On computing the thermal-slip coefficient from Kramers' problem

C. E. Siewert
Mathematics Department, North Carolina State University, Raleigh, North Carolina 27695-8205

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Classical techniques are used to derive a variant of an Onsager relation (used typically for Poiseuille flow and thermal-creep flow) that yields a convenient relationship between the heat flow of Kramers' problem and the thermal-slip coefficient. The analysis is based on the linearized Boltzmann equation for rigid-sphere interactions, and wall interactions are described by a general law that includes, for example, the Maxwell model (a mixture of specular and diffuse reflection) and the Cercignani–Lampis model. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1728157]

In a first-draft version of some recent work Sharipov communicated an interesting expression that relates the heat flow from Kramers' problem (viscous-slip problem) and the thermal-slip coefficient. Sharipov's result was deduced from physical arguments and was (in the first-draft version) presented in terms of the S model[1] that is used frequently in the general area of rarefied gas dynamics. Having seen that Sharipov's expression provides a useful way to simplify some computations, or alternatively that the result can be used as a measure of the accuracy obtained from a numerical algorithm, we generalize Sharipov's work to the case of the linearized Boltzmann equation (for rigid-sphere interactions). The approach used here, in contrast to one focused on physical arguments, is based on the defining balance equations, the boundary conditions, and known exact components of the solutions of the two problems (Kramers and thermal creep). It is noted that subsequent to the work reported here, and after many e-mail communications with the current author, Sharipov, in a second-draft version of his work, extended his analysis to obtain a generalized, but less explicit, version of his first-draft work.

We consider the linearized Boltzmann equation (for rigid-sphere interactions) written (essentially) in the Pekeris form[2–4]

$$c(1-\mu^2)^{1/2}\cos\chi(c^2-5/2)k_T + c\mu\frac{\partial}{\partial\tau}h(\tau,\mathbf{c}) = \varepsilon L\{h\}(\tau,\mathbf{c}), \tag{1}$$

where

$$L\{h\}(\tau,\mathbf{c}) = -\nu(c)h(\tau,\mathbf{c}) + \int_0^\infty\int_{-1}^1\int_0^{2\pi} e^{-c'^2}h(\tau,\mathbf{c}')\times K(\mathbf{c}':\mathbf{c})c'^2 d\chi'\, d\mu'\, dc'. \tag{2}$$

Here $K(\mathbf{c}':\mathbf{c})$ is the scattering kernel and

$$\nu(c) = \frac{2c^2+1}{c}\int_0^c e^{-x^2}dx + e^{-c^2} \tag{3}$$

is the collision frequency. In Eq. (1) we have used

$$\varepsilon = \sigma_0^2 n_0 \pi^{1/2} l, \tag{4}$$

where l is (at this point) an unspecified mean-free path, n_0 is the density, and σ_0 is the scattering diameter of the gas particles. In this work, the spatial variable τ is measured in units of the mean-free path l and $c(2kT_0/m)^{1/2}$ is the magnitude of the particle velocity. Also, k is the Boltzmann constant, m is the mass of a gas particle, and T_0 is a reference temperature. It can be noted that we have included in Eq. (1) an inhomogeneous driving term that is required for the thermal-creep problem (when the imposed temperature gradient is k_T). Note also that we use spherical coordinates $(c', \arccos\mu', \chi')$ and $(c, \arccos\mu, \chi)$ to define the (dimensionless) velocity vectors $\mathbf{c}'$ and $\mathbf{c}$. In addition to Eq. (1), we consider the boundary condition at the wall $(\tau=0)$ written as

$$h(0,c,\mu,\chi) = \int_0^\infty\int_0^1\int_0^{2\pi} e^{-c'^2}h(0,c',-\mu',\chi')\times R(\mathbf{c}':\mathbf{c})c'^2 d\chi'\, d\mu'\, dc', \tag{5}$$

for $\mu\in(0,1]$ and all c and χ. Here $R(\mathbf{c}':\mathbf{c})$ describes the manner in which the gas particles interact with the wall. In this notation the bulk velocity and the heat-flow profiles are written as

$$u(\tau) = \frac{1}{\pi^{3/2}}\int_0^\infty\int_{-1}^1\int_0^{2\pi} e^{-c^2}h(\tau,\mathbf{c})\times c^3(1-\mu^2)^{1/2}\cos\chi\, d\chi\, d\mu\, dc \tag{6}$$

and

$$q(\tau) = \frac{1}{\pi^{3/2}}\int_0^\infty\int_{-1}^1\int_0^{2\pi} e^{-c^2}h(\tau,\mathbf{c})(c^2-5/2)\times c^3(1-\mu^2)^{1/2}\cos\chi\, d\chi\, d\mu\, dc. \tag{7}$$

And so (in general) we seek, for the two considered problems, solutions of Eq. (1) that satisfy the boundary condition written as Eq. (5). In addition, for the thermal-creep problem the solution must be bounded as τ tends to infinity, while for Kramers' problem, since there is no driving term in Eq. (1), the solution must diverge (in a certain way) as τ tends to infinity.

