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Models of boundary condition for the Boltzmann equation based on kinetic approach

in memory of Giampiero Spiga

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Abstract

Models of the boundary conditions for the Boltzmann equation were constructed systematically in a recent paper by the present authors (K. Aoki *et al.*, in: Phys. Rev. E 106:035306, 2022) using an iteration scheme for the half-space problem of a linear kinetic equation describing the behavior of gas and physisorbed molecules in a thin layer adjacent to a solid surface (physisorbate layer). In the present paper, special attention is focused on the model based on the second iteration that was only touched on in the above reference. The model is presented in an explicit form, and its properties are investigated numerically. In particular, it is shown by the comparison with the numerical solution of the half-space problem that the model is a significant improvement compared with the model based on the first iteration and is accurate and useful.

Keywords. gas-surface interaction, adsorbate layer, kinetic theory, Boltzmann equation, boundary conditions.

Mathematics Subject Classification: 76P05, 82D05, 35Q49.

1 Introduction

The study of the boundary condition for the Boltzmann equation has been one of the important subjects in kinetic theory and gas-surface interaction. The boundary condition generally describes the relation between the velocity distribution function of the incident molecules and that of the reflected molecules on the boundary. The most conventional models of the boundary condition are specular reflection, diffuse reflection, and the Maxwell-type condition, which is a linear combination of specular and diffuse reflection [17, 27]. In addition to these conventional models, more general models have been proposed [19, 22, 18, 17, 24, 28]. However, most of the models are of mathematical or empirical nature and lack the relation to the physical properties, such as the characteristics of the gas and surface molecules and interaction potentials. A more physical approach is provided by molecular dynamics simulations, which help to understand the relation between the velocity distribution functions of the incident and reflected gas molecules [29, 25, 31, 30]. However, this approach is in general not useful to construct new models of the boundary condition though it is helpful to assess the existing models.

Another physical approach is the *kinetic* approach based on kinetic equations that describe the behavior of gas molecules interacting with the surface molecules [14, 13, 10, 12, 20, 1, 15, 16, 6, 2, 3, 4, 7, 5]. The kinetic equations contain a potential generated by fixed crystal molecules and a collision term with surface and bulk phonons describing the fluctuating part of the potential of the crystal molecules.

In a recent paper [7], we proposed a kinetic equation for gas-surface interaction, following the line of [14, 13, 10, 12, 20, 1, 15, 16, 6, 2, 3, 4], and applied it to the construction of the boundary condition for the Boltzmann equation. The kinetic equation contains an attractive-repulsive potential that is appreciable in the vicinity of the solid surface and grows indefinitely on the surface. This potential produces a thin layer of physisorbed molecules (physisorbate layer). The kinetic equation also contains the interaction term between gas molecules (the Boltzmann collision term) and that between gas molecules and phonons. Here, the term “gas molecules” also indicates the physisorbed gas molecules. In [7], the following assumptions were made: (i) the gas-phonon interaction is dominant in comparison with the gas-gas interaction inside the physisorbate layer; (ii) the thickness of the physisorbate layer is much smaller than the mean free path of the gas molecules; and (iii) the gas-phonon interaction is described by a simple collision model of relaxation type. Under these assumptions, an asymptotic analysis was performed, and a linear kinetic equation for the physisorbate layer was derived together with its boundary condition at infinity. The resulting kinetic equation and the boundary condition at infinity form a half-space problem, in which no boundary condition is imposed on the solid surface because the potential prevents the gas molecules from reaching the surface.

The half-space problem has a unique solution if the velocity distribution function of the gas molecule toward the surface is assigned at infinity. This property was first shown numerically [7] and then proved rigorously [5]. This means that the velocity distribution function of the outgoing gas molecules at infinity is determined by that of the incoming gas molecules there. Since the thickness of the physisorbate layer is much smaller than the mean free path, the infinity in the scale of the layer can be regarded as the very surface of the solid wall in the scale of the mean free path. Therefore, in this scale, the distribution function of the reflected molecules is determined by that of the incident molecules on the surface. In other words, the half-space problem plays the role of the boundary condition on the surface for the Boltzmann equation that is valid outside the physisorbate layer [7].

One of the main purposes of [7] was to establish models of the boundary condition for the Boltzmann equation by solving the half-space problem for the physisorbate layer approximately. In fact, an analytical model was constructed on the basis of an iteration scheme and its first iteration, and the effectiveness of the model was shown by its numerical assessment. Another model based on the second iteration was also mentioned briefly in the same reference, but it was not discussed numerically.

The aim of the present paper is to perform further investigation of the model based on the second iteration. The velocity distribution function for the reflected molecules on the surface based on the model is compared with that based on the numerical solution of the half-space problem for the physisorbate layer. According to the result, the second-iteration model gives a significant improvement and shows almost the same result as that based on the numerical solution.

The paper is organized as follows. The kinetic model for gas-surface interaction proposed in [7] and the resulting half-space problem for the physisorbate layer are summarized in Sec. 2. The iteration scheme based on the half-space problem and the models based on the first and second iterations are shown in Sec. 3. Section 4 is devoted to the numerical assessment of the second-iteration model. Finally, some concluding remarks are given in Sec. 5.

2 Summary of kinetic models for gas-surface interaction and physisorbate layer

In this section, we summarize the kinetic model for gas-surface interaction proposed in [7] and the resulting half-space problem for the physisorbate layer.

2.1 Kinetic model for gas-surface interaction

Consider a single monatomic gas in a half space ($z > 0$) interacting with a plane crystal surface located at $z = 0$, where $\mathbf{x} = (x, y, z)$ indicates the space coordinates, and assume that the gas molecules are subject to an interaction potential W generated by the *fixed* crystal molecules. The interaction potential W is assumed to depend only on the normal coordinate z for simplicity and is written in the form

$$(2.1) \quad W(z) = W_s(z/\delta) = W_s(\zeta),$$

where δ is a characteristic range of the surface potential and $\zeta = z/\delta$ denotes the rescaled normal coordinate, which is dimensionless. The rescaled potential W_s is such that

$$(2.2) \quad \lim_{\zeta \rightarrow 0} W_s(\zeta) = +\infty, \quad \lim_{\zeta \rightarrow +\infty} W_s(\zeta) = 0,$$

and involves an attractive zone and a repulsing zone as Lennard-Jones potentials as illustrated in Fig. 1. To be more specific, the following assumptions are made:

- (i) the potential $W_s(\zeta)$ is a smooth function of ζ and has a single minimum $W_{\min} (< 0)$ at $\zeta = \zeta_{\min} (> 0)$, i.e. $W_{\min} = W_s(\zeta_{\min})$;
- (ii) in the interval $(0, \zeta_{\min})$, $W_s(\zeta)$ decreases from $+\infty$ to W_{\min} monotonically, so that $(0, \zeta_{\min})$ is the repulsive zone;
- (iii) in the interval (ζ_{\min}, ∞) , $W_s(\zeta)$ increases from W_{\min} to 0 monotonically, so that (ζ_{\min}, ∞) is the attractive zone;
- (iv) in the repulsive zone $(0, \zeta_{\min})$, $W_s(\zeta)$ is convex downward.

The gas molecules that are trapped by the potential well are called the physisorbed molecules, and the set of such molecules forms the physisorbate.

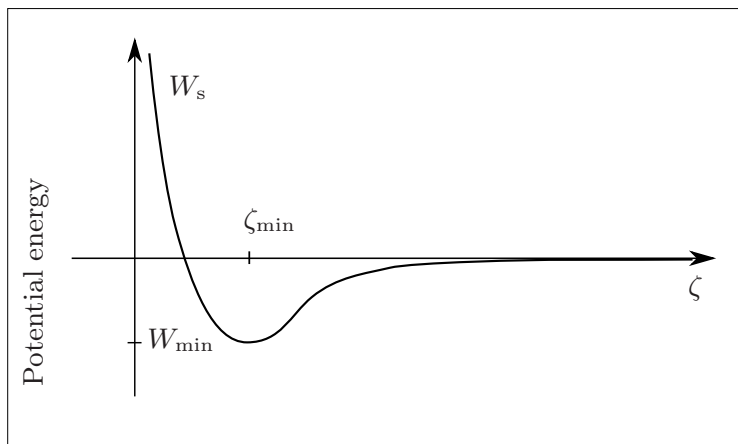


Figure 1: Typical surface interaction potential W_s as function of ζ .

The kinetic equation governing the behavior of the gas molecules is as follows [14, 13, 12, 1, 2, 3, 4, 6, 7]:

$$(2.3) \quad \frac{\partial f}{\partial t} + \mathbf{c} \cdot \frac{\partial f}{\partial \mathbf{x}} - \frac{1}{m} \frac{dW}{dz} \frac{\partial f}{\partial c_z} = J(f, f) + J_{\text{ph}}(f),$$

where m is the mass of a gas molecule, $f(t, \mathbf{x}, \mathbf{c})$ is the velocity distribution function of the gas molecules (including the physisorbed molecules), t is the time variable, $\mathbf{c} = (c_x, c_y, c_z)$ is the velocity of the gas molecules with c_x , c_y , and c_z being its x , y , and z components, $J(f, f)$ is the Boltzmann collision operator describing the gas-gas collision, and $J_{\text{ph}}(f)$ is the gas-phonon collision operator.

The explicit form of the Boltzmann collision operator $J(f, f)$, which is not relevant to this paper, is omitted here. In [7], under the assumption that the phonons are in equilibrium, a simple model of relaxation type is assumed for the gas-phonon collision operator $J_{\text{ph}}(f)$, i.e.,

$$(2.4) \quad J_{\text{ph}}(f) = \frac{1}{\tau_{\text{ph}}} (nM - f).$$

Here, τ_{ph} is the relaxation time of gas-phonon interaction and n and M are, respectively, the molecular number density and the wall Maxwellian given by

$$(2.5a) \quad n = \int_{\mathbf{R}^3} f \, d\mathbf{c},$$

$$(2.5b) \quad M = \left(\frac{m}{2\pi k_{\text{B}} T_{\text{w}}} \right)^{3/2} \exp \left(-\frac{m|\mathbf{c}|^2}{2k_{\text{B}} T_{\text{w}}} \right),$$

where k_{B} is the Boltzmann constant, T_{w} is the temperature of the solid wall, and the domain of integration in (2.5a) is the whole space of \mathbf{c} . The model (2.4), inspired by [14, 13], was used in [1, 2, 3, 4, 6, 7]. We further assume that τ_{ph} is a function of z and has the same length scale of variation as the potential W , i.e., it is a function of the scaled normal coordinate ζ :

$$(2.6) \quad \tau_{\text{ph}}(z) = \tau_{\text{ph},s}(z/\delta) = \tau_{\text{ph},s}(\zeta).$$

Since there is no interaction between molecules and phonons far away from the surface, we assume that

$$(2.7) \quad \lim_{z \rightarrow \infty} \tau_{\text{ph}}(z) = \lim_{\zeta \rightarrow \infty} \tau_{\text{ph},s}(\zeta) = \infty.$$

It is also natural to assume that $\tau_{\text{ph},s}(\zeta)$ is an increasing function of ζ in $[0, +\infty)$ with a finite positive $\tau_{\text{ph},s}(0)$.

