

Numerical analysis of the shear flow of a binary mixture of hard-sphere gases over a plane wall

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The shear flow of a binary mixture of rarefied gases over a plane wall is investigated on the basis of the linearized Boltzmann equation for hard-sphere molecules with the diffuse reflection boundary condition. This fundamental problem in rarefied gas dynamics is analyzed numerically by a finite-difference method, in which the complicated collision integrals are computed by the extension to the case of a gas mixture of the method proposed by Sone, Ohwada, and Aoki [Phys. Fluids A **1**, 363 (1989)]. As a result, the behavior of the mixture is clarified not only at the level of the macroscopic variables but also at the level of the velocity distribution function. In addition, an accurate formula of the shear-slip (viscous-slip) coefficient for arbitrary values of the concentration of a component gas is constructed by the use of the Chebyshev polynomial approximation. © 2004 American Institute of Physics. [DOI: 10.1063/1.1714665]

I. INTRODUCTION

Consider a slightly rarefied gas around bodies with a smooth boundary. In such a system, the Knudsen number, which is the ratio of the mean free path of gas molecules to the reference length of the system, is small. A general theory describing the steady behavior of the gas for small Knudsen numbers has been established by a systematic asymptotic analysis of the Boltzmann equation by Sone (e.g., Refs. 1–4). According to the theory, the overall behavior of the gas can be described by a set of fluid-dynamic-type equations, but, in contrast to the conventional treatment in fluid dynamics, the slip condition for the flow velocity and the jump condition for the temperature must be used at the surface of the body because of the gas rarefaction effect. That is, the flow velocity of the gas is no longer the same as that of the body (the so-called “velocity slip” phenomenon), and the temperature of the gas is different from that of the body (the so-called “temperature jump” phenomenon) at the surface. Moreover, the fluid-dynamic-type description mentioned above is to be corrected near the surface of the body in a thin layer with the thickness of the order of the mean free path. This thin layer is called the Knudsen layer. The problem of obtaining the slip and jump boundary conditions and the corrections to the fluid-dynamic description in the Knudsen layer is reduced to slip and jump problems in a half space.

These half-space problems are important fundamental problems in rarefied gas dynamics and have been investigated by many researchers. Here, mention should be made of the contributions by Sone, Cercignani, Loyalka, and their co-workers. The reader is referred to Refs. 4, 7, and 8 and the references therein for the details of their works. The recent works by Sharipov and by Siewert on this subject, which

should also be noted, will be cited on appropriate occasions in the sequel.

The general theory by Sone has been established for a single-component gas, but the situation mentioned in the first paragraph is the same for gas mixtures. In the case of gas mixtures, up to the order of the Knudsen number, there are three origins that cause the velocity slip, i.e., (1) the shear flow of the mixture, (2) the temperature gradient of the mixture, and (3) the concentration gradient of a component gas along the surface of a body. The velocity slips caused by them are called the shear slip (viscous slip), the thermal slip, and the diffusion slip, respectively. The present paper is concerned with the shear-slip phenomenon, i.e., the velocity-slip phenomenon caused by the shear flow along the surface of a body. The others have already been investigated in Refs. 5 and 6.

The analysis of the shear-slip phenomenon is reduced to the spatially one-dimensional half-space problem of the linearized Boltzmann equation in the situation where a gas flows along a plane wall with a velocity that grows linearly with respect to the distance from the wall. Since the pioneer work by Maxwell,⁹ this fundamental problem has been studied by various approaches^{10–22} (see also Refs. 4, 23, and 24, and the references therein). As a result, for a single-component gas, an accurate numerical solution of the original Boltzmann equation, as well as that of model Boltzmann equations, was established more than a decade ago at the level of the velocity distribution function.^{14,19}

Recently, in connection with micro-device engineering, a flow in micro-systems attracts a deal of attention.²⁵ Since the Knudsen number is no longer negligibly small in such systems, the velocity slip is significant in the analysis of the flow, which puts the shear-slip problem, especially that for gas mixtures, in the limelight again.^{20–22,26–30} Existing works for gas mixtures are, however, based on model Boltzmann equations or on the moment and the variational

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methods.^{10–13,16–18,20–22} Such approaches are handy but of an approximate nature. In order to assess the validity of those results, something that can be used as the standard is desired. Not only from an academic interest but also from such a practical viewpoint, we are going to carry out an accurate numerical analysis of the shear-slip problem on the basis of the original Boltzmann equation for hard-sphere molecules and to establish the standard solution of this fundamental problem for gas mixtures. The numerical method is the combination of the finite-difference and the numerical kernel methods, the latter of which was first proposed in Ref. 31 for the computation of the complicated collision integral in the case of a single-component gas and was extended to gas mixtures in Ref. 5. The method has already been applied to the diffusion-slip and the thermal-slip problems successfully.^{5,6}

In this paper, we first formulate the problem in Sec. II and then perform a preliminary analysis in Sec. III. The numerical method is explained only briefly in Sec. IV because it is described in detail in Ref. 6. The results and discussions are given in Sec. V, and finally concluding remarks are made in Sec. VI.

II. FORMULATION OF THE PROBLEM

A. Problem

We consider a semi-infinite expanse of a binary mixture of gases, gas A and gas B, over a plane wall at rest with a uniform temperature T_0 . The wall is located at $X_1=0$, and the mixture occupies the region $X_1>0$, where X_i is the rectangular coordinate system. Far away from the wall, the pressure and temperature of the mixture and the concentration of gas A (the number fraction of the molecules of gas A) are uniform, but the flow velocity v_2 of the mixture in the X_2 -direction grows linearly in X_1 . Hereinafter, the former three are denoted by p_0 , T_0 , and X_0^A , respectively. The Greek letters α and β are symbolically used to represent the gas species, i.e., $\alpha, \beta = A, B$.

We will investigate the steady behavior of the mixture under the following assumptions: (i) The molecules of gas α are hard spheres of mass m^α and diameter d^α , and they collide elastically with each other; (ii) the behavior of the mixture is described by the Boltzmann equation and the diffuse reflection condition for the reflected molecules on the wall; and (iii) the growing rate of the flow velocity v_2 with respect to X_1 is so small that the equations and boundary conditions can be linearized around the reference equilibrium state at rest with temperature T_0 and pressure p_0 of the mixture and concentration X_0^A of gas A.

B. Basic equation and boundary condition

We first summarize the main notation used in the paper. The n_0 is the reference molecular number density of the mixture and is defined by $n_0 = p_0/kT_0$, where k is Boltzmann's constant. The l_0 is the mean free path of the molecules in the equilibrium state at rest with the molecular number density n_0 and temperature T_0 when gas B is absent (i.e., $l_0 = 1/[\sqrt{2}\pi(d^A)^2n_0]$). The x_i is the nondimensional co-

ordinate system defined by $x_i = X_i l_0^{-1}(\sqrt{\pi}/2)^{-1}$. The $(2kT_0/m^A)^{1/2}\zeta_i$ [or $(2kT_0/m^A)^{1/2}\xi$] is the molecular velocity, $n_0(2kT_0/m^A)^{-3/2}(X_0^\alpha + \phi^\alpha)E^\alpha$ is the velocity distribution function of the molecules of gas α , where $E^\alpha(\xi) = (\hat{m}^\alpha/\pi)^{3/2} \exp(-\hat{m}^\alpha|\xi|^2)$ with $\hat{m}^\alpha = m^\alpha/m^A$, and $\hat{d}^\alpha = d^\alpha/d^A$. The molecular number density, density, pressure, temperature, flow velocity, stress tensor, and heat-flow vector of gas α are denoted, respectively, by $n_0(X_0^\alpha + N^\alpha)$, $n_0 m^A(\hat{m}^\alpha X_0^\alpha + \omega^\alpha)$, $p_0(X_0^\alpha + P^\alpha)$, $T_0(1 + \tau^\alpha)$, $(2kT_0/m^A)^{1/2}u_i^\alpha$, $p_0(X_0^\alpha \delta_{ij} + P_{ij}^\alpha)$, and $p_0(2kT_0/m^A)^{1/2}Q_i^\alpha$, where δ_{ij} is Kronecker's delta. Those of the mixture are denoted by $n_0(1 + N)$, $n_0 m^A(\sum_{\beta=A,B} \hat{m}^\beta X_0^\beta + \omega)$, $p_0(1 + P)$, $T_0(1 + \tau)$, $(2kT_0/m^A)^{1/2}u_i$, $p_0(\delta_{ij} + P_{ij})$, and $p_0(2kT_0/m^A)^{1/2}Q_i$.

The linearized Boltzmann equation in the present case ($\partial/\partial t = \partial/\partial x_2 = \partial/\partial x_3 = 0$) is written as^{32–34}

$$\zeta_1 \frac{\partial \phi^\alpha}{\partial x_1} = \sum_{\beta=A,B} K^{\beta\alpha} \tilde{L}^{\beta\alpha}(X_0^\alpha \phi^\beta, X_0^\beta \phi^\alpha), \quad (1)$$

where $\tilde{L}^{\beta\alpha}$ is the linearized collision integral defined by

$$\begin{aligned} \tilde{L}^{\beta\alpha}(f, g) = & \frac{1}{4\sqrt{2}\pi} \int [f(\xi'_*) - f(\xi_*) + g(\xi') - g(\xi)] \\ & \times E^\beta(\xi'_*) |\mathbf{e} \cdot \hat{\mathbf{V}}| d\Omega(\mathbf{e}) d^3 \xi_*, \end{aligned} \quad (2)$$

with

$$\xi' = \xi + \frac{\hat{\mu}^{\beta\alpha}}{\hat{m}^\alpha} (\mathbf{e} \cdot \hat{\mathbf{V}}) \mathbf{e}, \quad \xi'_* = \xi_* - \frac{\hat{\mu}^{\beta\alpha}}{\hat{m}^\beta} (\mathbf{e} \cdot \hat{\mathbf{V}}) \mathbf{e}, \quad (3a)$$

$$\hat{\mathbf{V}} = \xi_* - \xi, \quad d^3 \xi_* = d\xi_{*1} d\xi_{*2} d\xi_{*3}, \quad (3b)$$

$$K^{\beta\alpha} = \left(\frac{\hat{d}^\alpha + \hat{d}^\beta}{2} \right)^2, \quad \hat{\mu}^{\beta\alpha} = \frac{2\hat{m}^\alpha \hat{m}^\beta}{\hat{m}^\alpha + \hat{m}^\beta}. \quad (3c)$$

Here $\mathbf{e}$ is a unit vector, ξ_* the variable of integration corresponding to ξ , and $d\Omega(\mathbf{e})$ the solid-angle element in the direction of $\mathbf{e}$. The integration in Eq. (2) is carried out over the whole space of ξ_* and over all the directions of $\mathbf{e}$.

