A two-surface problem of the electron flow in a semiconductor on the basis of kinetic theory

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A steady flow of electrons in a semiconductor between two parallel plane Ohmic contacts is studied on the basis of the semiconductor Boltzmann equation, assuming a relaxation-time collision term, and the Poisson equation for the electrostatic potential. A systematic asymptotic analysis of the Boltzmann-Poisson system for small Knudsen numbers (scaled mean free paths) is carried out in the case when the Debye length is of the same order as the distance between the contacts and when the applied potential is of the same order as the thermal potential. A system of drift-diffusion-type equations and its boundary conditions is obtained up to second order in the Knudsen number. A numerical comparison is made between the obtained system and the original Boltzmann-Poisson system.

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I. INTRODUCTION

Precise simulations of classical carrier transport in modern semiconductor devices are usually performed using the semiconductor Boltzmann equation. However, this equation requires large computing times and is therefore inconvenient for the solution of real problems in semiconductor production mode. Therefore, simpler models have been derived which focus only on the first few moments of the velocity distribution function. For instance, the drift-diffusion model [1] comprises the first two moments, whereas the hydrodynamic model [2] contains three moments and the energy-transport model [3] four moments (see also Refs. [4, 5]). Also higher-order models have been investigated [6, 7].

The drift-diffusion equations and their variants are the most utilized model in semiconductor simulations since there exist very efficient numerical schemes and since it gives reasonable results even in far-from-equilibrium situations for moderate device lengths. Moreover, higher-order transport models have not been widely accepted as a viable substitute since they are numerically more complex and they contain several transport parameters, which are not always easy to determine or to fit to Monte-Carlo data.

Besides of the choice of the model equations, the modeling of accurate boundary conditions is another problem which is rarely addressed in the existing literature. Yamnahakki [8] derived for the drift-diffusion model improved boundary conditions of Robin type and showed that the current densities for a Schottky diode are closer to the analytic current values than the corresponding drift-diffusion values. However, no comparison with the current density resulting from the solution of the Boltzmann equation has been made. Improved inflow-type boundary conditions for the kinetic models have been suggested in Refs. [9, 10] but no macroscopic boundary conditions have been derived. In this paper, we derive for the first time boundary conditions up to second order in the Knudsen number, i.e.,

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the mean free path scaled by the characteristic length, for drift-diffusion-type equations and compare the results with the direct solution of the Boltzmann-Poisson system.

Our main result can be briefly described as follows. The current density from the macroscopic model with higher-order boundary conditions, computed for an n^+nn^+ ballistic diode, agrees well with the corresponding current values obtained from the original Boltzmann-Poisson system even for Knudsen numbers which are not too small (i.e., Kn = 0.05). Notice that the standard drift-diffusion model only gives sufficiently accurate results for much smaller Knudsen numbers. In fact, we take into account corrections due to small (but nonzero) Knudsen numbers, inspired from kinetic gas theory, which enables us to obtain the stated improved results.

Our approach is related to the asymptotic analysis of the Boltzmann equation for small Knudsen numbers employed in kinetic gas theory, developed by Sone and coworkers [11–18]. In these works, no external force has been imposed. Recently, the same asymptotic analysis has been used to investigate a rarefied gas flow between two parallel plates driven by a *uniform* external force parallel to the plate [19] on the basis of the Bhatnagar-Gross-Krook (BGK) model [20–22] of the Boltzmann equation.

It should be mentioned that, in the present study, we make rather strong assumptions in order to simplify the boundary-value problem. First, we assume that the collision operator is given by a relaxation model similar to the BGK model. A more general collision term can be employed (see Ref. [8]), but a specific choice has to be made in order to compute the Milne problem arising in the asymptotic analysis. Second, we suppose a simple geometry of two parallel plane Ohmic contacts. The asymptotic method also works for a more general geometry but the direct solution of the Boltzmann equation, which is needed for comparison, becomes much more complicate. Third, for the asymptotic analysis, we assume that the Debye length is of the same order as the distance between the contacts and that the applied voltage is of the same order as the thermal potential. The latter condition is not restricting in practice since the drift-diffusion model gives reasonable results even for larger applied voltages. However, the former assumption imposes a condition on the magnitude of the doping profile, which should not be too large. In fact, our results are valid in or close to the channel region of a ballistic diode (where the doping concentration is indeed small) and could in particular help for the derivation of interface conditions for hybrid models in which the highly doped regions and the channel region are described by different models.

The paper is organized as follows. After formulating the problem (Sec. II), we carry out a systematic asymptotic analysis of the Boltzmann-Poisson system for small Knudsen numbers (Sec. III). We derive a system of fluid-dynamic equations and their boundary conditions on the contacts up to second order of the Knudsen number. In Sec. IV, we perform a numerical comparison between the solutions of the derived fluid-dynamic systems and the direct solution of the original Boltzmann-Poisson system on a simple n^+nn^+ diode.

II. FORMULATION OF THE PROBLEM

A. Problem and basic assumptions

We consider a semiconductor between two plane Ohmic contacts located at $X_1 = 0$ (contact A) and $X_1 = L$ (contact B), where X_i is a rectangular space coordinate system. Let T_0 be the temperature of the semiconductor lattice as well as that of the contacts, and let ϕ_A and ϕ_B be the electric potentials applied at the contacts A and B, respectively. We investigate the steady behavior of the electron flow in the X_1 direction induced in the semiconductor under the following assumptions: (i) The behavior of the electrons is described by the semiconductor Boltzmann equation in the parabolic band approximation, employing a relaxation-time collision operator. The electrostatic potential is self-consistently computed from the Poisson equation. (ii) The velocity distribution of the electrons leaving the contact is described by the corresponding part of the Maxwellian distribution with temperature T_0 and zero flow velocity, fulfilling the charge-neutral condition. In the following, we restrict ourselves to the following physical situation: (i) The Knudsen number is small. (ii) The Debye length is of the same order as the distance between the contacts. (iii) The potential difference between the contacts is of the same order as the thermal potential. Thanks to these assumptions, a diffusion approximation of the Boltzmann equation can be performed. This approximation can be made mathematically rigorous; see, e.g., Refs. [23, 24].

B. Basic equations

Let v_i be the electron velocity, $f(X_1, v_i)$ the velocity distribution function of the electrons, $(E(X_1), 0, 0)$ the electric field, m^* the effective electron mass, q the elementary charge, and k the Boltzmann constant. Then, under the parabolic band approximation, the Boltzmann equation with a relaxation-time collision operator is written for the present stationary one-dimensional problem as

$$v_1 \frac{\partial f}{\partial X_1} - \frac{q}{m^*} E \frac{\partial f}{\partial v_1} = \frac{1}{\tau}(\rho M - f), \quad (1)$$

where

$$M = \frac{1}{(2\pi k T_0/m^*)^{3/2}} \exp\left(-\frac{v_i^2}{2kT_0/m^*}\right) \quad (2)$$

is the Maxwellian,

$$\rho = \int f d^3v, \quad (3)$$

the electron number density, $\tau(X_1)$ is the electron relaxation time, and $d^3v = dv_1 dv_2 dv_3$. The summation convention is employed. Here and in the following, the integral with respect to v_i is carried out over the whole space. The electric field E is calculated from the electrostatic potential $\phi(X_1)$ by

$$E = -\frac{d\phi}{dX_1}, \quad (4)$$

where $\phi(X_1)$ solves the Poisson equation

$$\epsilon_s \frac{d^2\phi}{dX_1^2} = q(\rho - C). \quad (5)$$

Here, ϵ_s is the permittivity of the semiconductor and $C(X_1)$ is the doping profile which is assumed to be smooth. We refer to Refs. [4, 5] for details on the modeling of semiconductors.

Under the charge neutral condition, the boundary condition on the contact A ($X_1 = 0$) is given by

$$f = C(0)M \quad \text{for } v_1 > 0, \quad (6)$$

$$\phi = \phi_A, \quad (7)$$

whereas the boundary condition on the contact B ($X_1 = L$) reads as

$$f = C(L)M \quad \text{for } v_1 < 0, \quad (8)$$

$$\phi = \phi_B. \quad (9)$$

Finally, let us define some macroscopic quantities. Let $(J(X_1), 0, 0)$ denote the electron current density, $(u(X_1), 0, 0)$ the electron mean velocity, and $T(X_1)$ the electron temperature. They are defined as

$$J = -q\rho u = -q \int v_1 f d^3v, \quad (10)$$

$$T = \frac{m^*}{3k\rho} \int (v_i - u\delta_{i1})^2 f d^3v. \quad (11)$$

Note that the particle flux in the positive X_1 direction is given by $-J/q$.

C. Dimensionless variables

Let ρ_0 and τ_0 be, respectively, characteristic values of the electron number density and of the relaxation time, and let $U_T = kT_0/q$ be the thermal potential related to the lattice temperature T_0. We introduce the following dimensionless quantities:

$$x_i = \frac{X_i}{L}, \quad \zeta_i = \frac{v_i}{(2kT_0/m^*)^{1/2}},$$
$$\hat{f} = \frac{(2kT_0/m^*)^{3/2}}{\rho_0} f, \quad \hat{\tau} = \frac{\tau}{\tau_0},$$
$$\hat{\phi} = \frac{\phi}{U_T}, \quad \hat{E} = \frac{E}{U_T/L}, \quad \hat{C} = \frac{C}{\rho_0},$$
$$\hat{\rho} = \frac{\rho}{\rho_0}, \quad \hat{J} = -\frac{J}{q\rho_0(2kT_0/m^*)^{1/2}},$$
$$\hat{u} = \frac{u}{(2kT_0/m^*)^{1/2}}, \quad \hat{T} = \frac{T}{T_0}.$$

Using these dimensionless quantities, the Boltzmann-Poisson system (1)–(5) becomes

$$\zeta_1 \frac{\partial \hat{f}}{\partial x_1} - \frac{1}{2}\hat{E}\frac{\partial \hat{f}}{\partial \zeta_1} = \frac{2}{\sqrt{\pi}}\frac{1}{\mathrm{Kn}}\frac{1}{\hat{\tau}}(\hat{\rho}\mathcal{M} - \hat{f}), \tag{12}$$

$$\mathcal{M} = \frac{1}{\pi^{3/2}}\exp(-\zeta_i^2), \tag{13}$$

$$\hat{\rho} = \int \hat{f} d^3\zeta, \tag{14}$$

$$\lambda^2 \frac{d^2\hat{\phi}}{dx_1^2} = \hat{\rho} - \hat{C}, \tag{15}$$

$$\hat{E} = -\frac{d\hat{\phi}}{dx_1}, \tag{16}$$

$$\mathrm{Kn} = \frac{l_0}{L} = \frac{2}{\sqrt{\pi}}\frac{(2kT_0/m^*)^{1/2}\tau_0}{L}, \tag{17}$$

$$\lambda = \frac{\lambda_0}{L} = \sqrt{\frac{\epsilon_s U_T}{q\rho_0 L^2}}, \tag{18}$$

where $d^3\zeta = d\zeta_1 d\zeta_2 d\zeta_3$. Again, here and in the following, the domain of integration with respect to ζ_i is the whole space. The dimensionless parameter Kn, which is defined by the ratio of the mean free path of an electron $l_0 = (2/\sqrt{\pi})(2kT_0/m^*)^{1/2}\tau_0$ to the distance L between the contacts, is called the Knudsen number (or scaled mean free path), and represents the frequency of collisions of an electron with other particles (phonons, impurities etc.). The dimensionless parameter λ, defined by the ratio of the Debye length $\lambda_0 = (\epsilon_s U_T/q\rho_0)^{1/2}$ of the semiconductor to the distance L between the contacts, is called the scaled Debye length. The dimensionless form of the boundary conditions is written as

$$\hat{f} = \hat{C}(0)\mathcal{M} \quad \text{for } \zeta_1 > 0, \tag{19}$$

$$\hat{\phi} = \hat{\phi}_A, \tag{20}$$

at $x_1 = 0$, and

$$\hat{f} = \hat{C}(1)\mathcal{M} \quad \text{for } \zeta_1 < 0, \tag{21}$$

$$\hat{\phi} = \hat{\phi}_B, \tag{22}$$

at $x_1 = 1$, where $(\hat{\phi}_A, \hat{\phi}_B) = (\phi_A/U_T, \phi_B/U_T)$. Finally, the dimensionless macroscopic quantities are expressed in terms of the dimensionless velocity distribution function as follows:

$$\hat{J} = \hat{\rho}\hat{u} = \int \zeta_1 \hat{f} d^3\zeta, \tag{23}$$

$$\hat{T} = \frac{2}{3\hat{\rho}}\int (\zeta_i - \hat{u}\delta_{i1})^2 \hat{f} d^3\zeta. \tag{24}$$

The functions $\hat{\tau}(x_1)$ and $\hat{C}(x_1)$ are specified according to the specific semiconductor device. The above boundary-value problem is characterized by the parameters

$$\mathrm{Kn}, \quad \lambda, \quad \hat{\phi}_A - \hat{\phi}_B.$$

In the present study, we investigate the behavior of the electron flow for small Knudsen numbers $\mathrm{Kn} \ll 1$ when both the scaled Debye length λ and the (dimensionless) potential difference $|\hat{\phi}_B - \hat{\phi}_A|$ are of the order of unity.

Incidentally, the integration of Eq. (12) with respect to ζ_i over the whole space leads to $d\hat{J}/dx_1 = 0$. and therefore, we have $\hat{J} =$ const for all $0 \le x_1 \le 1$.

III. ASYMPTOTIC ANALYSIS AND FLUID-DYNAMIC EQUATIONS

In this section, we carry out an asymptotic analysis of the Boltzmann-Poisson system described in the previous section when the scaled Debye length λ and the potential difference $|\hat{\phi}_B - \hat{\phi}_A|$ are of the order of unity. In the course of the analysis, we derive some drift-diffusion-type equations, coupled with the Poisson equation, as well as their boundary conditions. In the following, we use

$$\epsilon = \frac{\sqrt{\pi}}{2}\mathrm{Kn}$$

as a small parameter rather than the Knudsen number Kn itself.