Since J_{ph} as well as the potential W vanishes far away from the surface, we may let $z \rightarrow \infty$ (or $\zeta \rightarrow \infty$) in (2.3) to obtain the kinetic equation in the gas phase

$$(2.8) \quad \frac{\partial f_{\text{g}}}{\partial t} + \mathbf{c} \cdot \frac{\partial f_{\text{g}}}{\partial \mathbf{x}} = J(f_{\text{g}}, f_{\text{g}}),$$

where $f_{\text{g}}(t, \mathbf{x}, \mathbf{c})$ denotes the velocity distribution function of the gas molecules in the far field. Equation (2.8) is the standard Boltzmann equation for a monatomic gas, and the distribution f must converge to f_{g} far away from the surface.

2.2 Nondimensionalization and parameters

In order to nondimensionalize the kinetic equation (2.3), we introduce characteristic quantities that are marked with the $*$ superscript. We denote by n^* the characteristic number density, $c^* = (k_{\text{B}} T_{\text{w}} / m)^{1/2}$ the characteristic thermal speed, $f^* = n^* / c^{*3}$ the characteristic molecular velocity

distribution, τ_{fr}^* the characteristic mean free time, $\lambda^* = \tau_{\text{fr}}^* c^*$ the characteristic mean free path, $W^* = mc^{*2} = k_{\text{B}}T_{\text{w}}$ the characteristic potential, and τ_{ph}^* the characteristic time for gas-phonon interaction. We recall that δ is the distance normal to the surface where the potential W is significant, so that $\tau_{\text{la}}^* = \delta/c^*$ indicates the corresponding characteristic time of transit through the potential.

With these characteristic quantities, we introduce the dimensionless quantities \hat{t} , $\hat{\mathbf{x}}$, $\hat{\mathbf{c}}$, \hat{n} , \hat{f} , \hat{f}_{g} , \hat{M} , \hat{W} , $\hat{\tau}_{\text{ph}}$, and \hat{W}_{min} , which correspond to t , \mathbf{x} , \mathbf{c} , n , f , f_{g} , M , W , τ_{ph} , and W_{min} , respectively, by the following relations:

$$(2.9) \quad \begin{aligned} \hat{t} &= t/\tau_{\text{fr}}^*, & \hat{\mathbf{x}} &= \mathbf{x}/\lambda^*, & \hat{\mathbf{c}} &= \mathbf{c}/c^*, & \hat{n} &= n/n^*, \\ \hat{f} &= f c^{*3}/n^*, & \hat{f}_{\text{g}} &= f_{\text{g}} c^{*3}/n^*, & \hat{M} &= M c^{*3}, \\ \hat{W}(\zeta) &= W(z)/W^* = W_{\text{s}}(\zeta)/k_{\text{B}}T_{\text{w}}, & \hat{\tau}_{\text{ph}}(\zeta) &= \tau_{\text{ph}}(z)/\tau_{\text{ph}}^* = \tau_{\text{ph,s}}(\zeta)/\tau_{\text{ph}}^*, \\ \hat{W}_{\text{min}} &= W_{\text{min}}/k_{\text{B}}T_{\text{w}}. \end{aligned}$$

Correspondingly, the collision operators $J(f, f)$ and $J_{\text{ph}}(f)$ are nondimensionalized as

$$(2.10) \quad J(f, f) = \frac{n^*}{\tau_{\text{fr}}^* c^{*3}} \hat{J}(\hat{f}, \hat{f}),$$

and

$$(2.11) \quad J_{\text{ph}}(f) = \frac{n^*}{\tau_{\text{ph}}^* c^{*3}} \hat{J}_{\text{ph}}(\hat{f}), \quad \hat{J}_{\text{ph}}(\hat{f}) = \frac{1}{\hat{\tau}_{\text{ph}}} (\hat{n} \hat{M} - \hat{f}),$$

where

$$(2.12a) \quad \hat{n} = \int_{\mathbf{R}^3} \hat{f} d\hat{\mathbf{c}},$$

$$(2.12b) \quad \hat{M} = (2\pi)^{-3/2} \exp(-|\hat{\mathbf{c}}|^2/2),$$

and the domain of integration is the whole space of $\hat{\mathbf{c}}$. The explicit form of $\hat{J}(\hat{f}, \hat{f})$, which is not relevant to this paper, is omitted.

Substituting (2.9)–(2.12) into (2.3), we obtain the dimensionless version of (2.3), which is characterized by the following two dimensionless parameters:

$$(2.13) \quad \epsilon_{\text{ph}} = \frac{\tau_{\text{ph}}^*}{\tau_{\text{fr}}^*}, \quad \epsilon = \frac{\delta}{\lambda^*} = \frac{\tau_{\text{la}}^*}{\tau_{\text{fr}}^*}.$$

In [7], it is assumed that

$$(2.14) \quad \epsilon_{\text{ph}} = \epsilon \ll 1.$$

This means that the effective range δ of the potential, which is also the effective range of the gas-phonon interaction, is much shorter than the characteristic mean free path λ^* . Therefore, the molecules trapped by the potential and interacting with the phonons form a thin layer, which may be called the physisorbate layer, in the scale of the mean free path. Equation (2.14) also indicates that the characteristic time for gas-phonon interaction τ_{ph}^* is the same as the transit time across the layer τ_{la}^* and is much smaller than the mean free time τ_{fr}^* . The parameter setting (2.14) may be the simplest *kinetic scaling* for the present model of the physisorbate layer. This differs from the *fluid scaling* used in the derivation of fluid-type boundary conditions [6, 2, 3, 4].

In summary, we obtain the dimensionless version of (2.3) in the following form:

$$(2.15) \quad \frac{\partial \hat{f}}{\partial \hat{t}} + \hat{\mathbf{c}}_{\parallel} \cdot \frac{\partial \hat{f}}{\partial \hat{\mathbf{x}}_{\parallel}} + \hat{c}_z \frac{\partial \hat{f}}{\partial \hat{z}} - \frac{1}{\epsilon} \frac{d\hat{W}}{d\zeta} \frac{\partial \hat{f}}{\partial \hat{c}_z} = \frac{1}{\epsilon} \hat{J}_{\text{ph}}(\hat{f}) + \hat{J}(\hat{f}, \hat{f}),$$

where $\hat{\mathbf{c}}_{\parallel} = (\hat{c}_x, \hat{c}_y)$ and $\hat{\mathbf{x}}_{\parallel} = (\hat{x}, \hat{y})$. By taking the limit $\zeta \rightarrow \infty$ of (2.15), we recover the dimensionless version of the Boltzmann equation (2.8) in the gas phase, i.e.

$$(2.16) \quad \frac{\partial \hat{f}_g}{\partial \hat{t}} + \hat{\mathbf{c}} \cdot \frac{\partial \hat{f}_g}{\partial \hat{\mathbf{x}}} = \hat{J}(\hat{f}_g, \hat{f}_g).$$

2.3 Physisorbate layer and boundary condition for the Boltzmann equation

In order to investigate the physisorbate layer, we assume

$$(2.17) \quad \hat{f} = \hat{f}(\hat{t}, \hat{\mathbf{x}}_{\parallel}, \zeta, \hat{\mathbf{c}}_{\parallel}, \hat{c}_z),$$

because $\zeta = z/\delta = \hat{z}/\epsilon$ is the appropriate normal coordinate for the layer. Then, (2.15) is recast as

$$(2.18) \quad \epsilon \left(\frac{\partial \hat{f}}{\partial \hat{t}} + \hat{\mathbf{c}}_{\parallel} \cdot \frac{\partial \hat{f}}{\partial \hat{\mathbf{x}}_{\parallel}} \right) + \hat{c}_z \frac{\partial \hat{f}}{\partial \zeta} - \frac{d\hat{W}}{d\zeta} \frac{\partial \hat{f}}{\partial \hat{c}_z} = \hat{J}_{\text{ph}}(\hat{f}) + \epsilon \hat{J}(\hat{f}, \hat{f}).$$

This form suggests that \hat{f} and thus \hat{f}_g be expanded as $\hat{f} = \hat{f}^{(0)} + O(\epsilon)$ and $\hat{f}_g = \hat{f}_g^{(0)} + O(\epsilon)$, respectively. It is obvious that $\hat{f}_g^{(0)}$ is also governed by the Boltzmann equation (2.16). In the following, we consider only the zeroth order terms in ϵ and identify $\hat{f}^{(0)}$ and $\hat{f}_g^{(0)}$ with \hat{f} and \hat{f}_g , respectively (or equivalently, we omit the superscript $\langle 0 \rangle$). From (2.18), (2.11), and (2.12), the equation for the zeroth order is obtained as

$$(2.19) \quad \hat{c}_z \frac{\partial \hat{f}}{\partial \zeta} - \frac{d\hat{W}(\zeta)}{d\zeta} \frac{\partial \hat{f}}{\partial \hat{c}_z} = \frac{1}{\hat{\tau}_{\text{ph}}(\zeta)} (\hat{n}\hat{M} - \hat{f}),$$

where \hat{n} and \hat{M} are given by (2.12a) and (2.12b), respectively. Note that \hat{n} here is the zeroth-order number density in the physisorbate layer. Equation (2.19) is the kinetic equation governing the physisorbate layer.

Integrating both sides of (2.19) with respect to $\hat{\mathbf{c}}$ over the whole space, we then obtain that $(\partial/\partial\zeta) \int_{\mathbf{R}^3} \hat{c}_z \hat{f} d\hat{\mathbf{c}} = 0$, which leads to

$$(2.20) \quad \int_{\mathbf{R}^3} \hat{c}_z \hat{f} d\hat{\mathbf{c}} = 0,$$

for any ζ because $\hat{f} \rightarrow 0$ as $\zeta \rightarrow 0$. This indicates the particle conservation.