The diffuse reflection condition on the wall ($x_1=0$) is written as

$$\phi^\alpha = -2(\pi \hat{m}^\alpha)^{1/2} \int_{\xi_1 < 0} \zeta_1 \phi^\alpha E^\alpha d^3 \xi, \quad \xi_1 > 0. \quad (4)$$

The macroscopic quantities N^α , ω^α , u_i^α , etc., of gas α are written in terms of ϕ^α as

$$N^\alpha = \int \phi^\alpha E^\alpha d^3 \xi, \quad (5a)$$

$$\omega^\alpha = \hat{m}^\alpha \int \phi^\alpha E^\alpha d^3 \xi (= \hat{m}^\alpha N^\alpha), \quad (5b)$$

$$u_i^\alpha = \frac{1}{X_0^\alpha} \int \zeta_i \phi^\alpha E^\alpha d^3 \xi, \quad (5c)$$

$$\tau^\alpha = \frac{2}{3} \frac{1}{X_0^\alpha} \int \left(\hat{m}^\alpha \xi_j^2 - \frac{3}{2} \right) \phi^\alpha E^\alpha d^3 \xi, \quad (5d)$$

$$P^\alpha = \frac{2}{3} \hat{m}^\alpha \int \zeta_j^2 \phi^\alpha E^\alpha d^3 \zeta (= N^\alpha + X_0^\alpha \tau^\alpha), \quad (5e)$$

$$P_{ij}^\alpha = 2 \hat{m}^\alpha \int \zeta_i \zeta_j \phi^\alpha E^\alpha d^3 \zeta, \quad (5f)$$

$$Q_i^\alpha = \hat{m}^\alpha \int \zeta_i \zeta_j^2 \phi^\alpha E^\alpha d^3 \zeta - \frac{5}{2} X_0^\alpha u_i^\alpha. \quad (5g)$$

Here and henceforth, unless otherwise stated, the integration with respect to ζ is performed over its whole space. The macroscopic quantities of the mixture are expressed in terms of those of component gases as

$$N = \sum_{\beta=A,B} N^\beta, \quad \omega = \sum_{\beta=A,B} \omega^\beta, \quad P = \sum_{\beta=A,B} P^\beta, \quad (6a)$$

$$u_i = \left(\sum_{\beta=A,B} \hat{m}^\beta X_0^\beta u_i^\beta \right) / \left(\sum_{\beta=A,B} \hat{m}^\beta X_0^\beta \right), \quad (6b)$$

$$\tau = \sum_{\beta=A,B} X_0^\beta \tau^\beta, \quad P_{ij} = \sum_{\beta=A,B} P_{ij}^\beta, \quad (6c)$$

$$Q_i = \sum_{\beta=A,B} \left[Q_i^\beta - \frac{5}{2} X_0^\beta (u_i - u_i^\beta) \right]. \quad (6d)$$

If we denote by $X_0^\alpha + \chi^\alpha$ the concentration of gas α , χ^α is expressed as

$$\chi^\alpha = N^\alpha - X_0^\alpha N. \quad (7)$$

Note that $\chi^A = -\chi^B$ because of the relations $N = N^A + N^B$ and $X_0^A + X_0^B = 1$.

III. PRELIMINARY ANALYSIS

A. Asymptotic solution away from the wall

Let us consider the function

$$\phi_{\text{asy}}^\alpha = X_0^\alpha [2 \hat{m}^\alpha \zeta_2 (x_1 + b) - \zeta_1 \zeta_2 B^\alpha(\zeta)], \quad (8)$$

where $\zeta = |\zeta| = \sqrt{\zeta_j^2}$. Here b is an undetermined constant, and the function B^α is the solution of the following integral equation:^{33–35}

$$\sum_{\beta=A,B} K^{\beta\alpha} X_0^\beta \tilde{L}^{\beta\alpha}(\zeta_{ij} B^\beta, \zeta_{ij} B^\alpha) = -2 \hat{m}^\alpha \zeta_{ij}, \quad (9a)$$

with

$$\zeta_{ij} = \zeta_i \zeta_j - \frac{1}{3} \zeta^2 \delta_{ij}. \quad (9b)$$

The function ϕ_{asy}^α satisfies the Boltzmann equation (1). The corresponding macroscopic quantities take the following form:

$$N^\alpha = \omega^\alpha = \chi^\alpha = \tau^\alpha = P^\alpha = Q_i^\alpha = 0, \quad (10a)$$

$$u_i^\alpha = (x_1 + b) \delta_{i2}, \quad P_{ij}^\alpha = -\hat{\mu}^\alpha X_0^\alpha (\delta_{i1} \delta_{j2} + \delta_{i2} \delta_{j1}), \quad (10b)$$

$$N = \omega = \tau = P = Q_i = 0, \quad (10c)$$

$$u_i = (x_1 + b) \delta_{i2}, \quad P_{ij} = -\hat{\mu} (\delta_{i1} \delta_{j2} + \delta_{i2} \delta_{j1}), \quad (10d)$$

where

$$\hat{\mu} = \sum_{\beta=A,B} X_0^\beta \hat{\mu}^\beta, \quad (11a)$$

$$\hat{\mu}^\alpha = \frac{8\pi}{15} \hat{m}^\alpha \int_0^\infty \zeta^6 B^\alpha(\zeta) E^\alpha(\zeta) d\zeta. \quad (11b)$$

Here $\hat{\mu}$ is a constant depending on X_0^A , m^B/m^A , and d^B/d^A , which is related to the viscosity μ of the mixture by the relation^{36,37}

$$\mu = \frac{\sqrt{\pi}}{2} \hat{\mu} p_0 (2kT_0/m^A)^{-1/2} l_0. \quad (12)$$

It is seen from the form of P , τ , u_2 , and χ^α in Eq. (10) that, if we denote by c the dimensionless growing rate of the flow velocity

$$c = \left(\frac{du_2}{dx_1} \right)_{x_1 \rightarrow \infty},$$

then ϕ_{asy}^α of (8) multiplied by c is the solution describing the state at infinity. The asymptotic solution $c\phi_{\text{asy}}^\alpha$ is seen to represent the state of the mixture described by the fluid-dynamic equation. Therefore, we call $c\phi_{\text{asy}}^\alpha$ the fluid-dynamic solution.

B. Knudsen-layer problem

Let us now seek the solution in the form

$$\phi^\alpha = c [\phi_{\text{asy}}^\alpha + \phi_K^\alpha(x_1, \zeta_i)]. \quad (13)$$

Substituting Eq. (13) into Eqs. (1) and (4) and taking into account that ϕ_{asy}^α satisfies the condition at infinity, we obtain the following equation and boundary condition for ϕ_K^α :

$$\zeta_1 \frac{\partial \phi_K^\alpha}{\partial x_1} = \sum_{\beta=A,B} K^{\beta\alpha} \tilde{L}^{\beta\alpha}(X_0^\alpha \phi_K^\beta, X_0^\beta \phi_K^\alpha), \quad (14)$$

$$\phi_K^\alpha = -2 \hat{m}^\alpha X_0^\alpha b \zeta_2 + X_0^\alpha \zeta_1 \zeta_2 B^\alpha(\zeta)$$

$$-2(\pi \hat{m}^\alpha)^{1/2} \int_{\zeta_1 < 0} \zeta_1 \phi_K^\alpha E^\alpha d^3 \zeta,$$

$$\zeta_1 > 0, \quad x_1 = 0, \quad (15)$$

$$\phi_K^\alpha \rightarrow 0, \quad \text{as } x_1 \rightarrow \infty. \quad (16)$$

We call the half-space problem (14)–(16) the Knudsen-layer problem for the shear slip. For the problem, there is a unique solution ϕ_K^α if and only if the constant b takes a special value, and ϕ_K^α decays exponentially as $x_1 \rightarrow \infty$. This is a consequence of the existence and uniqueness theorem for the Knudsen-layer problem for a binary mixture of hard-sphere gases (Ref. 38; see also Refs. 39–44). It should be noted that the constant b in the fluid-dynamic solution $c\phi_{\text{asy}}^\alpha$ is determined by the analysis of the Knudsen-layer problem.

Since $\hat{m}^A = \hat{d}^A = 1$ and $X_0^A + X_0^B = 1$, the problem is characterized by the three parameters,

$$\hat{m}^B (\text{or } m^B/m^A), \quad \hat{d}^B (\text{or } d^B/d^A), \quad X_0^A.$$

Multiplying Eq. (14) by $\hat{m}^\alpha \zeta_2 E^\alpha$ for $\alpha = A, B$, adding the resulting equations, and taking into account the condition (16), one obtains the relation

$$\sum_{\beta=A,B} \hat{m}^\beta \int \zeta_1 \zeta_2 \phi_K^\beta E^\beta d^3 \zeta = 0. \quad (17)$$

This is the conservation law of the x_2 -component of the momentum.

