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Kullback-Leibler entropy in the electron distribution shape relaxation for electron-atom thermalization

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We study the thermalization of energetic electrons dilutely dispersed in inert gas atomic moderators, with and without the presence of an external electric field. We investigate the shape relaxation of the electron distribution function relative to the steady-state distribution by means of the Kullback-Leibler entropy. The departure of the distribution function from a local Maxwellian parametrized by the temperature of the electrons is also considered with a functional analogous to the Kullback-Leibler entropy. For neon and argon as moderators, we found no evidence for the formation of a local Maxwellian followed by a slower relaxation to equilibrium. The momentum-transfer cross section for e-Ne collisions is almost constant with energy, whereas the e-Ar momentum-transfer cross section has a deep Ramsauer-Townsend minimum and a strong energy dependence. The role of the Ramsauer minimum in the relaxation processes is investigated. The time-dependent Lorentz-Fokker-Planck equation is solved for the speed distribution of the electrons with a finite difference method. A pseudospectral method is also used to investigate the spectral properties of the Fokker-Planck operator. In spite of the multi-exponential time dependence of the speed distribution function, we show that a single average relaxation time can be defined to characterize the relaxation to equilibrium.

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I. INTRODUCTION

The relaxation of energetic electrons in a background gas at equilibrium at a fixed temperature T_b is an important fundamental problem in kinetic theory with equally important applications to numerous devices in plasma processing of materials, plasma displays, and other technologies [1–3]. There has been extensive work done to date on both atomic [4–9] and molecular moderators [10–13] including electronegative gases [14,15] with a strong affinity for electrons. In this latter case, owing to large electron attachment cross sections, there can be electron heating effects arising from the removal of thermal electrons. In atomic moderators, there have been two noticeable effects that occur, namely, the transient negative mobility effect predicted by McMahon and Shizgal [4] and observed experimentally by Warman *et al.* [16] and discussed since then by other researchers [17–19]. There is also the unexpected negative differential conductivity effect in mixtures of inert gases [20] that was previously thought to occur only for polyatomic gases with internal degrees of freedom [21,22].

Mozumder [23] studied the relaxation of electrons in the inert gases by assuming that the distribution function remains a local Maxwellian with a time-dependent temperature. The instantaneous electron temperature that defines the local Maxwellian is calculated in terms of the energy exchange determined with an integration of the Maxwellian and the electron-atom momentum-transfer cross section. Keizer [24] proposed an analysis of hot atom chemistry based on a time-dependent local Maxwellian as discussed later by Shizgal [25]. There are many additional examples such as in plasma physics [26] where the time scale for different rate processes is estimated with a local Maxwellian assumption. However, the exact preservation of a local Maxwellian in physically realistic systems is the exception rather than the rule. The maintenance of a local Maxwellian during the approach to equilibrium occurs only for a small number of systems such as the hard-sphere Rayleigh gas [27] and electron-atom systems whose interaction is given by the Maxwell molecule model [28]. It can be readily shown that these two systems are equivalent. They have the property that an initial Maxwellian at temperature $T(0)$ will relax to the equilibrium Maxwellian at T_b through a continuous sequence of Maxwellian distributions parametrized by $T(t)$, a feature that is referred to as canonical invariance [27,29].

For binary systems where no one component is present in large excess, the relaxation to equilibrium can occur on three distinctly different time scales, that is, two time scales for each component to approach Maxwellians at different temperatures via self-collisions and then complete equilibration of the two components via cross collisions on a third time scale. This “epochal” relaxation behavior of such binary systems with disparate mass ratios has been discussed previously [30–32]. In molecular systems with electronic, vibrational, rotational, and translational states, there can be a sharp separation in the relaxation times of the different degrees of freedom [33,34]. In plasma physics, electrons can attain a Maxwellian distribution on a short time scale, whereas ions and neutrals remain far from equilibrium. For each of these physical systems there can exist a spectrum of relaxation times within each time scale [26].

The main objective of this paper is to study the shape relaxation of the electron distribution function and the associated time scale for this electron-atom relaxation process without electron-electron interactions. The shape relaxation of the distribution function is studied in terms of the Kullback-Leibler entropy [35–39], which provides a global measure of the departure of the distribution function from the steady-state Maxwellian or from the steady Davydov distribution when a finite electric field is considered. In the absence of an external electric field, we also investigate the departure of the distribution function from a local Maxwellian and verify whether an intermediate local Maxwellian is established on a short time scale followed by a slow relaxation to equilibrium. The time dependence of the electron distribution function is given by a Fokker-Planck equation defined in terms of the electron-atom momentum-transfer cross section and the strength of an external uniform electric field if present. This is a linear time-dependent problem, and often it is useful to express the solution in terms of the time eigenmodes of the linear Fokker-Planck operator that defines the problem as discussed in Sec. II. Thus, the time evolution of the electron distribution function can be expressed as a sum of exponential terms involving the eigenvalues of the Fokker-Planck operator.

Experimental measurements of electron energy relaxation times are usually reported in terms of the times $\tau_{1.1}$ and $\tau_{1.01}$ required for the average electron energy to decay to within either 10% or 1%, respectively, of the thermal energy, which is $3k_BT_b/2$ where k_B is the Boltzmann constant. Owing to the multi-exponential nature of the relaxation process, it is of interest to reexamine these definitions and discuss the manner in which a single average relaxation time can be defined as a representative of the time scale for the approach to equilibrium [40]. We consider the relaxation time of the distribution function in terms of the Kullback-Leibler entropy and compare it with the relaxation time of the average energy.

The Fokker-Planck equation is presented in Sec. II together with a brief description of the methods of solution used. We employ the pseudospectral method [4,41–43] to investigate the spectral properties of the Fokker-Planck operator and the finite difference method by Chang and Cooper [44] to solve the time-dependent Fokker-Planck equation. The shape relaxation of the distribution function is studied in terms of the Kullback-Leibler relative entropy [35–39] as discussed in Sec. III. The results and discussions are presented in Sec. IV. The interpretation of the multi-exponential representation of the temperature relaxation and the other quantities studied in terms of a single relaxation time is given in Sec. V. The conclusion of this work is that a single relaxation time can be defined that is representative of the time scale for the relaxation of the distribution function and the temperature. No evidence was found for the formation of an intermediate local Maxwellian during the relaxation process.