A. Hilbert solution

First, putting aside the boundary conditions, we look for a solution ($\hat{f}_H$, $\hat{\phi}_H$) to Eqs. (12)–(16) which varies moderately over the distance between the contacts, i.e., $\partial\hat{f}_H/\partial x_1 = O(\hat{f}_H)$ and $d\hat{\phi}_H/dx_1 = O(\hat{\phi}_H)$. Such a solution is called the *Hilbert solution* and is denoted by the subscript H. We assume that $\hat{f}_H$ and $\hat{\phi}_H$ can be expressed in powers of ϵ, i.e.,

$$\hat{f}_H = \hat{f}_{H0} + \hat{f}_{H1}\epsilon + \hat{f}_{H2}\epsilon^2 + \cdots, \quad (25)$$

$$\hat{\phi}_H = \hat{\phi}_{H0} + \hat{\phi}_{H1}\epsilon + \hat{\phi}_{H2}\epsilon^2 + \cdots. \quad (26)$$

Correspondingly, the macroscopic variables h (where $h = \hat{\rho}_H$, $\hat{J}_H$, $\hat{u}_H$, or $\hat{T}_H$) as well as the electric field $\hat{E}_H$ are expanded in ϵ as

$$h_H = h_{H0} + h_{H1}\epsilon + h_{H2}\epsilon^2 + \cdots, \quad (27)$$

$$\hat{E}_H = \hat{E}_{H0} + \hat{E}_{H1}\epsilon + \hat{E}_{H2}\epsilon^2 + \cdots. \quad (28)$$

The relation between $\hat{f}_{Hm}$ and h_m is obtained by substituting Eqs. (25) and (27) into Eqs. (14), (23), and (24) with $h = h_H$ and $\hat{f} = \hat{f}_H$ and equating the coefficients with the same power of ϵ. For $h = \hat{\rho}_H$ or $\hat{J}_H$, we find

$$\hat{\rho}_{Hm} = \int \hat{f}_{Hm} d^3\zeta, \quad (29)$$

$$\hat{J}_{Hm} = \int \zeta_1 \hat{f}_{Hm} d^3\zeta \quad (m = 0, 1, \ldots). \quad (30)$$

The results for $\hat{u}_H$ and $\hat{T}_H$ up to order three are given in Appendix A. Similarly, the relation between $\hat{\phi}_{Hm}$ and $\hat{E}_{Hm}$ is obtained by substituting Eqs. (26) and (28) into Eq. (16) with $\hat{E} = \hat{E}_H$ and $\hat{\phi} = \hat{\phi}_H$ and equating the coefficients with the same power of ϵ. [Here, we keep in mind the property $d\hat{\phi}_H/dx_1 = O(\hat{\phi}_H)$.] Thus, we have

$$\hat{E}_{Hm} = -\frac{d\hat{\phi}_{Hm}}{dx_1} \quad (m = 0, 1, \ldots). \quad (31)$$

Since our collision term conserves the number of particles, it holds

$$\int (\hat{\rho}_H \mathcal{M} - \hat{f}_H) d^3\zeta = 0,$$

and hence,

$$\int (\hat{\rho}_{Hm} \mathcal{M} - \hat{f}_{Hm}) d^3\zeta = 0 \quad (m = 0, 1, \ldots). \quad (32)$$

Substituting Eqs. (25), (27) (with $h = \hat{\rho}$), and (28) into Eq. (12) and taking into account the property $\partial\hat{f}_H/\partial x_1 = O(\hat{f}_H)$ gives the following expressions for $\hat{f}_{Hm}$:

$$\hat{f}_{H0} = \hat{\rho}_{H0}\mathcal{M}, \quad (33)$$

$$\hat{f}_{Hm} = \hat{\rho}_{Hm}\mathcal{M} - \hat{\tau}\Big(\zeta_1 \frac{\partial \hat{f}_{Hm-1}}{\partial x_1} - \frac{1}{2}\sum_{n=0}^{m-1} \hat{E}_{Hn} \frac{\partial \hat{f}_{Hm-n-1}}{\partial \zeta_1}\Big) \quad (m \geq 1). \quad (34)$$

Equation (32) provides the compatibility conditions for Eq. (34), i.e.,

$$\int \Big(\zeta_1 \frac{\partial \hat{f}_{Hm-1}}{\partial x_1} - \sum_{n=0}^{m-1} \frac{\hat{E}_{Hn}}{2} \frac{\partial \hat{f}_{Hm-n-1}}{\partial \zeta_1}\Big) d^3\zeta = 0 \quad (m \geq 1), \quad (35)$$

which reduces to

$$\frac{d}{dx_1} \int \zeta_1 \hat{f}_{Hm-1} d^3\zeta = 0 \quad (m \geq 1). \quad (36)$$

When we use in Eq. (36) the explicit expressions for $\hat{f}_{Hn}$ ($n = 0, 1, \ldots$) in terms of $\hat{\rho}_{Hs}$ ($s \leq n$) and $\hat{E}_{Hs}$ ($s \leq n - 1$), which are obtained successively from Eqs. (33) and (34), we derive ordinary differential equations for $\hat{\rho}_{Hn}$ and $\hat{E}_{Hn}$, called here *fluid-dynamic equations.*

Furthermore, when we substitute Eqs. (26) and (27) (with $h = \hat{\rho}$) into

Eq. (15) with $\hat{\phi} = \hat{\phi}_H$ and $\hat{\rho} = \hat{\rho}_H$ and take into account the property $d\hat{\phi}_H/dx_1 = O(\hat{\phi}_H)$ as well as $\lambda = O(1)$, we obtain the following sequence of equations:

$$\lambda^2 \frac{d^2\hat{\phi}_{H0}}{dx_1^2} = \hat{\rho}_{H0} - \hat{C},$$

$$\lambda^2 \frac{d^2\hat{\phi}_{Hm}}{dx_1^2} = \hat{\rho}_{Hm} \quad (m \geq 1).$$

These equations are coupled with the fluid-dynamic equations through Eq. (31).

Now let us derive the explicit form of the fluid-dynamic equations. First, we note that the compatibility condition (36) is equivalent to

$$\frac{d}{dx_1}\hat{J}_{Hm-1} = 0 \quad (m \geq 1). \tag{37}$$

by the definition of $\hat{J}_{Hm}$ [Eq. (30)]. The explicit form of $\hat{J}_{Hm}$ $(m = 0, 1, \ldots)$ is obtained by substituting the explicit expression for $\hat{f}_{Hm}$, derived successively from the lowest order with the aid of Eqs. (33) and (34) and of the compatibility conditions, into the definition of $\hat{J}_{Hm}$ [Eq. (30)]. Thus, we obtain

$$\hat{J}_{H0} = 0, \tag{38}$$

$$\hat{J}_{H1} = -\frac{1}{2}\hat{\tau}\Big(\frac{d\hat{\rho}_{H0}}{dx_1} + \hat{\rho}_{H0}\hat{E}_{H0}\Big), \tag{39}$$

$$\hat{J}_{H2} = -\frac{1}{2}\hat{\tau}\Big(\frac{d\hat{\rho}_{H1}}{dx_1} + \hat{\rho}_{H0}\hat{E}_{H1} + \hat{\rho}_{H1}\hat{E}_{H0}\Big), \tag{40}$$

$$\hat{J}_{H3} = -\frac{1}{2}\hat{\tau}\Big(\frac{d\hat{\rho}_{H2}}{dx_1} + \hat{\rho}_{H0}\hat{E}_{H2} + \hat{\rho}_{H1}\hat{E}_{H1} + \hat{\rho}_{H2}\hat{E}_{H0}\Big) + \hat{\tau}\frac{d}{dx_1}\big(\hat{\tau}\hat{E}_{H0}\hat{J}_{H1}\big). \tag{41}$$

We observe that Eq. (37) for $m = 1$, together with Eq. (38), does not give any condition for the macroscopic quantities. Equation (37) for $m \geq 2$, together with Eqs. (38)–(41), gives the desired fluid-dynamic equations.

In summary, we obtain the following systems of fluid-dynamic equations: for $m = 0$,

$$\frac{d}{dx_1}\hat{J}_{H1} = 0, \tag{42a}$$

$$\hat{J}_{H1} = -\frac{1}{2}\hat{\tau}\Big(\frac{d\hat{\rho}_{H0}}{dx_1} + \hat{\rho}_{H0}\hat{E}_{H0}\Big), \tag{42b}$$

$$\hat{E}_{H0} = -\frac{d\hat{\phi}_{H0}}{dx_1}, \tag{42c}$$

$$\lambda^2 \frac{d^2\hat{\phi}_{H0}}{dx_1^2} = \hat{\rho}_{H0} - \hat{C}, \tag{42d}$$

for $m = 1$,

$$\frac{d}{dx_1}\hat{J}_{H2} = 0, \tag{43a}$$

$$\hat{J}_{H2} = -\frac{1}{2}\hat{\tau}\Big(\frac{d\hat{\rho}_{H1}}{dx_1} + \hat{\rho}_{H1}\hat{E}_{H0} + \hat{\rho}_{H0}\hat{E}_{H1}\Big), \tag{43b}$$

$$\hat{E}_{H1} = -\frac{d\hat{\phi}_{H1}}{dx_1}, \tag{43c}$$

$$\lambda^2 \frac{d^2\hat{\phi}_{H1}}{dx_1^2} = \hat{\rho}_{H1}, \tag{43d}$$

and for $m = 2$,

$$\frac{d}{dx_1}\hat{J}_{H3} = 0, \tag{44a}$$

$$\hat{J}_{H3} = -\frac{1}{2}\hat{\tau}\Big(\frac{d\hat{\rho}_{H2}}{dx_1} + \hat{\rho}_{H0}\hat{E}_{H2} + \hat{\rho}_{H1}\hat{E}_{H1} + \hat{\rho}_{H2}\hat{E}_{H0}\Big) + \hat{\tau}\frac{d}{dx_1}\big(\hat{\tau}\hat{E}_{H0}\big)\hat{J}_{H1}, \tag{44b}$$

$$\hat{E}_{H2} = -\frac{d\hat{\phi}_{H2}}{dx_1}, \tag{44c}$$

$$\lambda^2 \frac{d^2\hat{\phi}_{H2}}{dx_1^2} = \hat{\rho}_{H2}. \tag{44d}$$

Equations (42a)–(42d) are the well-known drift-diffusion equations for the leading-order quantities $\hat{\rho}_{H0}$, $\hat{E}_{H0}$, and $\hat{\phi}_{H0}$. Equations (43a)–(43d) for the variables $\hat{\rho}_{H1}$, $\hat{E}_{H1}$, and $\hat{\phi}_{H1}$ also correspond to a drift-diffusion model, since they can be obtained from a drift-diffusion system (with the mobility given by $\mu = q\tau/m^*$) by means of the expansion corresponding to Eqs. (25)–(28). However, the next-order equations (44a)–(44d) for the variables $\hat{\rho}_{H2}$, $\hat{E}_{H2}$, and $\hat{\phi}_{H2}$

do not constitute a drift-diffusion model due to the last term in Eq. (44b).

The presence of the last term in Eq. (44b) [or in Eq. (41)] can be understood in the following way. Suppose that the first order current density (or the particle flux) $\hat{J}_{H1}$ has been established. Since each electron is accelerated by the electric field and thus obtains a momentum, this produces a momentum flux (or *stress*) in the positive X_1 direction, which is given by $-2\hat{\tau}\hat{E}_{H0}\hat{J}_{H1}$ multiplied by $k\rho_0 T_0 \epsilon^2$. Therefore, if the last term of Eq. (44b) is nonzero, the force is exerted on the fluid by the stress, resulting in the induction of a current flow.

When the compatibility conditions (or the fluid-dynamic equations) are satisfied, the velocity distribution functions are expressed as

$$\hat{f}_{H0} = \hat{\rho}_{H0}\mathcal{M}, \tag{45}$$

$$\hat{f}_{H1} = \mathcal{M}\big(\hat{\rho}_{H1} + 2\hat{J}_{H1}\zeta_1\big), \tag{46}$$

$$\hat{f}_{H2} = \mathcal{M}\Big[\hat{\rho}_{H2} + 2\hat{J}_{H2}\zeta_1 - 2\hat{\tau}\hat{E}_{H0}\hat{J}_{H1}\Big(\zeta_1^2 - \frac{1}{2}\Big)\Big], \tag{47}$$

$$\hat{f}_{H3} = \mathcal{M}\Big\{\hat{\rho}_{H3} + 2\hat{J}_{H3}\zeta_1 - 2\hat{\tau}\left(\hat{E}_{H0}\hat{J}_{H2} + \hat{E}_{H1}\hat{J}_{H1}\right)\left(\zeta_1^2 - \frac{1}{2}\right) + 2\hat{\tau}\Big(\frac{d}{dx_1}\big(\hat{\tau}\hat{E}_{H0}\hat{J}_{H1}\big) + \hat{\tau}\hat{E}_{H0}^2\hat{J}_{H1}\Big) \times \left(\zeta_1^3 - \frac{3}{2}\zeta_1\right)\Big\}. \tag{48}$$

Using these expressions, we readily obtain the equations for the mean flow velocity $\hat{u}_{Hm}$ and the electron temperature $\hat{T}_{Hm}$. The results up to $m = 3$ are given in Appendix B.

B. Knudsen layers and boundary conditions for fluid-dynamic equations

In this section we derive the boundary conditions for the fluid-dynamic equations. Suppose that $\hat{\rho}_{H0}$ and $\hat{\phi}_{H0}$ take the following values on the boundary:

$$\hat{\rho}_{H0} = \hat{C}(0),\ \hat{\phi}_{H0} = \hat{\phi}_A \quad \text{at } x_1 = 0 \tag{49}$$

$$\hat{\rho}_{H0} = \hat{C}(1),\ \hat{\phi}_{H0} = \hat{\phi}_B \quad \text{at } x_1 = 1. \tag{50}$$

With this choice of values, the leading-order velocity distribution function $\hat{f}_{H0}$ [Eq. (45)] and the leading-order electrostatic potential $\hat{\phi}_{H0}$ satisfy the boundary conditions (19)–(22). Therefore, Eqs. (49) and (50) give consistent boundary conditions for the leading-order fluid-dynamic equations (42a)–(42d). For the higher-order quantities, however, the Hilbert solution does not have enough freedom to satisfy the boundary conditions. For example, in order for $\hat{f}_{H1}$ [Eq. (46)] to satisfy the corresponding boundary condition, i.e., $\hat{f}_{H1} = 0$ on the boundary, we need to impose the condition $\hat{J}_{H1} = 0$ as well as $\hat{\rho}_{H1} = 0$ on the boundary. The former condition cannot be satisfied in general except in the trivial case of the thermal equilibrium state. Therefore, we need to introduce a so-called Knudsen-layer correction near the boundary.