C. Similarity solution and macroscopic quantities

Let us assume that ϕ_K^α is of the form

$$\phi_K^\alpha = (\zeta_2 / \zeta_\rho) \Phi^\alpha(x_1, \zeta_1, \zeta_\rho), \quad (18)$$

where $\zeta_\rho = \sqrt{\zeta_2^2 + \zeta_3^2}$. This ϕ_K^α is compatible with Eqs. (14)–(16), which can be seen by using the spherical symmetry⁴ of the collision operator $\tilde{L}^{\beta\alpha}$. Therefore, using the notations

$$\Psi^\alpha(x_1, \zeta_1, \zeta_\rho) = \Phi^\alpha(x_1, \zeta_1, \zeta_\rho) E^\alpha, \quad (19a)$$

$$\tilde{L}^{\beta\alpha}(\Psi^\beta, \Psi^\alpha) = (\zeta_\rho / \zeta_2) \tilde{L}^{\beta\alpha} \left(\frac{\zeta_2}{\zeta_\rho} \Phi^\beta, \frac{\zeta_2}{\zeta_\rho} \Phi^\alpha \right) E^\alpha, \quad (19b)$$

we can transform the boundary-value problem (14)–(16) for ϕ_K^α into that for Ψ^α :

$$\zeta_1 \frac{\partial \Psi^\alpha}{\partial x_1} = \sum_{\beta=A,B} K^{\beta\alpha} \tilde{L}^{\beta\alpha}(X_0^\alpha \Psi^\beta, X_0^\beta \Psi^\alpha), \quad (20)$$

$$\Psi^\alpha = X_0^\alpha \zeta_\rho (-2\hat{m}^\alpha b + \zeta_1 B^\alpha) E^\alpha,$$

$$\zeta_1 > 0, \quad x_1 = 0, \quad (21)$$

$$\Psi^\alpha \rightarrow 0, \quad \text{as } x_1 \rightarrow \infty. \quad (22)$$

Here E^α and B^α are regarded as the functions of ζ_1 and ζ_ρ because $\zeta = |\zeta| = (\zeta_1^2 + \zeta_\rho^2)^{1/2}$. The integral $\tilde{L}^{\beta\alpha}$ can be expressed in terms of integral kernels:

$$\tilde{L}^{\beta\alpha}(f, g) = \tilde{L}_1^{\beta\alpha}(f) + \tilde{L}_2^{\beta\alpha}(g) - \tilde{L}_3^{\beta\alpha}(f) - \nu^\beta(\zeta)g, \quad (23)$$

with

$$\begin{aligned} \tilde{L}_J^{\beta\alpha}(f) &= E^\alpha \int_0^\infty d\xi_\rho \int_{-\infty}^\infty d\xi_1 \mathcal{K}_J^{\beta\alpha}(\xi_1, \xi_\rho, \zeta_1, \zeta_\rho) f(\xi_1, \xi_\rho) \\ (J &= 1, 2, 3), \end{aligned} \quad (24a)$$

$$\begin{aligned} \nu^\alpha(\zeta) &= \frac{1}{2\sqrt{2}} \left[\frac{1}{\sqrt{\hat{m}^\alpha}} \exp(-\hat{m}^\alpha \zeta^2) \right. \\ &\quad \left. + \left(2\zeta + \frac{1}{\hat{m}^\alpha \zeta} \right) \int_0^{\sqrt{\hat{m}^\alpha} \zeta} \exp(-y^2) dy \right]. \end{aligned} \quad (24b)$$

The explicit form of integral kernels $\mathcal{K}_J^{\beta\alpha}$ ($J=1, 2, 3$) is given in Appendix B of Ref. 6.

Substituting Eq. (13) with the similarity solution (18) [and (19a)] into Eqs. (5)–(7), we have the following expression for the macroscopic quantities:

$$N^\alpha = \omega^\alpha = \chi^\alpha = \tau^\alpha = P^\alpha = 0, \quad (25a)$$

$$u_i^\alpha = c(x_1 + b + U^\alpha) \delta_{i2}, \quad (25b)$$

$$P_{ij}^\alpha = c(-\hat{\mu}^\alpha X_0^\alpha + S^\alpha)(\delta_{i1} \delta_{j2} + \delta_{i2} \delta_{j1}), \quad (25c)$$

$$Q_i^\alpha = cH^\alpha \delta_{i2}, \quad (25d)$$

$$N = \omega = \tau = P = 0, \quad (25e)$$

$$u_i = c(x_1 + b + U) \delta_{i2}, \quad (25f)$$

$$P_{ij} = -c\hat{\mu}(\delta_{i1} \delta_{j2} + \delta_{i2} \delta_{j1}), \quad (25g)$$

$$Q_i = cH \delta_{i2}, \quad (25h)$$

where

$$U^\alpha(x_1) = \frac{\pi}{X_0^\alpha} \int_0^\infty \int_{-\infty}^\infty \zeta_\rho^2 \Psi^\alpha d\zeta_1 d\zeta_\rho, \quad (26a)$$

$$U(x_1) = \left(\sum_{\beta=A,B} \hat{m}^\beta X_0^\beta U^\beta \right) / \left(\sum_{\beta=A,B} \hat{m}^\beta X_0^\beta \right), \quad (26b)$$

$$S^\alpha(x_1) = 2\pi \hat{m}^\alpha \int_0^\infty \int_{-\infty}^\infty \zeta_1 \zeta_\rho^2 \Psi^\alpha d\zeta_1 d\zeta_\rho, \quad (26c)$$

$$H^\alpha(x_1) = \pi \int_0^\infty \int_{-\infty}^\infty \zeta_\rho^2 \left(\hat{m}^\alpha (\zeta_1^2 + \zeta_\rho^2) - \frac{5}{2} \right) \Psi^\alpha d\zeta_1 d\zeta_\rho, \quad (26d)$$

$$H(x_1) = \sum_{\beta=A,B} \left(H^\beta + \frac{5}{2} X_0^\beta (U^\beta - U) \right). \quad (26e)$$

In deriving the expression of P_{ij} in Eq. (25g), the relation

$$S^A + S^B = 0, \quad (27)$$

which is deduced from the property (17), has been used. This relation will be used as a measure of accuracy of the numerical solution (see Appendix A).

The functions U^α , U , S^α , H^α , and H , which we call the Knudsen-layer functions, decay exponentially as $x_1 \rightarrow \infty$. In Eq. (25), they appear only in the x_2 -component of the flow velocities u_2^α and u_2 , in that of the heat-flow vectors Q_2^α and Q_2 , and in the $x_1 x_2$ -component of the stress tensors P_{12}^α (or P_{21}^α). In other words, except u_2^α , u_2 , Q_2^α , Q_2 , and P_{12}^α (or P_{21}^α), the macroscopic quantities are expressed only by the fluid-dynamic solution: Equation (10) multiplied by c .

The expression of u_i in Eq. (25f) shows that, if the Knudsen-layer function is neglected, the flow velocity of the mixture on the wall ($x_1 = 0$) is expressed as

$$u_2 = bc = b \left(\frac{du_2}{dx_1} \right). \quad (28)$$

This means that the flow velocity of the fluid-dynamic solution is subject to the slip on the wall caused by the gradient of flow velocity (or the shear stress). From this point of view, the constant b is called the coefficient of shear slip (or viscous slip).

IV. NUMERICAL ANALYSIS

As in Ref. 6, we solve the boundary-value problem (20)–(22) by the use of the following technique. This method was devised in Ref. 14.

Consider the function $\tilde{\Psi}^\alpha$ and the constant b_* given by

$$\tilde{\Psi}^\alpha(x_1, \zeta_1, \zeta_\rho) = \Psi^\alpha(x_1, \zeta_1, \zeta_\rho) + 2\hat{m}^\alpha X_0^\alpha \delta \zeta_\rho E^\alpha, \quad (29a)$$

$$b_* = b - \delta, \quad (29b)$$

where δ is an undetermined constant. The function $\tilde{\Psi}^\alpha$ satisfies Eq. (20) and the boundary condition on the wall (21) with b replaced by b_* , i.e.,

$$\zeta_1 \frac{\partial \tilde{\Psi}^\alpha}{\partial x_1} = \sum_{\beta=A,B} K^{\beta\alpha} \tilde{\mathcal{L}}^{\beta\alpha}(X_0^\alpha \tilde{\Psi}^\beta, X_0^\beta \tilde{\Psi}^\alpha), \quad (30)$$

$$\tilde{\Psi}^\alpha = X_0^\alpha \zeta_\rho (-2\hat{m}^\alpha b_* + \zeta_1 B^\alpha) E^\alpha, \quad \zeta_1 > 0, \quad x_1 = 0. \quad (31)$$

At a large distance d for which Ψ^α is negligibly small, $\tilde{\Psi}^\alpha$ satisfies the reflection condition

$$\tilde{\Psi}^\alpha(d, \zeta_1, \zeta_\rho) = \tilde{\Psi}^\alpha(d, -\zeta_1, \zeta_\rho), \quad (32)$$

and δ is related to the following moment of $\tilde{\Psi}^\alpha$:

$$\delta = \tilde{U}(d), \quad (33)$$

where $\tilde{U}(x_1)$ is the quantity defined by Eqs. (26a) and (26b) with Ψ^α replaced by $\tilde{\Psi}^\alpha$. We solve the boundary-value problem (30)–(32) for a given b_* under a proper choice of d . Once $\tilde{\Psi}^\alpha$ is obtained, δ is determined by Eq. (33). Then Ψ^α and b are obtained from Eqs. (29a) and (29b). In the actual computation, we repeat this solution process by putting b as new b_* in order to avoid the accumulation of the numerical errors caused by the computation of the collision integrals of the second term of Eq. (29a) in the wide region of x_1 -space.

The numerical method is the same as that in Ref. 6, except that the third-order finite-difference scheme is used for $\partial/\partial x_1$ in place of the second-order one in Ref. 6 (see Appendix B). Corresponding to this change, the following new lattice system is used for x_1 :

$$x_1^{(i)} = 20 \ln(p^{(\bar{N}_x)} / (p^{(\bar{N}_x)} - 0.7p^{(i)})) + 10^{-4} \left(\frac{i}{\bar{N}_x} \right) \quad (i=0, 1, \dots, N_x), \quad (34)$$

with

$$p^{(i)} = 25(i^4/\bar{N}_x^3) / [1 + 25(i/\bar{N}_x)^3], \quad (35)$$

where $x_1^{(i)}$ denotes the i th lattice point in x_1 -space, and $\bar{N}_x$ and $N_x (\geq \bar{N}_x)$ are given positive integers. We will denote by $\overline{S1}$ the system with $N_x = \bar{N}_x = 300$, by $\overline{S2}$ that with $N_x = \bar{N}_x = 600$, by $\overline{S3}$ that with $N_x = 320$ and $\bar{N}_x = 300$, and by $\overline{S4}$ that with $N_x = 340$ and $\bar{N}_x = 300$, respectively. For the molecular velocity, (ζ_1, ζ_ρ) -space is truncated in the region $-Z_1 \leq \sqrt{\hat{m}^\alpha} \zeta_1 \leq Z_1$ and $0 \leq \sqrt{\hat{m}^\alpha} \zeta_\rho \leq Z_\rho$ for gas α , and the same lattice system as that in Ref. 6 is used.