As discussed in [7], the connection condition between the inner physisorbate layer and the outer gas domain at the zeroth order is given by

$$(2.21) \quad \hat{f}(\hat{t}, \hat{\mathbf{x}}_{\parallel}, \zeta \rightarrow \infty, \hat{\mathbf{c}}_{\parallel}, \hat{c}_z) = \hat{f}_g(\hat{t}, \hat{\mathbf{x}}_{\parallel}, \hat{z} = 0, \hat{\mathbf{c}}_{\parallel}, \hat{c}_z).$$

Note that \hat{f}_g and thus (2.16) have been extended to the crystal surface $\hat{z} = 0$. Condition (2.21) means physically that the outer edge of the inner physisorbate layer may be identified with the solid surface for the outer gas domain (see [7] for a more quantitative argument).

As shown in [5], (2.19) has a unique solution when \hat{f} for the molecules toward the surface ($\hat{c}_z < 0$) is imposed at infinity, that is,

$$(2.22) \quad \hat{f}(\hat{t}, \hat{\mathbf{x}}_{\parallel}, \zeta, \hat{\mathbf{c}}_{\parallel}, \hat{c}_z) \rightarrow \hat{f}_{\infty}(\hat{t}, \hat{\mathbf{x}}_{\parallel}, \hat{\mathbf{c}}_{\parallel}, \hat{c}_z), \quad \text{as } \zeta \rightarrow \infty, \quad \text{for } \hat{c}_z < 0,$$

where \hat{f}_{∞} is an arbitrary function of \hat{t} , $\hat{\mathbf{x}}_{\parallel}$, $\hat{\mathbf{c}}_{\parallel}$, and \hat{c}_z decaying fast as $|\hat{\mathbf{c}}| \rightarrow \infty$, more specifically, satisfying $\hat{f}_{\infty} \leq (2\pi)^{-3/2} A(\hat{t}, \hat{\mathbf{x}}_{\parallel}) \exp(-|\hat{\mathbf{c}}|^2/2)$ with A being an arbitrary function of \hat{t} and $\hat{\mathbf{x}}_{\parallel}$. In other words, the kinetic equation (2.19) with the boundary condition (2.22) determines the solution

\hat{f} and thus \hat{f} for $\hat{c}_z > 0$ at infinity, and this constitutes the physisorbate-layer problem. This means that the solution defines the operator Λ that maps \hat{f} for $\hat{c}_z < 0$ to \hat{f} for $\hat{c}_z > 0$ at infinity, i.e.,

$$(2.23) \quad \hat{f}(\hat{t}, \hat{\mathbf{x}}_{\parallel}, \zeta \rightarrow \infty, \hat{\mathbf{c}}_{\parallel}, \hat{c}_z > 0) = \Lambda \hat{f}(\hat{t}, \hat{\mathbf{x}}_{\parallel}, \zeta \rightarrow \infty, \hat{\mathbf{c}}_{\parallel}, \hat{c}_z < 0),$$

or equivalently, because of (2.21),

$$(2.24) \quad \hat{f}_g(\hat{t}, \hat{\mathbf{x}}_{\parallel}, \hat{z} = 0, \hat{\mathbf{c}}_{\parallel}, \hat{c}_z > 0) = \Lambda \hat{f}_g(\hat{t}, \hat{\mathbf{x}}_{\parallel}, \hat{z} = 0, \hat{\mathbf{c}}_{\parallel}, \hat{c}_z < 0).$$

This relation indicates that the operator Λ provides the boundary condition for the Boltzmann equation on the surface $\hat{z} = 0$.

In the following, we construct models of the boundary condition (2.24) by solving the half-space problem (2.19) and (2.22) iteratively. It should be noted here that the structure of this half-space problem differs from that of the traditional half-space problem of the linearized Boltzmann equation relevant to Knudsen layer [8, 21, 9]. For instance, in the problem (2.19) and (2.22), the gas molecules are subject to an external attractive-repulsive potential, and no boundary condition is imposed on the boundary $\zeta = 0$.

2.4 Change of variables

In order to investigate (2.19) and (2.22), we transform these equations into a more convenient form. Let us put

$$(2.25) \quad \varepsilon = \frac{1}{2} \hat{c}_z^2 + \hat{W}(\zeta).$$

Then, it follows from the properties of $\hat{W}(\zeta)$ that, for each $\varepsilon \in [\hat{W}_{\min}, \infty)$, the range of ζ is as follows:

$$(2.26) \quad \begin{cases} [\zeta_a(\varepsilon), \infty) & \text{for } \varepsilon \geq 0, \\ [\zeta_a(\varepsilon), \zeta_b(\varepsilon)] & \text{for } \hat{W}_{\min} \leq \varepsilon < 0, \end{cases}$$

where $\zeta_a(\varepsilon)$ is the solution of $\varepsilon = \hat{W}(\zeta)$ for $\varepsilon \geq 0$, and $\zeta_a(\varepsilon)$ and $\zeta_b(\varepsilon)$ are the two solutions of the same equation satisfying $\zeta_a(\varepsilon) \leq \zeta_{\min} \leq \zeta_b(\varepsilon)$ for $\hat{W}_{\min} \leq \varepsilon < 0$.

We now transform the independent variables from (ζ, \hat{c}_z) to (ζ, ε) and define

$$(2.27) \quad \hat{f}_{\pm}(\hat{t}, \hat{\mathbf{x}}_{\parallel}, \zeta, \hat{\mathbf{c}}_{\parallel}, \varepsilon) = \hat{f}\left(\hat{t}, \hat{\mathbf{x}}_{\parallel}, \zeta, \hat{\mathbf{c}}_{\parallel}, \pm \sqrt{2[\varepsilon - \hat{W}(\zeta)]}\right).$$

Note that \hat{f}_+ corresponds to $\hat{c}_z > 0$, and \hat{f}_- to $\hat{c}_z < 0$.

Then, (2.19), (2.12), and (2.22) are transformed to

$$(2.28a) \quad \pm \sqrt{2[\varepsilon - \hat{W}(\zeta)]} \frac{\partial \hat{f}_{\pm}(\zeta, \varepsilon)}{\partial \zeta} = \frac{1}{\hat{\tau}_{\text{ph}}(\zeta)} [\hat{n}(\zeta) \hat{M}(\zeta, \varepsilon) - \hat{f}_{\pm}(\zeta, \varepsilon)],$$

$$(2.28b) \quad \hat{n}(\zeta) = \int_{\hat{W}(\zeta)}^{\infty} \left[\int \int_{-\infty}^{\infty} [\hat{f}_-(\zeta, \varepsilon) + \hat{f}_+(\zeta, \varepsilon)] d\hat{c}_x d\hat{c}_y \right] \frac{1}{\sqrt{2[\varepsilon - \hat{W}(\zeta)]}} d\varepsilon,$$

$$(2.28c) \quad \hat{M}(\zeta, \varepsilon) = (2\pi)^{-3/2} \exp\left(-|\hat{\mathbf{c}}_{\parallel}|^2/2 - \varepsilon + \hat{W}(\zeta)\right),$$

$$(2.28d) \quad \hat{f}_-(\zeta, \varepsilon) \rightarrow \hat{f}_{\infty}(-\sqrt{2\varepsilon}) \quad \text{as } \zeta \rightarrow \infty, \quad \text{for } \varepsilon > 0,$$

where $\hat{M}(\zeta, \varepsilon)$ is the expression of \hat{M} in (2.12b) in terms of ζ and ε . In (2.28), the arguments \hat{t} , $\hat{\mathbf{x}}_{\parallel}$, and $\hat{\mathbf{c}}_{\parallel}$ in \hat{f}_{\pm} , \hat{f}_{∞} , and \hat{M} and the arguments \hat{t} and $\hat{\mathbf{x}}_{\parallel}$ in \hat{n} are not shown explicitly. This convention applies in the sequel unless otherwise stated.

In addition, we need to assume the continuity conditions

$$(2.29a) \quad \hat{f}_+(\zeta_a(\varepsilon), \varepsilon) = \hat{f}_-(\zeta_a(\varepsilon), \varepsilon), \quad \text{for } \varepsilon \geq \hat{W}_{\min},$$

$$(2.29b) \quad \hat{f}_-(\zeta_b(\varepsilon), \varepsilon) = \hat{f}_+(\zeta_b(\varepsilon), \varepsilon), \quad \text{for } \hat{W}_{\min} < \varepsilon < 0,$$

at $\zeta = \zeta_a(\varepsilon)$ and $\zeta = \zeta_b(\varepsilon)$ to complete the half-space problem in the new variables (ζ, ε) .

Incidentally, the particle conservation (2.20) is transformed to

$$(2.30) \quad \int_{\hat{W}(\zeta)}^{\infty} \iint_{-\infty}^{\infty} [\hat{f}_+(\zeta, \varepsilon) - \hat{f}_-(\zeta, \varepsilon)] d\hat{c}_x d\hat{c}_y d\varepsilon = 0.$$

3 Models of boundary condition for the Boltzmann equation

In this section, we construct models of the boundary condition for the Boltzmann equation on the basis of the half-space problem (2.28) and (2.29), which is equivalent to the problem (2.19) and (2.22).

3.1 Iteration scheme

On the basis of (2.28) and (2.29), we define the following iteration scheme:

$$(3.1a) \quad \pm \sqrt{2[\varepsilon - \hat{W}(\zeta)]} \frac{\partial \hat{f}_{\pm}^{(k)}(\zeta, \varepsilon)}{\partial \zeta} = \frac{1}{\hat{\tau}_{\text{ph}}(\zeta)} [\hat{n}^{(k-1)}(\zeta) \hat{M}(\zeta, \varepsilon) - \hat{f}_{\pm}^{(k)}(\zeta, \varepsilon)],$$

$$(3.1b) \quad \hat{n}^{(k)}(\zeta) = \int_{\hat{W}(\zeta)}^{\infty} \left[\iint_{-\infty}^{\infty} [\hat{f}_-^{(k)}(\zeta, \varepsilon) + \hat{f}_+^{(k)}(\zeta, \varepsilon)] d\hat{c}_x d\hat{c}_y \right] \times \frac{1}{\sqrt{2[\varepsilon - \hat{W}(\zeta)]}} d\varepsilon,$$

$$(3.1c) \quad \hat{M}(\zeta, \varepsilon) = (2\pi)^{-3/2} \exp\left(-|\hat{\mathbf{c}}|^2/2 - \varepsilon + \hat{W}(\zeta)\right),$$

$$(3.1d) \quad \hat{f}_-^{(k)}(\zeta, \varepsilon) \rightarrow \hat{f}_{\infty}(-\sqrt{2\varepsilon}) \quad \text{as } \zeta \rightarrow \infty, \quad \text{for } \varepsilon > 0,$$

$$(3.1e) \quad \hat{f}_+^{(k)}(\zeta_a(\varepsilon), \varepsilon) = \hat{f}_-^{(k)}(\zeta_a(\varepsilon), \varepsilon), \quad \text{for } \varepsilon \geq \hat{W}_{\min},$$

$$(3.1f) \quad \hat{f}_-^{(k)}(\zeta_b(\varepsilon), \varepsilon) = \hat{f}_+^{(k)}(\zeta_b(\varepsilon), \varepsilon), \quad \text{for } \hat{W}_{\min} < \varepsilon < 0,$$

where $\hat{f}_{\pm}^{(k)}$ and $\hat{n}^{(k)}$ are, respectively, the k th iteration corresponding to \hat{f}_{\pm} and \hat{n} .