II. FOKKER-PLANCK EQUATION

The formalism for the calculations in the present paper follows closely the work in previous papers [4–6,8], and only a brief summary is presented here. The dependence of the distribution function is expressed in reduced speed, $x = v\sqrt{m_e/2k_BT_b}$, where v and m_e are the speed and mass of the electron, T_b is the temperature of the atomic moderator, and k_B denotes the Boltzmann constant. The time t' is expressed in units of t_0, that is, $t = t'/t_0$, where

$$\frac{1}{t_0} = \frac{nm_e}{2M}\sigma_0\sqrt{\frac{2k_BT_b}{m_e}}. \tag{1}$$

In Eq. (1), n and M are the density and mass of the moderator particles, respectively, and σ_0 is a convenient hard-sphere cross section. In terms of these dimensionless variables, the isotropic portion of the distribution function is given by the Fokker-Planck equation:

$$\frac{\partial f(x,t)}{\partial t}=\frac{1}{x^2}\frac{\partial}{\partial x}\left[2x^4\widehat{\sigma}(x)f(x,t)+x^2B(x)\frac{\partial f(x,t)}{\partial x}\right], \tag{2}$$

where $\widehat{\sigma}(x) = \sigma(x)/\sigma_0$ and

$$B(x) = x\widehat{\sigma}(x) + \frac{\alpha^2}{x\widehat{\sigma}(x)}. \tag{3}$$

The function $\sigma(x)$ denotes the electron-atom momentum-transfer cross section and α measures the strength of the uniform external electric field E and is defined by

$$\alpha^2 = \frac{M}{6m_e}\left[\frac{eE}{n\sigma_0k_BT_b}\right]^2, \tag{4}$$

where e is the electron charge. The steady-state distribution function, $f_{\rm SS}(x)$, at infinite time is the Davydov distribution function derived from Eq. (2) and given by

$$f_{\rm SS}(x) = C\exp[-d(x)], \tag{5}$$

where

$$d(x) = 2\int_0^x \frac{y^2\widehat{\sigma}(y)}{B(y)}dy. \tag{6}$$

The normalization constant C is determined from $4\pi\int_0^\infty x^2 f_{\rm SS}(x)\,dx = 1$. In the absence of an electric field, $f_{\rm SS}(x)$ corresponds to the Maxwellian distribution function at T_b. A finite electric field will heat the electrons above the moderator temperature.

We now express the distribution function in terms of the deviation from $f_{\rm SS}$ and write the Fokker-Planck equation in terms of $g(x,t) = f(x,t)/f_{\rm SS}(x)$, namely,

$$\frac{\partial g(x,t)}{\partial t}=Lg(x,t)=\frac{1}{x^2f_{\rm SS}(x)}\frac{\partial}{\partial x}\left[x^2f_{\rm SS}(x)B(x)\frac{\partial g(x,t)}{\partial x}\right], \tag{7}$$

where we have defined the linear Fokker-Planck operator L. We determine the distribution function by the finite difference method on a uniform grid, which guarantees the positivity of the distribution function [44]. The finite difference method provides very good results for the distribution function with a relatively small number of grid points. We also investigate the spectral properties of the Fokker-Planck operator by using a pseudospectral method based on a nonuniform grid that is defined as the quadrature points associated with the weight function $w(x) = x^2e^{-x^2}$, developed elsewhere [41–43]. The discretization of the Fokker-Planck equation with the pseudospectral method gives the representation

$$L_{ij} = \sum_{k=1}^{N} B(x_k)[D_{ki} + h(x_k)\delta_{ik}][D_{kj} + h(x_k)\delta_{jk}], \tag{8}$$

where

$$\begin{aligned} h(x) &= \frac{w'(x)}{2w(x)} - \frac{[x^2f_{\rm SS}(x)]'}{2x^2f_{\rm SS}(x)} \\ &= \frac{d'(x)}{2} - x, \end{aligned} \tag{9}$$

and D_{ij} is the discrete representation of the derivative operator [41,42]. As shown in Ref. [5], the Fokker-Planck operator has an entirely discrete eigenvalue spectrum. The eigenvalue problem $L\phi_n(x) = \lambda_n \phi_n(x)$ is solved by the numerical diagonalization of the $N \times N$ representative matrix L_{ij} of L. The pseudospectral approach provides a rapid convergence of the eigenvalues and eigenfunctions versus the number of quadrature points N. The time dependence of the distribution function is then obtained by expanding $g(x,t)$ in the eigenfunctions of L,

$$g(x,t) = \sum_{n=0}^{N} a_n e^{-\lambda_n t} \phi_n(x), \tag{10}$$

where

$$a_n = \int_0^\infty x^2 \phi_n(x) f(x,0)\, dx.$$

It is important to note that the lowest eigenvalue is $\lambda_0 = 0$ owing to conservation of particle number [$4\pi \int_0^\infty x^2 f(x,t) dx = 1$] and the existence of a steady distribution at infinite time.

The moments of the distribution function and in particular the temperature, which in reduced speed is given by $T(t) = (8\pi/3) T_b \int_0^\infty x^4 f(x,t)\, dx$, can be expressed in terms of the multi-exponential decay:

$$\frac{T(t)}{T_b} = \sum_{n=0}^{N} b_n e^{-\lambda_n t}. \tag{11}$$

The coefficients b_n are expressed in terms of the a_n and the projection of x^2 on the eigenfunctions, that is,

$$b_n = \frac{8\pi}{3} a_n \int_0^\infty f_{\mathrm{SS}}(x) x^4 \phi_n(x)\, dx. \tag{12}$$

For the Maxwell molecule (MM) model and zero electric field, $B(x)$ is independent of the speed of the particles, and the solution to the Fokker-Planck equation Eq. (2) can be given in a closed form. For this model, the interaction potential is

$$V(r) = \frac{pe^2}{2a_0}\left(\frac{a_0}{r}\right)^4,$$

where pa_0^3 is the polarizability of the atomic moderator, a_0 is the Bohr radius, and e denotes the charge of the electron. Then it can be shown that the reduced MM momentum-transfer cross section is given by $\widehat{\sigma}(x) = a/x$, where

$$a = Q^{(1)} \frac{a_0^2}{\sigma_0} \sqrt{\frac{V_0}{k_B T_b}}, \tag{13}$$

and $V_0 = V(a_0)$. The quantity $Q^{(1)} = 3.748$ results from an appropriate angular average of the MM differential cross section. Therefore, for MM we have $B(x) = a$, and the solution of Eq. (2) [27,28,45] is given by Eq. (10) with $\phi_n(x) = L_n^{(\frac{1}{2})}(x^2)$ being the nth generalized Laguerre polynomial of order one-half and $\lambda_n = 4an$, that is,

$$f(x,t) = f_{\mathrm{SS}}(x) \sum_{n=0}^{\infty} a_n L_n^{(\frac{1}{2})}(x^2) e^{-4ant}. \tag{14}$$

Here $f_{\mathrm{SS}}(x)$ is the Maxwellian distribution function at T_b, and the expansion coefficients are

$$a_n = \frac{2n!}{\Gamma\left(n+\frac{3}{2}\right)} \int_0^\infty x^2 f(x,0) L_n^{(\frac{1}{2})}(x^2)\, dx.$$

Moreover, the temperature of the electrons relaxes as a single exponential

$$\frac{T(t) - T_b}{T(0) - T_b} = e^{-4at}, \tag{15}$$

independent of the initial distribution chosen. If the initial distribution $f(x,0)$ is a Maxwellian with temperature $T(0)$, then the solution (14) has the closed form of a local Maxwellian $f_{\mathrm{LM}}[x,T(t)] = [T_b/\pi T(t)]^{3/2} \exp[-x^2 T_b/T(t)]$ evaluated at the temperature $T(t)$; that is, for the MM model Eq. (2) satisfies the canonical invariance property. These are well-known results [27,28,45] that we use to check the numerical methods implemented in this work.