From now on, we seek the solution in the form

$$\hat{f} = \hat{f}_H + \hat{f}_K, \tag{51}$$

$$\hat{\phi} = \hat{\phi}_H + \hat{\phi}_K, \tag{52}$$

where $(\hat{f}_K, \hat{\phi}_K)$, which is called the *Knudsen-layer part*, is the correction to the Hilbert solution $(\hat{f}_H, \hat{\phi}_H)$ appreciable only in thin layers of thickness of order ϵ (or of the mean free path in the dimensional X_1 variable) adjacent to the boundary. In order to analyze the Knudsen layers near $x_1 = 0$ and $x_1 = 1$ simultaneously, it is convenient to introduce the following new variables:

$$y = x_1, \quad \eta = y/\epsilon, \quad \zeta_y = \zeta_1,$$

around $x_1 = 0$ and

$$y = 1 - x_1, \quad \eta = y/\epsilon, \quad \zeta_y = -\zeta_1,$$

around $x_1 = 1$. Here, y, whose origin is on the boundary, is the coordinate normal to the boundary pointing to the semiconductor, η is the stretched coordinate normal to the boundary, and ζ_y is the component of ζ_1

in the positive y direction. We assume that the variations of $(\hat{f}_K, \hat{\phi}_K)$ are of the order ϵ, i.e.,

$$\hat{f}_K = \hat{f}_K(\eta, \zeta_y, \zeta_2, \zeta_3), \quad \hat{\phi}_K = \hat{\phi}_K(\eta), \tag{53}$$

or $\partial \hat{f}_K/\partial\eta = O(\hat{f}_K)$ and $d\hat{\phi}_K/d\eta = O(\hat{\phi}_K)$, and that $(\hat{f}_K, \hat{\phi}_K)$ vanishes rapidly as $\eta \to \infty$. We further suppose that $(\hat{f}_K, \hat{\phi}_K)$ is expanded in ϵ as

$$\hat{f}_K = \hat{f}_{K1}\epsilon + \hat{f}_{K2}\epsilon^2 + \cdots, \tag{54}$$

$$\hat{\phi}_K = \hat{\phi}_{K1}\epsilon + \hat{\phi}_{K2}\epsilon^2 + \cdots. \tag{55}$$

The expansion starts from order ϵ because $(\hat{f}_{H0}, \hat{\phi}_{H0})$ already satisfies the boundary condition. Corresponding to Eqs. (51), (52), (54), and (55), the macroscopic quantity h (where $h = \hat{\rho}$, $\hat{J}$, $\hat{u}$, or $\hat{T}$) and the electric field $\hat{E}$ are expressed as

$$h = h_H + h_K, \tag{56}$$

$$\hat{E} = \hat{E}_H + \hat{E}_K \tag{57}$$

with

$$h_K = h_{K1}\epsilon + h_{K2}\epsilon^2 + \cdots, \tag{58}$$

$$\hat{E}_K = \hat{E}_{K0} + \hat{E}_{K1}\epsilon + \hat{E}_{K2}\epsilon^2 + \cdots. \tag{59}$$

The expansion of $\hat{E}_K$ starts from order ϵ^0 for the following reason. If we substitute Eqs. (52) and (57) into Eq. (16) and take into account that $\hat{E}_H$ and $\hat{\phi}_H$ solve the Poisson equation, we obtain

$$\hat{E}_K = \mp\frac{1}{\epsilon}\frac{d\hat{\phi}_K}{d\eta}, \tag{60}$$

where the minus (plus) sign corresponds to the Knudsen layer around $x_1 = 0$ ($x_1 = 1$). This convention is used throughout the paper. Since $\hat{\phi}_K = O(\epsilon)$ and $d\hat{\phi}_K/d\eta = O(\hat{\phi}_K)$ [see the sentence that contains Eq. (53)], we conclude that $\hat{E}_K = O(1)$ and therefore, the $\hat{E}_{K0}$ term in the expansion (59) is not zero.

Substituting the expansions (55) and (59) into Eq. (60) and equating the coefficients of the same power of ϵ yields the following expression of $\hat{E}_{Km}$ in terms of $\hat{\phi}_{Km}$:

$$\hat{E}_{Km-1} = \mp\frac{d\hat{\phi}_{Km}}{d\eta} \quad (m \geq 1). \tag{61}$$

In order to obtain the relation between h_{Km} and $\hat{f}_{Km}$, we substitute Eq. (51) [with Eqs. (25) and (54)] and Eq. (56) [with Eqs. (27) and (57)] into Eqs. (14), (23), and (24) and take into account the relation between h_{Hm} and $\hat{f}_{Hm}$ [Eqs. (29), (30), (A1a)–(A4b)]. Thus, for $\hat{\rho}_{Km}$ and $\hat{J}_{Km}$, we obtain the expressions

$$\hat{\rho}_{Km} = \int \hat{f}_{Km} d^3\bar{\zeta}, \;\; \hat{J}_{Km} = \int \zeta_1 \hat{f}_{Km} d^3\bar{\zeta}, \tag{62}$$

where $d^3\bar{\zeta} = d\zeta_y d\zeta_2 d\zeta_3$. In order to compute $\hat{u}_{Km}$ and $\hat{T}_{Km}$, we employ the following expansion of the Hilbert part around the boundary ($y = 0$):

$$h_{Hn} = (h_{Hn})_B + \Big(\frac{dh_{Hn}}{dy}\Big)_B \eta\epsilon + \frac{1}{2}\Big(\frac{d^2 h_{Hn}}{dy^2}\Big)_B \eta^2\epsilon^2 \cdots, \tag{63}$$

where $(\;)_B$ denotes the value on the boundary. Then, after equating the terms with the same power of ϵ, we obtain the desired expressions for $\hat{u}_{Km}$ and $\hat{T}_{Km}$. The results for $m = 1$ and $m = 2$ are summarized in Appendix C.

Now let us derive the equations for $(\hat{f}_K, \hat{\phi}_K)$. When we substitute Eqs. (51), (52) and (58) (with $h = \hat{\rho}$) into Eqs. (12) [with Eq. (16)] and (15) and take into account the length scale of variation of $(\hat{f}_K, \hat{\phi}_K)$ as well as the fact that $(\hat{f}_H, \hat{\phi}_H)$ is a solution of Eqs. (12) and (15), we obtain

$$\zeta_y\frac{\partial \hat{f}_K}{\partial\eta} + \frac{1}{2}\Big(\frac{d\hat{\phi}_H}{dy}\frac{\partial \hat{f}_K}{\partial\zeta_y}\epsilon + \frac{d\hat{\phi}_K}{d\eta}\frac{\partial \hat{f}_H}{\partial\zeta_y} + \frac{d\hat{\phi}_K}{d\eta}\frac{\partial \hat{f}_K}{\partial\zeta_y}\Big) = \frac{1}{\hat{\tau}}(\hat{\rho}_K\mathcal{M} - \hat{f}_K),$$

$$\lambda^2\frac{d^2\hat{\phi}_K}{d\eta^2} = \epsilon^2\hat{\rho}_K.$$

Inserting the expansions (25), (26), (54), (55), and (58) and using the following expansion for $(\hat{f}_H, \hat{\phi}_H)$ and $\hat{\tau}$ near the boundary,

$$\hat{g}_H = (\hat{g}_{H0})_B + \left[(\hat{g}_{H1})_B + \left(\frac{\partial \hat{g}_{H0}}{\partial y} \right)_B \eta \right] \epsilon + \cdots \quad \text{with } g = f, \phi, \tag{64}$$

$$\frac{1}{\hat{\tau}} = \frac{1}{(\hat{\tau})_B} - \frac{1}{(\hat{\tau})_B^2} \left(\frac{d\hat{\tau}}{dy} \right)_B \eta\epsilon + \cdots , \tag{65}$$

yields a sequence of equations for ($\hat{f}_{Km}$, $\hat{\phi}_{Km}$) ($m \geq 1$). On the other hand, the boundary conditions for $(\hat{f}_{Km}, \hat{\phi}_{Km})$ are derived from the requirements $(\hat{f}_{Hm})_B + (\hat{f}_{Km})_B = 0$ (for $\zeta_y > 0$) and $(\hat{\phi}_H)_B + (\hat{\phi}_{Km})_B = 0$ on the boundary. Furthermore, the condition $(\hat{f}_{Km}, \hat{\phi}_{Km}) \to (0, 0)$ as $\eta \to \infty$ needs to be imposed.

In the following, we present the explicit equations and boundary conditions for ($\hat{f}_{K1}$, $\hat{\phi}_{K1}$) and ($\hat{f}_{K2}$, $\hat{\phi}_{K2}$):

$$\zeta_y \frac{\partial \hat{f}_{Km}}{\partial \eta} + \frac{1}{2} \frac{d\hat{\phi}_{Km}}{d\eta} \frac{\partial}{\partial \zeta_y} (\hat{f}_{H0})_B = \frac{1}{(\hat{\tau})_B} (\hat{\rho}_{Km} \mathcal{M} - \hat{f}_{Km}) + I_m, \tag{66}$$

$$\lambda^2 \frac{d^2 \hat{\phi}_{Km}}{d\eta^2} = 0, \tag{67}$$

$$\hat{f}_{Km} = -\mathcal{M} \left[(\hat{\rho}_{Hm})_B + L_m \right] \ (\text{for } \zeta_y > 0), \tag{68}$$

$$\hat{\phi}_{Km} = -(\hat{\phi}_{Hm})_B \tag{69}$$

at $\eta = 0$, and

$$\hat{f}_{Km} \to 0, \quad \hat{\phi}_{Km} \to 0 \tag{70}$$

as $\eta \to \infty$. Here, $m = 1, 2$, and I_m and L_m are given by

$$I_1 = 0, \tag{71a}$$

$$I_2 = -\frac{1}{2} \left(\frac{d\hat{\phi}_{H0}}{dy} \right)_B \frac{\partial \hat{f}_{K1}}{\partial \zeta_y} + \frac{d\hat{\phi}_{K1}}{d\eta} \frac{\partial}{\partial \zeta_y} \left[(\hat{f}_{H1})_B + \left(\frac{d\hat{f}_{H0}}{dy} \right)_B \eta + \hat{f}_{K1} \right] - \frac{1}{(\hat{\tau})_B^2} \left(\frac{d\hat{\tau}}{dy} \right)_B \eta (\hat{\rho}_{K1} \mathcal{M} - \hat{f}_{K1}), \tag{71b}$$

and

$$L_1 = 2(\widetilde{J}_{H1})_B \zeta_y, \tag{72a}$$

$$L_2 = 2(\widetilde{J}_{H2})_B \zeta_y + 2(\hat{\tau})_B \left(\frac{d\hat{\phi}_{H0}}{dy} \right)_B (\widetilde{J}_{H1})_B \left(\zeta_y^2 - \frac{1}{2} \right), \tag{72b}$$

where

$$\widetilde{J}_{H1} = -\frac{1}{2} \hat{\tau} \left(\frac{d\hat{\rho}_{H0}}{dy} - \hat{\rho}_{H0} \frac{d\hat{\phi}_{H0}}{dy} \right), \tag{73}$$

$$\widetilde{J}_{H2} = -\frac{1}{2} \hat{\tau} \left(\frac{d\hat{\rho}_{H1}}{dy} - \hat{\rho}_{H0} \frac{d\hat{\phi}_{H1}}{dy} - \hat{\rho}_{H1} \frac{d\hat{\phi}_{H0}}{dy} \right). \tag{74}$$

We observe that the equations and boundary conditions for $\hat{\phi}_{Km}$ ($m = 1, 2$), i.e., Eqs. (67), (69), and (70), are in closed form. Therefore, we first consider the problem for $\hat{\phi}_{Km}$. We claim that $(\hat{\phi}_{Hm})_B$ vanishes. Indeed, integrating Eq. (67) and employing the condition (70), we find

$$\hat{\phi}_{Km} = 0, \tag{75}$$

for all $\eta \geq 0$. Therefore, in order for the boundary-value problem to have a solution, $(\hat{\phi}_{Hm})_B$ in Eq. (69) must satisfy

$$(\hat{\phi}_{Hm})_B = 0 \tag{76}$$

($m = 1, 2$). This gives the boundary condition for Eqs. (43d) and (44d). Moreover, it implies, by (61), that

$$\hat{E}_{K0} = \hat{E}_{K1} = 0.$$

Next, we consider the problem for $\hat{f}_{Km}$ ($m = 1, 2$). Let us introduce the following variables:

$$\Phi_{Km} = \frac{\hat{f}_{Km}}{\mathcal{M}}, \ \eta' = \frac{\eta}{(\hat{\tau})_B}, \ y' = \frac{y}{(\hat{\tau})_B}.$$

Then the equation and boundary conditions for $\hat{f}_{Km}$, Eqs. (66) [with Eq. (76)], (68), (70), can be transformed into

$$\zeta_y \frac{\partial \Phi_{Km}}{\partial \eta'} = \hat{\rho}_{Km} - \Phi_{Km} + \mathcal{I}_m, \tag{77}$$

$$\Phi_{Km} = -(\hat{\rho}_{Hm})_B + \mathcal{L}_m \quad (\text{for } \zeta_y > 0, \text{ at } \eta' = 0), \tag{78}$$

$$\Phi_{Km} \to 0 \quad (\text{as } \eta' \to \infty), \tag{79}$$

where

$$\mathcal{I}_1 = 0, \tag{80a}$$

$$\mathcal{I}_2 = -\frac{1}{2}\Big(\frac{d\hat{\phi}_{H0}}{dy'}\Big)_B\Big(\frac{\partial\Phi_{K1}}{\partial\zeta_y} - 2\zeta_y\Phi_{K1}\Big) - \frac{1}{(\hat{\tau})_B}\Big(\frac{d\hat{\tau}}{dy'}\Big)_B\eta'(\hat{\rho}_{K1} - \Phi_{K1}), \tag{80b}$$

and

$$\mathcal{L}_1 = -2(\widetilde{J}_{H1})_B\zeta_y, \tag{81a}$$

$$\mathcal{L}_2 = -2(\widetilde{J}_{H1})_B\zeta_y - 2\Big(\frac{d\hat{\phi}_{H0}}{dy'}\Big)_B(\widetilde{J}_{H1})_B\Big(\zeta_y^2 - \frac{1}{2}\Big). \tag{81b}$$

Equations (77)–(79) form a one-dimensional boundary-value problem (half-space problem) of the linear semiconductor Boltzmann equation with a relaxation-time collision operator. The problem is also called the Milne problem. Concerning the problem with more general $\mathcal{I}_m$ and $\mathcal{L}_m$ [not necessarily restricted to the forms of $\mathcal{I}_m$ and $\mathcal{L}_m$ given in Eqs. (80) and (81)], the following statements holds: (i) For a given function $\mathcal{I}_m(\eta', \zeta_y, \zeta_2, \zeta_3)$ which satisfies $\int \mathcal{I}_m \mathcal{M} d^3\bar{\zeta} = 0$ and $\mathcal{I}_m \to 0$ (rapidly) as $\eta' \to 0$ and a given function $\mathcal{L}_m(\eta', \zeta_y, \zeta_2, \zeta_3)$, the solution Φ_{Km} is determined together with the constant $(\hat{\rho}_{Hm})_B$ contained in the boundary condition (78). (ii) $\int \zeta_y \Phi_{Km}\mathcal{M} d^3\bar{\zeta} = 0$ holds [this is obvious from (77) and (79)]. The boundary value $(\hat{\rho}_{Hm})_B$ thus determined gives the boundary condition for the fluid-dynamic equations (43a), (43b), (44a), and (44b). We mention that the property of the half-space problem described above has been proved for the linear semiconductor Boltzmann equation with a general collision operator in the homogeneous case (i.e., $\mathcal{I}_m = 0$) in Ref. [24]. It follows from (ii) and Eq. (62) that

$$\hat{J}_{Km} = 0 \quad (m = 1, 2). \tag{82}$$

In view of the expressions for $\mathcal{I}_m$ and $\mathcal{L}_m$, we can seek the solutions Φ_{K1} and Φ_{K2} in the form

$$\begin{bmatrix} \Phi_{K1} \\ (\hat{\rho}_{H1})_B \end{bmatrix} = \begin{bmatrix} \psi_1 \\ \xi_1 \end{bmatrix} (\widetilde{J}_{H1})_B \tag{83}$$

and

$$\begin{bmatrix} \Phi_{K2} \\ (\hat{\rho}_{H2})_B \end{bmatrix} = \begin{bmatrix} \psi_{2a} \\ \xi_{2a} \end{bmatrix} (\widetilde{J}_{H2})_B - \begin{bmatrix} \psi_{2b} \\ \xi_{2b} \end{bmatrix} \Big(\frac{d\hat{\phi}_{H0}}{dy'}\Big)_B(\widetilde{J}_{H1})_B + \begin{bmatrix} \psi_{2c} \\ \xi_{2c} \end{bmatrix} \frac{1}{(\hat{\tau})_B}\Big(\frac{d\hat{\tau}}{dy'}\Big)_B(\widetilde{J}_{H1})_B, \tag{84}$$

where ξ_1, ξ_{2a}, ξ_{2b}, and ξ_{2c} are constants to be determined together with the solutions. Each problem is analyzed numerically to determine $(\xi_\alpha, \psi_\alpha)$ $(\alpha = 1, 2a, 2b, 2c)$. We refer to Appendix D for a brief comment on the numerical solution of this problem. Once we obtain $(\xi_\alpha, \psi_\alpha)$ and thus Φ_{K1} and Φ_{K2}, the Knudsen-layer parts of the electron number density, the mean flow velocity, and the electron temperature are calculated with the aid of Eqs. (C1a)–(C2b).