In this work, we make use of the Pekeris[2] form of the scattering kernel, viz.

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$$K(\mathbf{c}':\mathbf{c})=\frac{1}{4\pi}\sum_{n=0}^{\infty}\sum_{m=0}^{n}(2n+1)(2-\delta_{0,m})P_n^m(\mu')\times P_n^m(\mu)k_n(c':c)\cos m(\chi'-\chi), \tag{8}$$

where the component functions $k_n(c',c)$ are reviewed in another work,[3] and where the *normalized* Legendre functions are given (in terms of the Legendre polynomials) by

$$P_n^m(\mu)=\left[\frac{(n-m)!}{(n+m)!}\right]^{1/2}(1-\mu^2)^{m/2}\frac{d^m}{d\mu^m}P_n(\mu),\quad n\geqslant m. \tag{9}$$

We note from Eqs. (6) and (7) that if we seek only the bulk velocity and the heat-flow profiles, then we can define our problems in terms of the azimuthal average

$$\psi(\tau,c,\mu)=\frac{1}{\pi}(1-\mu^2)^{-1/2}\int_0^{2\pi}h(r,\mathbf{c})\cos\chi\,d\chi. \tag{10}$$

And so we multiply Eqs. (1) and (5) by $\cos\chi$ and integrate to find the balance equation

$$c(c^2-5/2)k_T+c\mu\frac{\partial}{\partial\tau}\psi(\tau,c,\mu)=\varepsilon L^*\{\psi\}(\tau,c,\mu) \tag{11}$$

and the boundary condition

$$\psi(0,c,\mu)=\int_0^{\infty}\int_0^1 e^{-c'^2}\psi(0,c',-\mu')\times r(c',\mu':c,\mu)c'^2\,d\mu'\,dc', \tag{12}$$

for $\mu\in(0,1]$ and all c. Here

$$L^*\{\psi\}(\tau,c,\mu)=-\nu(c)\psi(\tau,c,\mu)+\int_0^{\infty}\int_{-1}^{1}e^{-c'^2}\psi(\tau,c',\mu')\times k(c',\mu':c,\mu)c'^2d\mu'\,dc', \tag{13}$$

where we see from Eq. (8) that we can write

$$\cos\chi'(1-\mu^2)^{1/2}k(c',\mu':c,\mu)=(1-\mu'^2)^{1/2}\int_0^{2\pi}K(\mathbf{c}':\mathbf{c})\cos\chi\,d\chi. \tag{14}$$

While we do not specify the wall kernel $R(\mathbf{c}':\mathbf{c})$, we assume that it has properties similar to those of $K(\mathbf{c}':\mathbf{c})$, i.e., we consider here that we can write

$$\cos\chi'(1-\mu^2)^{1/2}r(c',\mu':c,\mu)=(1-\mu'^2)^{1/2}\int_0^{2\pi}R(\mathbf{c}':\mathbf{c})\cos\chi\,d\chi. \tag{15}$$

We add subscripts K for Kramers' problem and T for the thermal-creep problem and state the two problems as

$$c\mu\frac{\partial}{\partial\tau}\psi_{\mathrm{K}}(\tau,c,\mu)=\varepsilon_a L^*\{\psi_{\mathrm{K}}\}(\tau,c,\mu) \tag{16}$$

and

$$c(c^2-5/2)k_T+c\mu\frac{\partial}{\partial\tau}\psi_T(\tau,c,\mu)=\varepsilon_b L^*\{\psi_T\}(\tau,c,\mu), \tag{17}$$

where both $\psi_{\mathrm{K}}(\tau,c,\mu)$ and $\psi_T(\tau,c,\mu)$ must satisfy Eq. (12). While $\psi_T(\tau,c,\mu)$ will be bounded as τ tends to infinity, $\psi_{\mathrm{K}}(\tau,c,\mu)$ must diverge in that same limit, but at the same time the resulting bulk velocity $u_{\mathrm{K}}(\tau)$ must satisfy