Since (3.1a) is an ODE for $\hat{f}_{\pm}^{(k)}$, it can be solved, under the boundary condition (3.1d), to express $\hat{f}_{\pm}^{(k)}$ in terms of $\hat{n}^{(k-1)}$, that is,

$$(3.2a) \quad \hat{f}_+^{(k)}(\zeta, \varepsilon) = \theta(\zeta_a(\varepsilon), \zeta; \varepsilon) \left(\hat{f}_-^{(k)}(\zeta_a(\varepsilon), \varepsilon) + \int_{\zeta_a(\varepsilon)}^{\zeta} \theta(s, \zeta_a(\varepsilon); \varepsilon) \frac{\hat{n}^{(k-1)}(s) \hat{M}(s, \varepsilon) ds}{\hat{\tau}_{\text{ph}}(s) \sqrt{2[\varepsilon - \hat{W}(s)]}} \right),$$

$$\hat{f}_-^{(k)}(\zeta, \varepsilon) = \mathbf{1}_{\varepsilon > 0} \theta(\zeta, \infty; \varepsilon) \left(\hat{f}_{\infty}(-\sqrt{2\varepsilon}) \right)$$

$$\begin{aligned}
& + \int_{\zeta}^{\infty} \theta(\infty, s; \varepsilon) \frac{\hat{n}^{(k-1)}(s) \hat{M}(s, \varepsilon) ds}{\hat{\tau}_{\text{ph}}(s) \sqrt{2[\varepsilon - \hat{W}(s)]}} \\
& + \mathbf{1}_{\hat{W}_{\min} < \varepsilon < 0} \theta(\zeta, \zeta_b(\varepsilon); \varepsilon) \left(\hat{f}_+^{(k)}(\zeta_b(\varepsilon), \varepsilon) \right. \\
(3.2b) \quad & \left. + \int_{\zeta}^{\zeta_b(\varepsilon)} \theta(\zeta_b(\varepsilon), s; \varepsilon) \frac{\hat{n}^{(k-1)}(s) \hat{M}(s, \varepsilon) ds}{\hat{\tau}_{\text{ph}}(s) \sqrt{2[\varepsilon - \hat{W}(s)]}} \right),
\end{aligned}$$

where

$$(3.3) \quad \theta(a, b; \varepsilon) = \exp \left(- \int_a^b \frac{ds}{\hat{\tau}_{\text{ph}}(s) \sqrt{2[\varepsilon - \hat{W}(s)]}} \right),$$

and $\mathbf{1}_{\mathcal{S}}$ is the indicator function of the set \mathcal{S} , that is, $\mathbf{1}_{\mathcal{S}} = 1$ for $\eta \in \mathcal{S}$ and $\mathbf{1}_{\mathcal{S}} = 0$ for $\eta \notin \mathcal{S}$ with η being the relevant variable.

We consider the first and second iterations $\hat{f}_{\pm}^{(1)}$ and $\hat{f}_{\pm}^{(2)}$ starting from the following zeroth guess:

$$(3.4) \quad \hat{f}_{\pm}^{(0)} = \hat{\beta} \mathbf{M}(\varepsilon), \quad \mathbf{M}(\varepsilon) = (2\pi)^{-3/2} \exp(-|\hat{\mathbf{c}}_{\parallel}|^2/2 - \varepsilon),$$

where $\hat{\beta}$ is a constant to be determined later. Note that (3.4) is an exact solution of (2.28) expressing the absolute equilibrium. Correspondingly, $\hat{n}^{(0)}$ is obtained as

$$(3.5) \quad \hat{n}^{(0)}(\zeta) = \hat{\beta} \exp(-\hat{W}(\zeta)).$$

3.2 Model based on first iteration

Let us consider the first iteration $\hat{f}_{\pm}^{(1)}$ and start with the case $\varepsilon > 0$. Since $\hat{n}^{(0)} \hat{M}(\zeta, \varepsilon) = \hat{\beta} \mathbf{M}(\varepsilon)$, the first integral in (3.2b) with $k = 1$ is recast as

$$\begin{aligned}
\int_{\zeta}^{\infty} \theta(\infty, s; \varepsilon) \frac{\hat{n}^{(0)}(s) \hat{M}(s, \varepsilon)}{\hat{\tau}_{\text{ph}}(s) \sqrt{2[\varepsilon - \hat{W}(s)]}} ds &= -\hat{\beta} \mathbf{M}(\varepsilon) \int_{\zeta}^{\infty} \frac{\partial}{\partial s} \theta(\infty, s; \varepsilon) ds \\
&= \hat{\beta} \mathbf{M}(\varepsilon) [\theta(\infty, \zeta; \varepsilon) - 1].
\end{aligned}$$

The integral in (3.2a) can be transformed in a similar way. Therefore, it follows from (3.2) (with $k = 1$) that

$$\begin{aligned}
(3.6a) \quad \hat{f}_-^{(1)}(\zeta, \varepsilon) &= \theta(\zeta, \infty; \varepsilon) \hat{f}_{\infty}(-\sqrt{2\varepsilon}) + [1 - \theta(\zeta, \infty; \varepsilon)] \hat{\beta} \mathbf{M}(\varepsilon), \\
\hat{f}_+^{(1)}(\zeta, \varepsilon) &= \theta(\zeta_a(\varepsilon), \zeta; \varepsilon) \hat{f}_-^{(1)}(\zeta_a(\varepsilon), \varepsilon) + [1 - \theta(\zeta_a(\varepsilon), \zeta; \varepsilon)] \hat{\beta} \mathbf{M}(\varepsilon) \\
&= \theta(\zeta_a(\varepsilon), \zeta; \varepsilon) \theta(\zeta_a(\varepsilon), \infty; \varepsilon) \hat{f}_{\infty}(-\sqrt{2\varepsilon}) \\
(3.6b) \quad &+ [1 - \theta(\zeta_a(\varepsilon), \zeta; \varepsilon) \theta(\zeta_a(\varepsilon), \infty; \varepsilon)] \hat{\beta} \mathbf{M}(\varepsilon),
\end{aligned}$$

for $\varepsilon > 0$.

On the other hand, for $\hat{W}_{\min} < \varepsilon < 0$, (3.2) leads to the following expressions for $\hat{f}_{\pm}^{(1)}$:

$$(3.7a) \quad \hat{f}_-^{(1)}(\zeta, \varepsilon) = \theta(\zeta, \zeta_b(\varepsilon); \varepsilon) \hat{f}_+^{(1)}(\zeta_b(\varepsilon), \varepsilon) + [1 - \theta(\zeta, \zeta_b(\varepsilon); \varepsilon)] \hat{\beta} \mathbf{M}(\varepsilon),$$

$$(3.7b) \quad \hat{f}_+^{(1)}(\zeta, \varepsilon) = \theta(\zeta_a(\varepsilon), \zeta; \varepsilon) \hat{f}_-^{(1)}(\zeta_a(\varepsilon), \varepsilon) + [1 - \theta(\zeta_a(\varepsilon), \zeta; \varepsilon)] \hat{\beta} \mathbf{M}(\varepsilon),$$

from which it follows

$$(3.8) \quad \hat{f}_+^{(1)}(\zeta, \varepsilon) = \hat{f}_-^{(1)}(\zeta, \varepsilon) = \hat{\beta} \mathbf{M}(\varepsilon),$$

for $\hat{W}_{\min} < \varepsilon < 0$.

With the first iteration $\hat{f}_\pm^{(1)}(\zeta, \varepsilon)$ obtained in (3.6) and (3.8), the corresponding number density $\hat{n}^{(1)}(\zeta)$ is obtained from (3.1b), i.e.,

- For $0 < \zeta \leq \zeta_a(0)$, where $\hat{W}(\zeta) \geq 0$,

$$(3.9) \quad \hat{n}^{(1)}(\zeta) = \int_{\hat{W}(\zeta)}^{\infty} \left\{ \Theta(\zeta, \varepsilon) \iint_{-\infty}^{\infty} \hat{f}_\infty(-\sqrt{2\varepsilon}) d\hat{c}_x d\hat{c}_y + \frac{1}{\sqrt{2\pi}} \hat{\beta} [2 - \Theta(\zeta, \varepsilon)] e^{-\varepsilon} \right\} \frac{d\varepsilon}{\sqrt{2[\varepsilon - \hat{W}(\zeta)]}}.$$

- For $\zeta > \zeta_a(0)$, where $\hat{W}(\zeta) < 0$,

$$(3.10) \quad \hat{n}^{(1)}(\zeta) = \int_0^{\infty} \left\{ \Theta(\zeta, \varepsilon) \iint_{-\infty}^{\infty} \hat{f}_\infty(-\sqrt{2\varepsilon}) d\hat{c}_x d\hat{c}_y + \frac{1}{\sqrt{2\pi}} \hat{\beta} [2 - \Theta(\zeta, \varepsilon)] e^{-\varepsilon} \right\} \frac{d\varepsilon}{\sqrt{2[\varepsilon - \hat{W}(\zeta)]}} + \hat{\beta} e^{-\hat{W}(\zeta)} \operatorname{erf}\left(\sqrt{-\hat{W}(\zeta)}\right).$$

Here

$$(3.11) \quad \begin{aligned} \Theta(\zeta, \varepsilon) &= \theta(\zeta, \infty; \varepsilon) \{1 + [\theta(\zeta_a(\varepsilon), \zeta; \varepsilon)]^2\} \\ &= \theta(\zeta_a(\varepsilon), \infty; \varepsilon) [\theta(\zeta_a(\varepsilon), \zeta; \varepsilon) + \theta(\zeta, \zeta_a(\varepsilon); \varepsilon)], \end{aligned}$$

and $\operatorname{erf}(x)$ is the error function,

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt.$$

Now, let us consider the boundary condition (2.24) [or (2.23)] for the Boltzmann equation on the basis of the first iteration. For this purpose, we take the limit $\zeta \rightarrow \infty$ in (3.6b) and replace $\hat{f}_\infty(-\sqrt{2\varepsilon})$ with the equivalent $\hat{f}_-^{(1)}(\infty, \varepsilon)$ for convenience. Then, we obtain

$$(3.12) \quad \hat{f}_+^{(1)}(\infty, \varepsilon) = [\theta(\zeta_a(\varepsilon), \infty; \varepsilon)]^2 \hat{f}_-^{(1)}(\infty, \varepsilon) + \{1 - [\theta(\zeta_a(\varepsilon), \infty; \varepsilon)]^2\} \hat{\beta} \mathbf{M}(\varepsilon).$$

We here go back from the (ζ, ε) representation to the original (ζ, \hat{c}_z) representation. We omit the superscript (1) of $\hat{f}_\pm^{(1)}$, supposing that $\hat{f}_\pm^{(1)}$ is an approximation of \hat{f}_\pm , and note that

$$(3.13a) \quad \hat{f}_+(\zeta, \varepsilon) = \hat{f}(\zeta, \hat{c}_z) \quad \text{for } \hat{c}_z > 0,$$

$$(3.13b) \quad \hat{f}_-(\zeta, \varepsilon) = \hat{f}(\zeta, \hat{c}_z) \quad \text{for } \hat{c}_z < 0,$$

$$(3.13c) \quad \varepsilon = \hat{c}_z^2/2 \quad \text{at } \zeta = \infty.$$

Furthermore, to be consistent with the boundary condition (2.24) for the Boltzmann equation, we replace $\hat{f}(\infty, \hat{c}_z)$ with the equivalent $\hat{f}_g(0, \hat{c}_z)$ recalling (2.21).