Notice that the Lorentz-Fokker-Planck equation for MM is equivalent to the hard-sphere Rayleigh gas discussed by Andersen and Shuler in Ref. [45]. Indeed, if we introduce the reduced energy $y = x^2$ and the distribution $P(y,t) = \sqrt{y} f(\sqrt{y},t)$, the Fokker-Planck equation (2) can be written as

$$\frac{\partial P(y,t)}{\partial t} = 4\frac{\partial}{\partial y}\left\{\left[y - \frac{3}{2}\right] P(y,t) + \frac{\partial}{\partial y}[yP(y,t)]\right\}. \tag{16}$$

This is the Fokker-Planck equation deduced in Ref. [45] for the relaxation of the hard-sphere Rayleigh gas, which satisfies the properties cited above. On the other hand, the function $P(y,t) = \sqrt{y} f(\sqrt{y},t)$ substituted into the Fokker-Planck equation (2) with the hard-sphere cross section, $\widehat{\sigma}(x) = 1$, yields

$$\frac{\partial P(y,t)}{\partial t} = 4\frac{\partial}{\partial y}\left\{(y-2)\sqrt{y}P(y,t) + \frac{\partial}{\partial y}[y\sqrt{y}P(y,t)]\right\}, \tag{17}$$

which is the Fokker-Planck equation deduced in Ref. [45] for the relaxation of the hard-sphere Lorentz gas. In contrast to the MM model, there is no closed-form solution for either $f(x,t)$ or $T(t)$.

III. DISTRIBUTION FUNCTION SHAPE RELAXATION AND CANONICAL INVARIANCE

The relaxation of the electron distribution function in inert gas moderators has a very long history [4,5,16,46,47]. The main objective for many of these previous investigations has been the determination of the electron thermalization times defined in terms of the relaxation of the electron temperature to the equilibrium temperature T_b of the background atoms. The definition of the relaxation times $\tau_{1.1}$ and $\tau_{1.01}$ used to interpret experimental studies are defined as the times required for the temperature $T(t)$ to be respectively within 10% and 1% of T_b. These definitions are somewhat arbitrary and in some sense misleading as the relaxation time can be made arbitrarily long by choosing a definition with $T(t)$ arbitrarily close to T_b. In addition, these definitions do not take into account the values of $T(t)$ at early times. On the other hand, the solution of the linear Fokker-Planck equation for the electron distribution as well as the temperature are expressed as sums of exponential terms of the eigenvalues of the Fokker-Planck operator, Eqs. (10) and (11). It has long been recognized that the determination of this multi-exponential time dependence from experiment or from simulation is an ill-defined problem [40,48–50]. Quite generally the temperature relaxation that has been reported to date does not show separate distinct time scales. One of the objectives of this paper is to consider the manner in which this multi-exponential decay can be characterized by a single relaxation time that provides the time scale for the approach to equilibrium for this system.

In this paper, we investigate the relaxation to equilibrium of the electron distribution function and the temperature. In particular, we follow the evolution of the shape of the distribution function relative to the time independent steady-state distribution in terms of the Kullback-Leibler entropy [35–39] defined by

$$\Sigma_{\mathrm{SS}}(t) = -4\pi \int_0^\infty x^2 f(x,t) \ln \frac{f(x,t)}{f_{\mathrm{SS}}(x)}\, dx. \tag{18}$$

The functional $\Sigma_{\mathrm{SS}}(t)$ is negative at $t = 0$ for an arbitrary initial distribution function and tends to zero monotonically as $t \to \infty$. For two Maxwellian distributions at different temperatures, in particular for an initial Maxwellian with temperature $T(0)$ and a steady-state Maxwellian at T_b, we have

$$\Sigma_{\mathrm{SS}}(0) = \frac{3}{2}\left[1 - \frac{T(0)}{T_b} + \ln \frac{T(0)}{T_b}\right], \tag{19}$$

which satisfies $\Sigma_{\mathrm{SS}}(0) < 0$ for all $T(0) \neq T_b$ and $\Sigma_{\mathrm{SS}}(0) = 0$ for $T(0) = T_b$. More generally, if we add to Eq. (18) the integral of $x^2[f_{\mathrm{SS}}(x) - f(x,t)]$, which is zero owing to the conservation of the particles number, we obtain

$$\Sigma_{\mathrm{SS}}(t) = -4\pi \int_0^\infty x^2 f_{\mathrm{SS}}(x)\left[\frac{f(x,t)}{f_{\mathrm{SS}}(x)} \ln \frac{f(x,t)}{f_{\mathrm{SS}}(x)} - \frac{f(x,t)}{f_{\mathrm{SS}}(x)} + 1\right] dx. \tag{20}$$

Then, since $X \ln X - X + 1 \geqslant 0$ with equality only if $X = 1$, we have that $\Sigma_{\mathrm{SS}}(t) \leqslant 0$ for all times and $\Sigma_{\mathrm{SS}}(t) = 0$ only when $f(x,t) = f_{\mathrm{SS}}(x)$. On the other hand, if we use $f(x,t) = g(x,t) f_{\mathrm{SS}}(x)$, the time derivative of $\Sigma_{\mathrm{SS}}(t)$ from Eq. (18) is

$$\frac{d\Sigma_{\mathrm{SS}}(t)}{dt} = -4\pi \int_0^\infty f_{\mathrm{SS}}(x) \frac{\partial g(x,t)}{\partial t} \ln g(x,t)\, dx, \tag{21}$$

where the time derivative of $\ln g(x,t)$ gives zero owing to particle conservation. With Eq. (2), an integration by parts and zero flux boundary conditions, we find that

$$\frac{d\Sigma_{\mathrm{SS}}(t)}{dt} = 4\pi \int_0^\infty x^2 B(x) f(x,t) \left|\frac{\partial}{\partial x} \ln \frac{f(x,t)}{f_{\mathrm{SS}}(x)}\right|^2 dx. \tag{22}$$

Therefore $d\Sigma_{\mathrm{SS}}(t)/dt \geqslant 0$ with equality only when $f(x,t) = f_{\mathrm{SS}}(x)$ at infinite time. This provides an H-theorem for the Fokker-Planck equation (2) [36–39].

In many studies, the assumption of local thermodynamic equilibrium is made and estimates of relaxation times are determined from the energy exchange process occurring with the maintenance of a Maxwellian distribution [23–26]. This procedure assumes that the system satisfies canonical invariance [27,28] to some degree. In the absence of an electric field, $\alpha = 0$, we also follow the evolution of $f(x,t)$ relative to a local Maxwellian $f_{\mathrm{LM}}[x,T(t)]$ and define the quantity

$$\Sigma_{\mathrm{LM}}(t) = -4\pi \int_0^\infty x^2 f(x,t) \ln \frac{f(x,t)}{f_{\mathrm{LM}}[x,T(t)]}\, dx, \tag{23}$$

analogous to Eq. (18). This functional measures the departure of the distribution function from a local Maxwellian during the relaxation process, and it is a useful tool to investigate the canonical invariance property. If the initial distribution is a Maxwellian and remains Maxwellian with a time-dependent temperature, then $\Sigma_{\mathrm{LM}}(t) = 0$ for all times. In general, $\Sigma_{\mathrm{LM}}(t) \leqslant 0$, which can be shown by replacing $f_{\mathrm{SS}}(x)$ with $f_{\mathrm{LM}}[x,T(t)]$ in Eq. (20) and using the inequality that follows Eq. (20). It is understood that the distributions $f(x,t)$ and $f_{\mathrm{LM}}[x,T(t)]$ in the resulting equation are normalized according to $4\pi \int_0^\infty x^2 f(x,t)\, dx = 1$. However, whereas $\Sigma_{\mathrm{SS}}(t)$ satisfies an H theorem [Eq. (22)], $\Sigma_{\mathrm{LM}}(t)$ does not. For an initial Maxwellian at $T(0)$, we have $\Sigma_{\mathrm{LM}}(0) = 0$, and we also have $\Sigma_{\mathrm{LM}}(\infty) = 0$ since $f(x,\infty) \equiv f_{\mathrm{LM}}[x,T(\infty)]$. Then, unless the system exhibits canonical invariance, $\Sigma_{\mathrm{LM}}(t)$ must attain a strict minimum at some intermediate time.