Various accuracy tests were performed by using the systems $\overline{S1}$ – $\overline{S3}$ for x_1 and the systems M1–M7 in Ref. 6 for (ζ_1, ζ_ρ) . They were intended to assess not only the appropriate size of the lattice intervals but also the appropriate size of the truncated region of $(x_1, \zeta_1, \zeta_\rho)$ -space. The results are

summarized in Appendix A. After the tests for different lattice systems, the pair ($\overline{S1}$, M1) is adopted as the standard lattice system for $m^B/m^A = 2, 4$, and 5. For $m^B/m^A = 10$, the pair ($\overline{S4}$, M1), which covers a wider region of x_1 , is used instead of ($\overline{S1}$, M1). All the results given in the next section are obtained by using these systems. For the system ($\overline{S1}$, M1) [or ($\overline{S4}$, M1)], the original regions of x_1 , ζ_1 , and ζ_ρ are limited to the regions $0 \leq x_1 \leq 24.08$ (or 32.49) [i.e., $d = 24.08$ (or 32.49)], $-4.5 \leq \sqrt{\hat{m}^\alpha} \zeta_1 \leq 4.5$ (i.e., $Z_1 = 4.5$), and $0 \leq \sqrt{\hat{m}^\alpha} \zeta_\rho \leq 4.5$ (i.e., $Z_\rho = 4.5$) for gas α , and there are 301 (or 341), 101, and 55 lattice points, respectively. Additional information about the accuracy test for the standard systems are also given in Appendix A.

Incidentally, the function B^α is often approximated by a few terms of the Sonine polynomial expansion³³ in the literature. In the present paper, however, we make use of the accurate numerical data of B^α that are obtained by a direct numerical computation of Eq. (9a) in Ref. 35.

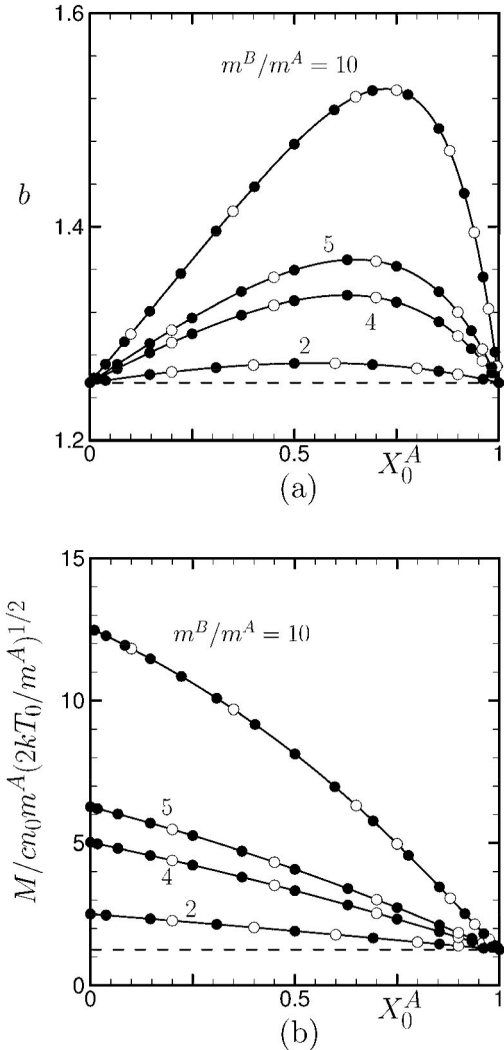


FIG. 1. Coefficient of shear slip and the corresponding momentum. (a) Slip coefficient b and (b) momentum $(0, M, 0)$ of the mixture per unit volume. Both closed and open circles indicate the present result. The solid line indicates the present result using the formula (37). The data used to construct the formula are marked with closed circles. The dashed line indicates the result for $m^B/m^A = 1$.

TABLE I. Data of $b^{(n)}$ ($n=0, \dots, N$) in Eq. (37).

n	m^B/m^A			
	2 (N=8)	4 (N=12)	5 (N=12)	10 (N=16)
0	1.894 35	3.228 36	3.915 05	7.486 58
1	-6.276 54(-1) ^a	-1.887 19	-2.517 48	-5.655 07
2	-1.351 92(-2)	-9.603 84(-2)	-1.583 81(-1)	-6.179 29(-1)
3	6.632 18(-4)	5.698 24(-3)	8.213 20(-3)	1.110 81(-4)
4	1.132 85(-4)	2.477 04(-3)	4.893 79(-3)	2.369 40(-2)
5	1.012 51(-5)	5.191 18(-4)	1.253 85(-3)	1.045 64(-2)
6	9.391 77(-7)	1.075 21(-4)	3.054 54(-4)	3.872 40(-3)
7	1.048 49(-6)	2.259 87(-5)	7.547 69(-5)	1.409 03(-3)
8	-7.375 01(-7)	4.944 17(-6)	1.924 14(-5)	5.187 87(-4)
9	...	1.095 29(-6)	4.984 96(-6)	1.937 82(-4)
10	...	2.469 68(-7)	1.313 92(-6)	7.320 91(-5)
11	...	5.877 42(-8)	3.695 48(-7)	2.789 92(-5)
12	...	1.273 07(-8)	9.202 34(-8)	1.070 59(-5)
13	...	...	...	4.140 01(-6)
14	...	...	...	1.633 83(-6)
15	...	...	...	7.152 63(-7)
16	...	...	...	2.421 03(-7)

^aRead as $-6.276\,54 \times 10^{-1}$.

The computation was performed by using a parallel code for 10 CPUs on the FUJITSU VPP800 in the Academic Center for Computing and Media Studies of Kyoto University. First the computation was carried out for a smaller lattice system with $301 \times 73 \times 21$ points in (x_1, ξ_1, ξ_ρ) -space [system (S1, M7)], and the resulting data were transformed into the data for the standard lattice system by interpolation. Then, the computation for the standard system (S1, M1) or (S4, M1) was performed by using the transformed data as the initial guess in the iterative solution process. For each set of parameters $(m^B/m^A, d^B/d^A, X_0^A)$, it takes about a half hour for the smaller system, 3 hours for system (S1, M1), and 3.5 hours for system (S4, M1). The computing time does not much depend on the values of the parameters.

V. RESULTS AND DISCUSSIONS

In the present paper, we carry out the computation for $m^B/m^A=2, 4, 5$, and 10 and for various values of X_0^A , restricting ourselves to the case $d^B/d^A=1$. Hereinafter, we assume that $m^B/m^A \geq 1$, because the results for $m^B/m^A < 1$ can be obtained from those for $m^B/m^A > 1$ by a simple transformation.

A. Slip coefficient

The coefficient of shear slip b versus the concentration X_0^A of gas A is shown in Fig. 1(a). Since b is positive, the slip is induced in the direction of the flow of the mixture far away from the wall. The b is larger for larger molecular mass ratio m^B/m^A . For $m^B/m^A=1$, it is independent of X_0^A because there is no difference (except “color” or “label”) between molecules of different kind. But, for $m^B/m^A \neq 1$, b is not uniform with respect to X_0^A and attains the maximum at an intermediate value of X_0^A in the interval of $0.5 < X_0^A < 1$. This value of X_0^A increases with m^B/m^A and, consequently, b changes steeply near $X_0^A=1$ for large m^B/m^A . It should be noted that the value of b at $X_0^A=0$ (the case of pure gas B) is

the same as that at $X_0^A=1$ (the case of pure gas A), irrespective of the value of m^B/m^A . This means that the slip coefficient is independent of the molecular mass in the case of one species gases.

The flow velocity of the fluid-dynamic solution along the wall is given by $u_2 = c(x_1 + b)$ [see Eq. (25f)], namely, the sum of the classical shear flow cx_1 and the uniform flow cb caused by the velocity slip. If we denote by $(0, M, 0)$ the momentum of the mixture of this uniform flow per unit volume, M is given by

$$M/cn_0m^A(2kT_0/m^A)^{1/2} = \hat{\rho}_0 b, \quad (36)$$

where $\hat{\rho}_0 (\equiv \hat{m}^A X_0^A + \hat{m}^B X_0^B) = (1 - \hat{m}^B)X_0^A + \hat{m}^B$. Figure 1(b) shows its dependence on X_0^A . The momentum is larger for larger m^B/m^A and decreases monotonically as X_0^A increases. It takes a common value at $X_0^A=1$ because there is no gas B in this case.

The numerical computations are performed for several values of X_0^A , the results of which are indicated by closed or open circles in Fig. 1. From the data shown by closed circles, following Ref. 6, we constructed the formula of b for arbitrary values of X_0^A by the use of the Chebyshev polynomial approximation (Ref. 45). Since the dependence of $\hat{\rho}_0 b$ on X_0^A is much simpler than that of b , the formula is constructed from the data of $\hat{\rho}_0 b$, not from the data of b itself. The resulting formula is given as

$$b = \sum_{n=0}^N b^{(n)} T_n(2X_0^A - 1) / \hat{\rho}_0, \quad (37)$$

where $T_n(x)$ ($n=0, 1, 2, \dots$) is the Chebyshev polynomial of degree n defined for $0 \leq \theta \leq \pi$ by the relation

$$T_n(\cos \theta) = \cos n\theta. \quad (38)$$

The data of $b^{(n)}$ are listed in Table I. The solid line in Fig. 1 is drawn by using Eq. (37). The accuracy of this formula is checked by comparing with the data shown by open circles

TABLE II. The values of the slip coefficients b by the formula (37).