Before presenting the boundary conditions and the Knudsen-layer parts of the fluid-dynamic equations (42a)–(44d), we comment on the second-order Knudsen-layer part of the electric field $\hat{E}_{K2}$. Since $\hat{E}_{K2}$ is determined by $\hat{\phi}_{K3}$ [see Eq. (61) with $m = 3$], we need some information from the Knudsen-layer problem of order ϵ^3 in order to obtain $\hat{E}_{K2}$. Namely, the Knudsen-layer equation for $\hat{\phi}_{K3}$ is given by

$$\lambda^2\frac{d^2\hat{\phi}_{K3}}{d\eta^2} = \hat{\rho}_{K1}.$$

Since $\hat{\rho}_{K1}$ is already known from the lower order Knudsen-layer problem, integration of the above equation under the boundary condition $\hat{\phi}_{K3} \to 0$ (as $\eta \to \infty$) yields an expression of $d\hat{\phi}_{K3}/d\eta$. Then, Eq. (61) for $m = 3$ immediately gives the desired formula for $\hat{E}_{K2}$. Incidentally, the integration of the Knudsen-layer equation for $\hat{f}_{K3}$ with respect to $(\zeta_y, \zeta_2, \zeta_3)$ over the whole space yields $\hat{J}_{K3} = \int \zeta_1 \hat{f}_{K3} d\bar{\zeta} = 0$. This relation (and the relation between $\hat{u}_{K3}$ and $\hat{f}_{K3}$ which is not given in Appendix C) is used to derive the expression of $\hat{u}_{K3}$ given in Eq. (91b) below. In general, from the analysis of the Knudsen-layer problem for $(\hat{f}_{Km}, \hat{\phi}_{Km})$, we obtain the boundary values $(\hat{\rho}_{Hm})_B$ and $(\hat{\phi}_{Hm})_B$ and the Knudsen-layer parts of $\hat{\phi}_{Km}$, h_{Km} ($h = \hat{\rho}$, $\hat{J}$, $\hat{u}$, or $\hat{T}$), and $\hat{E}_{Km-1}$.

Finally, we summarize the boundary conditions for the fluid-dynamic equations and the computed Knudsen-layer parts. The boundary conditions for Eqs. (43a)–(44d) are given by

$$(\hat{\rho}_{H1})_B = \xi_1(\widetilde{J}_{H1})_B, \tag{85a}$$

$$(\hat{\phi}_{H1})_B = 0, \tag{85b}$$

and

$$(\hat{\rho}_{H2})_B = \xi_{2a}(\widetilde{J}_{H2})_B - \xi_{2b}(\hat{\tau})_B\Big(\frac{d\hat{\phi}_{H0}}{dy}\Big)_B \times (\widetilde{J}_{H1})_B + \xi_{2c}\Big(\frac{d\hat{\tau}}{dy}\Big)_B(\widetilde{J}_{H1})_B, \tag{86a}$$

$$(\hat{\phi}_{H2})_B = 0, \tag{86b}$$

where the numerical values of the slip coefficients ξ_1, ξ_{2a}, ξ_{2b}, and ξ_{2c} are given by

$$\xi_1 = \xi_{2a} = -2.03238284, \quad \xi_{2b} = 1.03264500, \quad \text{and} \quad \xi_{2c} = 0. \tag{87}$$

The Knudsen-layer parts are as follows. For $m = 0$ we have

$$\hat{E}_{K0} = 0; \tag{88}$$

for $m = 1$,

$$\hat{\rho}_{K1} = \Omega_1(\eta')(\widetilde{J}_{H1})_B, \tag{89a}$$

$$\hat{T}_{K1} = -\frac{1}{3}\frac{(\widetilde{J}_{H1})_B}{(\hat{\rho}_{H0})_B}\Omega_1(\eta'), \tag{89b}$$

$$\hat{\phi}_{K1} = \hat{E}_{K1} = \hat{J}_{K1} = \hat{u}_{K1} = 0; \tag{89c}$$

for $m = 2$,

$$\hat{\rho}_{K2} = \Omega_1(\eta')(\widetilde{J}_{H2})_B - [\Omega_2(\eta') + \Omega_3(\eta')](\hat{\tau})_B\Big(\frac{d\hat{\phi}_{H0}}{dy}\Big)_B \times (\widetilde{J}_{H1})_B + \Omega_4(\eta')\Big(\frac{d\hat{\tau}}{dy}\Big)_B(\widetilde{J}_{H1})_B, \tag{90a}$$

$$\begin{aligned}\hat{T}_{K2} = -\frac{1}{3(\hat{\rho}_{H0})_B}\Big\{&\Omega_1(\eta')(\widetilde{J}_{H2})_B \\ &- \Big[\Omega_2(\eta') + \Omega_3(\eta') - \int_{\eta'}^{\infty}\Omega_1(s)ds\Big] \\ &\times (\hat{\tau})_B\Big(\frac{d\hat{\phi}_{H0}}{dy}\Big)_B(\widetilde{J}_{H1})_B \\ &+ \Omega_4(\eta')\Big(\frac{d\hat{\tau}}{dy}\Big)_B(\widetilde{J}_{H1})_B \\ &- \Big[(\hat{\rho}_{H1})_B + \big(\frac{d\hat{\rho}_{H0}}{dy}\big)_B\eta \\ &+ \Omega_1(\eta')(\widetilde{J}_{H1})_B\Big]\frac{(\widetilde{J}_{H1})_B}{(\hat{\rho}_{H0})_B}\Omega_1(\eta')\Big\},\end{aligned} \tag{90b}$$

$$\hat{u}_{K2} = -\Omega_1(\eta')(\hat{u}_{H1})_B(\widetilde{J}_{H1})_B/(\hat{\rho}_{H0})_B, \tag{90c}$$

$$\hat{E}_{K2} = \pm\frac{(\hat{\tau})_B}{\lambda^2}(\widetilde{J}_{H1})_B\int_{\eta'}^{\infty}\Omega_1(s)ds, \tag{90d}$$

$$\hat{\phi}_{K2} = \hat{J}_{K2} = 0; \tag{90e}$$

and for $m = 3$,

$$\hat{J}_{K3} = 0, \tag{91a}$$

$$\begin{aligned}\hat{u}_{K3} = -\Omega_1(\eta')\frac{(\hat{u}_{H1})_B}{(\hat{\rho}_{H0})_B}\Big\{&(\widetilde{J}_{H2})_B \\ &- \Big[\frac{(\hat{\rho}_{H1})_B}{(\hat{\rho}_{H0})_B} - \frac{(\hat{u}_{H2})_B}{(\hat{u}_{H1})_B} \\ &+ 2\Big(\frac{d\ln\hat{\rho}_{H0}}{dy}\Big)_B\eta\Big](\widetilde{J}_{H1})_B\Big\} \\ &+ [\Omega_2(\eta') + \Omega_3(\eta')](\hat{\tau})_B\Big(\frac{d\hat{\phi}_{H0}}{dy}\Big)_B \\ &\times \frac{(\hat{u}_{H1})_B}{(\hat{\rho}_{H0})_B}(\widetilde{J}_{H1})_B \\ &- \Omega_4(\eta')\Big(\frac{d\hat{\tau}}{dy}\Big)_B\frac{(\hat{u}_{H1})_B}{(\hat{\rho}_{H0})_B}(\widetilde{J}_{H1})_B \\ &+ (\hat{u}_{H1})_B\Big[\frac{(\widetilde{J}_{H1})_B}{(\hat{\rho}_{H0})_B}\Omega_1(\eta')\Big]^2.\end{aligned} \tag{91b}$$

The values of the so-called Knudsen-layer functions $\Omega_m(\eta')$ ($m = 1, 2, 3, 4$) as well as those of the integral $\int_{\eta'}^{\infty}\Omega_1(s)ds$ are displayed in Table I.

IV. NUMERICAL SIMULATION OF THE ELECTRON FLOW IN AN n^+nn^+ DIODE FOR SMALL KNUDSEN NUMBERS

In this section, we consider an electron flow induced in a semiconductor with a doping profile corresponding to a one-dimensional n^+nn^+ diode. We make a numerical comparison between the asymptotic solution of the fluid-dynamic system obtained in the previous section and the direct numerical solution of the Boltzmann-Poisson system.

A. Comments on the numerical method

The similarity between the present relaxation-time semiconductor Boltzmann equation and the Boltzmann equation for rarefied gases with relaxation collision terms, like the BGK model [20–22], allows us to employ numerical techniques developed for the BGK-Boltzmann equation in order to solve the semiconductor problem. For example, we can eliminate the independent variables ζ_2 and ζ_3 from the system (see Ref. [25]). For this, let us introduce a function (the so-called marginal velocity distribution function) $\mathcal{G}(x_1, \zeta_1)$ by

$$\mathcal{G}(x_1, \zeta_1) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \hat{f} d\zeta_2 d\zeta_3.$$

Integrating Eq. (12) with respect to ζ_2 and ζ_3 over the whole range of the variables gives a system of equations for $(\mathcal{G}, \hat{\phi})$. The corresponding boundary conditions for $\mathcal{G}$ are obtained from Eqs. (19) and (21) in a similar way. The resulting system for $(\mathcal{G}, \hat{\phi})$ is given by

$$\zeta_1 \frac{\partial \mathcal{G}}{\partial x_1} - \frac{1}{2}\hat{E}\frac{\partial \mathcal{G}}{\partial \zeta_1} = \frac{2}{\sqrt{\pi}\mathrm{Kn}} \frac{1}{\hat{\tau}} (\frac{\hat{\rho} e^{-\zeta_1^2}}{\pi^{1/2}} - \mathcal{G}), \tag{92}$$

$$\hat{\rho} = \int_{-\infty}^{\infty} \mathcal{G} d\zeta_1, \tag{93}$$

$$\lambda^2 \frac{d^2 \hat{\phi}}{dx_1^2} = \hat{\rho} - \hat{C}, \tag{94}$$

$$\hat{E} = -\frac{d\hat{\phi}}{dx_1} \tag{95}$$

with the boundary conditions

$$\mathcal{G} = \frac{\hat{C}(0)}{\pi^{1/2}} \exp(-\zeta_1^2) \quad \text{for } \zeta_1 > 0, \tag{96}$$

$$\hat{\phi} = \hat{\phi}_A \tag{97}$$

at $x_1 = 0$ and

$$\mathcal{G} = \frac{\hat{C}(1)}{\pi^{1/2}} \exp(-\zeta_1^2) \quad \text{for } \zeta_1 < 0, \tag{98}$$

$$\hat{\phi} = \hat{\phi}_B \tag{99}$$

at $x_1 = 1$. The system (92)–(99) is solved numerically by a finite difference method similar to that used in Ref. [26] but including an additional step to solve the Poisson equation.

It should be noted that $\hat{T}$ cannot be expressed in terms of $\mathcal{G}$ alone [cf. Eq. (24)]. In order to compute $\hat{T}$, we introduce, in addition to $\mathcal{G}$, the marginal velocity distribution function $\mathcal{H} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(\zeta_2^2+\zeta_3^2)\hat{f}d\zeta_2\zeta_3$. The equation and the boundary conditions for $\mathcal{H}$ are obtained in the same way as those for $\mathcal{G}$. It turns out that the form of the equation and boundary condition for $\mathcal{H}$ coincides with that for $\mathcal{G}$, and therefore, $\mathcal{H} = \mathcal{G}$ holds. Thus, we can compute $\hat{T}$ from the solution $\mathcal{G}$.

B. Numerical results

The semiconductor device is specified by the doping profile $C(X_1)$ and the relaxation time $\tau(X_1)$. We choose

$$C(X_1) = N_d + \frac{N_d - N_c}{2} \times \left[\tanh\left(40\frac{X_1 - L + D}{L}\right) - \tanh\left(40\frac{X_1 - D}{L}\right)\right], \quad (100)$$

[see Fig. 1(a)] modeling an n^+nn^+ diode. Here, the positive constants N_d, $N_c(< N_d)$, and $D(< L/2)$ denote the doping concentration of the highly doped (n^+) region, that of the channel (n) region, and the position of the junctions (the doping profile is symmetric with respect to $X_1 = L/2$), respectively. The relaxation time is assumed to be constant, $\tau = \tau_0$, such that $\hat{\tau} = 1$.

We take N_d as the reference value of the electron number density, i.e., $\rho_0 = N_d$ (see the first sentence of Sec. II C). The present problem is then characterized by the following parameters:

$$\mathrm{Kn}, \quad \lambda, \quad \frac{\phi_B - \phi_A}{U_T}, \quad \frac{N_c}{N_d}, \quad \frac{D}{L}. \quad (101)$$

For convenience, we introduce $\phi_{app} = \phi_B - \phi_A$.

We first present some numerical results for a doping profile with $N_c/N_d = 0.2$ and $D/L = 0.25$ [the solid line in Fig. 1(b)]. Figures 2–4 show the solutions of the fluid-dynamic equations (42a)–(44d) under the boundary conditions (49), (50), (85a)–(86b) for various values of ϕ_{app} and for $\lambda = 1$ and $\lambda = 0.5$.

Once we obtain $\hat{\rho}_{Hm}$, $\hat{E}_{Hm}$, and $\hat{\phi}_{Hm}$, the asymptotic solution is readily obtained from Eqs. (56), (57), (52), (27), (28), (26), (58), (59), and (55) by specifying ϵ (or Kn). The result is shown in Figs. 5 and 6 for $\phi_{app}/U_T = 1$ and 3 in the cases $\lambda = 1$ (Fig. 5) and $\lambda = 0.5$ (Fig. 6), where the asymptotic solution of u (up to order Kn^3) and that of T (up to order Kn^2) are also included [the corresponding Hilbert solutions are obtained from $\hat{\rho}_{Hm}$ and $\hat{E}_{Hm}$ ($m = 0, 1, 2$) with the aid of the formulas given in Appendix B]. In Figs. 5 and 6, the direct numerical solutions of the original Boltzmann-Poisson system (12)–(16), (19)–(22) are also shown.

The numerical results show that the asymptotic solutions are in good agreement with the direct numerical solutions of the Boltzmann-Poisson system. However, there are some appreciable differences in the case Kn = 0.1. The difference increases with the applied potentials ϕ_{app} and is more pronounced at the right boundary. This can be explained as follows.