$$\lim_{\tau\to\infty}\frac{d}{d\tau}u_{\mathrm{K}}(\tau)=\mathcal{K}, \tag{18}$$

where $\mathcal{K}$ is a normalizing constant. Since there is a choice between using a mean-free path based, for example, on viscosity or one based on thermal conductivity, and since these and other choices have been made in the literature, we have used ε_a in Eq. (16) and ε_b in Eq. (17). In this way, we can have a general result that allows free choice of mean-free paths for each of the two problems. In Eq. (16) let $\tau\to\eta\tau$, where $\eta=\varepsilon_b/\varepsilon_a$, and in Eq. (17) let $\mu\to-\mu$, so we can write

$$c\mu\frac{\partial}{\partial\tau}\psi_{\mathrm{K}}(\eta\tau,c,\mu)=\varepsilon_b L^*\{\psi_{\mathrm{K}}\}(\eta\tau,c,\mu) \tag{19}$$

and

$$c(c^2-5/2)k_T-c\mu\frac{\partial}{\partial\tau}\psi_T(\tau,c,-\mu)=\varepsilon_b L^*\{\psi_T\}(\tau,c,-\mu). \tag{20}$$

We now multiply Eq. (19) by

$$f_T(\tau,c,\mu)=c^2e^{-c^2}(1-\mu^2)\psi_T(\tau,c,-\mu), \tag{21}$$

multiply Eq. (20) by

$$f_{\mathrm{K}}(\tau,c,\mu)=c^2e^{-c^2}(1-\mu^2)\psi_{\mathrm{K}}(\eta\tau,c,\mu) \tag{22}$$

and integrate the resulting equations over all c and μ. Subtracting the resulting equations, one from the other, we find

$$\pi^{1/2}k_Tq_{\mathrm{K}}(\eta\tau)=\int_0^{\infty}\int_{-1}^{1}e^{-c^2}c^3\mu(1-\mu^2)\times\frac{\partial}{\partial\tau}[\psi_{\mathrm{K}}(\eta\tau,c,\mu)\psi_T(\tau,c,-\mu)]d\mu\,dc. \tag{23}$$

In obtaining Eq. (23), we have used the fact that the basic scattering kernel is invariant under time reversal, i.e.,

$$K(c',\mu',\chi':c,\mu,\chi)=K(c,-\mu,\chi:c',-\mu',\chi'), \tag{24}$$

for all $\mathbf{c}$ and $\mathbf{c}'$. We now integrate Eq. (23) from $\tau=0$ to $\tau=\tau_0$ to find

$$\pi^{1/2}k_T\int_0^{\tau_0} q_{\rm K}(\eta\tau)d\tau$$
$$=\int_0^\infty\int_{-1}^1 e^{-c^2}c^3\mu(1-\mu^2)$$
$$\times\psi_{\rm K}(\eta\tau_0,c,\mu)\psi_T(\tau_0,c,-\mu)d\mu\,dc. \quad (25)$$

To arrive at Eq. (25) we have assumed that the wall scattering function has the basic property

$$c\mu R(\mathbf{c}':\mathbf{c})=c'\mu' R(\mathbf{c}:\mathbf{c}'), \quad (26)$$

for μ, $\mu'\in[0,1]$ and all c, c', χ', and χ. Kramers' problem and the half-space thermal-creep problem were solved in other works[3,4] to yield

$$\psi_{\rm K}(\tau,c,\mu)=\mathcal{K}\{cA_{\rm K}+2c\tau-(2\mu/\varepsilon_a)B(c)+\cdots\} \quad (27)$$

and

$$\psi_T(\tau,c,\mu)=k_T\{cA_T-(1/\varepsilon_b)A(c)+\cdots\}, \quad (28)$$

where the $\cdots$ are used to indicate terms that vanish as τ tends to infinity. In addition, $A(c)$ and $B(c)$ are solutions of the Chapman–Enskog integral equations[5,6] related to thermal conductivity and viscosity. We also note that $A_{\rm K}$ and A_T are to be determined from the boundary condition at the wall, and so these two constants depend on the particular wall kernel $R(\mathbf{c}':\mathbf{c})$ that is used. Now use Eqs. (27) and (28) in Eq. (25) and let $\tau_0\to\infty$ to find

$$\frac{1}{\mathcal{K}}\int_0^\infty q_{\rm K}(\eta\tau)d\tau=\frac{8}{15\pi^{1/2}\varepsilon_a\varepsilon_b}\int_0^\infty e^{-c^2}A(c)B(c)c^3\,dc$$
$$-(A_T/2)(\varepsilon_p/\varepsilon_a). \quad (29)$$