Then, (3.12) is recast as

$$(3.14) \quad \hat{f}_g(0, \hat{c}_z) = [1 - \hat{\alpha}(\hat{c}_z^2)] \hat{f}_g(0, -\hat{c}_z) + \hat{\alpha}(\hat{c}_z^2) \hat{\beta} \hat{M}(\hat{c}), \quad \text{for } \hat{c}_z > 0,$$

where

$$(3.15) \quad \begin{aligned} \hat{\alpha}(\hat{c}_z^2) &= 1 - [\theta(\zeta_a(\hat{c}_z^2/2), \infty; \hat{c}_z^2/2)]^2 \\ &= 1 - \exp\left(-\sqrt{2} \int_{\zeta_a(\hat{c}_z^2/2)}^{\infty} \frac{ds}{\hat{\tau}_{\text{ph}}(s) \sqrt{\hat{c}_z^2/2 - \hat{W}(s)}}\right), \end{aligned}$$

and $\hat{M}(\hat{c})$ is given by (2.12b). It should be noted that the number of molecules is not conserved for each step of iteration. Therefore, $\hat{\beta}$ in (3.14) is chosen in such a way that the particle conservation (2.20) is satisfied for $\hat{f}(\infty, \hat{c}_z)$ or equivalently for $\hat{f}_g(0, \hat{c}_z)$. As the result, $\hat{\beta}$ is obtained as follows:

$$(3.16) \quad \begin{aligned} \hat{\beta} &= -\sqrt{2\pi} \left[\int_0^{\infty} v \hat{\alpha}(v^2) \exp(-v^2/2) dv \right]^{-1} \\ &\quad \times \int_{-\infty}^0 v \hat{\alpha}(v^2) \left(\iint_{-\infty}^{\infty} \hat{f}_g(0, v) d\hat{c}_x d\hat{c}_x \right) dv, \end{aligned}$$

where v indicates the integration variable for \hat{c}_z .

Equation (3.14) with (3.15) and (3.16) provides a model of the operator Λ in the boundary condition (2.24) for the Boltzmann equation. If the input distribution $\hat{f}_g(0, \hat{c}_z)$ ($\hat{c}_z < 0$) is the (dimensionless) wall Maxwellian $\hat{M} = (2\pi)^{-3/2} \exp(-|\hat{c}|^2/2)$, then it follows immediately from (3.14) and (3.16) that the output distribution $\hat{f}_g(0, \hat{c}_z)$ ($\hat{c}_z > 0$) is also equal to \hat{M} . This is an important property of the boundary condition for the Boltzmann equation. The dimensional form of this model, which is given in Sec. VB in [7], is summarized in Appendix A.

3.3 Model based on second iteration

To obtain the model based on the second iteration, it suffices to consider the case $\varepsilon > 0$. It follows from (3.2b) that

$$(3.17) \quad \begin{aligned} \hat{f}_-^{(2)}(\zeta_a(\varepsilon), \varepsilon) &= \theta(\zeta_a(\varepsilon), \infty; \varepsilon) \hat{f}_\infty(-\sqrt{2\varepsilon}) \\ &\quad + \int_{\zeta_a(\varepsilon)}^{\infty} \theta(\zeta_a(\varepsilon), s; \varepsilon) \frac{\hat{n}^{(1)}(s) \hat{M}(s, \varepsilon) ds}{\hat{\tau}_{\text{ph}}(s) \sqrt{2[\varepsilon - \hat{W}(s)]}}. \end{aligned}$$

Therefore, (3.2a) gives

$$\begin{aligned} \hat{f}_+^{(2)}(\infty, \varepsilon) &= \theta(\zeta_a(\varepsilon), \infty; \varepsilon) \left(\hat{f}_-^{(2)}(\zeta_a(\varepsilon), \varepsilon) \right. \\ &\quad \left. + \int_{\zeta_a(\varepsilon)}^{\infty} \theta(s, \zeta_a(\varepsilon); \varepsilon) \frac{\hat{n}^{(1)}(s) \hat{M}(s, \varepsilon) ds}{\hat{\tau}_{\text{ph}}(s) \sqrt{2[\varepsilon - \hat{W}(s)]}} \right) \\ &= [\theta(\zeta_a(\varepsilon), \infty; \varepsilon)]^2 \hat{f}_-^{(2)}(\infty, \varepsilon) \\ &\quad + \theta(\zeta_a(\varepsilon), \infty; \varepsilon) \int_{\zeta_a(\varepsilon)}^{\infty} [\theta(\zeta_a(\varepsilon), s; \varepsilon) + \theta(s, \zeta_a(\varepsilon); \varepsilon)] \\ &\quad \times \frac{\hat{n}^{(1)}(s) \hat{M}(s, \varepsilon) ds}{\hat{\tau}_{\text{ph}}(s) \sqrt{2[\varepsilon - \hat{W}(s)]}} \end{aligned}$$

$$(3.18) \quad = [\theta(\zeta_a(\varepsilon), \infty; \varepsilon)]^2 \hat{f}_-^{(2)}(\infty, \varepsilon) + \int_{\zeta_a(\varepsilon)}^{\infty} \Theta(s, \varepsilon) \frac{\hat{n}^{(1)}(s) \hat{M}(s, \varepsilon) ds}{\hat{\tau}_{\text{ph}}(s) \sqrt{2[\varepsilon - \hat{W}(s)]}},$$

where $\hat{f}_\infty(-\sqrt{2\varepsilon})$ in (3.17) has been replaced with the equivalent $\hat{f}_-^{(2)}(\infty, \varepsilon)$ as was done in (3.12).

We now go back from the (ζ, ε) representation to the original (ζ, \hat{c}_z) representation. As was done in the derivation of (3.14), we omit the superscript (2) of $\hat{f}_\pm^{(2)}$, supposing that $\hat{f}_\pm^{(2)}$ is an approximation of \hat{f}_\pm , recall the relations (3.13), and then replace $\hat{f}(\infty, \hat{c}_z)$ with the equivalent $\hat{f}_g(0, \hat{c}_z)$ [cf. (2.21)]. Then, using (3.15), we obtain the following expression:

$$(3.19) \quad \begin{aligned} \hat{f}_g(0, \hat{c}_z) &= [1 - \hat{\alpha}(\hat{c}_z^2)] \hat{f}_g(0, -\hat{c}_z) \\ &+ \hat{M}(\hat{c}) \int_{\zeta_a(\hat{c}_z^2/2)}^{\infty} \Theta(s, \hat{c}_z^2/2) \frac{\hat{n}^{(1)}(s) e^{\hat{W}(s)} ds}{\hat{\tau}_{\text{ph}}(s) \sqrt{2[\hat{c}_z^2/2 - \hat{W}(s)]}}, \quad \text{for } \hat{c}_z > 0, \end{aligned}$$

where $\hat{n}^{(1)}(s)$ is given by (3.9) and (3.10) (with ζ being replaced with s). However, (3.9) and (3.10) are expressed in terms of the variables (ζ, ε) . To be consistent with (3.19), these should be transformed into the expression in terms of the original variables (ζ, \hat{c}_z) . This can be done straightforwardly, and after some algebra, we obtain the following expression of $\hat{n}^{(1)}(\zeta)$:

$$(3.20) \quad \hat{n}^{(1)}(\zeta) = \mathcal{K}_1[\hat{f}_g(0, \cdot)](\zeta) + \hat{\beta} e^{-\hat{W}(\zeta)} [1 - K_2(\zeta)],$$

where the operator \mathcal{K}_1 , which operates on $\hat{f}_g(0, \hat{c}_z)$ for $\hat{c}_z < 0$, and the function K_2 are defined by

$$(3.21a) \quad \begin{aligned} \mathcal{K}_1[\hat{f}_g(0, \cdot)](\zeta) &= \int_{-\infty}^{-\sqrt{\max\{0, -2\hat{W}(\zeta)\}}} \Theta\left(\zeta, \frac{v^2}{2} + \hat{W}(\zeta)\right) \\ &\times \left(\iint_{-\infty}^{\infty} \hat{f}_g\left(0, -\sqrt{v^2 + 2\hat{W}(\zeta)}\right) d\hat{c}_x d\hat{c}_y \right) dv, \end{aligned}$$

$$(3.21b) \quad K_2(\zeta) = \frac{1}{\sqrt{2\pi}} \int_{\sqrt{\max\{0, -2\hat{W}(\zeta)\}}}^{\infty} \Theta\left(\zeta, \frac{v^2}{2} + \hat{W}(\zeta)\right) e^{-v^2/2} dv.$$

Here, the integration variable v corresponds to \hat{c}_z , and $\hat{f}_\infty(-\sqrt{2\varepsilon})$ in (3.9) and (3.10) has been replaced with $\hat{f}_g\left(0, -\sqrt{v^2 + 2\hat{W}(\zeta)}\right)$.

