim_{r \to \infty} \int_{|\mathbf{x}|=r} \varepsilon \langle \zeta_n \zeta_1 A(|\boldsymbol{\zeta}|) \phi^{\mathrm{II}} \rangle \mathrm{dS}$$

$$= -\lim_{r \to \infty} \int_{|\mathbf{x}|=r} \varepsilon \langle \zeta_n \zeta_1 A(|\boldsymbol{\zeta}|) \phi^{\mathrm{II}}_{\mathrm{H}} \rangle \mathrm{dS}$$

$$= -2\pi \gamma_3 \bigg[1 + k_0 \bigg(1 - 5\frac{\gamma_2}{\gamma_3} \frac{d_4}{k_0} \bigg) \varepsilon \bigg] \varepsilon^2 + o(\varepsilon^3).$$

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Remember that $\varepsilon = (\sqrt{\pi}/2)$ Kn. Thus, our first representation (3) is reduced to

$$F_1^{\rm I} = 30\pi\gamma_2 d_4 \left(\frac{\sqrt{\pi}}{2}{\rm Kn}\right)^3 + o({\rm Kn}^3) \quad ({\rm Kn} \le 1),$$
 (16)

while Sharipov's formula (6) is reduced to

$$F_{1}^{I} = 2\pi\gamma_{3}\left[1 + \left(k_{0} + 10\frac{\gamma_{2}}{\gamma_{3}}d_{4}\right)\frac{\sqrt{\pi}}{2}\mathrm{Kn}\right]\left(\frac{\sqrt{\pi}}{2}\mathrm{Kn}\right)^{2} + o(\mathrm{Kn}^{3}) \quad (\mathrm{Kn} \ll 1).$$
(17)

IV. DISCUSSIONS

On comparing Eq. (17) with Eq. (11), we notice that the term of $O(Kn^2)$ in the former is absent from the latter. That is, Sharipov's formula (6) fails to recover the results of Refs. 6–8 and 11.

On the other hand, Eq. (16) is consistent with Eq. (11) in the sense that the thermal force is the quantity of $O(\text{Kn}^3)$. A closer observation of Eqs. (11) and (16) shows that the following relation is required to hold:

$$a_4 = \frac{5}{2} \frac{\gamma_2}{\gamma_1} d_4, \tag{18}$$

for the consistency of these equations. In order to check this consistency, we use the data of a_4 and d_4 for the BGK model with diffuse reflection condition, which were obtained accurately by a faithful direct solution of different half-space Knudsen-layer problems.²⁵ The data are

$$a_4 = 0.279 \ 22, \quad d_4 = 0.111 \ 69.$$

The substitution of these values, together with $\gamma_1 = 1$ and $\gamma_2 = 1$, shows that the relation (18) holds actually for BGK model. This is a numerical evidence of the consistency between Eqs. (16) and (11). That is, the asymptotic theory numerically supports the validity of our representation (3). Incidentally, as far as the present specific problems are concerned, the relation reported by Roldughin, ${}^{20} \lambda_{12} = \lambda_{21}^T$ in his notation, is consistent with Eq. (18), though it was criticized by Sharipov.^{22,23,34}

As seen from Eq. (13f), the coefficient d_4 is essential for the investigation of the thermal polarization phenomenon, the temperature field induced by a slow uniform flow past a body, for small Kn. Nevertheless, the numerical value of d_4 has not been reported except for the BGK model. Here we can report its value for a hard-sphere gas based on the original Boltzmann equation by the use of Eq. (18), because fortunately the numerical data of a_4 for a hard-sphere gas are available from Ref. 8. The result is shown in Table I (remember that $\gamma_1 = 1.270\ 042$ and $\gamma_2 = 1.922\ 284$ for a hard-sphere gas). The value of d_4 in Table I is smaller than the counterpart for the BGK model roughly by one digit. It implies that the thermal polarization in the slip flow regime (Kn \ll 1) will be overestimated by the use of the BGK model, when compared with the original Boltzmann equation. This observation agrees with the results of direct numerical computation in the literature.¹⁸

TABLE I. Slip coefficients d_4 and a_4 for hard-sphere gases under the Maxwell-type boundary condition. Here α is the accommodation coefficient (α =1 corresponds to the diffuse reflection). The data of a_4 are taken from Ref. 8, while those of d_4 are newly obtained from them by the use of Eq. (18).