$X_0^A \backslash m^B/m^A$	b			
	2	4	5	10
0	1.2540	1.2540	1.2540	1.2540
0.1	1.2594	1.2734	1.2792	1.2995
0.3	1.2678	1.3075	1.3253	1.3919
0.5	1.2720	1.3307	1.3593	1.4772
0.7	1.2707	1.3336	1.3677	1.5282
0.9	1.2619	1.2977	1.3202	1.4507
1	1.2540	1.2540	1.2540	1.2540

in the figure. The results are summarized at the end of Appendix A. Some of the values of b obtained by Eq. (37) are shown in Table II.

The shear-slip problem has been studied by various approximation methods (the variational method, the moment method, etc.) or by direct computation of model Boltzmann equations. In contrast, in the present paper, the problems are analyzed faithfully and accurately on the basis of the Boltzmann equation. As a result, the validity of the existing results can be assessed by the present result. The results for a mixture of hard-sphere gases in Refs. 18 and 20–22 are compared with the present result in Fig. 2 and in Table III. Naturally a comparison is made only among the results for hard-sphere gases. The formulas in Refs. 20 and 21 are derived by a special kind of half-space moment method, the former of which is evaluated by the use of the first order Chapman–Enskog expansions while the latter of which is evaluated by the use of the second-order Chapman–Enskog expansions. The result based on the second-order approximation (Ref. 21) agrees less well with the present result than that based on the first-order approximation (Ref. 20). However, the devia-

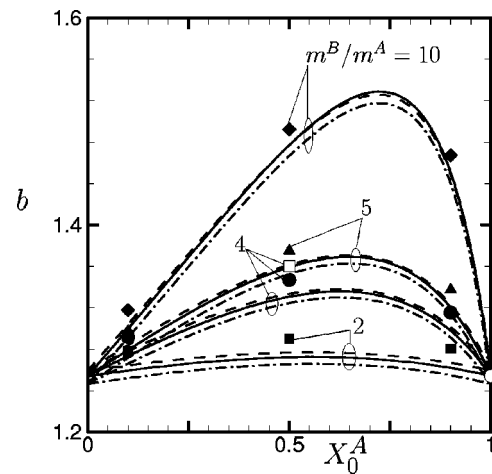


FIG. 2. A comparison with the previous results: b vs X_0^A . The solid line indicates the present result, the dashed line the formula in Ref. 20, and the dot-dash line that in Ref. 21. The closed symbols $\blacksquare$, $\bullet$, $\blacktriangle$, and $\blacklozenge$ indicate the result of Ref. 22 for $m^B/m^A=2, 4, 5$, and 10 , respectively. The open square $\square$ indicates the result of Ref. 18 for $m^B/m^A=4$ and $X_0^A=0.5$. The open circle $\circ$ indicates the result of Ref. 14 for a single-component gas.

tions from the present result are both very small (less than 1%). In particular, the result in Ref. 20 agrees quite well. The results obtained by the direct computation on the basis of the McCormack model⁴⁶ by Sharipov and Kalempa²² are also close to the present results. They overestimate the values about 1–1.5%. The result by Yalamov, Yushkanov, and Savkov¹⁸ (half-space moment method) shown in Fig. 2 overestimates the value by 2.2%. Table III suggests that their results for other molecular mass ratio would overestimate the value by the same degree. In Fig. 2, the shear-slip coefficient for a single-component gas obtained by a finite-difference method,¹⁴ on which the present method is based, is also

TABLE III. A comparison with the previous results for the shear-slip coefficient b .

m^B/m^A	$X_0^A=0.1$				
	Present result	Ref. 18	Ref. 20	Ref. 21	Ref. 22
2	1.2594	...	1.2644	1.2520	1.2781
4	1.2734	...	1.2781	1.2660	1.2917
5	1.2792	...	1.2838	1.2716	1.2975
10	1.2995	...	1.3039	1.2912	1.3177
m^B/m^A	$X_0^A=0.5$				
	Present result	Ref. 18	Ref. 20	Ref. 21	Ref. 22
1.5	...	1.27	1.2650	1.2528	...
2	1.2720	...	1.2765	1.2654	1.2901
7/3	...	1.29	1.2855	1.2750	...
4	1.3307	1.36	1.3335	1.3246	1.3470
5	1.3593	...	1.3614	1.3526	1.3751
9	...	1.48	1.4569	1.4470	...
10	1.4772	...	1.4771	1.4668	1.4923
m^B/m^A	$X_0^A=0.9$				
	Present result	Ref. 18	Ref. 20	Ref. 21	Ref. 22
2	1.2619	...	1.2668	1.2548	1.2805
4	1.2977	...	1.3013	1.2912	1.3153
5	1.3202	...	1.3230	1.3135	1.3374
10	1.4507	...	1.4488	1.4403	1.4672

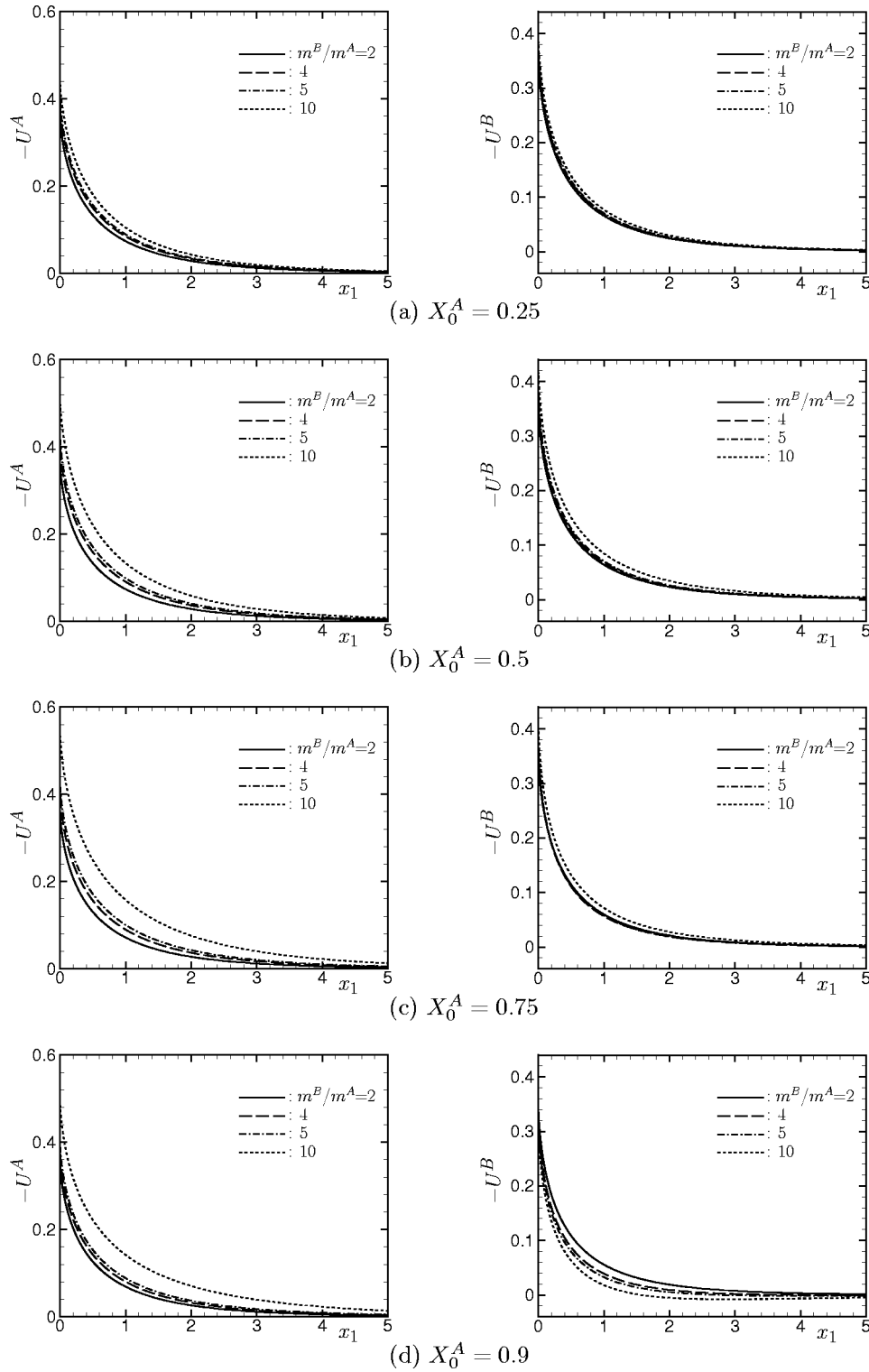


FIG. 3. Knudsen-layer functions U^A and U^B of species gases. (a) $X_0^A = 0.25$, (b) $X_0^A = 0.5$, (c) $X_0^A = 0.75$, and (d) $X_0^A = 0.9$.

shown by an open circle. Incidentally, essentially the same value is obtained in Refs. 15 and 28 for a single-component gas. The approaches in these references are based on the expansion of the kernel of collision integral in terms of associate Legendre functions.