First, the values of $\hat{\rho}_{H1}$ and $\hat{\rho}_{H2}$ as well as their gradients near $X_1 = L$ are increasing in ϕ_{app}/U_T. This results in a large value of $\hat{u}_{H2}$ and $\hat{u}_{H3}$ [see Eqs. (B3) and (B4)]. Second, the second-order Knudsen-layer correction contains product terms depending on $(d\hat{\phi}_{H0}/dy)_B$, $(\tilde{J}_{H1})_B$, and $(\hat{u}_{H1})_B$ which are increasing in ϕ_{app}/U_T. Therefore, the Knudsen-layer part for Kn = 0.1 is not well confined near the boundary. For these reasons, the validity of the asymptotic expansion is resticted to rather small values of Kn. We mention that this situation is very similar to that in Ref. [19], where a similar type of asymptotic expansion is carried out on the basis of the BGK model to investigate the behavior of a rarefied gas flow between two parallel plates driven by a uniform external force parallel to the plates.

In Figs. 7 and 8, the current-voltage characteristics obtained from the asymptotic solutions are compared with those obtained from the numerical solution of the Boltzmann-Poisson system for various Kn and λ. For the doping profile we choose again $N_c/N_d = 0.2$ and $D/L = 0.25$.

In the figures, we have included not only the asymptotic solution up to the order Kn^3, i.e., $\hat{J}^{(3)} = \hat{J}_{H1}\epsilon + \hat{J}_{H2}\epsilon^2 + \hat{J}_{H3}\epsilon^3$, but also the asymptotic solutions up to first and second order, $\hat{J}^{(1)} = \hat{J}_{H1}\epsilon$ and $\hat{J}^{(2)} = \hat{J}_{H1}\epsilon + \hat{J}_{H2}\epsilon^2$, for comparison. For Kn = 0.02, the current density $\hat{J}^{(3)}$ gives a result very close to the current-voltage characteristic obtained from the Boltzmann-Poisson system in the entire range of ϕ_{app} shown in the figures. For Kn = 0.05 and 0.1, the difference between $\hat{J}^{(3)}$ and the current density from the Boltzmann-Poisson system becomes noticeable for smaller values of ϕ_{app} (roughly $\phi_{app}/U_T > 5$). The current density $\hat{J}^{(1)}$, which corresponds to the solution of the drift-diffusion equation under the conventional non-slip boundary condition, does not predict correctly the current density of the Boltzmann-Poisson system except for very small values of ϕ_{app}.

Next, we show some results for a different doping profile. In Fig. 9, we show the asymptotic solution of (ρ, E, ϕ) up to order Kn^2, together with the corresponding numerical solution of the Boltzmann-Poisson system, for various values of Kn with $(N_c/N_d, D/L) = (0.1, 0.25)$ [the dashed line in Fig. 1 (b)]. In Fig. 10, we show the same quantities for the same values of Kn with $(N_c/N_d, D/L) = (0.2, 0.1)$ [the dash-dotted line in Fig. 1 (b)]. The dependence of these quantities on N_c/N_d and D/L is rather weak except for the electric field E, whose profile clearly depends strongly on the position of the junctions given by D/L. The asymptotic solutions u (up to order Kn^3) and T (up to order Kn^2) as well as the Boltzmann-Poisson solutions, computed with the parameters used in Figs. 9 and 10, are similar to those presented in Fig. 5.

Finally, we show some results when λ is relatively small. Figure 11 shows the asymptotic solution of (ρ, E, ϕ, u, T) (up to order Kn^2 for ρ, E, ϕ, and T, and up to order Kn^3 for u), as well as the Boltzmann-Poisson solutions, for various values of Kn for $\lambda = 0.2$. In Fig. 12, the corresponding current-voltage characteristics are displayed. We recall that the asymptotic analysis carried out in Sec. III assumes that the scaled Debye length is of order one. Therefore, the present asymptotic expansion is theoretically not applicable to the case of small λ. In spite of this fact, the asymptotic solutions presented in Figs. 11 and 12 exhibit good agreements with the corresponding numerical solutions of the Boltzmann-Poisson system.

V. CONCLUSION

In this paper, we have considered the flow of electrons induced in a semiconductor between two parallel plane contacts. The distribution of the electrons is given by the semiconductor Boltzmann equation with a relaxation-time collision operator of BGK-type. Applying a Hilbert expansion method and Knudsen-layer corrections to the Boltzmann equation, we have derived a drift-diffusion system with higher-order boundary conditions improving results of Ref. [8]. The numerical results show a good agreement between the solution of the drift-diffusion model up to order Kn^2 and that of the Boltzmann-Poisson system if the Knudsen number is not too large and if the Debye length is of the same order as the device length.

This is the first step of deriving higher-order boundary conditions for fluid-dynamic equations for semiconductors. We expect that our results can be improved by considering more moments in the Boltzmann equation – leading to energy-transport or hydrodynamic models –, a more general geometry, or improved kinetic inflow boundary conditions [10], for instance.

VI. ACKNOWLEDGEMENT

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APPENDIX A: EXPLICIT FORM OF $\hat{u}_{Hm}$ AND $\hat{T}_{Hm}$

We present the macroscopic variables $\hat{u}_{Hm}$ and $\hat{T}_{Hm}$ in terms of the distribution functions $\hat{f}_{Hm}$. For $m = 0$, we obtain

$$\hat{u}_{H0} = \frac{1}{\hat{\rho}_{H0}} \int \zeta_1 \hat{f}_{H0} d^3\zeta, \tag{A1a}$$

$$\hat{T}_{H0} = \frac{2}{3\hat{\rho}_{H0}} \int (\zeta_i - \hat{u}_{H0}\delta_{i1})^2 \hat{f}_{H0} d^3\zeta; \tag{A1b}$$

for $m=1$,

$$\hat{u}_{H1} = \frac{1}{\hat{\rho}_{H0}} \int (\zeta_1 - \hat{u}_{H0}) \hat{f}_{H1} d^3\zeta, \quad \text{(A2a)}$$

$$\hat{T}_{H1} = \frac{2}{3\hat{\rho}_{H0}} \int (\zeta_i - \hat{u}_{H0}\delta_{i1})^2 \hat{f}_{H1} d^3\zeta - \Big(\frac{\hat{\rho}_{H1}}{\hat{\rho}_{H0}}\Big)\hat{T}_{H0}; \quad \text{(A2b)}$$

for $m=2$,

$$\hat{u}_{H2} = \frac{1}{\hat{\rho}_{H0}} \int (\zeta_1 - \hat{u}_{H0}) \hat{f}_{H2} d^3\zeta - \Big(\frac{\hat{\rho}_{H1}}{\hat{\rho}_{H0}}\Big)\hat{u}_{H1}, \quad \text{(A3a)}$$

$$\hat{T}_{H2} = \frac{2}{3\hat{\rho}_{H0}} \int (\zeta_i - \hat{u}_{H0}\delta_{i1})^2 \hat{f}_{H2} d^3\zeta - \frac{2}{3}(\hat{u}_{H1})^2 - \Big(\frac{\hat{\rho}_{H1}}{\hat{\rho}_{H0}}\Big)\hat{T}_{H1} - \Big(\frac{\hat{\rho}_{H2}}{\hat{\rho}_{H0}}\Big)\hat{T}_{H0}; \quad \text{(A3b)}$$

and finally, for $m=3$,

$$\hat{u}_{H3} = \frac{1}{\hat{\rho}_{H0}} \int (\zeta_1 - \hat{u}_{H0}) \hat{f}_{H3} d^3\zeta - \Big(\frac{\hat{\rho}_{H1}}{\hat{\rho}_{H0}}\Big)\hat{u}_{H2} - \Big(\frac{\hat{\rho}_{H2}}{\hat{\rho}_{H0}}\Big)\hat{u}_{H1}, \quad \text{(A4a)}$$

$$\hat{T}_{H3} = \frac{2}{3\hat{\rho}_{H0}} \int (\zeta_i - \hat{u}_{H0}\delta_{i1})^2 \hat{f}_{H3} d^3\zeta - \frac{2}{3}\Big(\frac{\hat{\rho}_{H1}}{\hat{\rho}_{H0}}\Big)(\hat{u}_{H1})^2 - \frac{4}{3}\hat{u}_{H1}\hat{u}_{H2} - \Big(\frac{\hat{\rho}_{H1}}{\hat{\rho}_{H0}}\Big)\hat{T}_{H2} - \Big(\frac{\hat{\rho}_{H2}}{\hat{\rho}_{H0}}\Big)\hat{T}_{H1} - \Big(\frac{\hat{\rho}_{H3}}{\hat{\rho}_{H0}}\Big)\hat{T}_{H0}. \quad \text{(A4b)}$$

APPENDIX B: MEAN FLOW VELOCITY AND ELECTRON TEMPERATURE OF THE HILBERT SOLUTION

We summarize the Hilbert part of the mean flow velocity,

$$\hat{u}_{H0} = 0, \quad \text{(B1)}$$

$$\hat{u}_{H1} = -\frac{1}{2}\hat{\tau}\Big(\frac{d\ln\hat{\rho}_{H0}}{dx_1} + \hat{E}_{H0}\Big), \quad \text{(B2)}$$

$$\hat{u}_{H2} = -\frac{1}{2}\hat{\tau}\Big(\frac{\hat{\rho}_{H1}}{\hat{\rho}_{H0}}\frac{d\ln(\hat{\rho}_{H1}/\hat{\rho}_{H0})}{dx_1} + \hat{E}_{H1}\Big), \quad \text{(B3)}$$

$$\hat{u}_{H3} = -\frac{1}{2}\hat{\tau}\Big[\frac{\hat{\rho}_{H2}}{\hat{\rho}_{H0}}\frac{d\ln(\hat{\rho}_{H2}/\hat{\rho}_{H0})}{dx_1} - \Big(\frac{\hat{\rho}_{H1}}{\hat{\rho}_{H0}}\Big)^2\frac{d\ln(\hat{\rho}_{H1}/\hat{\rho}_{H0})}{dx_1} + \hat{E}_{H2} - 2\hat{u}_{H1}\frac{d}{dx_1}(\hat{\tau}\hat{E}_{H0})\Big], \quad \text{(B4)}$$

and of the electron temperature,

$$\hat{T}_{H0} = 1, \quad \text{(B5)}$$

$$\hat{T}_{H1} = 0, \quad \text{(B6)}$$

$$\hat{T}_{H2} = -\frac{2}{3}\hat{\tau}\hat{E}_{H0}\hat{u}_{H1} - \frac{2}{3}\hat{u}_{H1}^2, \quad \text{(B7)}$$

$$\hat{T}_{H3} = -\frac{2}{3}\hat{\tau}\big(\hat{E}_{H0}\hat{u}_{H2} + \hat{E}_{H1}\hat{u}_{H1}\big) - \frac{4}{3}\hat{u}_{H1}\hat{u}_{H2}. \quad \text{(B8)}$$

APPENDIX C: EXPLICIT FORM OF $\hat{u}_{Km}$ AND $\hat{T}_{Km}$

We summarize the expressions for $\hat{u}_{Km}$ and $\hat{T}_{Km}$ when $m=1$ and $m=2$. In the following expressions, Eqs. (B1), (B5), and (B6) are used. It holds for $m=1$,

$$\hat{u}_{K1} = \frac{1}{(\hat{\rho}_{H0})_B} \int \zeta_1 \hat{f}_{K1} d^3\bar{\zeta}, \quad \text{(C1a)}$$

$$\hat{T}_{K1} = \frac{2}{3(\hat{\rho}_{H0})_B} \int (\zeta^2 - \frac{3}{2})\hat{f}_{K1} d^3\bar{\zeta}; \quad \text{(C1b)}$$

and for $m = 2$,

$$\hat{u}_{K2} = \frac{1}{(\hat{\rho}_{H0})_B}\bigg\{ \int \zeta_1 \hat{f}_{K2} d^3\bar{\zeta} - \bigg[(\hat{\rho}_{H1})_B + \Big(\frac{d\hat{\rho}_{H0}}{dy}\Big)_B \eta\bigg] \hat{u}_{K1} - (\hat{u}_{H1})_B \hat{\rho}_{K1} - \hat{\rho}_{K1}\hat{u}_{K1}\bigg\}, \quad \text{(C2a)}$$

$$\hat{T}_{K2} = \frac{1}{(\hat{\rho}_{H0})_B}\bigg\{ \frac{2}{3}\int (\zeta^2 - \frac{3}{2})\hat{f}_{K2} d^3\bar{\zeta} - \bigg[(\hat{\rho}_{H1})_B + \Big(\frac{d\hat{\rho}_{H0}}{dy}\Big)_B \eta\bigg] \hat{T}_{K1} - \hat{\rho}_{K1}\hat{T}_{K1}\bigg\} - \frac{4}{3}(\hat{u}_{H1})_B \hat{u}_{K1} - \frac{2}{3}\hat{u}_{K1}^2. \quad \text{(C2b)}$$

Here, $\zeta^2 = \zeta_y^2 + \zeta_2^2 + \zeta_3^2$, $d^3\bar{\zeta} = d\zeta_y d\zeta_2 d\zeta_3$, and $(\ )_B$ denotes the value on the boundary ($y = 0$).

APPENDIX D: COMMENTS ON THE NUMERICAL SOLUTION OF THE KNUDSEN-LAYER PROBLEMS

Let us introduce the functions $g_m(\eta', \zeta_y, \zeta_2, \zeta_3)$ ($m = 1, 2, 3, 4$) which are the solutions of the following half-space boundary-value problems:

$$\zeta_y \frac{\partial g_m}{\partial \eta'} = \Omega_m - g_m + Ih_m, \quad \text{(D1)}$$

$$\Omega_m(\eta') = \int g_m \mathcal{M} d^3\bar{\zeta}, \quad \text{(D2)}$$

$$g_m = -a_m + \mathcal{J}_m \ (\text{for } \zeta_y > 0,\ \text{at } \eta' = 0), \quad \text{(D3)}$$

$$g_m \to 0, \quad (\text{as } \eta' \to \infty), \quad \text{(D4)}$$

with

$$Ih_1 = Ih_2 = 0, \quad Ih_3 = \frac{1}{2}\frac{\partial g_1}{\partial \zeta_y} - \zeta_y g_1, \quad Ih_4 = -\eta'(\Omega_1 - \psi_1)$$

and

$$\mathcal{J}_1 = -2\zeta_y, \quad \mathcal{J}_2 = 2\zeta_y^2, \quad \mathcal{J}_3 = \mathcal{J}_4 = 0.$$

Here, a_m are constants to be determined together with the solutions. Then (ξ_1, ψ_1), (ξ_{2a}, ψ_{2a}), (ξ_{2b}, ψ_{2b}), and (ξ_{2c}, ψ_{2c}) introduced in the main text [Eqs. (83) and (84)] are given by

$$(\xi_1, \psi_1) = (\xi_{2a}, \psi_{2a}) = (a_1, g_1),$$
$$(\xi_{2b}, \psi_{2b}) = (a_2 + a_3 - 1, g_2 + g_3),$$
$$(\xi_{2c}, \psi_{2c}) = (a_4, g_4).$$

Our aim is to obtain the slip coefficients a_m and the Knudsen-layer functions $\Omega_m(\eta')$ numerically. In this appendix, we give a brief comment on the numerical method.