The input distribution $\hat{f}_g(0, \hat{c}_z)$ ($\hat{c}_z < 0$) is contained in (3.19) as well as (3.20). The constant $\hat{\beta}$ is determined in such a way that $\hat{f}_g(0, \hat{c}_z)$ for $\hat{c}_z > 0$ and that for $\hat{c}_z < 0$ satisfy the particle conservation (2.20). In summary, with (3.20) and the resulting $\hat{\beta}$, (3.19) is recast as

$$(3.22a) \quad \begin{aligned} \hat{f}_g(0, \hat{c}_z) &= [1 - \hat{\alpha}(\hat{c}_z^2)] \hat{f}_g(0, -\hat{c}_z) + \hat{M}(\hat{c}) \mathcal{L}_1[\hat{f}_g(0, \cdot)](\hat{c}_z) \\ &+ \hat{\beta} \hat{M}(\hat{c}) [\hat{\alpha}(\hat{c}_z^2) - L_2(\hat{c}_z)], \quad \text{for } \hat{c}_z > 0, \end{aligned}$$

$$(3.22b) \quad \begin{aligned} \hat{\beta} &= - \left[\int_0^{\infty} v [\hat{\alpha}(v^2) - L_2(v)] e^{-v^2/2} dv \right]^{-1} \\ &\times \left[\sqrt{2\pi} \int_{-\infty}^0 v \hat{\alpha}(v^2) \left(\iint_{-\infty}^{\infty} \hat{f}_g(0, v) d\hat{c}_x d\hat{c}_y \right) dv \right. \\ &\left. + \int_0^{\infty} v \mathcal{L}_1[\hat{f}_g(0, \cdot)](v) e^{-v^2/2} dv \right], \end{aligned}$$

where v indicates the integration variable for \hat{c}_z . In addition, the operator $\mathcal{L}_1[\hat{f}_g(0, \cdot)](\hat{c}_z)$, which operates on $\hat{f}_g(0, \hat{c}_z)$ for $\hat{c}_z < 0$, and the function $L_2(\hat{c}_z)$ are defined by

$$\mathcal{L}_1[\hat{f}_g(0, \cdot)](\hat{c}_z) = \int_{\zeta_a(\hat{c}_z^2/2)}^{\infty} \Theta(s, \hat{c}_z^2/2) \mathcal{K}_1[\hat{f}_g(0, \cdot)](s) e^{\hat{W}(s)}$$

$$(3.23a) \quad \times \frac{ds}{\hat{\tau}_{\text{ph}}(s)\sqrt{2[\hat{c}_z^2/2 - \hat{W}(s)]}},$$

$$(3.23b) \quad L_2(\hat{c}_z) = \int_{\zeta_a(\hat{c}_z^2/2)}^{\infty} \Theta(s, \hat{c}_z^2/2) K_2(s) \frac{ds}{\hat{\tau}_{\text{ph}}(s)\sqrt{2[\hat{c}_z^2/2 - \hat{W}(s)]}}.$$

In deriving (3.22), use has been made of the following equality:

$$\begin{aligned} & \int_{\zeta_a(\hat{c}_z^2/2)}^{\infty} \Theta(s, \hat{c}_z^2/2) \frac{ds}{\hat{\tau}_{\text{ph}}(s)\sqrt{2[\hat{c}_z^2/2 - \hat{W}(s)]}} \\ &= \int_{\zeta_a(\hat{c}_z^2/2)}^{\infty} \theta(\zeta_a(\hat{c}_z^2/2), \infty; \hat{c}_z^2/2) \\ & \quad \times \frac{\theta(\zeta_a(\hat{c}_z^2/2), s; \hat{c}_z^2/2) + \theta(s, \zeta_a(\hat{c}_z^2/2); \hat{c}_z^2/2)}{\hat{\tau}_{\text{ph}}(s)\sqrt{2[\hat{c}_z^2/2 - \hat{W}(s)]}} ds \\ &= \int_{\zeta_a(\hat{c}_z^2/2)}^{\infty} \theta(\zeta_a(\hat{c}_z^2/2), \infty; \hat{c}_z^2/2) \\ & \quad \times \left[-\frac{\partial}{\partial s} \theta(\zeta_a(\hat{c}_z^2/2), s; \hat{c}_z^2/2) + \frac{\partial}{\partial s} \theta(s, \zeta_a(\hat{c}_z^2/2); \hat{c}_z^2/2) \right] ds \\ &= \theta(\zeta_a(\hat{c}_z^2/2), \infty; \hat{c}_z^2/2) [-\theta(\zeta_a(\hat{c}_z^2/2), \infty; \hat{c}_z^2/2) + \theta(\infty, \zeta_a(\hat{c}_z^2/2); \hat{c}_z^2/2)] \\ &= 1 - [\theta(\zeta_a(\hat{c}_z^2/2), \infty; \hat{c}_z^2/2)]^2 \\ &= \hat{\alpha}(\hat{c}_z^2). \end{aligned}$$

If the input distribution $\hat{f}_g(0, \hat{c}_z)$ ($\hat{c}_z < 0$) is the (dimensionless) wall Maxwellian $\hat{M} = (2\pi)^{-3/2} \exp(-|\hat{c}|^2/2)$, then, we obtain $\mathcal{K}_1[\hat{f}_g(0, \cdot)](\zeta) = K_2(\zeta) \times \exp(-\hat{W}(\zeta))$ from (3.21) and thus $\mathcal{L}_1[\hat{f}_g(0, \cdot)](\hat{c}_z) = L_2(\hat{c}_z)$ from (3.23). Therefore, (3.22b) gives $\hat{\beta} = 1$, so that it follows from (3.22a) that the output distribution $\hat{f}_g(0, \hat{c}_z)$ ($\hat{c}_z > 0$) is also equal to \hat{M} . Thus, the model (3.22) based on the second iteration is seen to satisfy the important property of the boundary condition for the Boltzmann equation. This model will be examined numerically in Sec. 4, and its dimensional form is shown in Appendix A.

4 Numerical assessment of the second-iteration model

In this section, we consider the model (3.22) based on the second iteration and assess it numerically by comparison with the result based on the numerical solution of the original half-space problem (2.19) and (2.22) [7]. The calculation of the right-hand side of (3.22) is straightforward though the operator $\mathcal{L}_1[\hat{f}_g(0, \cdot)]$ and L_2 in (3.23) contain singular integrals. In addition, the numerical solution method for the half-space problem (2.19) and (2.22) is described in detail in [7]. Therefore, we omit the description of the numerical methods and show only the results.

4.1 Preparations

In order to investigate the models (3.14) and (3.22) numerically, one first has to specify the interaction potential $\hat{W}(\zeta)$ as well as the relaxation time $\hat{\tau}_{\text{ph}}(\zeta)$ explicitly. We adopt the Lennard-Jones (LJ) (9, 3) potential [7]:

$$(4.1) \quad \hat{W}(\zeta) = \frac{3\sqrt{3}}{2} \kappa \left(\frac{1}{\zeta^9} - \frac{1}{\zeta^3} \right),$$

and the relaxation times of algebraic type [7]:

$$(4.2) \quad \hat{\tau}_{\text{ph}}(\zeta) = \kappa_{\tau} \left(1 + \frac{\sigma}{\nu} \zeta\right)^{\nu},$$

where κ , κ_{τ} , ν , and σ are parameters. It should be noted that (4.1) and (4.2) are in dimensionless form and correspond to (88) and (91) in [7], respectively. The reader is referred to [7] for the related properties; for instance, $\zeta_a(\varepsilon)$ and $\zeta_b(\varepsilon)$ for (4.1) are given by (89) there. The LJ(9, 3) potential (4.1) is known to be realistic as a potential of interaction between a gas molecule and a crystal surface [26, 11, 23]. In fact, it results from a continuous model of the crystal after volume integration.

In addition, the input velocity distribution $\hat{f}_{\text{g}}(0, \hat{c}_z)$ in (3.14) or in (3.22) should be specified. As can be seen from the first-iteration model (3.14), the dependence on \hat{c}_x and \hat{c}_y of the reflected distribution $\hat{f}_{\text{g}}(0, \hat{c}_z)$ ($\hat{c}_z > 0$) is determined partially by that of the incident distribution $\hat{f}_{\text{g}}(0, \hat{c}_z)$ ($\hat{c}_z < 0$) and partially by the thermalizing term $\hat{M}(\hat{\mathbf{c}})$. This tendency is more or less the same for the second-iteration model (3.22). This means that the models determine the \hat{c}_z -dependence of the reflected molecules crucially but not the \hat{c}_x - and \hat{c}_y -dependence.

For this reason, we only consider the reduced distribution function $\hat{F}_{\text{g}}(0, \hat{c}_z)$ defined by

$$(4.3) \quad \hat{F}_{\text{g}}(0, \hat{c}_z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \hat{f}_{\text{g}}(0, \hat{\mathbf{c}}_{\parallel}, \hat{c}_z) d\hat{c}_x d\hat{c}_y,$$

and assume the following shifted Maxwellian

$$(4.4) \quad \hat{F}_{\text{g}}(0, \hat{c}_z) = \frac{1}{\sqrt{2\pi\hat{T}_*}} \exp\left(-\frac{(\hat{c}_z - \hat{v}_{z*})^2}{2\hat{T}_*}\right), \quad (\hat{c}_z < 0),$$

for the input distribution function, where \hat{v}_{z*} and \hat{T}_* are the parameters to be specified.

In this Sec. 4, the parameters κ in (4.1) and κ_{τ} , σ , and ν in (4.2) are set to be

$$(4.5) \quad (\kappa, \kappa_{\tau}, \sigma, \nu) = (1, 1, 1, 4)$$

as in [7], and the parameters $(\hat{T}_*, \hat{v}_{z*})$ in (4.4) are assumed to be

$$(\hat{T}_*, \hat{v}_{z*}) = (1, -1), (1, 1), (0.3, 0), (0.3, -0.5), \text{ and } (2, 0).$$

4.2 Numerical results

In Figs. 2–6, the reduced distribution function $\hat{F}_{\text{g}}(0, \hat{c}_z)$ for the reflected molecules ($\hat{c}_z > 0$) in response to that for the incident molecules ($\hat{c}_z < 0$) is shown versus \hat{c}_z for $\kappa = \kappa_{\tau} = \sigma = 1$ and $\nu = 4$: Fig. 2 is for $\hat{T}_* = 1$ and $\hat{v}_{z*} = -1$, Fig. 3 for $\hat{T}_* = 1$ and $\hat{v}_{z*} = 1$, Fig. 4 for $\hat{T}_* = 0.3$ and $\hat{v}_{z*} = 0$, Fig. 5 for $\hat{T}_* = 0.3$ and $\hat{v}_{z*} = -0.5$, and Fig. 6 for $\hat{T}_* = 2$ and $\hat{v}_{z*} = 0$. In each figure, panel (b) is the magnified figure of panel (a) for the range $-0.1 \leq \hat{c}_z \leq 1.1$. The thick line for $\hat{c}_z < 0$ indicates the incident distribution (4.4). The thick line for $\hat{c}_z > 0$ indicates $\hat{F}_{\text{g}}(0, \hat{c}_z)$ for the reflected molecules obtained from the second-iteration model (3.22), the thin line indicates that obtained from the first-iteration model (3.14), and the circles indicate that based on the numerical solution of the original half-space problem (2.19) and (2.22).