In the case of a nonzero field, $\alpha \neq 0$, the situation is different as the steady state is the Davydov distribution function [Eq. (5)] with a temperature that can be greater than T_b as a consequence of the heating of the electrons by the external electric field. In this case, the study of $\Sigma_{\mathrm{LM}}(t)$ is meaningless.

IV. CALCULATIONS AND RESULTS

The time evolution of the electron distribution function is determined by the energy variation of the electron-atom momentum-transfer cross section. We consider here a comparison of the behavior for e-Ne and e-Ar relaxation for which the cross section data is shown in Fig. 1 of Ref. [6]. For e-Ne, the momentum-transfer cross section exhibits a weak dependence on the relative energy, whereas for e-Ar it has a very deep Ramsauer-Townsend minimum. The initial electron distribution is chosen either as a Maxwellian at $T(0) > T_b$ or as the Gaussian $f(x,0) = Ae^{-\beta(x-x_0)^2}$ where A is a normalization constant such that $4\pi \int_0^\infty f(x,0)x^2\, dx = 1$. The solution of the Fokker-Planck equation is determined with the finite difference algorithm developed by Chang and Cooper [44]. We interpret these results with the spectral approach in terms of the eigenvalues and eigenfunctions of the Fokker-Planck operator. The Chang and Cooper code is robust and preserves the positivity of the distribution. It has been employed in the solution of partial differential equations describing many different physical problems [51–53].

We show in Fig. 1 the time evolution of the electron distribution function, the relaxation of the temperature ratio, and time dependence of $\Sigma_{\mathrm{SS}}(t)$ and $\Sigma_{\mathrm{LM}}(t)$ for electrons in Ne

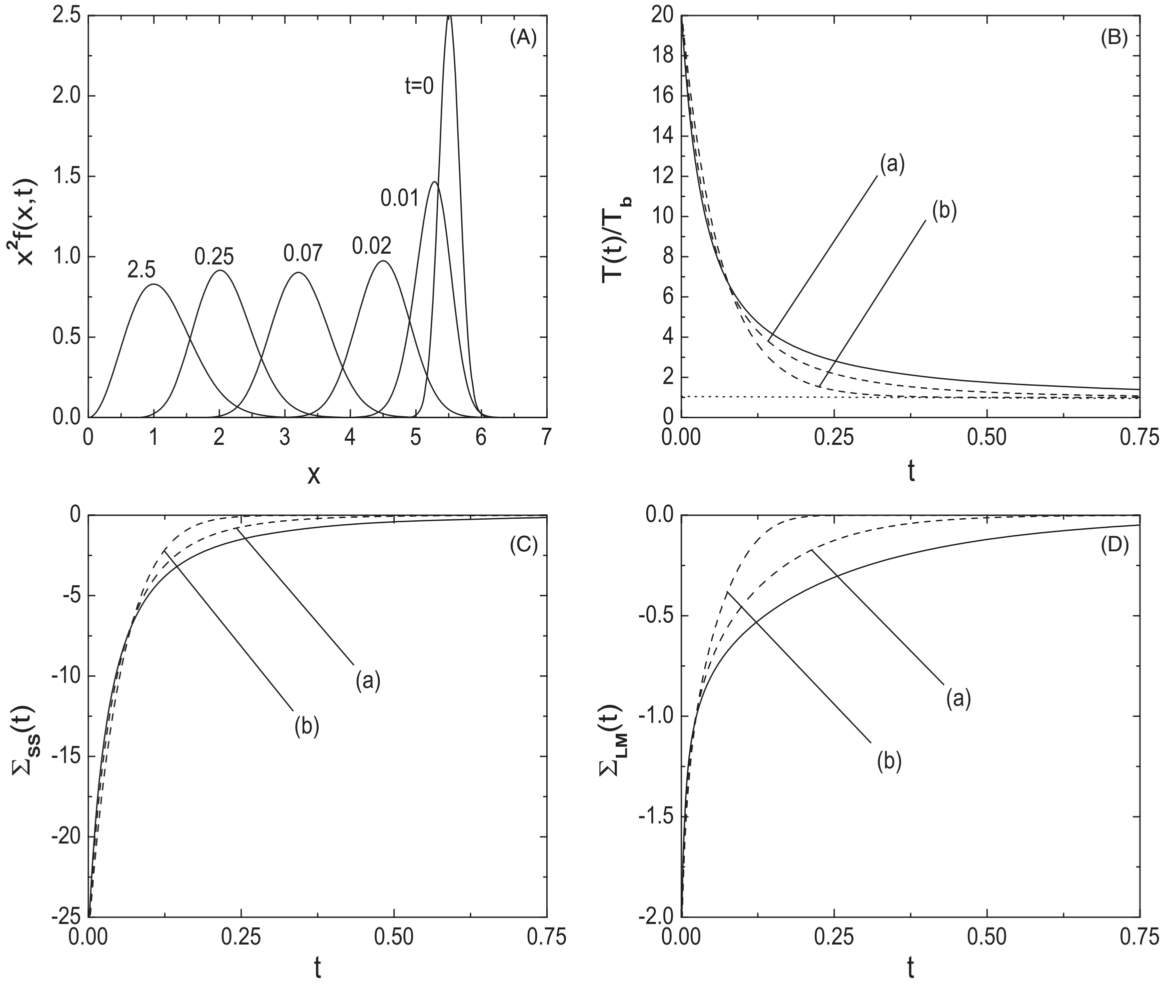

FIG. 1. The time dependence of $x^2 f(x,t)$, $T(t)/T_b$, $\Sigma_{\mathrm{SS}}(t)$ and $\Sigma_{\mathrm{LM}}(t)$ for electrons in Ne (solid curves); $E/n = 0$, $f(x,0) = Ae^{-\beta(x-x_0)^2}$ with $\beta = 20$ and $x_0 = 5.5$; $t = t'/t_0$ with $t_0 = 666$ in units of 10^{11} cm^{-3} s; $T_b = 290.1$K; (a) hard sphere ($\sigma_0 = 1.18$ Å^2); (b) Maxwell molecules ($a = 4$, $\sigma_0 = 10$ Å^2).

without an external electric field. The distribution function in Fig. 1(A) evolves as a sequence of unimodal distributions from an initial Gaussian to the final Maxwellian distribution at T_b, which is essentially attained at $t = 2.5$. Since the momentum-transfer cross section is slowly varying with energy, a hard-sphere cross section should approximate the behavior for electrons in Ne. This is indeed the case with $\sigma_0 = 1.18$ Å^2, as we show for the temperature relaxation by the dashed curve (a) in Fig. 1(B). This particular choice corresponds to the value of the momentum-transfer cross section for e-Ne at the energy $3k_B\bar{T}/2$, where $\bar{T} = (T(0) + T_b)/2$ and $T(0)$ is the temperature of the initial Gaussian. Also shown by the dashed curve (b) is the temperature relaxation for the MM model for which $\widehat{\sigma}(x) = a/x$. The constant a for Ne is determined by Eq. (13) with $p = 1.38$. For convenience, we choose $\sigma_0 = 10$ Å^2 with $k_B T_b = 0.025$ eV such that $a = 4$. Whereas the time dependence with the real cross section and the hard-sphere cross section is multi-exponential, the relaxation of the temperature for MM is a single exponential as discussed in Sec. II.