In comparing the results by different authors, one needs a conversion relation between the reference mean free paths. For instance, the “slip coefficient” σ_P in Ref. 22 is related to b as

$$b = \frac{l_{SK}}{l_0} \sigma_P, \quad (39)$$

where l_{SK} is the reference mean free path used in Ref. 22 (ℓ_0 in the notation there). The l_{SK} is defined as

$$l_{SK} = \frac{\mu_{SK}}{p_0} \left(\frac{2kT_0}{m} \right)^{1/2}, \quad (40)$$

with

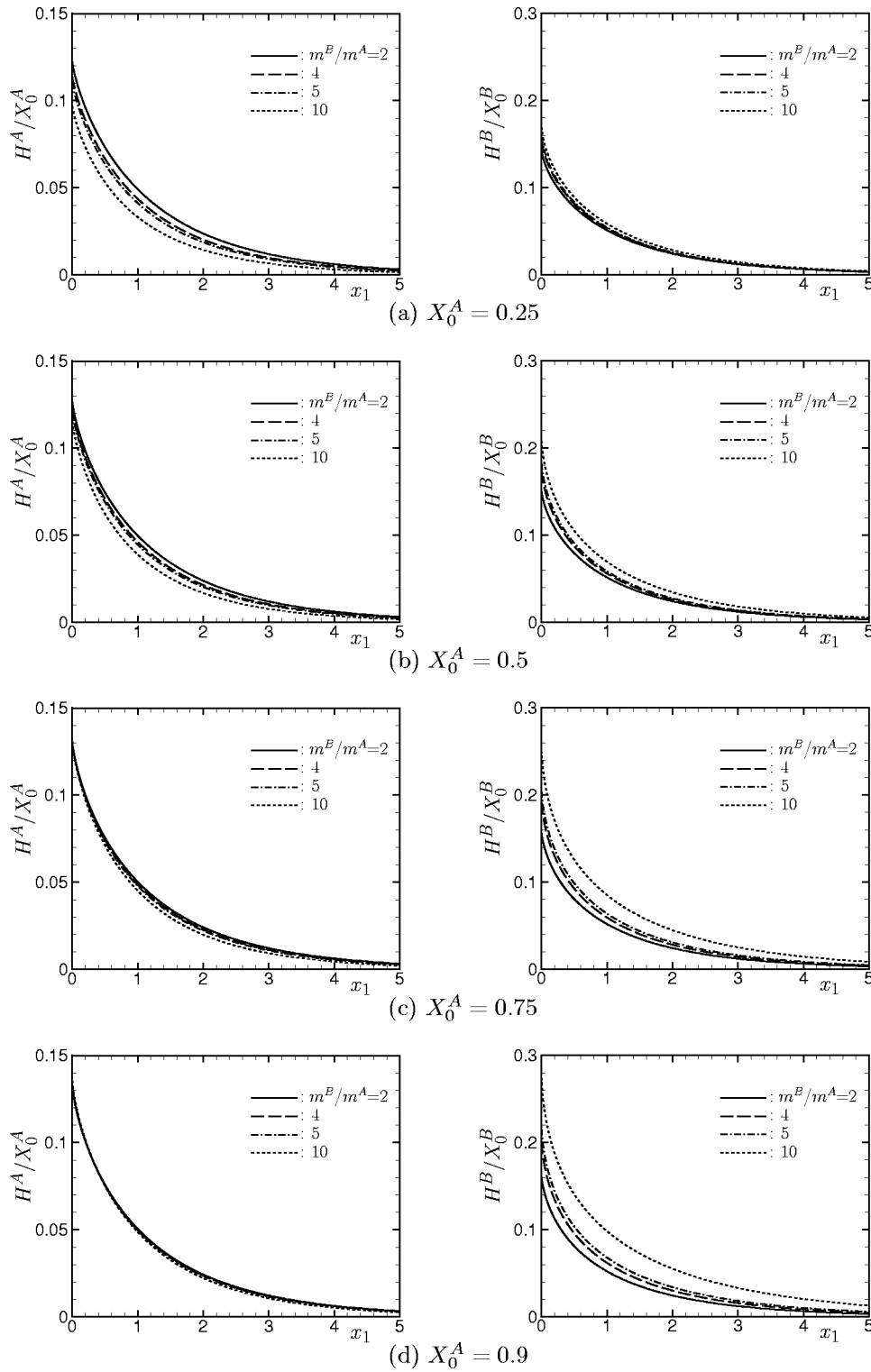


FIG. 4. Knudsen-layer functions H^A/X_0^A and H^B/X_0^B of species gases. (a) $X_0^A=0.25$, (b) $X_0^A=0.5$, (c) $X_0^A=0.75$, and (d) $X_0^A=0.9$.

$$m = m^A X_0^A + (1 - X_0^A) m^B, \quad (41)$$

where μ_{SK} is the Chapman–Enskog approximation of the viscosity whose explicit form is given in Ref. 22 (μ in the notation there). Eliminating p_0 from Eq. (40) by using the definition of l_0 , i.e., $l_0 = [\sqrt{2} \pi (d^A)^2 n_0]^{-1}$, one has the conversion relation

$$l_{SK} = \frac{2 \pi (d^A)^2}{(m k T_0)^{1/2} \mu_{SK} l_0}. \quad (42)$$

Substitution of this relation into Eq. (39) gives the conversion of the data from σ_P to b . The results of the other references (Refs. 18, 20, and 21) were converted in a similar way.

B. Knudsen-layer functions and velocity distribution functions

The Knudsen-layer functions of species gases for some cases are shown in Figs. 3–5 and Tables IV and V; that is,

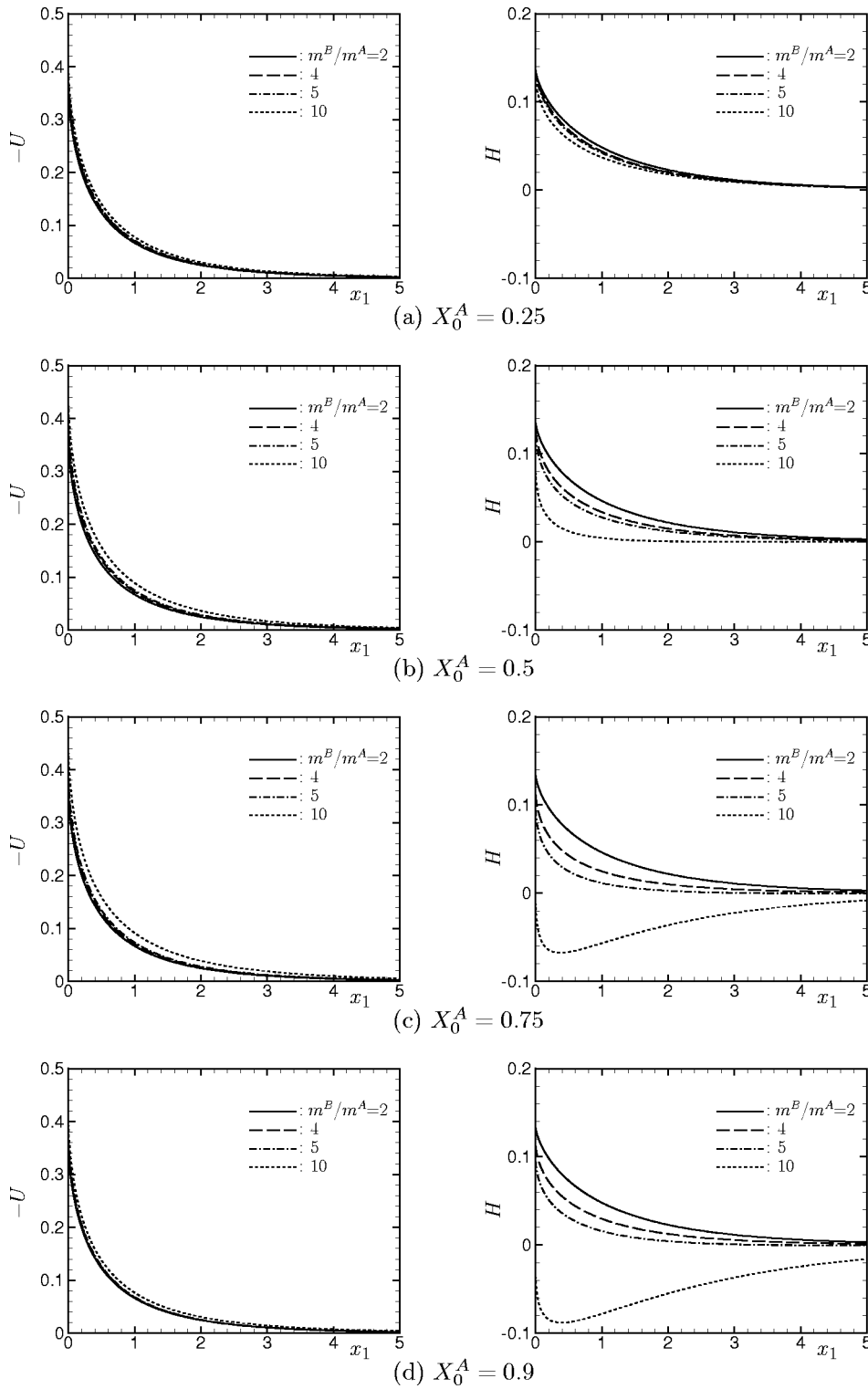


FIG. 6. Knudsen-layer functions U and H of the mixture. (a) $X_0^A=0.25$, (b) $X_0^A=0.5$, (c) $X_0^A=0.75$, and (d) $X_0^A=0.9$.

U^A and U^B are shown in Fig. 3 and Tables IV and V, H^A/X_0^A and H^B/X_0^B are in Fig. 4 and Tables IV and V, and S^A is in Fig. 5. Each function decays rapidly to zero as the distance from the wall increases. The dependence on X_0^A is larger for larger m^B/m^A . It is remarkable that, for large m^B/m^A and X_0^A close to 1, U^B changes its sign from minus to plus as the distance from the wall increases. Note that the function S^A (or S^B) is identically zero when $X_0^A=0$ and 1.

The Knudsen-layer functions U and H of the mixture for

some cases are shown in Fig. 6. Corresponding to the features of U^α and H^α , each function decays rapidly to zero as the distance from the wall increases, and the dependence on X_0^A is larger for larger m^B/m^A . It should be noted that the profiles of U and H at $X_0^A=0$ are the same as those at $X_0^A=1$.