α	0.5	0.75	1
a_4	0.1547	0.0700	0.0330
<i>a</i> ₄	0.040 88	0.0185	0.008 72

Finally, we briefly explain the reason of failure of the formula (6) [or Eq. (17)]. As mentioned before, the source of error in Ref. 21 is the missing of the last term of Eq. (3), which further comes from the fact that the last term containing $A(|\boldsymbol{\zeta}|)$ is missing in the far field condition (1c) at the stage of formulation of problem I. Unfortunately, this is not a careless mistake and unveils a fatal error of the theory in Ref. 31, on which the consequences of Ref. 21 are fully relying. In Ref. 31, the linearization is made around a resting local Maxwellian and the Onsager-Casimir reciprocity is discussed by assuming that the perturbation from that local Maxwellian approaches a certain uniform equilibrium distribution at a far distance. However, it should be reminded that the local Maxwellian is not necessarily a solution of the Boltzmann equation. The above assumption is allowed only for a special class of local Maxwellians (see, e.g., Appendix A.8 of Ref. 27) and the present thermophoresis problem (problem I) is not the case. This is the reason why the term containing $A(|\boldsymbol{\zeta}|)$ is dropped in the formulation in Ref. 21. In short, at least for the systems without external forces, the theory in Ref. 31 does not give a correct result in general for unbounded domain systems if the linearization around a local Maxwellian is required. The reader is referred to Sec. 7 of Ref. 35 for more detailed comments on this issue.

V. CONCLUSION

In the present paper, we discussed the relation between the problem of thermophoresis of a sphere and that of a uniform flow past a sphere on the basis of the linearized Boltzmann equation. We first presented a relation predicted by the representation theorem²⁴ and pointed out the disagreement with the prediction of the existing theory²¹ by Sharipov. Then, we assessed the two contradicting predictions by the use of the consequence of the asymptotic theory for small Knudsen numbers. The result numerically supports the prediction of the former and reveals the failure of the latter. Finally, by the use of the former representation, we obtained, for the hard-sphere Boltzmann equation, new data of the slip coefficient that is predominantly responsible for the thermal polarization phenomenon in slightly rarefied gases.

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APPENDIX A: LINEARIZED COLLISION OPERATOR \mathcal{L} AND REFLECTION KERNEL *R*

The linearized collision operator is required to have the following properties:

(i) \mathcal{L} commutes with the parity operator acting on $\boldsymbol{\zeta}$:

 $\mathcal{L}(\Phi)^- = \mathcal{L}(\Phi^-) \quad \text{for any } \Phi,$

where $\Psi^{-}(\boldsymbol{x},\boldsymbol{\zeta}) \equiv \Psi(\boldsymbol{x},-\boldsymbol{\zeta}).$

(ii) \mathcal{L} is self-adjoint,

 $\langle \Phi \mathcal{L}(\Psi) \rangle \,{=}\, \langle \Psi \mathcal{L}(\Phi) \rangle \quad \text{for any } \Phi \ \text{and} \ \Psi,$

where the brackets $\langle \cdots \rangle$ indicate the moment (5) of the quantity inside.

- (iii) $\mathcal{L}(\Phi)=0$ holds if and only if Φ is a linear combination of 1, ζ , and $|\zeta|^2$.
- (iv) \mathcal{L} is nonpositive,

$$\langle \Phi \mathcal{L}(\Phi) \rangle \leq 0$$
 for any Φ ,

and the equality holds if and only if Φ is a linear combination of 1, ζ , and $|\zeta|^2$.

In the present paper, we assume the kernel R to have the properties listed below:

(1) Non-negativity:

$$R(\boldsymbol{\zeta}^*, \boldsymbol{\zeta}; \boldsymbol{x}) \ge 0 \quad \text{for } \boldsymbol{\zeta}_n > 0, \quad \boldsymbol{\zeta}_n^* < 0.$$

(2) Condition of no net flow:

$$\int_{\zeta_n>0} R(\boldsymbol{\zeta}^*,\boldsymbol{\zeta};\boldsymbol{x}) \mathrm{d}\boldsymbol{\zeta} = 1 \quad \text{for } \boldsymbol{\zeta}_n^* < 0.$$