Noting Eq. (10), we can use Eq. (28) in Eq. (6) to find

$$u_T(\tau)=k_T\{(1/2)A_T+\cdots\}, \quad (30)$$

where we have used the fact[5,6] that $A(c)$ is normalized such that

$$\int_0^\infty e^{-c^2}A(c)c^3\,dc=0. \quad (31)$$

The thermal-slip coefficient is defined by

$$\zeta_T=u_T(\infty)/k_T, \quad (32)$$

and so since Eq. (29) is independent of $\mathcal{K}$ (we use $\mathcal{K}=1$ to normalize Kramers' problem), we can rewrite Eq. (29) as

$$\int_0^\infty q_{\rm K}(\tau)d\tau=\frac{\varepsilon_p\varepsilon_t}{\varepsilon_a^2}[\beta-(\varepsilon_b/\varepsilon_t)\zeta_T], \quad (33)$$

where

$$\beta=\frac{8}{15\pi^{1/2}\varepsilon_p\varepsilon_t}\int_0^\infty e^{-c^2}A(c)B(c)c^3\,dc. \quad (34)$$

To be clear, we note that if we wish to use in a problem a mean-free path based on viscosity, we should use $\varepsilon=\varepsilon_p$; on the other hand, if we wish to base the mean-free path on thermal conductivity, we should use $\varepsilon=\varepsilon_t$. These two basic constants are given[5,6] in terms of the Chapman–Enskog functions $A(c)$ and $B(c)$ as

$$\varepsilon_p=\frac{16}{15\pi^{1/2}}\int_0^\infty e^{-c^2}B(c)c^4\,dc=0.449\,027\,806... \quad (35)$$

and

$$\varepsilon_t=\frac{16}{15\pi^{1/2}}\int_0^\infty e^{-c^2}A(c)c^5\,dc=0.679\,630\,049.... \quad (36)$$

We have evaluated Eq. (34) to find

$$\beta=0.398\,935\,128.... \quad (37)$$

We note that the conditions listed as Eqs. (15) and (26) are satisfied by both the Maxwell model (a mixture of specular and diffuse reflection) and the Cercignani–Lampis model[7] for defining the boundary condition at the wall.

The CES model[8] of the linearized Boltzmann equation uses the exact Chapman–Enskog functions $A(c)$ and $B(c)$, and so Eq. (33), with Eqs. (35)–(37), is valid. On the other hand, the required approximations for the S model are

$$B(c)=c^2,\quad A(c)=\varepsilon_t c(c^2-5/2),\quad \varepsilon_p=1,\quad \varepsilon_t=3/2, \quad (38)$$

which lead to $\beta=1/2$ for the S model. For the BGK model, the relevant expressions are

$$B(c)=c^2,\quad A(c)=c(c^2-5/2),\quad \varepsilon_p=1,\quad \varepsilon_t=1, \quad (39)$$

which lead to $\beta=1/2$ also for the BGK model.

The purpose of this work was to establish Eq. (33) that relates the heat flow from Kramers' problem to the thermal-slip coefficient. This result can be used to find one of the two quantities in terms of the other, or the expression can be used to support confidence in results obtained from numerical algorithms used to solve the two problems.

While we have based our derivation of Eq. (33) on the linearized Boltzmann equation for rigid-sphere interactions and the Maxwell or the Cercignani–Lampis boundary condition, a justification of Eq. (33) for other interaction laws is possible. To be clear, we note that Eqs. (14), (15), (24), and (26) are the properties of the interaction laws we have used in this work. If these (reasonable) properties are valid for other laws, and if the general forms of the solutions, as listed in Eqs. (27) and (28), are available, then Eq. (33) will also be valid.

To conclude this work, we note that we have used the FORTRAN code written to establish the numerical results (based on the linearized Boltzmann equation and the Cercignani–Lampis boundary condition) previously reported[4] to confirm the usefulness of the basic result given by Eq. (33). Using, as was done before, $\varepsilon_a=\varepsilon_p$ and $\varepsilon_b=\varepsilon_t$, we were able to confirm with six figures of accuracy the results for the thermal-slip coefficient given in Table III of the previous work.[4] In carrying out this numerical work, one special case was found noteworthy. For Kramers' problem with the Cercignani–Lampis accommodation coefficients $\alpha_t=2$ and $\alpha_n=0$, the heat flow is zero. And so for this special case, Eq. (33) yields the interesting (and correct) result $\zeta_T=\beta$.

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