The departure of the shape of the distribution function from the equilibrium Maxwellian at T_b is shown in Fig. 1(C) in terms of the Kullback-Leibler entropy $\Sigma_{\mathrm{SS}}(t)$, which is initially negative and increases monotonically to zero at infinite time in accordance with the H-theorem, Eq. (22). In Fig. 1(D), we show the evolution of $\Sigma_{\mathrm{LM}}(t)$, which measures the departure of a nonequilibrium distribution function from a local Maxwellian parametrized by $T(t)$. As can be seen from the results shown, the time it takes for $\Sigma_{\mathrm{LM}}(t)$ and $\Sigma_{\mathrm{SS}}(t)$ to approach zero is very similar. This is clear from the results in Table I(a), where we show that the ratio of the $\tau_{0.01}$ values for the approach of $\Sigma_{\mathrm{SS}}(t)$ and $\Sigma_{\mathrm{LM}}(t)$ to within 0.01 of zero is of the order of unity. Note that in this analysis we only have to report the times at which these functions are close enough to zero, and no information on the behavior at early times are needed. Thus, we do not regard these values as relaxation times but merely as indicators for the approach of the distribution functions to a local and steady-state Maxwellians. In Sec. V we define the relaxation times as measures of the average history of the processes in comparison with the spectral properties of the systems.

These results imply that there is no initial fast relaxation to a local Maxwellian in this system since the distribution relaxes to the local Maxwellian approximately at the same

TABLE I. Times $\tau_{0.01}$ in units of $10^{11}\mathrm{cm}^{-3}\,\mathrm{s}$ defined as the time for which if $t > \tau_{0.01}$ then $|\Sigma_{\mathrm{LM}}(t)| < 0.01$ [analogously for $\Sigma_{\mathrm{SS}}(t)$]; $E/n = 0$; $T_b = 290.1\mathrm{K}$; (a) $f(x,0) = A\exp[-\beta(x-x_0)^2]$ with $\beta = 20$ and $x_0 = 5.5$, (b) initial Maxwellian with $T(0) = 20T_b$; bold numbers denote the ratio of the bottom row to the top row.

	(a)			(b)	
Process	Ne	Ar		Ne	Ar
			$\tau_{0.01}$		
$\Sigma_{\mathrm{LM}}(t)$	793	2579		761	2451
$\Sigma_{\mathrm{SS}}(t)$	989	2802		960	2667
	1.3	**1.1**		**1.3**	**1.1**

time that it relaxes to the steady-state Maxwellian. Zhang *et al.* [54] suggested that for atom-atom relaxation, the sharply peaked forward scattering quantum differential cross section that characterizes these systems will result in the relaxation of the distribution function to a local Maxwellian at $T(t)$ in a time approximately 10 times shorter than the time for $T(t)$ to reach within 5% of T_b. In Ref. [55], they cited a previous work [47] on electron-atom relaxation that demonstrated a similar two-stage relaxation. However, this "epochal" relaxation occurs owing to the inclusion of electron-electron collisions as done in Ref. [47]. On the other hand, for electron-atom systems it is only the momentum-transfer cross section computed from an average over scattering angle of the differential cross section that determines the relaxation behavior rather than the full differential cross section.

We now compare the relaxation process in Fig. 1 for electrons in Ne, a system with a nearly constant momentum-transfer cross section, with the relaxation of electrons in Ar, for which the momentum-transfer cross section has a deep Ramsauer-Townsend minimum and thus a strong energy dependence. The evolution of the electron distribution function from an initial Gaussian shown in Fig. 2(A) exhibits bimodal distributions at intermediate times that do not occur for electrons in Ne. This behavior is better understood if we define $h(x,t) = x^2 f(x,t)$ and rewrite the Fokker-Planck equation Eq. (2) as

$$\frac{\partial h(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[A(x)h(x,t) + B(x)\frac{\partial h(x,t)}{\partial x}\right]. \qquad (24)$$