The functions U and H at $X_0^A=0$ (or 1) are shown in Table VI. They are the functions for a single-component gas, which have already been obtained in Ref. 14 by the same

TABLE VI. Knudsen-layer functions U and H for single-species gases, i.e., $X_0^A = 0$ (or 1).

x_1	$-U$	H
0.0000	0.3452	0.1338
0.0271	0.3023	0.1261
0.0988	0.2456	0.1138
0.2011	0.1973	0.1012
0.3838	0.1448	0.0845
0.5833	0.1090	0.0708
0.7967	0.0834	0.0594
1.1424	0.0565	0.0454
1.6669	0.0334	0.0309
2.4139	0.0171	0.0183
3.3368	0.0081	0.0099
4.7525	0.0028	0.0040
7.6134	0.0004	0.0007
11.4643	0.0000	0.0001
15.3020	0.0000	0.0000

numerical method, i.e., the combination of the finite-difference and the numerical kernel methods. In the present work, they are obtained with a higher accuracy. The difference is, at most, 6.3×10^{-5} for U and 2.8×10^{-5} for H .

Some of the results for $X_0^A = 0.25, 0.75$, and 0.9 in the figures and tables in this section are obtained by the use of Chebyshev polynomial approximation from the data of U^A , U^B , H^A/X_0^A , H^B/X_0^B , and S^A/X_0^A at the values of X_0^A indicated by closed circles in Fig. 1. The FORTRAN code generating the Knudsen-layer functions for an arbitrary value of X_0^A is available from the authors.

Figures 7 and 8 show the reduced velocity distribution functions Ψ^A and Ψ^B and their contour plots in the case of $m^B/m^A = 5$ and $X_0^A = 0.5$. There is a discontinuity at $\zeta_1 = 0$ on the wall ($x_1 = 0$) [see Figs. 7(a) and 8(a)]. The discontinuity disappears immediately inside the gas,⁴⁷ but its trace remains as a steep gradient around $\zeta_1 = 0$ near the wall [see Figs. 7(b)

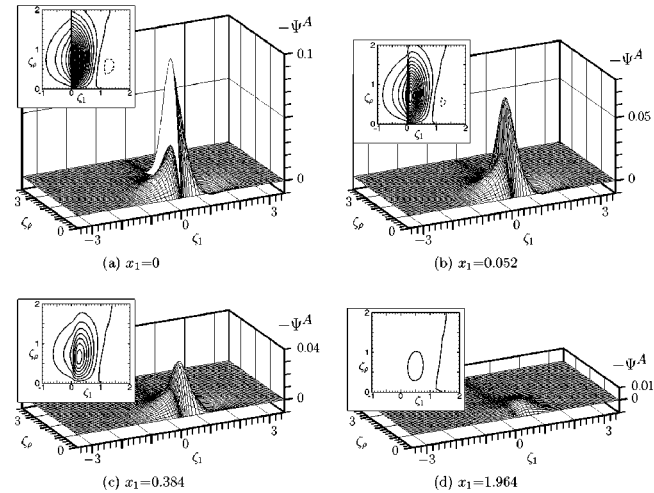


FIG. 7. Reduced velocity distribution function Ψ^A of gas A and its contour plots for $m^B/m^A = 5$ and $X_0^A = 0.5$. (a) $x_1 = 0$, (b) $x_1 = 0.052$, (c) $x_1 = 0.384$, and (d) $x_1 = 1.964$. In the contour plots the curves are drawn with the interval 0.005. The contour of positive values of $-\Psi^A$ is indicated by a solid line and that of negative values of $-\Psi^A$ by a dashed line. The nonclosed curve shown by a solid line indicates the contour $\Psi^A = 0$.

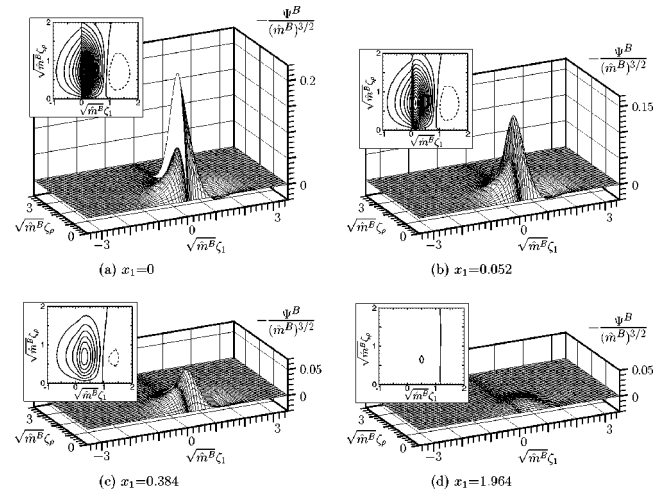


FIG. 8. Reduced velocity distribution function $\Psi^B/(\hat{m}^B)^{3/2}$ of gas B and its contour plots for $m^B/m^A = 5$ and $X_0^A = 0.5$. (a) $x_1 = 0$, (b) $x_1 = 0.052$, (c) $x_1 = 0.384$, and (d) $x_1 = 1.964$. In the contour plots the curves are drawn with the interval 0.01. See the caption of Fig. 7.

and 8(b)]. As the distance from the wall increases, Ψ^A decays to zero with keeping the distinct difference in the shape between the positive and the negative regions of ζ_1 [see the transition of the contour plots from Figs. 7(a)–7(d) and from Figs. 8(a)–8(d)]. These features are the same as those of thermal-slip and diffusion-slip problems studied in Ref. 6. A new feature of the present case is that there is an appreciable hollow in the positive region of ζ_1 . The hollow is more remarkable in Ψ^B than in Ψ^A . For the former, according to the observation of the other cases, it is larger for larger m^B/m^A and for larger X_0^A ; for the latter, it is little affected by m^B/m^A and X_0^A .

VI. CONCLUDING REMARKS

In the present paper, by the use of the finite-difference method developed in Ref. 6, we have established an accurate numerical solution of the shear-slip problem for the original linearized Boltzmann equation for a binary mixture of hard-sphere gases. The obtained solution would serve as the standard to assess the validity of approximate solution methods used for practical applications.

The hard-sphere model is chosen in the present study because it is a simple but the most fundamental model in kinetic theory. The present method can, in principle, be extended to more realistic models such as the Lennard-Jones potential, since the linearized collision integrals can generally be expressed in terms of integral kernels. For such models, however, we need to handle more complicated kernels. Another complexity arises from the fact that the problem, in general, has a complicated dependence on the temperature as well as on the concentration. For hard-sphere molecules, the temperature dependence can be factorized, so that the number of parameters in the problem is reduced. This simplicity also motivated us to study this model at the present stage. Maxwell's molecular model can be another target of the present method because the temperature dependence can be factorized for this model too. The extension to the variable

TABLE VII. A comparison of b among the different lattice systems for $m^B/m^A=2$. The comparison was made at five sample values of X_0^A .

Lattice systems	Maximum relative error of b
($\overline{S1}$, M7) vs ($\overline{S3}$, M7)	3.2×10^{-8}
($\overline{S1}$, M5) vs ($\overline{S1}$, M6)	5.1×10^{-8}
($\overline{S1}$, M7) vs ($\overline{S2}$, M7)	8.1×10^{-6}
($\overline{S1}$, M3) vs ($\overline{S1}$, M4)	1.8×10^{-6}
($\overline{S1}$, M3) vs ($\overline{S1}$, M1)	7.2×10^{-6}
($\overline{S1}$, M1) vs ($\overline{S1}$, M2)	1.2×10^{-5}

hard sphere (VHS) or variable soft sphere (VSS) models would also be worth trying because those models, which are still simple enough, can describe some of the basic macroscopic properties of real gases. Such extensions are, however, left to future work.

ACKNOWLEDGMENTS

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APPENDIX A: DATA OF COMPUTATION

We summarize the data of accuracy of the numerical computation.

- (i) Comparisons among the results for different lattice systems were made for various purposes in the case of $m^B/m^A=2$. A part of the results are shown in Table VII. Here information about the lattice system for the molecular velocity would be in order. For the systems M1–M5, the truncation of the velocity space is commonly set as $Z_1=Z_\rho=4.5$. There are, respectively, 101×55 , 101×73 , 101×49 , 113×49 , and 113×37 points in the truncation region of (ζ_1, ζ_ρ) -space in system M1, M2, M3, M4, and M5. System M6 is the same as M5 in the region of $[-4.5, 4.5] \times [0, 4.5]$ and covers a wider region ($Z_1=5$ and $Z_\rho=5.25$) than M5. System M7 is a rather small system compared to M1–M6. It has 73×21 points in the truncation region with $Z_1=Z_\rho=4$. (See Sec. 6 in Ref. 6 for the complete information about the lattice systems for the molecular velocity.) These systems as well as those for x_1 -space are made not only to assess the appropriate size of the lattice intervals but also to assess the appropriate size of the truncation region. For example, the comparison between the systems ($\overline{S1}$, M7) and ($\overline{S3}$, M7) is made for an estimate of the appropriate value of d . Similarly the comparison between ($\overline{S1}$,

TABLE VIII. Maximum error of the integrals $\tilde{\mathcal{L}}^{\beta\alpha}(f^\beta, f^\alpha)$ with $f^\alpha = \hat{m}^\alpha \zeta_\rho E^\alpha$ for system M1. The maximum value of $\nu^\beta f^\alpha$ is also shown for comparison in parentheses.

(β, α)	m^B/m^A			
	2	4	5	10
(A,A)	3.51×10^{-6} (0.064)	3.51×10^{-6} (0.064)	3.51×10^{-6} (0.064)	3.51×10^{-6} (0.064)
(B,A)	1.89×10^{-6} (0.053)	2.64×10^{-6} (0.047)	3.03×10^{-6} (0.046)	5.06×10^{-6} (0.043)
(A,B)	6.15×10^{-6} (0.237)	3.24×10^{-5} (0.908)	5.94×10^{-5} (1.407)	4.11×10^{-4} (5.528)
(B,B)	9.93×10^{-6} (0.182)	2.81×10^{-5} (0.514)	3.93×10^{-5} (0.719)	1.11×10^{-4} (2.033)

M5) and ($\overline{S1}$, M6) is made for an estimate of the appropriate values of Z_1 and Z_ρ . The comparison between ($\overline{S1}$, M7) and ($\overline{S2}$, M7) is for determining the number of lattice points N_x in x_1 . The comparisons among ($\overline{S1}$, M1), ($\overline{S1}$, M2), ($\overline{S1}$, M3), and ($\overline{S1}$, M4) are for determining the number of points (N_1, N_ρ) in (ζ_1, ζ_ρ) . After such a series of tests, the system ($\overline{S1}$, M1) is chosen as the standard lattice system for $m^B/m^A=2, 4$, and 5. For $m^B/m^A=10$, we used the system ($\overline{S4}$, M1) that covers a wider range of x_1 than ($\overline{S1}$, M1).