The reduced velocity distribution for the reflected molecules based on the first-iteration model agrees well on the whole with that obtained by the numerical solution of the physisorbate-layer problem. However, it shows some discrepancies for \hat{c}_z in the range $0 \leq \hat{c}_z \lesssim 0.5$. In contrast, the second-iteration model reproduces the velocity distribution of the reflected molecules obtained by the numerical solution quite well for the whole range of $\hat{c}_z \geq 0$. In particular, it describes the sharp change for small $\hat{c}_z (> 0)$ very well. Therefore, it is a significant improvement compared to the

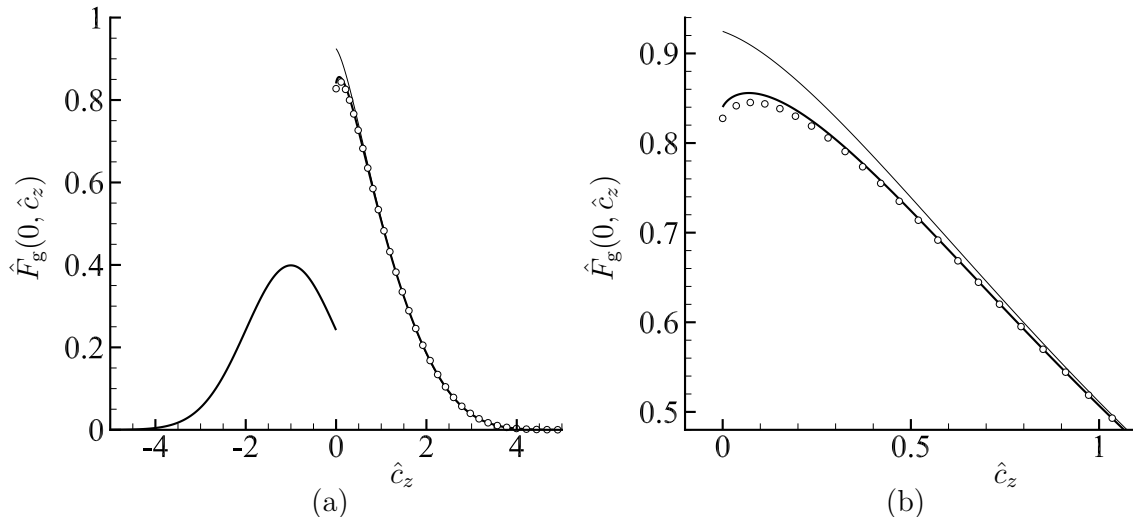


Figure 2: $\hat{F}_g(0, \hat{c}_z)$ versus \hat{c}_z for $\hat{T}_* = 1$ and $\hat{v}_{z*} = -1$ ($\kappa = \kappa_\tau = \sigma = 1$ and $\nu = 4$). Panel (b) is the magnified figure of panel (a) for the range $-0.1 \leq \hat{c}_z \leq 1.1$. The thick line for $\hat{c}_z < 0$ indicates the incident distribution (4.4). The thick line for $\hat{c}_z > 0$ indicates $\hat{F}_g(0, \hat{c}_z)$ for the reflected molecules obtained from the second-iteration model (3.22), the thin line indicates that obtained from the first-iteration model (3.14), and the circles indicate that based on the numerical solution of the original half-space problem (2.19) and (2.22).

first-iteration model. The figures similar to panel (a)s in Figs. 2–6 for other sets of parameter values are shown in Fig. 11 in [5] and show the same behavior. In conclusion, the model (3.22) based on the second iteration is a good model of the boundary condition for the Boltzmann equation with physical basis.

5 Concluding remarks

In our previous paper [7], we proposed a kinetic model of gas surface interaction, from which a kinetic equation describing the behavior of the gas molecules in a thin layer on the solid surface (physisorbate layer) was derived by an asymptotic analysis. It was shown both numerically [7] and mathematically [5] that the solution of the kinetic equation for the physisorbate layer provides a boundary condition for the Boltzmann equation, which is the governing equation outside the physisorbate layer.

One of the main results in [7] was that an iteration scheme, based on the kinetic equation for the physisorbate layer, was proposed and used to construct physical models of the boundary condition for the Boltzmann equation systematically. To be more specific, the model constructed by the first iteration is a Maxwell-type condition (i.e., a linear combination of specular and diffuse reflections) with an accommodation coefficient depending on the molecular velocity. It was shown that the model well reproduced the velocity distribution of the reflected molecules obtained by the numerical solution of the kinetic equation for the physisorbate layer. At the same time, it was expected that the model based on the second iteration, which was shown in a rather implicit form in [7], would provide a further improvement.

The present study focuses its attention on the model based on the second iteration. We first tried to express the model in an explicit form that is convenient for practical applications. Then, the velocity distribution for the reflected gas molecules obtained from the model was compared with

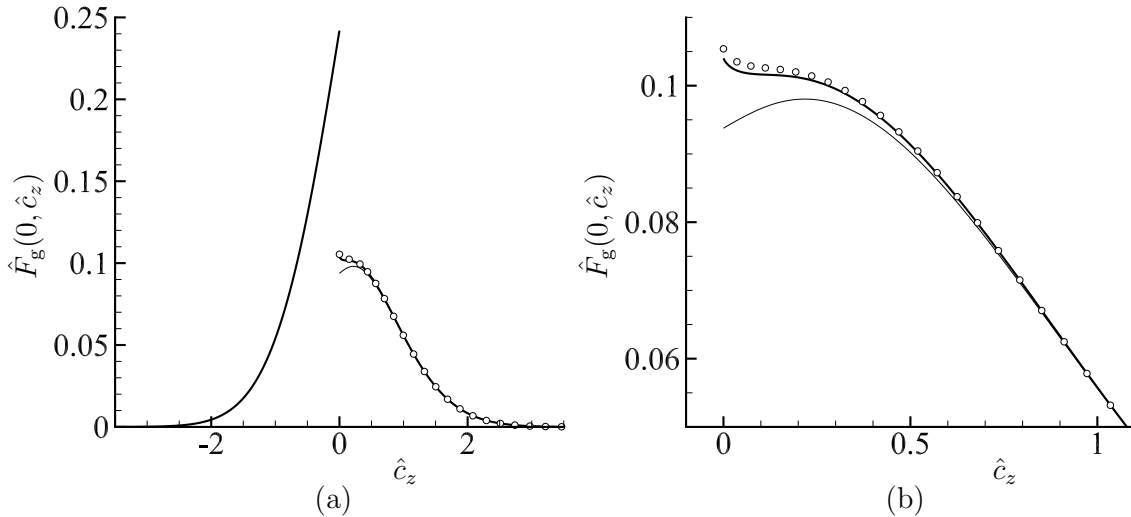


Figure 3: $\hat{F}_g(0, \hat{c}_z)$ versus \hat{c}_z for $\hat{T}_* = 1$ and $\hat{v}_{z*} = 1$ ($\kappa = \kappa_\tau = \sigma = 1$ and $\nu = 4$). See the caption of Fig. 2.

that provided by the numerical solution of the physisorbate-layer kinetic equation. It was shown that the second-iteration model reproduced the latter velocity distribution significantly better than the first-iteration model. Although the second-iteration model has a more complex structure than the first-iteration model, it is still explicit in terms of the interaction potential and the gas-phonon relaxation time. Thus, it can easily be incorporated in the numerical schemes for the Boltzmann and its model equations. Application of the first and second-iteration models of the boundary condition for practical rarefied gas flows is an interesting and important subject, which will be a target of our future research.

A Dimensional form of (3.14) and (3.22)

It is straightforward to express the models (3.14) and (3.22) in terms of the dimensional quantities. The results are summarized in this appendix. Here, we denote the boundary value $f_g(t, \mathbf{x}_\parallel, z = 0, \mathbf{c}_\parallel, c_z)$ by $f_g(0, c_z)$ omitting the variables t , \mathbf{x}_\parallel , and \mathbf{c}_\parallel , as in the dimensionless forms (3.14) and (3.22).

- *First-iteration model* (3.14)

The first-iteration model (3.14) is transformed into the following dimensional form [7]:

$$(A.1) \quad f_g(0, c_z) = [1 - \alpha(c_z^2)] f_g(0, -c_z) + \alpha(c_z^2) \beta M(\mathbf{c}), \quad \text{for } c_z > 0,$$

where

$$(A.2a) \quad M(\mathbf{c}) = \left(\frac{m}{2\pi k_B T_w} \right)^{3/2} \exp\left(-\frac{m|\mathbf{c}|^2}{2k_B T_w} \right),$$

$$(A.2b) \quad \alpha(c_z^2) = 1 - \exp\left(-\sqrt{2m} \delta \int_{\zeta_a(m c_z^2 / 2k_B T_w)}^{\infty} \frac{ds}{\tau_{\text{ph},s}(s) \sqrt{m c_z^2 / 2 - W_s(s)}} \right),$$

$$\beta = - \left(\frac{2\pi k_B T_w}{m} \right)^{1/2} \left[\int_0^{\infty} w \alpha(w^2) \exp\left(-\frac{m w^2}{2k_B T_w} \right) dw \right]^{-1}$$

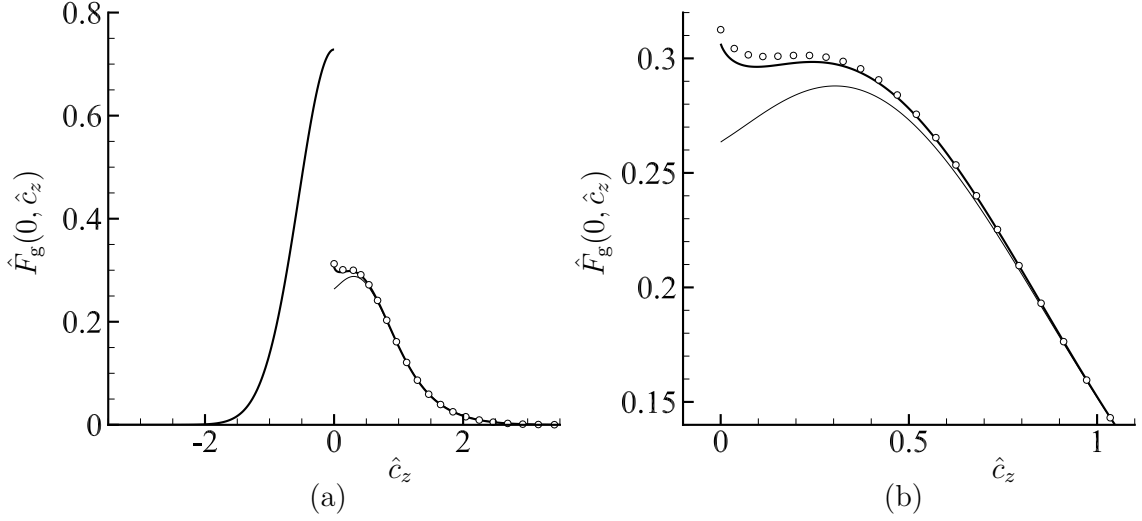


Figure 4: $\hat{F}_g(0, \hat{c}_z)$ versus \hat{c}_z for $\hat{T}_* = 0.3$ and $\hat{v}_{z*} = 0$ ($\kappa = \kappa_\tau = \sigma = 1$ and $\nu = 4$). See the caption of Fig. 2.

$$(A.2c) \quad \times \int_{-\infty}^0 w \alpha(w^2) \left(\iint_{-\infty}^{\infty} f_g(0, w) dc_x dc_y \right) dw.$$

Here, s is the integration variable for the dimensionless normal coordinate $\zeta = z/\delta$ [cf. (2.1)], and w is the integration variable for c_z . Recall that $\zeta_a(mc_z^2/2k_B T_w)$ is the solution of $\tilde{W}(\zeta) = mc_z^2/2k_B T_w$, i.e., that of $W_s(\zeta) = mc_z^2/2$.