By taking advantage of the simple expression of the relaxation-time collision operator, we can transform the equation and boundary conditions (D1)–(D4) to an integral equation for $\Omega_m(\eta')$. This is done by integrating Eq. (D1) formally under the boundary conditions (D3) and (D4), inserting the result into Eq. (D2), and carrying out the integration with respect to the velocity space. The result reads as

$$\pi^{1/2}\Omega_m(\eta') = \int_0^\infty \Omega_m(s) J_{-1}(|\eta' - s|) ds - a_m J_0(\eta') + S_m(\eta') \quad \text{(D6)}$$

with

$$S_1(\eta') = -2J_1(\eta'), \quad \text{(D7a)}$$

$$S_2(\eta') = 2J_2(\eta'), \quad \text{(D7b)}$$

$$S_3(\eta') = \frac{\pi^{1/2}}{2}\int_{\eta'}^\infty \Omega_1(s) ds - a_1 J_1(\eta') - 4J_2(\eta') + J_0(\eta'), \quad \text{(D7c)}$$

$$S_4(\eta') = \pi^{1/2}\int_{\eta'}^\infty \int_{s_2}^\infty \int_{s_1}^\infty \Omega_1(s_0) d^3s - \pi^{1/2}\int_{\eta'}^\infty \Omega_1(s) ds - \pi^{1/2}\eta'\Omega_1(\eta') - 2J_2(\eta'), \quad \text{(D7d)}$$

where $d^3s = ds_0 ds_1 ds_2$ and $J_n(x)$ is given by [27]

$$J_n(x) = \int_0^\infty t^n \exp\Big(-t^2 - \frac{x}{t}\Big) dt.$$

In deriving Eqs. (D7c) and (D7d), Eq. (D6) with $m = 1$ has been used. Since we have to deal with a function only depending on η', the problem simplifies significantly. Moreover, we can avoid the singularity contained in Ih_3 of the original form [note that g_1 or, in general, g_m has a discontinuity at $\eta' = 0$ with respect to ζ_y, i.e. $\lim_{\zeta_y \to 0+} g_1(0, \zeta_y, \zeta_2, \zeta_3) \neq \lim_{\zeta_y \to 0-} g_1(0, \zeta_y, \zeta_2, \zeta_3)$].

The integral equations (D6) for $m = 1$ and $m = 2$ are identical with those for the Knudsen-layer problems of rarefied gas flows around a boundary, derived from the linearized BGK model of the Boltzmann equation. More precisely, Eq. (D6) with $m = 1$ and $m = 2$, respectively, are identical with the equation for the Knudsen layer in shear flow over a flat wall [28–31] and in thermal-creep flow over a flat wall [32]. The numerical solutions to these equations are obtained in Refs. [12, 29–31] (also see Refs. [11, 17, 33]). Concerning $m = 3$, the same type of equation as Eq. (D6) has been solved numerically in Ref. [34]. Therefore, we can make use of the numerical data given in these references. For example, $[a_1, \Omega_1(x)] = [2k_0, 2Y_0(x)]$ in Refs. [11, 17, 33], $[a_2, \Omega_2(x)] = [1 - 4K_1, -2Y_1(x)]$ in Refs. [17, 33], and $[a_3, \Omega_3(x)] = [a_2 + 2k_0^2 + 8K_1, -2\widetilde{Y}_0(x) + 2k_0 Y_0(x) + 4Y_1(x)]$ in Ref. [17]. In the cited works, the integral equations are solved by means of a moment method devised by Sone [29, 35] and improved by Sone and Onishi [33, 36]. We employ this method in order to obtain the numerical solution of Eq. (D6) for $m = 4$ in the present study.

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TABLE I: Knudsen-layer functions. The Knudsen-layer functions generally have the singularity $\eta' \ln \eta'$ at $\eta' = 0$. Their coefficients are also shown.

η'	Ω_1	$-\Omega_2$	Ω_3	Ω_4	$\int_{\eta'}^{\infty} \Omega_1(s) ds$
0.00	0.61817	1.09553	0.78144	0.00000	0.46736
0.05	0.51453	0.96234	0.68806	0.00174	0.43948
0.10	0.45655	0.87923	0.62444	0.00492	0.41529
0.20	0.37755	0.75753	0.52794	0.01288	0.37386
0.30	0.32227	0.66650	0.45441	0.02147	0.33901
0.40	0.28006	0.59357	0.39526	0.02996	0.30898
0.50	0.24632	0.53303	0.34629	0.03804	0.28272
0.60	0.21858	0.48163	0.30500	0.04557	0.25951
0.70	0.19529	0.43730	0.26973	0.05248	0.23885
0.80	0.17546	0.39864	0.23931	0.05876	0.22034
0.90	0.15836	0.36460	0.21287	0.06442	0.20367
1.00	0.14349	0.33441	0.18975	0.06948	0.18859
1.20	0.11895	0.28333	0.15152	0.07790	0.16245
1.40	0.09965	0.24193	0.12154	0.08429	0.14066
1.60	0.08418	0.20788	0.09776	0.08892	0.12234
1.80	0.07160	0.17956	0.07874	0.09205	0.10680
2.00	0.06127	0.15580	0.06341	0.09392	0.09355
2.50	0.04235	0.11103	0.03657	0.09440	0.06799
3.00	0.02996	0.08056	0.02041	0.09079	0.05012
3.50	0.02157	0.05929	0.01059	0.08483	0.03737
4.00	0.01574	0.04413	0.00464	0.07770	0.02813
5.00	0.00867	0.02512	−0.00097	0.06263	0.01631
6.00	0.00494	0.01471	−0.00263	0.04878	0.00969
8.00	0.00173	0.00537	−0.00242	0.02798	0.00361
10.00	0.00065	0.00208	−0.00148	0.01543	0.00142
12.00	0.00026	0.00084	−0.00082	0.00835	0.00059
15.00	0.00007	0.00023	−0.00031	0.00328	0.00016
coeff. of $\eta' \ln \eta'$	0.79788	0.81080	0.40540	0	0

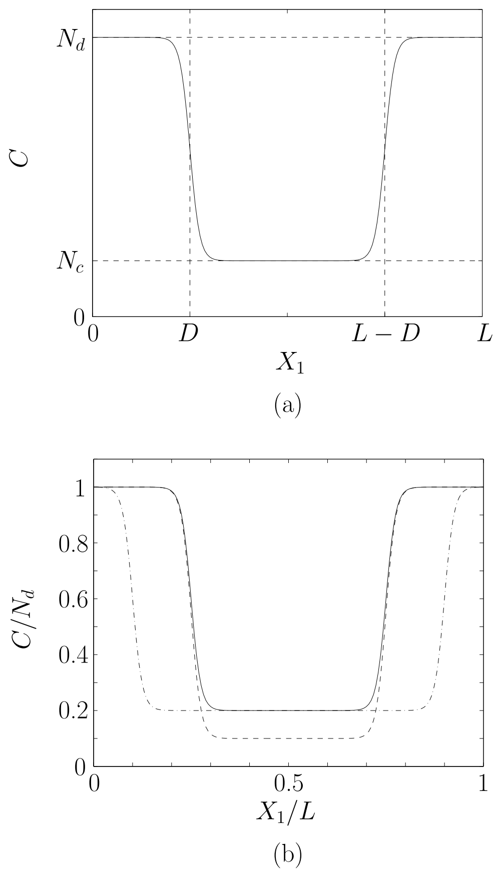


FIG. 1: (a) The doping profile C. (b) The doping profile C normalized by N_d with $N_c/N_d = 0.2$, $D/L = 0.25$ (solid line); $N_c/N_d = 0.1$, $D/L = 0.25$ (dashed line); $N_c/N_d = 0.2$, $D/L = 0.1$ (dash-dotted line).

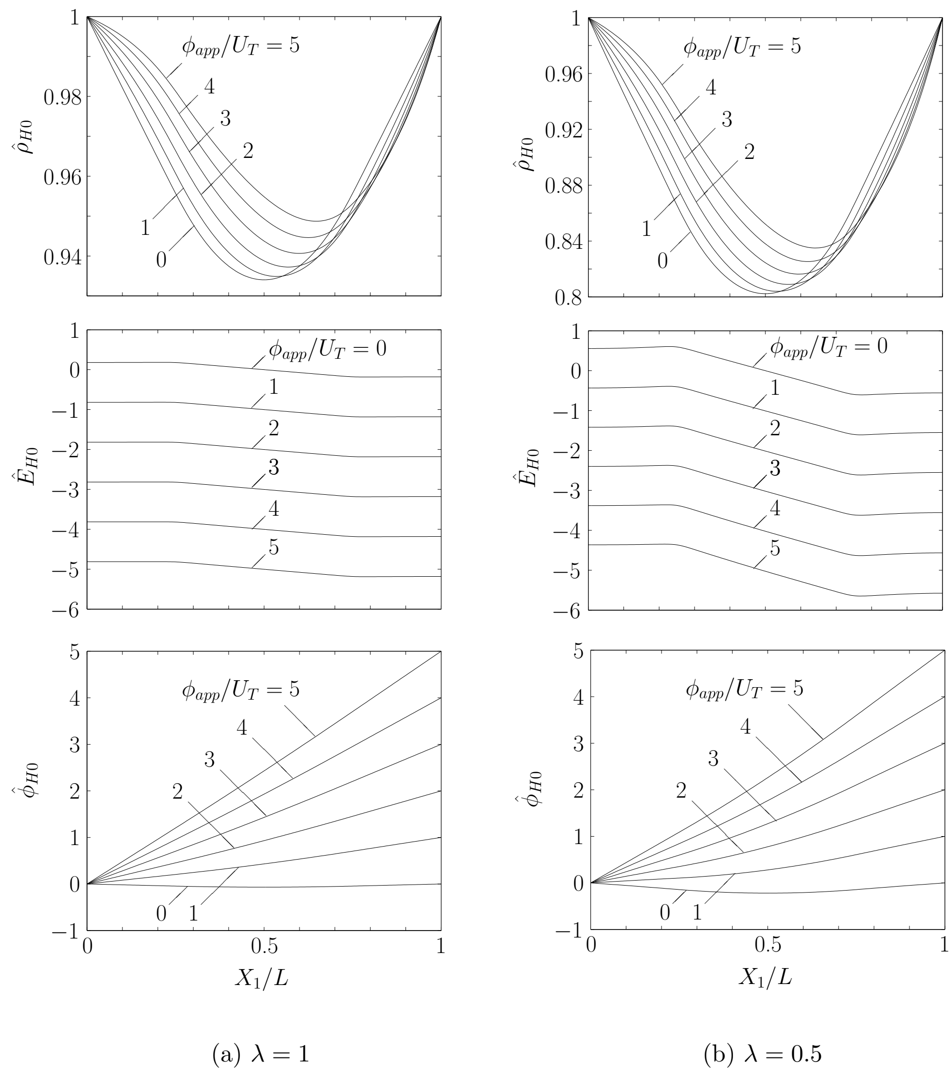
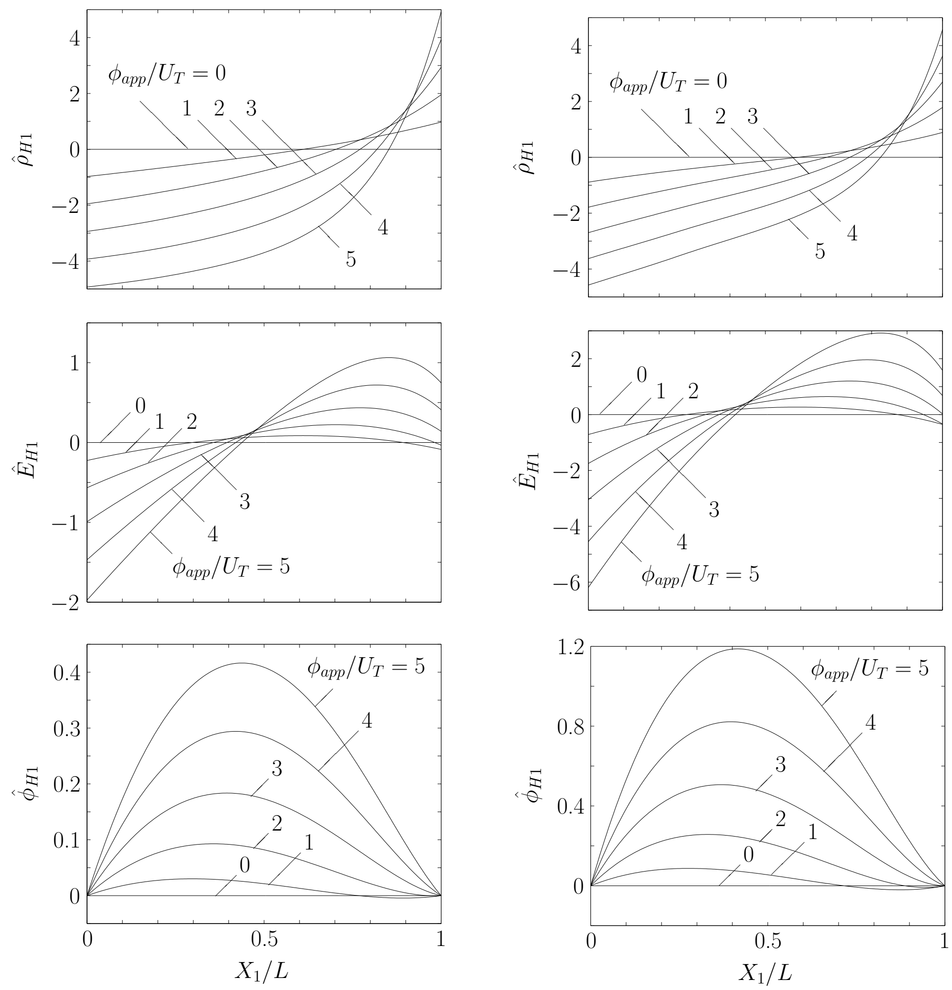
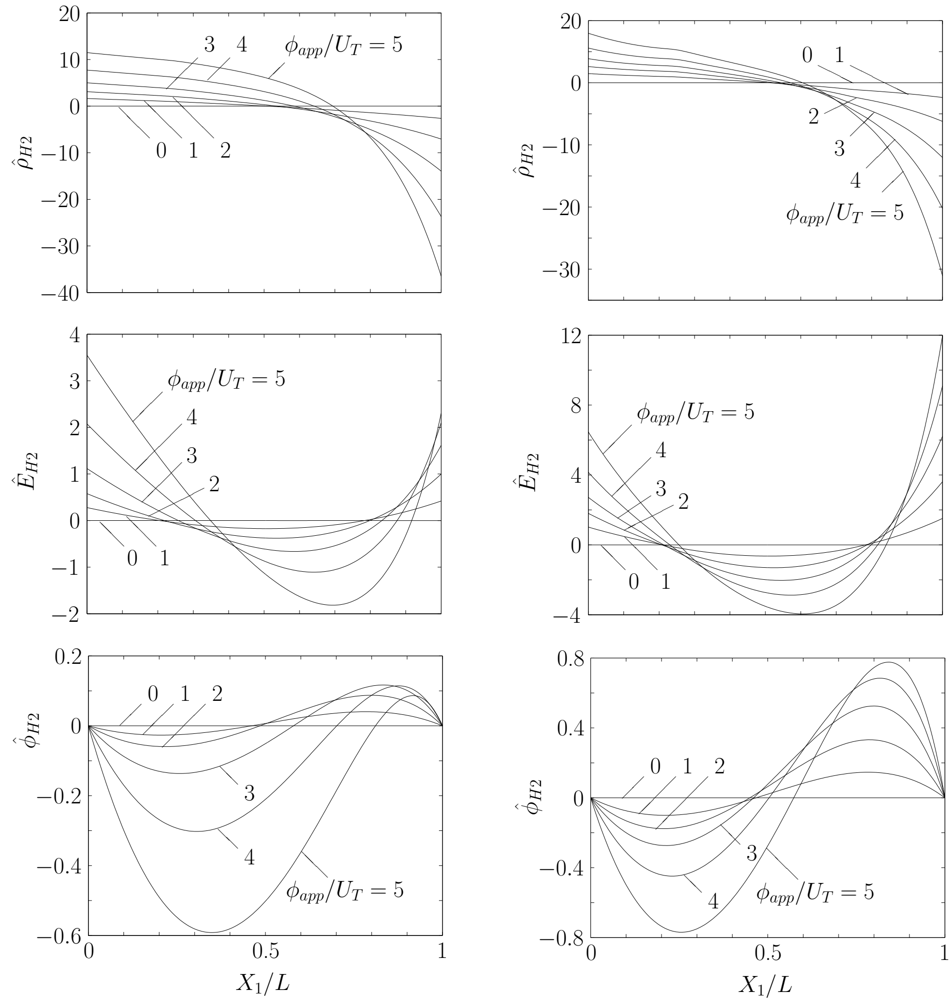