- (ii) Two properties of $\tilde{\mathcal{L}}^{\beta\alpha}$ are used as accuracy tests of the collision integrals for the standard lattice system M1. The first is the relation $\tilde{\mathcal{L}}^{\beta\alpha}(\hat{m}^\beta \zeta_\rho E^\beta, \hat{m}^\alpha \zeta_\rho E^\alpha) = 0$, which corresponds to the fact that the original linearized collision integrals vanish when the collision invariants are substituted. Table VIII shows the maximum error of the quantity on the left. The error comes from the part $\tilde{\mathcal{L}}_1^{\beta\alpha} + \tilde{\mathcal{L}}_2^{\beta\alpha} - \tilde{\mathcal{L}}_3^{\beta\alpha}$ [see Eq. (23)] because ν^β can be computed exactly [note that the integral in Eq. (24b) is the error function]. The maximum value of $|\hat{m}^\alpha \zeta_\rho E^\alpha \nu^\beta|$ is, therefore, shown in parentheses in the table. The second is the relation

$$\sum_{\beta=A,B} K^{\beta\alpha} X_0^\beta \tilde{\mathcal{L}}^{\beta\alpha}(\zeta_1 \zeta_\rho B^\beta E^\beta, \zeta_1 \zeta_\rho B^\alpha E^\alpha) + 2\hat{m}^\alpha \zeta_1 \zeta_\rho E^\alpha = 0, \quad (\text{A1})$$

which comes from Eq. (9a). The maximum error of the quantity on the left is shown in Table IX, together with the maximum value of $|2\hat{m}^\alpha \zeta_1 \zeta_\rho E^\alpha|$ in parentheses.

TABLE IX. Maximum error of the left-hand side of Eq. (A1) at six sample values of X_0^A for system M1. The maximum value of $|2\hat{m}^\alpha \zeta_1 \zeta_\rho E^\alpha|$ is also shown for comparison in parentheses just below the data.

α	m^B/m^A			
	2	4	5	10
A	5.77×10^{-6} (0.066)	5.77×10^{-6} (0.066)	5.77×10^{-6} (0.066)	5.77×10^{-6} (0.066)
B	1.63×10^{-5} (0.19)	5.69×10^{-5} (0.53)	1.12×10^{-4} (0.74)	1.01×10^{-3} (2.08)

- (iii) As mentioned in Sec. III C, Eq. (27) provides another measure of accuracy. For the standard lattice system, the value of $|S^A + S^B|$, which should theoretically be zero, is calculated at nine ($m^B/m^A=2$), thirteen ($m^B/m^A=4,5$) or seventeen ($m^B/m^A=10$) sample values of X_0^A . The resulting value is bounded as follows:

$$|S^A + S^B| < \begin{cases} 3.15 \times 10^{-6} & (m^B/m^A=2,4,5), \\ 2.64 \times 10^{-5} & (m^B/m^A=10). \end{cases}$$

- (iv) For the same values of X_0^A as (iii), we compared the maximum values of $|\Psi^\alpha(d, \cdot, \cdot)|$, $|\Psi^\alpha(\cdot, \pm Z_1^\alpha, \cdot)|$, and $|\Psi^\alpha(\cdot, \cdot, Z_\rho^\alpha)|$ to the maximum value of $|\Psi^\alpha|$, where $Z_1^\alpha = Z_1 / \sqrt{\hat{m}^\alpha}$ and $Z_\rho^\alpha = Z_\rho / \sqrt{\hat{m}^\alpha}$. The former three values should be negligible in order that the computation in the finite region of $(x_1, \zeta_1, \zeta_\rho)$ is justified. The results are

$$\frac{|\Psi^A(d, \cdot, \cdot)|}{\max|\Psi^A|} < \begin{cases} 4.1 \times 10^{-8} & (m^B/m^A=2), \\ 1.1 \times 10^{-7} & (m^B/m^A=4,5,10), \end{cases}$$

$$\frac{|\Psi^B(d, \cdot, \cdot)|}{\max|\Psi^B|} < \begin{cases} 4.0 \times 10^{-8} & (m^B/m^A=2), \\ 6.7 \times 10^{-7} & (m^B/m^A=4,5,10), \end{cases}$$

$$\frac{\max(|\Psi^A(\cdot, \pm Z_1^A, \cdot)|, |\Psi^A(\cdot, \cdot, Z_\rho^A)|)}{\max|\Psi^A|} < 1.7 \times 10^{-8},$$

$$\frac{\max(|\Psi^B(\cdot, \pm Z_1^B, \cdot)|, |\Psi^B(\cdot, \cdot, Z_\rho^B)|)}{\max|\Psi^B|} < 1.7 \times 10^{-8}.$$

- (v) The accuracy of the Chebyshev polynomial approximation with respect to X_0^A was checked. The b obtained by the formula (37) with the coefficient $b^{(n)}$ in Table I is compared with that computed directly. The comparison was made at five sample values of X_0^A for $m^B/m^A=2, 4$, and 5 , and at eight values for $m^B/m^A=10$. The sample values are indicated by an open circle in Fig. 1. The relative errors to the directly computed data are, at most, 9.4×10^{-7} , 2.8×10^{-9} , 2.4×10^{-8} , and 8.9×10^{-8} , respectively.

APPENDIX B: THIRD-ORDER FINITE-DIFFERENCE SCHEME

As is mentioned in Sec. IV, we use a third-order finite-difference scheme for $\partial/\partial x_1$. That is, in the present work, we use the formula

$$\nabla_{ijk} \tilde{\Psi}^{\alpha(n)} = \begin{cases} (\tilde{\Psi}_{(1,j,k)}^{\alpha(n)} - \tilde{\Psi}_{(0,j,k)}^{\alpha(n)})/h_1 & (i=1), \\ \frac{h_1+2h_2}{h_2(h_1+h_2)} \tilde{\Psi}_{(2,j,k)}^{\alpha(n)} - \frac{h_1+h_2}{h_1 h_2} \tilde{\Psi}_{(1,j,k)}^{\alpha(n)} + \frac{h_2}{h_1(h_1+h_2)} \tilde{\Psi}_{(0,j,k)}^{\alpha(n)} & (i=2), \\ w_0(h_i, h_{i-1}, h_{i-2}) \tilde{\Psi}_{(i,j,k)}^{\alpha(n)} - w_1(h_i, h_{i-1}, h_{i-2}) \tilde{\Psi}_{(i-1,j,k)}^{\alpha(n)} \\ + w_2(h_i, h_{i-1}, h_{i-2}) \tilde{\Psi}_{(i-2,j,k)}^{\alpha(n)} - w_3(h_i, h_{i-1}, h_{i-2}) \tilde{\Psi}_{(i-3,j,k)}^{\alpha(n)} & (3 \leq i \leq N_x), \end{cases} \quad (B1)$$

in place of that in Eq. (37a) of Ref. 6 and the formula

$$\nabla_{ijk} \tilde{\Psi}^{\alpha(n)} = \begin{cases} -w_0(h_{N_x}, h_{N_x}, h_{N_x-1}) \tilde{\Psi}_{(N_x-1,j,k)}^{\alpha(n)} + w_1(h_{N_x}, h_{N_x}, h_{N_x-1}) \tilde{\Psi}_{(N_x,j,k)}^{\alpha(n)} \\ - w_2(h_{N_x}, h_{N_x}, h_{N_x-1}) \tilde{\Psi}_{(N_x-1,-j,k)}^{\alpha(n)} + w_3(h_{N_x}, h_{N_x}, h_{N_x-1}) \tilde{\Psi}_{(N_x-2,-j,k)}^{\alpha(n)} & (i=N_x-1), \\ -w_0(h_{N_x-1}, h_{N_x}, h_{N_x}) \tilde{\Psi}_{(N_x-2,j,k)}^{\alpha(n)} + w_1(h_{N_x-1}, h_{N_x}, h_{N_x}) \tilde{\Psi}_{(N_x-1,j,k)}^{\alpha(n)} \\ - w_2(h_{N_x-1}, h_{N_x}, h_{N_x}) \tilde{\Psi}_{(N_x,j,k)}^{\alpha(n)} + w_3(h_{N_x-1}, h_{N_x}, h_{N_x}) \tilde{\Psi}_{(N_x-1,-j,k)}^{\alpha(n)} & (i=N_x-2), \\ -w_0(h_{i+1}, h_{i+2}, h_{i+3}) \tilde{\Psi}_{(i,j,k)}^{\alpha(n)} + w_1(h_{i+1}, h_{i+2}, h_{i+3}) \tilde{\Psi}_{(i+1,j,k)}^{\alpha(n)} \\ - w_2(h_{i+1}, h_{i+2}, h_{i+3}) \tilde{\Psi}_{(i+2,j,k)}^{\alpha(n)} + w_3(h_{i+1}, h_{i+2}, h_{i+3}) \tilde{\Psi}_{(i+3,j,k)}^{\alpha(n)} & (0 \leq i \leq N_x-3), \end{cases} \quad (B2)$$

in place of that in Eq. (37b) of Ref. 6, where

$$h_i = x_1^{(i)} - x_1^{(i-1)},$$

$$w_0(a, b, c) = \frac{1}{a} + \frac{1}{a+b} + \frac{1}{a+b+c},$$

$$w_1(a, b, c) = \frac{(a+b)(a+b+c)}{ab(b+c)}, \quad (B3)$$

$$w_2(a, b, c) = \frac{a(a+b+c)}{bc(a+b)},$$

$$w_3(a, b, c) = \frac{a(a+b)}{c(b+c)(a+b+c)}.$$

Equation (B1) is the scheme when $\zeta_1 > 0$ and Eq. (B2) is that when $\zeta_1 \leq 0$.

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