- *Second-iteration model* (3.22)

The second-iteration model (3.22) is transformed into the following dimensional form:

$$(A.3) \quad \begin{aligned} f_g(0, c_z) = & [1 - \alpha(c_z^2)] f_g(0, -c_z) + M(\mathbf{c}) \tilde{\mathcal{L}}_1[f_g(0, \cdot)](c_z) \\ & + \beta_* M(\mathbf{c}) [\alpha(c_z^2) - \tilde{L}_2(c_z)], \quad \text{for } c_z > 0, \end{aligned}$$

where $\alpha(c_z^2)$ is given by (A.2b) and

$$(A.4a) \quad \begin{aligned} \tilde{\mathcal{L}}_1[f_g(0, \cdot)](c_z) = & \sqrt{\frac{m}{2}} \delta \int_{\zeta_a(mc_z^2/2k_B T_w)}^{\infty} \Theta(s, mc_z^2/2k_B T_w) \\ & \times \tilde{\mathcal{K}}_1[f_g(0, \cdot)](s) \frac{e^{W_s(s)/k_B T_w} ds}{\tau_{\text{ph},s}(s) \sqrt{mc_z^2/2 - W_s(s)}}, \end{aligned}$$

$$(A.4b) \quad \begin{aligned} \tilde{L}_2(c_z) = & \sqrt{\frac{m}{2}} \delta \int_{\zeta_a(mc_z^2/2k_B T_w)}^{\infty} \Theta(s, mc_z^2/2k_B T_w) \tilde{K}_2(s) \\ & \times \frac{ds}{\tau_{\text{ph},s}(s) \sqrt{mc_z^2/2 - W_s(s)}}, \end{aligned}$$

$$(A.4c) \quad \begin{aligned} \tilde{\mathcal{K}}_1[f_g(0, \cdot)](s) = & \int_{-\infty}^{-\sqrt{\max\{0, -2W_s(s)/m\}}} \Theta\left(s, \frac{mw^2/2 + W_s(s)}{k_B T_w}\right) \\ & \times \left[\iint_{-\infty}^{\infty} f_g\left(0, -\sqrt{w^2 + 2W_s(s)/m}\right) dc_x dc_y \right] dw, \end{aligned}$$

$$(A.4d) \quad \begin{aligned} \tilde{K}_2(s) = & \frac{1}{\sqrt{2\pi}} \sqrt{\frac{m}{k_B T_w}} \int_{\sqrt{\max\{0, -2W_s(s)/m\}}}^{\infty} \Theta\left(s, \frac{mw^2/2 + W_s(s)}{k_B T_w}\right) \\ & \times e^{-mw^2/2k_B T_w} dw, \end{aligned}$$

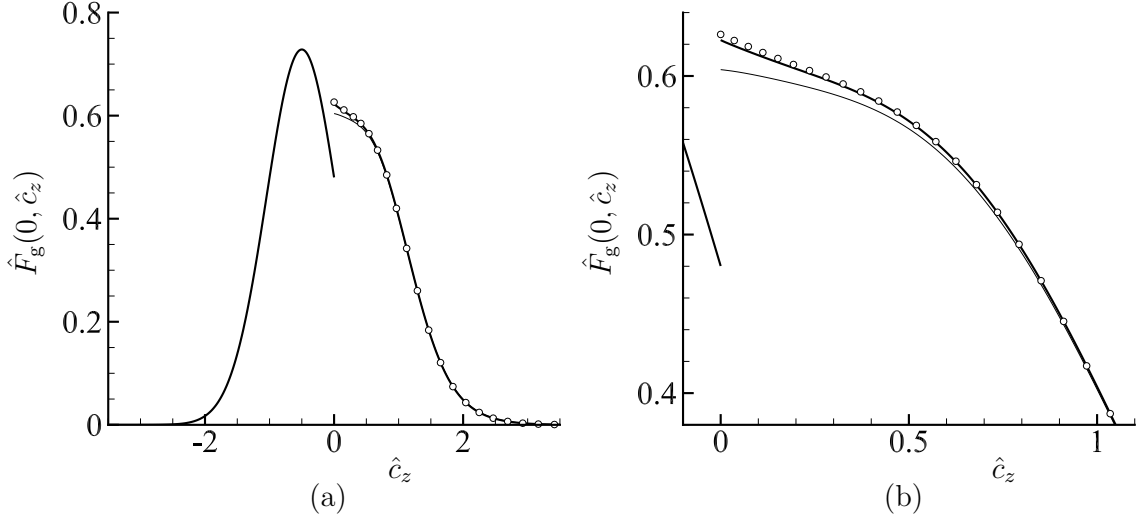


Figure 5: $\hat{F}_g(0, \hat{c}_z)$ versus \hat{c}_z for $\hat{T}_* = 0.3$ and $\hat{v}_{z*} = -0.5$ ($\kappa = \kappa_\tau = \sigma = 1$ and $\nu = 4$). See the caption of Fig. 2.

$$\begin{aligned}
 \beta_* = & - \left[\int_0^\infty w[\alpha(w^2) - \tilde{L}_2(w)]e^{-mw^2/2k_B T_w} dw \right]^{-1} \\
 & \times \left[\sqrt{2\pi} \sqrt{\frac{k_B T_w}{m}} \int_{-\infty}^0 w\alpha(w^2) \left(\iint_{-\infty}^\infty f_g(0, w) dc_x dc_y \right) dw \right. \\
 (A.4e) \quad & \left. + \int_0^\infty w \tilde{\mathcal{L}}_1[f_g(0, \cdot)](w) e^{-mw^2/2k_B T_w} dw \right].
 \end{aligned}$$

Here, the variable s corresponds to the dimensionless normal coordinate $\zeta = z/\delta$ [cf. (2.1)], and w is the integration variable for c_z . The explicit form of the function $\Theta(s, [mw^2/2 + W_s(s)]/k_B T_w)$ occurring in (A.4c) and (A.4d), which can be obtained straightforwardly from (3.11), is shown here for convenience:

$$\begin{aligned}
 & \Theta \left(s, \frac{mw^2/2 + W_s(s)}{k_B T_w} \right) \\
 & = \exp \left(-\sqrt{\frac{m}{2}} \delta \int_s^\infty \frac{d\xi}{\tau_{\text{ph},s}(\xi) \sqrt{mw^2/2 + W_s(s) - W_s(\xi)}} \right) \\
 (A.5) \quad & \times \left\{ 1 + \exp \left(-\sqrt{2m} \delta \int_{\zeta_a^*}^s \frac{d\xi}{\tau_{\text{ph},s}(\xi) \sqrt{mw^2/2 + W_s(s) - W_s(\xi)}} \right) \right\},
 \end{aligned}$$

with

$$\zeta_a^* = \zeta_a \left(\frac{mw^2/2 + W_s(s)}{k_B T_w} \right).$$

The function $\Theta(s, mc_z^2/2k_B T_w)$ appearing in (A.4a) and (A.4b) is obtained readily from (A.5) with the replacement $(w, W_s(s)) \Rightarrow (c_z, 0)$.

In our previous paper [7], the generalization of the first-iteration model (A.1) and (A.2) to more general cases, such as the cases of varying wall temperature and curved boundary, is discussed. The reader is referred to Sec. VB in [7] for the details. We should note that the same generalization can be made for the second-iteration model (A.3) and (A.4).

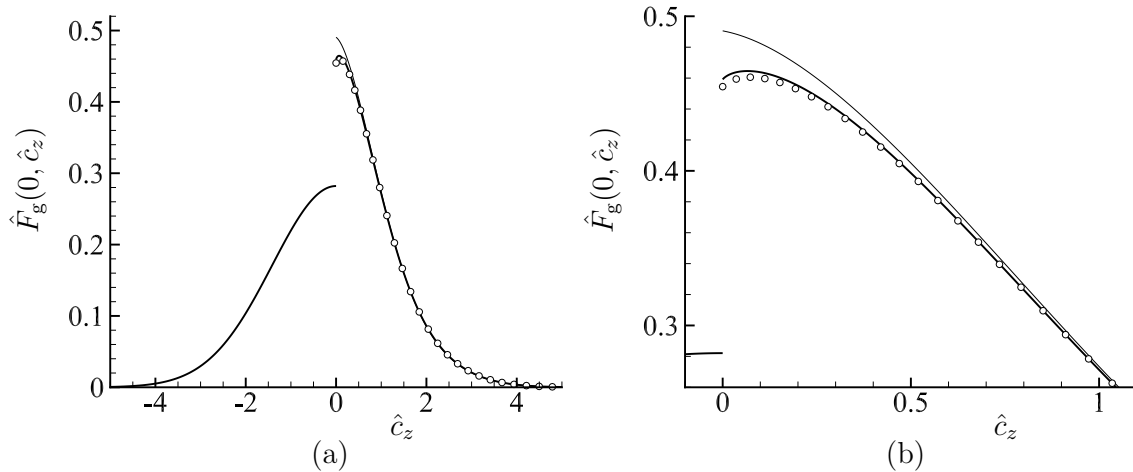


Figure 6: $\hat{F}_g(0, \hat{c}_z)$ versus \hat{c}_z for $\hat{T}_* = 2$ and $\hat{v}_{z*} = 0$ ($\kappa = \kappa_\tau = \sigma = 1$ and $\nu = 4$). See the caption of Fig. 2.

Acknowledgments.

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