FIG. 2: The solution $\hat{\rho}_{H0}$, $\hat{E}_{H0}$, and $\hat{\phi}_{H0}$ for various applied potentials ϕ_{app} with $N_c/N_d = 0.2$, $D/L = 0.25$, and (a) $\lambda = 1$, (b) $\lambda = 0.5$.



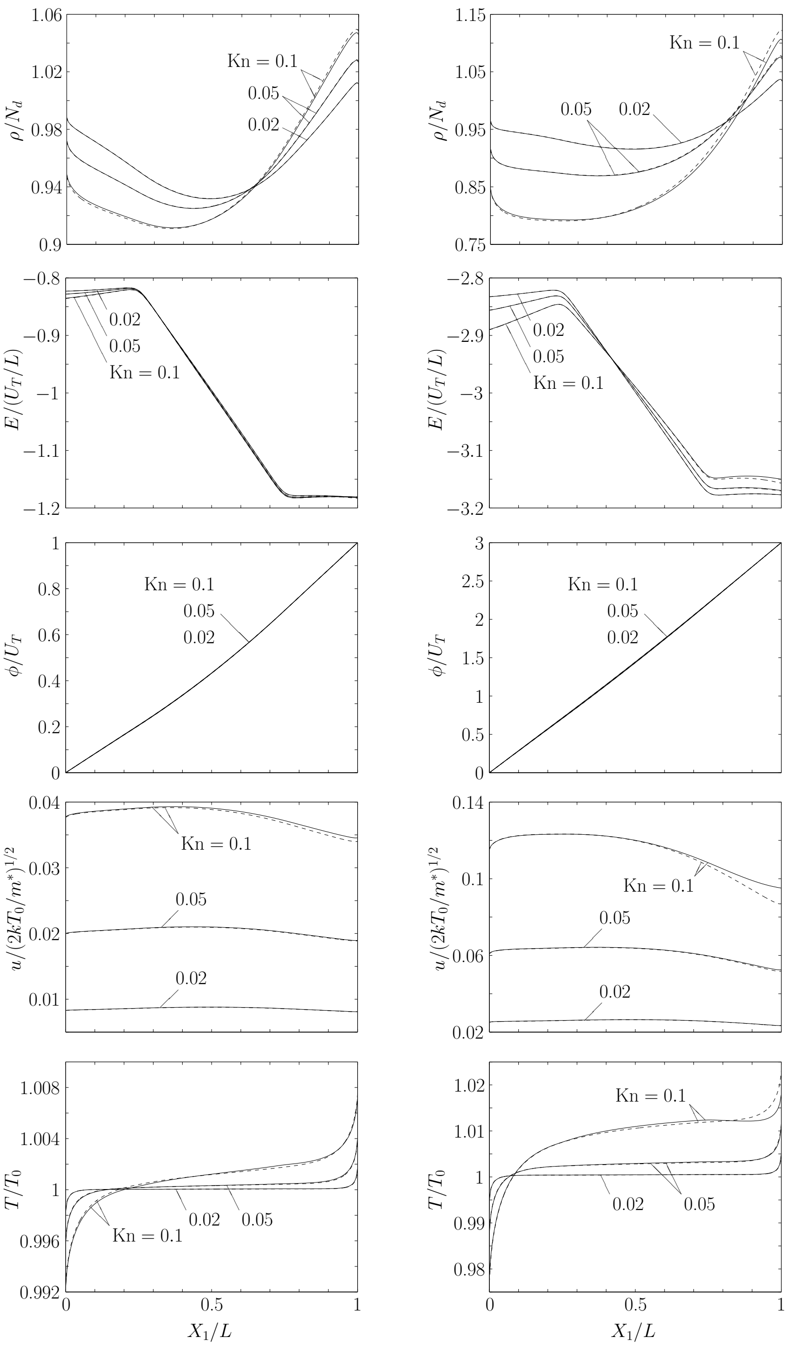
(a) $\lambda = 1$ (b) $\lambda = 0.5$

FIG. 3: The solution $\hat{\rho}_{H1}$, $\hat{E}_{H1}$, and $\hat{\phi}_{H1}$ for various applied potentials ϕ_{app} with $N_c/N_d = 0.2$, $D/L = 0.25$, and (a) $\lambda = 1$, (b) $\lambda = 0.5$.



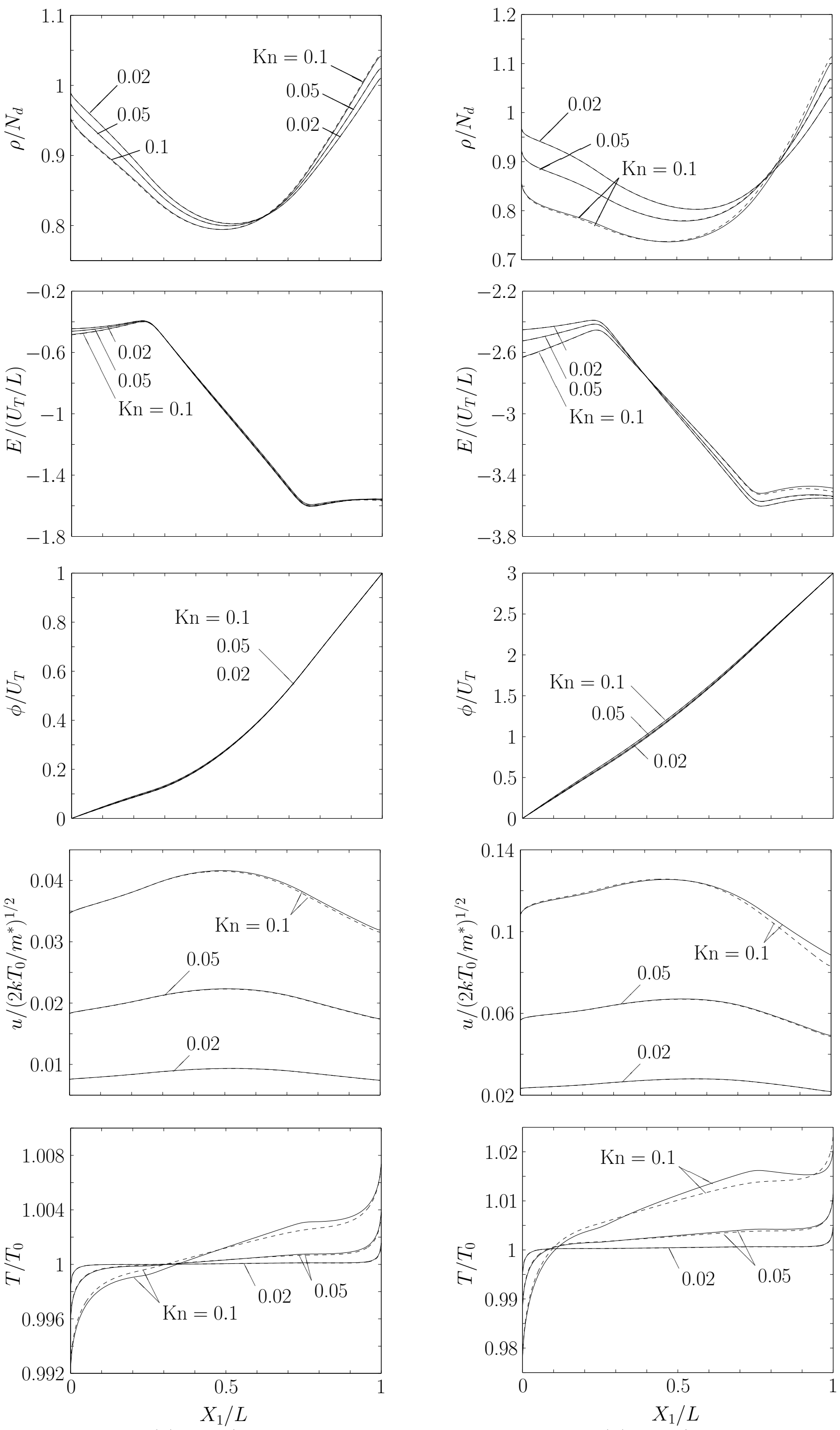
(a) $\lambda = 1$ (b) $\lambda = 0.5$

FIG. 4: The solution $\hat{\rho}_{H2}$, $\hat{E}_{H2}$, and $\hat{\phi}_{H2}$ for various applied potentials ϕ_{app} with $N_c/N_d = 0.2$, $D/L = 0.25$, and (a) $\lambda = 1$, (b) $\lambda = 0.5$.



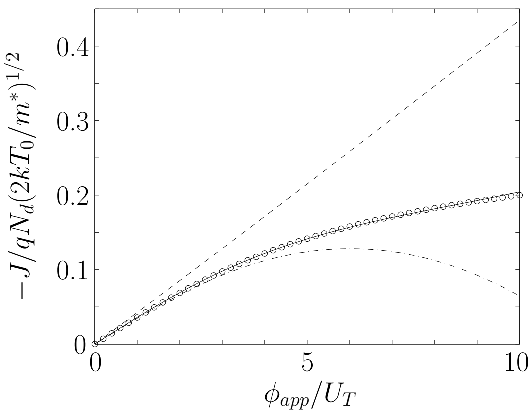
(a) $\phi_{app}/U_T = 1$ (b) $\phi_{app}/U_T = 3$

FIG. 5: The profiles of the electron density ρ, electric field E, electrostatic potential ϕ, mean flow velocity u, and electron temperature T for Kn = 0.1, 0.05, and 0.02 with $\lambda = 1$, $N_c/N_d = 0.2$, and $D/L = 0.25$. The solid line indicates the asymptotic solution up to order Kn^2 (up to order Kn^3 in the case of u), and the dashed lines indicate the corresponding numerical solutions of the original Boltzmann-Poisson system.

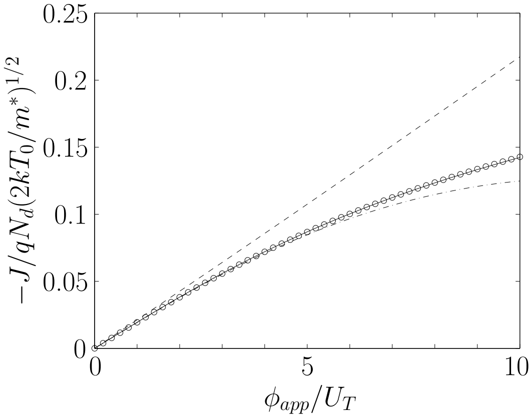


(a) $\phi_{app}/U_T = 1$ (b) $\phi_{app}/U_T = 3$

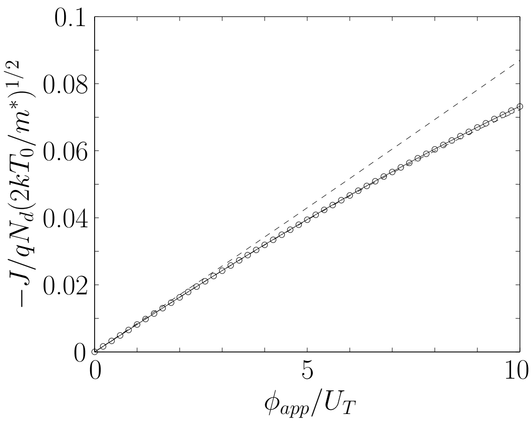
FIG. 6: The profiles of the electron density ρ, electric field E, electrostatic potential ϕ, mean flow velocity u, and electron temperature T for Kn = 0.1, 0.05, and 0.02 with $\lambda = 0.5$, $N_c/N_d = 0.2$, and $D/L = 0.25$. See the caption of Fig. 5.



(a) Kn = 0.1

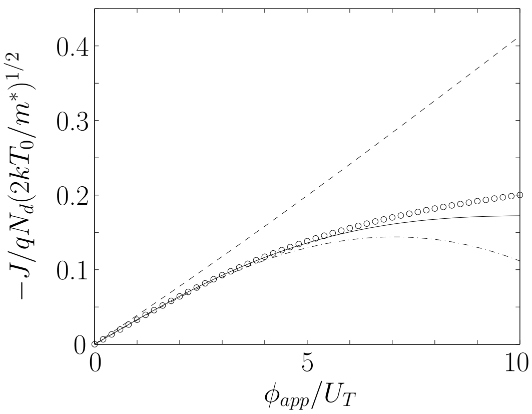


(b) Kn = 0.05

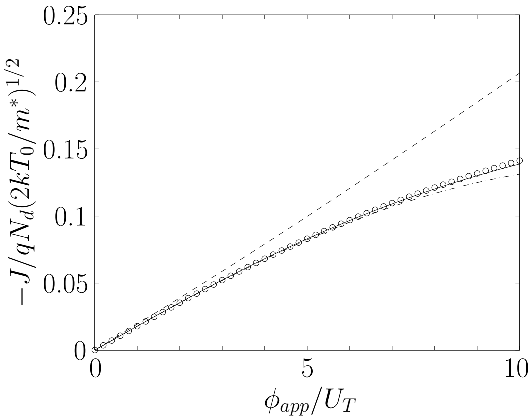


(c) Kn = 0.02

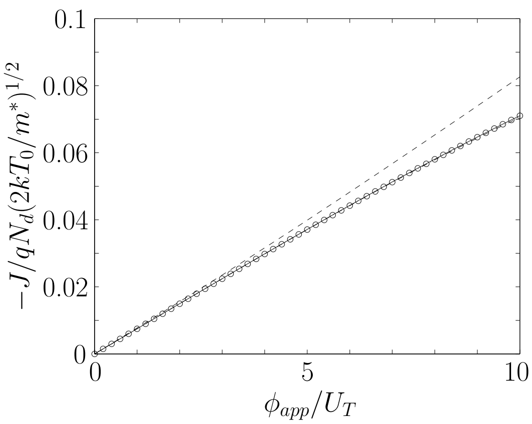
FIG. 7: Current density J versus applied potential ϕ_{app} for various Kn with $\lambda = 1$, $N_c/N_d = 0.2$, and $D/L = 0.25$. The asymptotic solutions up to order Kn^3 (solid line), Kn^2 (dashed line), and Kn (dash-dotted line) are shown. The direct numerical solution of the Boltzmann-Poisson system is indicated by the symbol "∘".