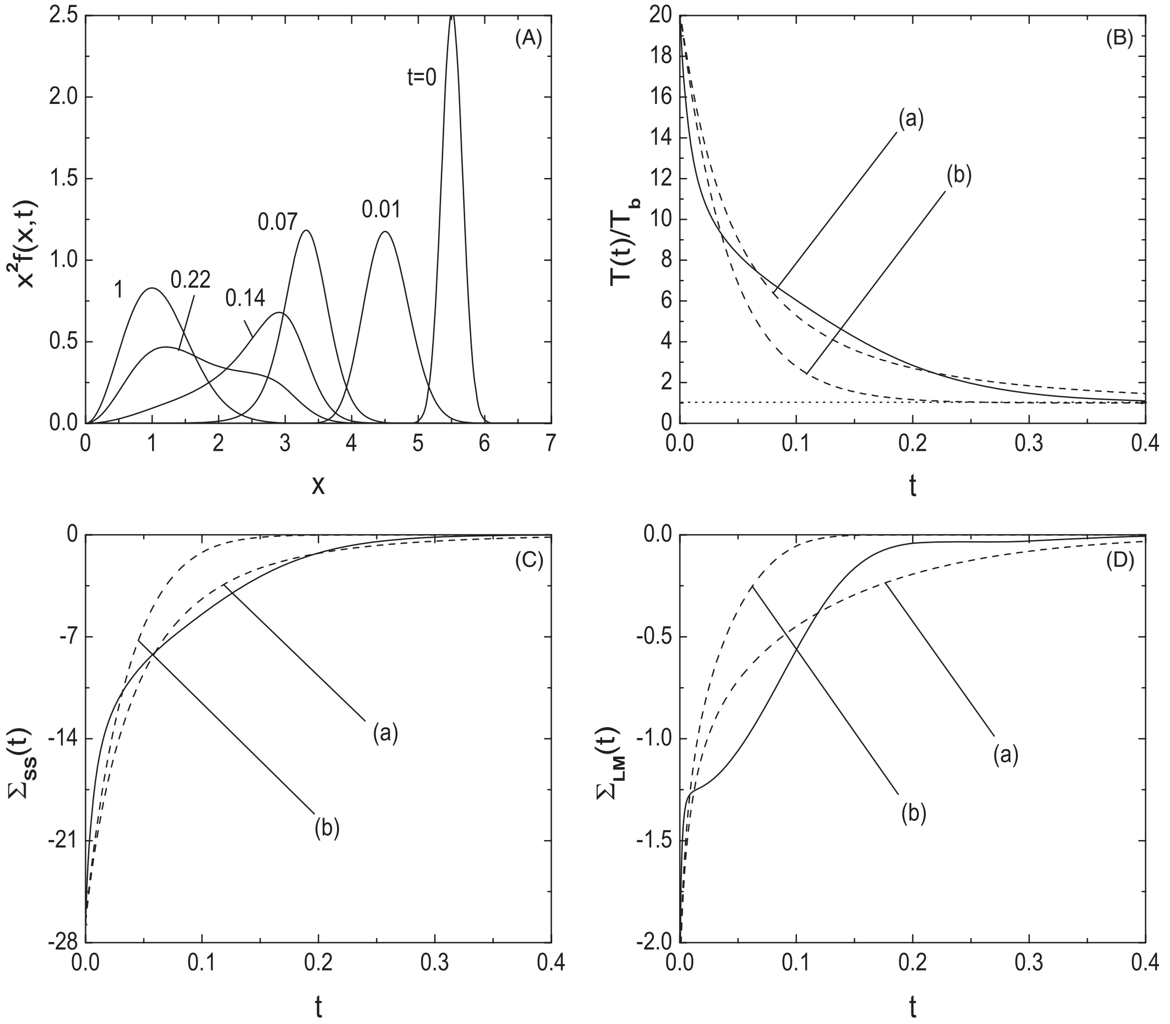

FIG. 2. Relaxation of electrons in Ar with an initial normalized Gaussian distribution; see caption to Fig. 1; $t_0 = 6752$ in units of $10^{11}\ \mathrm{cm}^{-3}$ s; $T_b = 290.1\mathrm{K}$; (a) hard sphere ($\sigma_0 = 0.23\ \text{Å}^2$); (b) Maxwell molecules ($a = 6$, $\sigma_0 = 13.57\ \text{Å}^2$).

For $E/n = 0$, the time evolution of $h(x,t)$ is determined by the coefficients $B(x) = x\widehat{\sigma}(x)$ and

$$A(x) = 2\left(1 - \frac{1}{x^2}\right) x B(x),$$

which for e-Ar are shown in Fig. 3 [curves (a)]. Due to the Ramsauer-Townsend minimum in the momentum-transfer cross section, the function $B(x)$ has a local minimum approximately at $x = 3.1$, and the function $A(x)$ has a local minimum and a maximum approximately at $x = 3$ and $x = 1.9$, respectively. These critical points lie within the interval limited by the dashed lines shown in the figure, which are the positions of the maximum for the initial Gaussian at $x = 5.5$ and the steady-state Maxwellian at $x = 1$. Since small absolute values of $A(x)$, $B(x)$ and their derivatives imply slow variation in time of h, the distribution function tends to vary faster at points lying outside a small neighborhood of the critical points. As a result, in the cooling process of electrons in Ar, the distribution function is first compressed close to $x = 3.1$, its maximum slowly decreases around this point, and then intermediate bimodal distributions appear when electrons with reduced speed higher than $x = 1.9$ migrate to lower values of x. In contrast, the function $B(x)$ for e-Ne is almost linear in x [similar to the hard-sphere case, for which $B(x) = x$], and $A(x)$ is almost parabolic with a minimum at $x = 0$, which lies outside the interval limited by the dashed lines. As a result, the relaxation of $h(x,t)$ occurs by unimodal distributions.

The relaxation of $T(t)/T_b$, $\Sigma_{\mathrm{SS}}(t)$ and $\Sigma_{\mathrm{LM}}(t)$ for e-Ar has a stronger departure from the hard-sphere cross section than in the e-Ne case. Moreover, there are changes in the concavity of $\Sigma_{\mathrm{LM}}(t)$ that are not present for the e-Ne system, as shown in Fig. 2(D). These differences between the two systems are a consequence of the deep Ramsauer-Townsend minimum in the momentum-transfer cross section for e-Ar mentioned above. Note that the computations for e-Ar were carried out with $\sigma_0 = 0.23\,\text{Å}^2$, which provides a better fit than the value obtained by the criterion used for the e-Ne system. For comparison, we also show for Ar the results for the MM cross section [curve (b)] with $a = 6$, obtained by Eq. (13) with $\sigma_0 = 13.57\,\text{Å}^2$ and $p = 11.1$.

Figure 4 shows the heating of electrons in Ne (left) and Ar (right) by the action of an external electric field $E/n \neq 0$. The curves (a)–(c) are for different values of E/n. The initial distribution function is a Maxwellian at $T_b = 290.1$K that evolves to the final Davydov distribution, Eqs. (5) and (6), at a temperature $T_{\mathrm{SS}} > T_b$, as shown in Figs. 4(A) and 4(B) in the case of $E/n = 0.15$ Td. For Ne, the initial Maxwellian evolves as a sequence of unimodal distributions, while for Ar the relaxation includes intermediate bimodal distributions. This difference is the result of the Ramsauer-Townsend minimum in the e-Ar momentum-transfer cross section. According to the Fokker-Planck equation (24), the time dependence of the distribution function is determined by $B(x)$ as given by Eq. (3), and

$$A(x) = 2\left[\frac{x\widehat{\sigma}(x)}{B(x)} - \frac{1}{x^2}\right] x B(x). \tag{25}$$

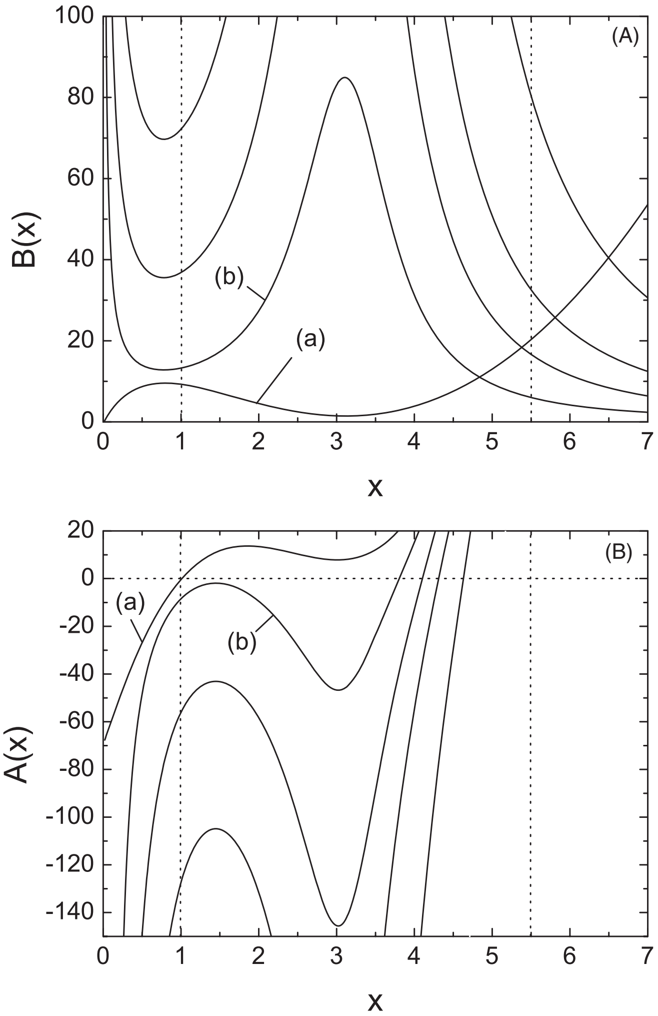

FIG. 3. Variation of (A) $B(x)$ [Eq. (3)] and (B) $A(x)$ [Eq. (25)] vs reduced speed for electrons in Ar with E/n in Td equal to (a) 0 and (b) 0.15; 1 Td = 10^{-17} V cm^2; other curves correspond to higher values of the field; curves (a) computed with $\sigma_0 = 0.23\,\text{Å}^2$ and other curves computed with $\sigma_0 = 155\,\text{Å}^2$; dashed lines indicate positions of the maximum for the initial Gaussian ($x_0 = 5.5$) and steady-state Maxwellian ($x_0 = 1$) distributions shown in Fig. 2(A); tabulated e-Ar momentum-transfer cross section [23] was fitted to an analytic expression.