(3) Uniqueness condition: Let ψ be ψ=c₀+c_iζ_i+c₄|ζ|², where c₀, c_i, and c₄ are independent of ζ. Among such ψ, only ψ=c₀ satisfies the relation

$$\psi = \int_{\zeta_n^* < 0} \frac{|\zeta_n^*| E^*}{|\zeta_n| E} R(\boldsymbol{\zeta}^*, \boldsymbol{\zeta}; \boldsymbol{x}) \psi^* \mathrm{d} \boldsymbol{\zeta}^* \text{ for } \boldsymbol{\zeta}_n > 0.$$

(4) Detailed balance:

$$\zeta_n^* | R(\boldsymbol{\zeta}^*, \boldsymbol{\zeta}; \boldsymbol{x}) E^* = | \zeta_n | R(-\boldsymbol{\zeta}, -\boldsymbol{\zeta}^*; \boldsymbol{x}) E$$

for $\zeta_n > 0, \quad \zeta_n^* < 0.$

- (5) Locally isotropic condition: At every fixed x on the boundary, R is invariant under the following transformations of ζ and ζ*:
 - (a) A rotation around the normal n of boundary.
 - (b) The reflection with respect to a plane containing n.

The properties (1)–(4) are required for the application of the representation theorem in Ref. 24. The property (5) is necessary for the application of the slip boundary condition in the form summarized in Appendix B. The reader is referred to Sec. 3.4 of Ref. 26 for further detailed descriptions for the last property.

It should be remarked that \mathcal{L} of the linearized BGK model has the properties (i)–(iv) and *R* of the Maxwell-type condition with nonzero accommodation coefficient, which includes the diffuse reflection as a special case, has the prop-

erties (1)–(5). Therefore, the results of the asymptotic theory in Secs. III and IV may be used for the assessment in the present work.

APPENDIX B: SLIP BOUNDARY CONDITION

The boundary condition on a rigid solid surface for the Stokes set of equations, Eq. (7), is summarized as follows:

$$u_{i\rm H0} = u_{i\rm w},\tag{B1a}$$

$$u_{i\mathrm{H}1}n_i = 0, \tag{B1b}$$

$$u_{iH1}t_i = k_0 S_{ijH0}n_i t_j + K_1 G_{iH0}t_i,$$
 (B1c)

$$u_{iH2}n_i = b_1 \partial_k S_{ijH0}n_i n_j n_k + b_2 (\partial_j G_{iH0}n_i n_j + 2\bar{\kappa} G_{iH0}n_i),$$
(B1d)

$$\begin{aligned} u_{iH2}t_i &= k_0 S_{ijH1} n_i t_j + a_1 \partial_k S_{ijH0} t_i n_j n_k + a_2 \kappa S_{ijH0} n_i t_j \\ &+ a_3 \kappa_{ij} S_{jkH0} n_k t_i + a_4 \partial_j G_{iH0} n_j t_i + a_5 \overline{\kappa} G_{iH0} t_i \\ &+ a_6 \kappa_{ij} G_{iH0} t_i, \end{aligned}$$
(B1e)

$$\tau_{\rm H0} = \tau_{\rm w},\tag{B1f}$$

$$\tau_{\rm H1} = -d_1 G_{i\rm H0} n_i, \tag{B1g}$$

$$\tau_{\rm H2} = -d_1 G_{i\rm H1} n_i - d_4 \partial_k S_{ij\rm H0} n_i n_j n_k - d_3 \partial_j G_{i\rm H0} n_i n_j - d_5 \overline{\kappa} G_{i\rm H0} n_i,$$
(B1h)

where

$$\begin{split} S_{ijH\ell} &= -\left(\partial_{j} u_{iH\ell} + \partial_{i} u_{jH\ell}\right), \\ G_{iH\ell} &= -\partial_{i} \tau_{H\ell} \quad (\ell = 0, 1), \end{split}$$

 $(2kT_0/m)^{1/2}u_{iw}$ and $T_0(1 + \tau_w)$ are the velocity and the temperature of the boundary, n_i is a unit normal to the boundary pointing to the gas side, and t_i is a unit tangential to the boundary. It should be remarked that $S_{ijH\ell}$, $G_{iH\ell}$, and their derivatives, as well as u_{iw} and τ_w , are evaluated at the boundary. The coefficients $\bar{\kappa}$ and κ_{ij} are defined as below in terms of the principal curvatures³⁶ of the boundary κ_1/L and κ_2/L and of the corresponding direction cosines of the principal directions l_i and m_i :

$$\overline{\kappa} = \frac{1}{2}(\kappa_1 + \kappa_2), \quad \kappa_{ij} = \kappa_1 l_i l_j + \kappa_2 m_i m_j.$$