(a) Kn = 0.1



(b) Kn = 0.05



(c) Kn = 0.02

FIG. 8: Current density J versus applied potential ϕ_{app} for various Kn with $\lambda = 0.5$, $N_c/N_d = 0.2$, and $D/L = 0.25$. See the caption of Fig. 7.

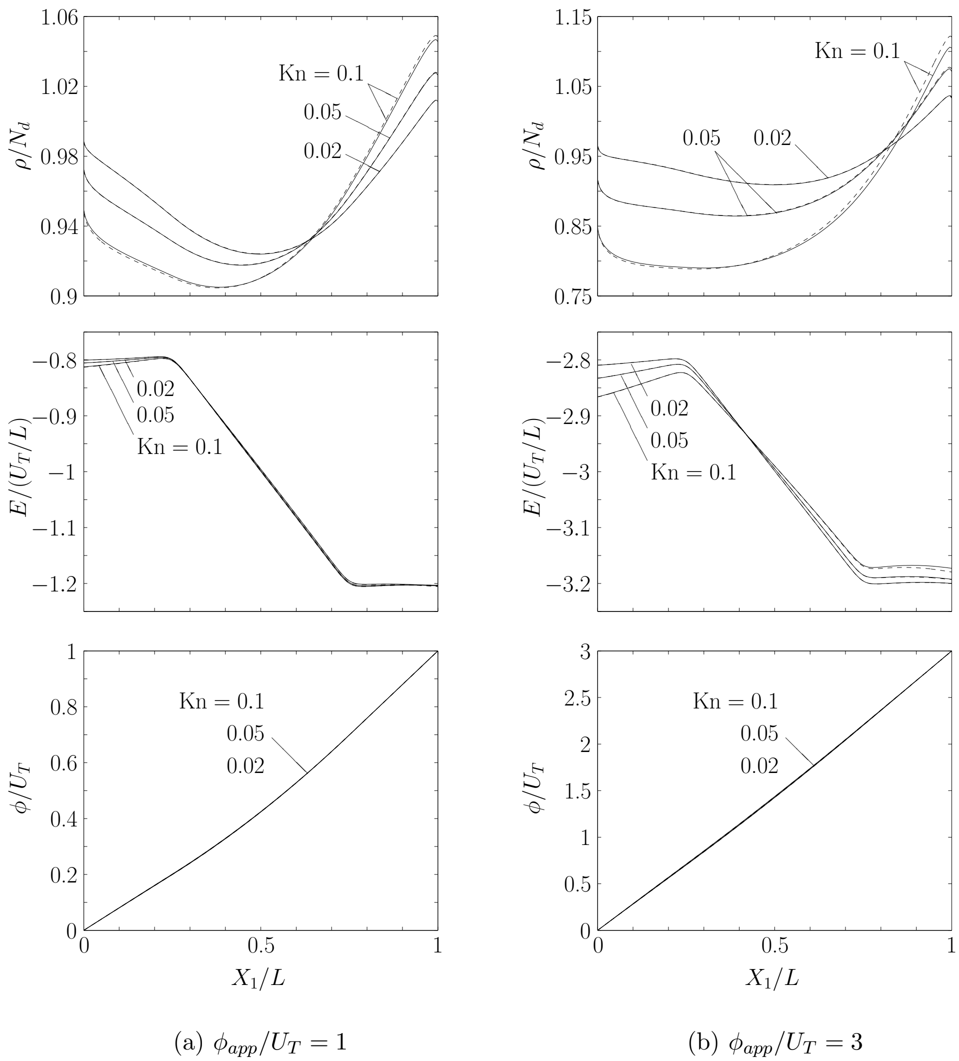


FIG. 9: The profiles of the electron density ρ, electric field E, electrostatic potential ϕ for Kn = 0.1, 0.05, and 0.02 with $\lambda = 1$, $N_c/N_d = 0.1$, and $D/L = 0.25$. The solid line indicates the asymptotic solution up to the order Kn^2 and the dashed line the numerical solution of the original Boltzmann-Poisson system.

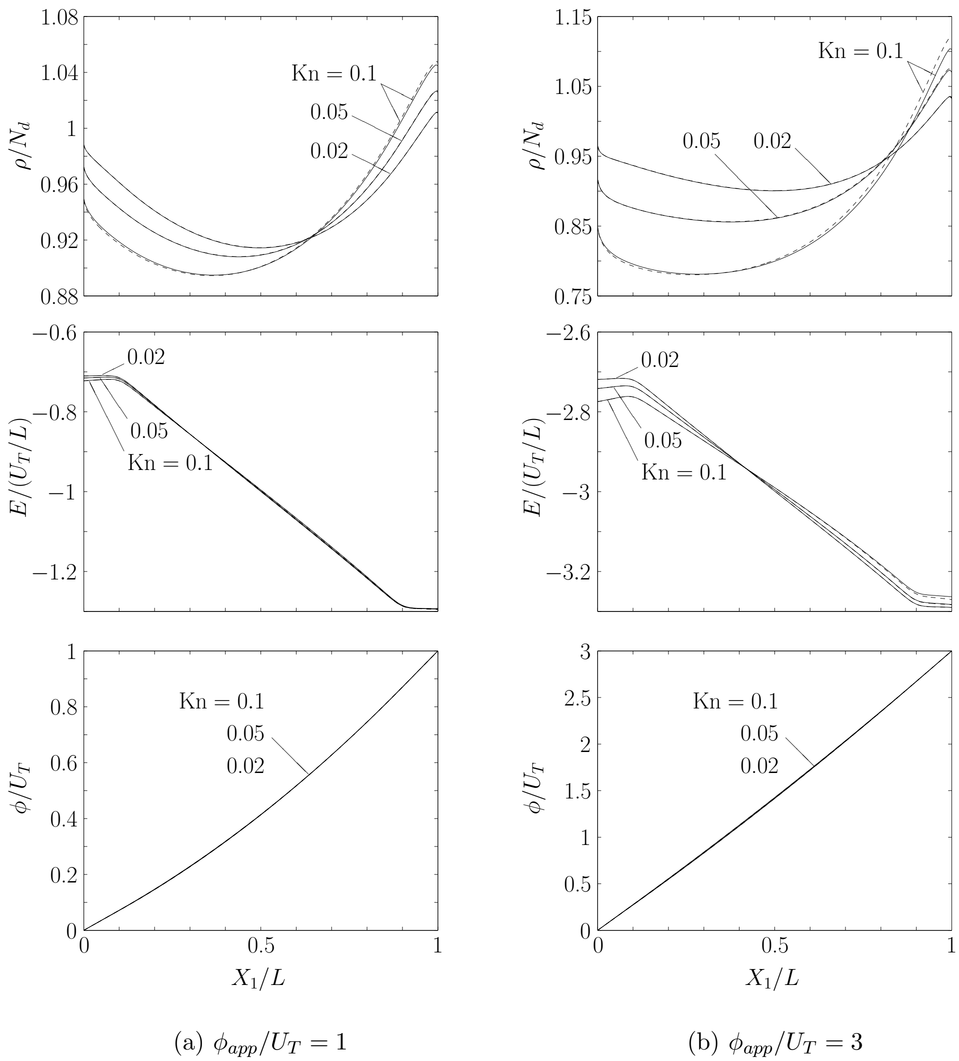


FIG. 10: The profiles of the electron density ρ, electric field E, electrostatic potential ϕ for Kn = 0.1, 0.05, and 0.02 with $\lambda = 1$, $N_c/N_d = 0.2$, and $D/L = 0.1$. See the caption of Fig. 9.

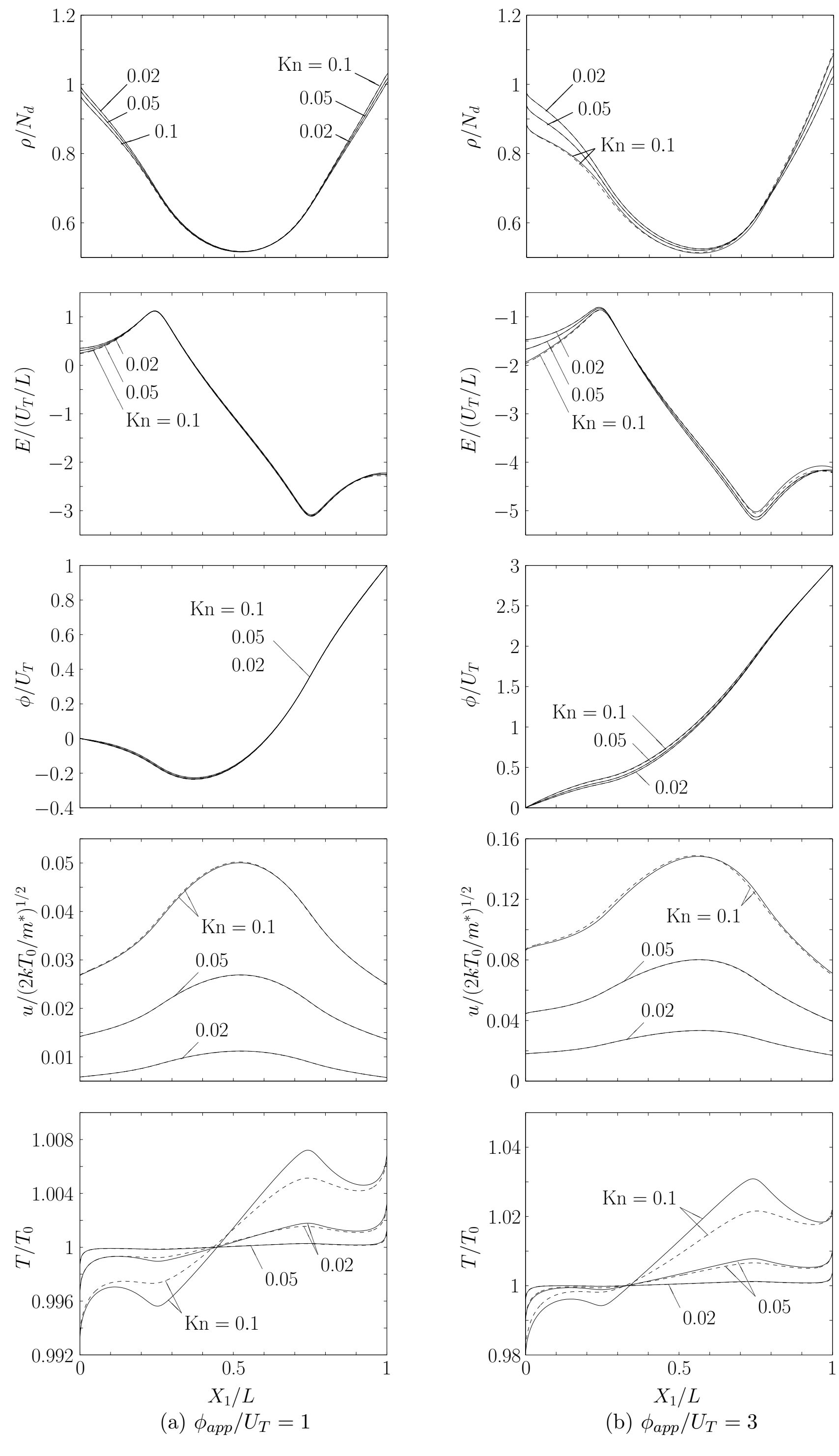
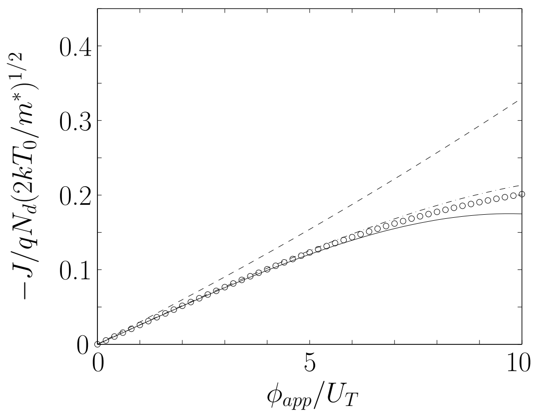
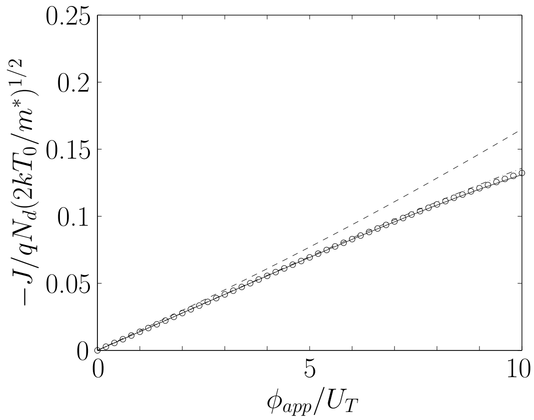


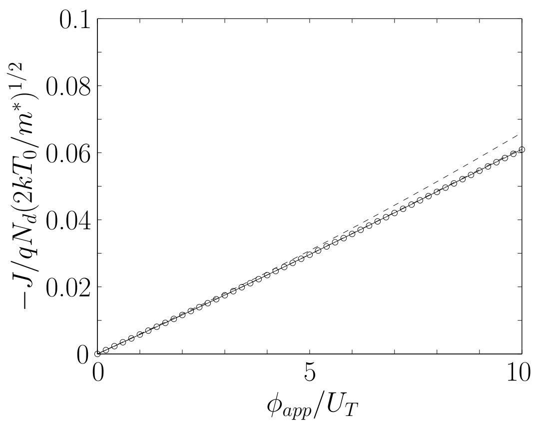
FIG. 11: The profiles of the electron density ρ, electric field E, electrostatic potential ϕ, mean flow velocity u, and electron temperature T for Kn = 0.1, 0.05, and 0.02 with $\lambda = 0.2$, $N_c/N_d = 0.2$, and $D/L = 0.25$. See the caption of Fig. 5.



(a) Kn = 0.1



(b) Kn = 0.05



(c) Kn = 0.02

FIG. 12: Current density J versus applied potential ϕ_{app} for various Kn with $\lambda = 0.2$, $N_c/N_d = 0.2$, and $D/L = 0.25$. See the caption of Fig. 7.