Both $A(x)$ and $B(x)$ are shown in Fig. 3 [curves (b)] for the e-Ar system. The action of the external electric field changes the concavity of $B(x)$ at $E/n = 0$ [Fig. 3(A) curve (a)], and in particular the minimum at $x = 3.1$ becomes a maximum. Also, $A(x)$ has a maximum and a minimum at approximately $x = 1.5$ and 3, respectively. Thus, the relaxation of electrons in Ar with an external electric field is somewhat reverse to the case discussed above for the zero field case. Initially the Maxwellian distribution function is peaked at $x = 1$ and is heated to a Dayvdov distribution with a maximum approximately at $x = 6$, after going through these critical points of $A(x)$ and $B(x)$. The maximum of the distribution slowly decreases around the reduced speed $x = 1$, and the fast migration of electrons coming into and leaving from

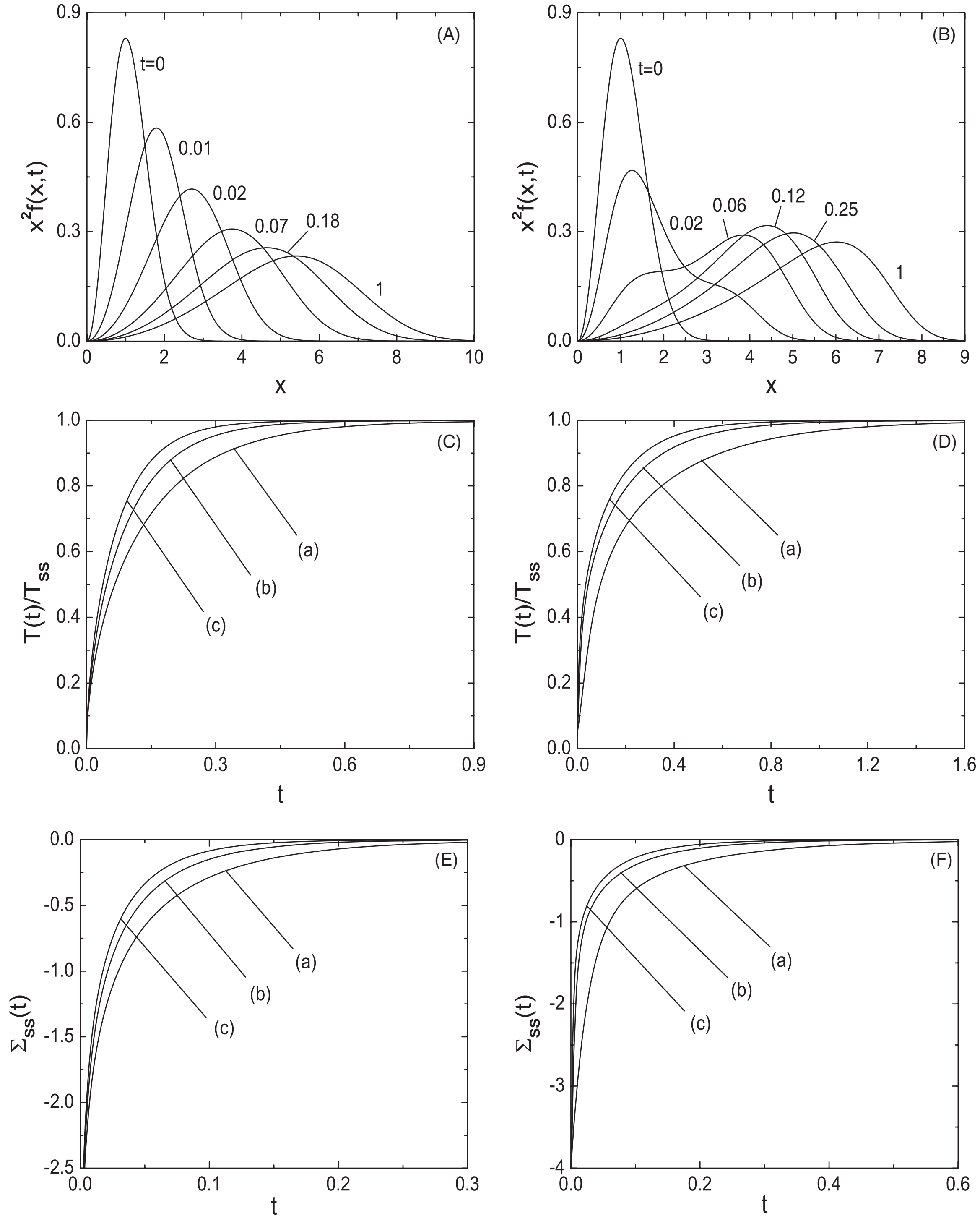

FIG. 4. The nonzero electric field time variation of $x^2 f(x,t)$, $T(t)/T_{\rm SS}$, and $\Sigma_{\rm SS}(t)$ for electrons in Ne (left) and Ar (right). E/n in Td is (a) 0.15, (b) 0.35, (c) 0.55; initial Maxwellian distribution at $T(0) = T_b = 290.1$ K; for Ne $t_0 = 44$, $\sigma_0 = 18.0$ Å^2 and $T_{\rm SS}$ in units of T_b is (a) 20, (b) 41, (c) 60; for Ar $t_0 = 10$, $\sigma_0 = 155$ Å^2 and $T_{\rm SS}$ in units of T_b is (a) 20, (b) 30, (c) 38; t_0 in units of 10^{11}cm^{-3} s.

a neighborhood of $x = 3$ produces intermediate bimodal distributions.

The time dependence of the electron temperature relative to $T_{\rm SS} > T_b$ is shown in Figs. 4(C) and 4(D) for several values of E/n. The increasing values of $T_{\rm SS}$ with E/n for Ne and Ar show the heating of the electrons by the electric field. The Kullback-Leibler entropy, $\Sigma_{\rm SS}(t)$, shown in Figs. 4(E) and 4(F) is initially negative and increases monotonically to zero in accordance with the H-theorem discussed in Sec. III.