The coefficients k_0 , K_1 , b_1 , b_2 , $a_1 \sim a_6$, d_1 , and $d_3 \sim d_5$ occurring in Eq. (B1) are the so-called slip (or jump) coefficients. Their concrete values depend on the choice of molecular model and reflection kernel *R* in the boundary condition at the microscopic level. For instance, the data for BGK model and diffuse reflection condition are

$$k_0 = -1.016 \ 19, \quad K_1 = -0.383 \ 16, \quad d_1 = 1.302 \ 72,$$

 $a_1 = 0.766 \ 32, \quad a_2 = 0.500 \ 00, \quad a_3 = -0.266 \ 32,$
 $a_4 = 0.279 \ 22, \quad a_5 = 0.266 \ 93, \quad a_6 = -0.766 \ 44,$
 $b_1 = 0.116 \ 84, \quad b_2 = 0.266 \ 93, \quad d_3 = 0,$

 $d_4 = 0.111\ 69, \quad d_5 = 1.821\ 81,$

and the counterparts for a hard-sphere gas based on the original Boltzmann equation are

$$k_0 = -1.2540, \quad K_1 = -0.6465, \quad d_1 = 2.4001,$$

$$a_4 = 0.0330, \quad b_1 = 0.1069, \quad b_2 = 0.4779.$$

These data are taken from Ref. 27, except that K_1 , b_1 , and b_2 have been updated.

- ¹J. Tyndall, "On dust and disease," Proc. Roy. Inst. **6**, 1 (1870).
- ²P. S. Epstein, "Zur Theorie das Radiometers," Z. Phys. 54, 537 (1929).
 ³S. P. Bakanov and B. V. Deryaguin, "On the theory of thermal precipita-
- tion of highly disperse aerosol systems," Kolloidn. Zh. **21**, 377 (1959). ⁴L. Waldmann, "Über die Kraft eines inhomogenen Gases auf kleine sus-
- pendierte Kugeln," Z. Naturforsch **14a**, 589 (1959).
- ⁵L. Talbot, "Thermophoresis—A review," in *Rarefied Gas Dynamics*, edited by S. S. Fisher (AIAA, New York, 1981), pp. 467–488.
- ⁶Y. Sone, "Flow induced by thermal stress in rarefied gas," Phys. Fluids **15**, 1418 (1972).
- ⁷Y. Sone and K. Aoki, "Negative thermophoresis: Thermal stress slip flow around a spherical particle in a rarefied gas," in *Rarefied Gas Dynamics*, edited by S. S. Fisher (AIAA, New York, 1981), pp. 489–503.
- ⁸T. Ohwada and Y. Sone, "Analysis of thermal stress slip flow and negative thermophoresis using the Boltzmann equation for hard-sphere molecules," Eur. J. Mech. B/Fluids **11**, 389 (1992).
- ⁹K. I. Borg and L. H. Söderholm, "Thermophoresis of axially symmetric bodies," in *Rarefied Gas Dynamics*, edited by T. J. Bartel and M. A. Gallis (AIP, Melville, 2001), pp. 867–874.
- ¹⁰F. Zheng, "Thermophoresis of spherical and non-spherical particles: A review of theories and experiments," Adv. Colloid Interface Sci. **97**, 253 (2002).
- ¹¹Y. Sone and K. Aoki, "Forces on a spherical particle in a slightly rarefied gas," in *Rarefied Gas Dynamics*, edited by J. L. Potter (AIAA, New York, 1979), pp. 417–433.
- ¹²A. Millikan, "The general law of fall of a small spherical body through a gas, and its bearing upon the nature of molecular reflection from surfaces," Phys. Rev. 22, 1 (1923).
- ¹³C. Cercignani, C. D. Pagani, and P. Bassanini, "Flow of a rarefied gas past an axisymmetric body. II. Case of a sphere," Phys. Fluids **11**, 1399 (1968).
- ¹⁴K. Aoki and Y. Sone, "Temperature field induced around a sphere in a uniform flow of a rarefied gas," Phys. Fluids **30**, 2286 (1987).
- ¹⁵I. A. Beresnev, V. G. Chernyak, and G. A. Fomyagin, "Motion of a spherical particle in a rarefied gas. Part 2. Drag and thermal polarization," J. Fluid Mech. **219**, 405 (1990).
- ¹⁶S. Takata, Y. Sone, and K. Aoki, "Drag and thermal force on a spherical particle in a rarefied gas-Numerical analysis for all Knudsen numbers," J. Vac. Soc. Jpn. **35**, 143 (1992) (in Japanese).
- ¹⁷S. K. Loyalka, "Motion of a sphere in a gas: Numerical solution of the linearized Boltzmann equation," Phys. Fluids A 4, 1049 (1992).

- ¹⁸S. Takata, Y. Sone, and K. Aoki, "Numerical analysis of a uniform flow of a rarefied gas past a sphere on the basis of the Boltzmann equation for hard-sphere molecules," Phys. Fluids A 5, 716 (1993).
- ¹⁹S. P. Bakanov, V. V. Vysotskij, B. J. Derjaguin, and V. I. Roldughin, "Thermal polarization of bodies in the rarefied gas flows," J. Non-Equilib. Thermodyn. 8, 75 (1983).
- ²⁰V. I. Roldughin, "On the theory of thermal polarization of bodies in a rarefied gas flow," J. Non-Equilib. Thermodyn. **19**, 349 (1994).
- ²¹F. Sharipov, "Onsager-Casimir reciprocity relations for open gaseous systems at arbitrary rarefaction. II. Application of the theory for single gas," Physica A 203, 457 (1994).
- ²²F. Sharipov, "Comments on 'On the theory of thermal polarization of bodies in a rarefied gas flow'," J. Non-Equilib. Thermodyn. **21**, 164 (1996).
- ²³V. I. Roldughin, "Reply to Comments of Sharipov on my paper 'On the theory of thermal polarization of bodies in a rarefied gas flow'," J. Non-Equilib. Thermodyn. **23**, 99 (1998).
- ²⁴S. Takata, "Symmetry of the linearized Boltzmann equation and its application," J. Stat. Phys. **136**, 751 (2009).
- ²⁵Y. Sone, "Asymptotic theory of flow of rarefied gas over a smooth boundary I," in *Rarefied Gas Dynamics*, edited by L. Trilling and H. Y. Wachman (Academic, New York, 1969), Vol. 1, pp. 243–253.
- ²⁶Y. Sone, *Kinetic Theory and Fluid Dynamics* (Birkhäuser, Boston, 2002); Supplementary Notes and Errata: Kyoto University Research Information Repository. http://hdl.handle.net/2433/66099.
- ²⁷Y. Sone, *Molecular Gas Dynamics* (Birkhäuser, Boston, 2007); Supplementary Notes and Errata: Kyoto University Research Information Repository. http://hdl.handle.net/2433/66098.
- ²⁸P. L. Bhatnagar, E. P. Gross, and M. Krook, "A model for collision processes in gases. I. Small amplitude processes in charged and neutral onecomponent systems," Phys. Rev. 94, 511 (1954).
- ²⁹P. Welander, "On the temperature jump in a rarefied gas," Ark. Fys. 7, 507 (1954).
- ³⁰It is called Boltzmann–Krook–Welander (BKW) model in Refs. 26 and 27 because of the independent contribution of Welander.
- ³¹F. Sharipov, "Onsager–Casimir reciprocity relations for open gaseous systems at arbitrary rarefaction. I. General theory for single gas," Physica A 203, 437 (1994).
- ³²If the boundary is convex, there exists a much thinner layer, the so-called S-layer, at the bottom of the Knudsen layer. However, this fact does not affect the consequence of the subsequent discussions. See, for example, Ref. 7, Chap. 3.7 of Ref. 26 and Ref. [178] therein. We merely ignore it in the present paper.
- ³³In Ref. 14, τ_{H2}^{lf} is expressed in terms of d_4^* by the use of the relation $d_4^* = -4d_4$ that exceptionally holds for BGK model. It should be noted that this relation does not hold in general.
- ³⁴It would be fair to explicitly state that we checked the consistency of Roldughin's relation only for the situation that the temperature of the sphere is uniform (or the case with a sphere of infinitely high thermal conductivity).
- ³⁵S. Takata, "Symmetry of the linearized Boltzmann equation II. Entropy production and Onsager–Casimir relation," J. Stat. Phys. 136, 945 (2009).
- ³⁶The curvature is defined so as to be negative when the corresponding center of curvature lies on the gas side.