In Fig. 5 we show the thermalization of electrons in Ne for $E/n = 0$ and with an initial Maxwellian distribution at $T(0) = 20T_b$. The distribution function evolves as sequence of unimodal distributions to the steady-state Maxwellian, as

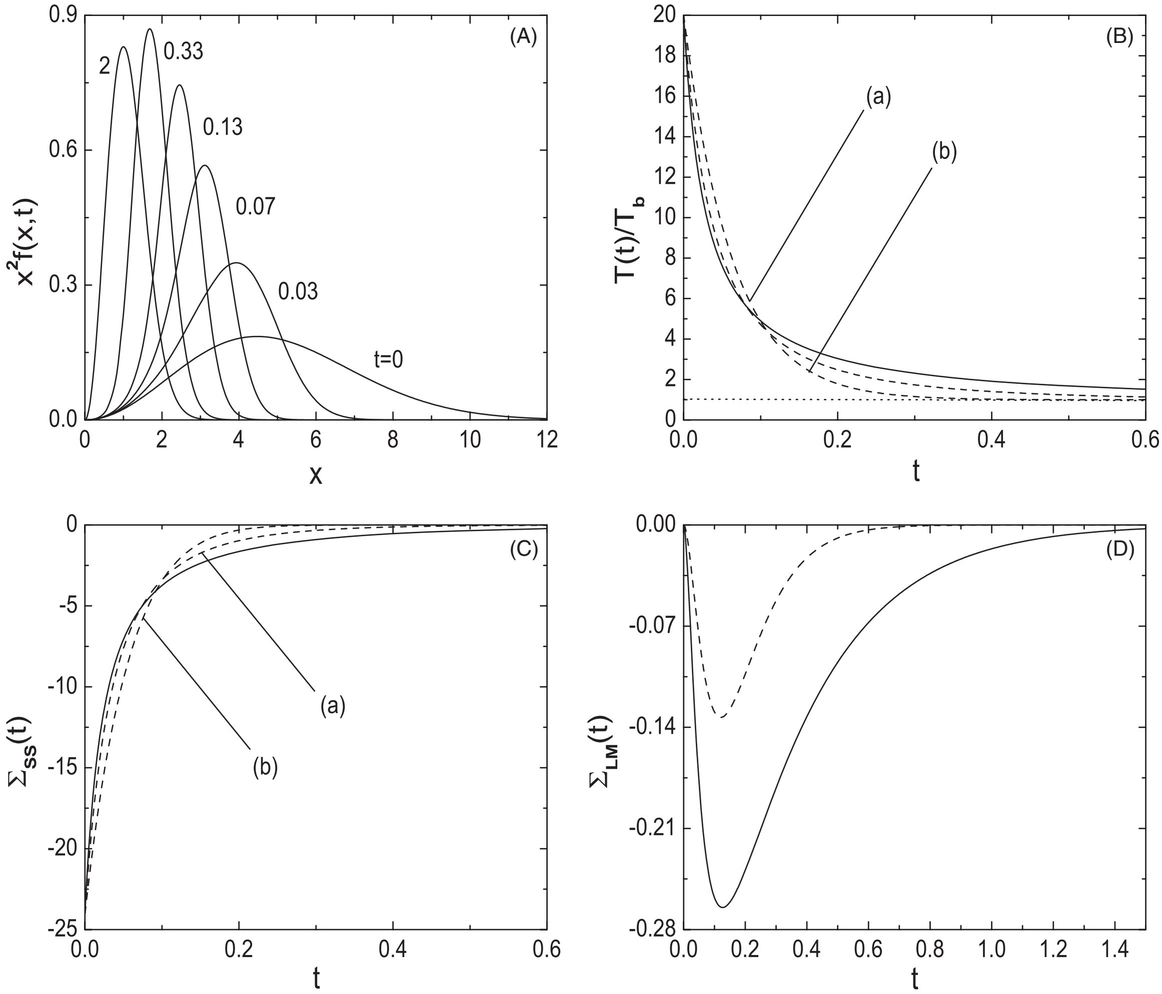

FIG. 5. The time dependence of $x^2 f(x,t)$, $T(t)/T_b$, $\Sigma_{\mathrm{SS}}(t)$, and $\Sigma_{\mathrm{LM}}(t)$ for electrons in Ne (solid curves); $E/n = 0$; initial Maxwellian distribution at $T(0) = 20T_b$ with $T_b = 290.1$ K; $t = t'/t_0$ with $t_0 = 669$ in units of 10^{11} cm^{-3} s; $T_b = 290.1$K; (a) hard sphere ($\sigma_0 = 1.18$ Å^2); (b) Maxwell molecules ($a = 4$, $\sigma_0 = 10$ Å^2); (D) (dashed line) hard-sphere cross section. For Maxwell molecules $\Sigma_{\mathrm{LM}}(t) = 0$ for all t.

shown in Fig. 5(A). The temperature relaxation is shown in Fig. 5(B), and the Kullback-Leibler entropy $\Sigma_{\mathrm{SS}}(t)$ is given in Fig. 5(C). The latter evolves from the initial value $\Sigma_{\mathrm{SS}}(0) = -24$ as given by Eq. (19) monotonically to zero. A good approximation is obtained by the hard-sphere model [dashed curve (a)] with $\sigma_0 = 1.17$ Å^2. This value was chosen by the same criterion used earlier for the relaxation of electrons in Ne with an initial Gaussian distribution.

In Fig. 5(D) we show the evolution of $\Sigma_{\mathrm{LM}}(t)$. Since the initial distribution function is a Maxwellian at $T(0)$, $\Sigma_{\mathrm{LM}}(0) = 0$. Electron-Ne collisions do not preserve the Maxwellian distribution during the relaxation process, and therefore $\Sigma_{\mathrm{LM}}(t) < 0$ for $t > 0$. The departure from the local Maxwellian is the result of the energy dependence of $B(x)$ in the Fokker-Planck equation, Eq. (7). It is a maximum at about $t = 0.13$ for which $\Sigma_{\mathrm{LM}}(t)$ attains a minimum shown in Fig. 5(D). For subsequent times, e-Ne collisions cause the distribution function to approach the global Maxwellian at the bath temperature T_b, in accordance with the H-theorem. As a consequence, $\Sigma_{\mathrm{LM}}(t)$ increases to zero after it reaches its minimum value. The relaxation of $\Sigma_{\mathrm{LM}}(t)$ takes approximately the same time as $\Sigma_{\mathrm{SS}}(t)$, which is shown in Table I(b). For the MM model $\Sigma_{\mathrm{LM}}(t) \equiv 0$ for all times due to the canonical invariance property.

A useful interpretation of the canonical invariance property arises from the unique feature of the Fokker-Planck operator for MM, which is defined by the right-hand side of Eq. (2), or equivalently Eq. (24), with $B(x) = 1$. The quantity in square brackets in Eq. (24) is a flux $J(x)$ in speed space, and the Fokker-Planck equation is thus a diffusion equation, namely, $\partial h/\partial t = \partial J/\partial x$. If we substitute the local Maxwellian $h_{\mathrm{LM}}(x,t) = x^2 f_{\mathrm{LM}}(x,T(t))$ into both sides of Eq. (24) with $B(x) = 1$, we have that

$$f_{\mathrm{LM}}[x,T(t)]\left[\frac{x^2}{T(t)/T_b} - \frac{3}{2}\right]\frac{1}{T(t)}\frac{dT(t)}{dt} = -4 f_{\mathrm{LM}}[x,T(t)]\left[\frac{x^2}{T(t)/T_b} - \frac{3}{2}\right]\left[1 - \frac{T_b}{T(t)}\right], \tag{26}$$

which yields

$$\frac{dT(t)}{dt} = -4\,[T(t) - T_b]\,. \tag{27}$$

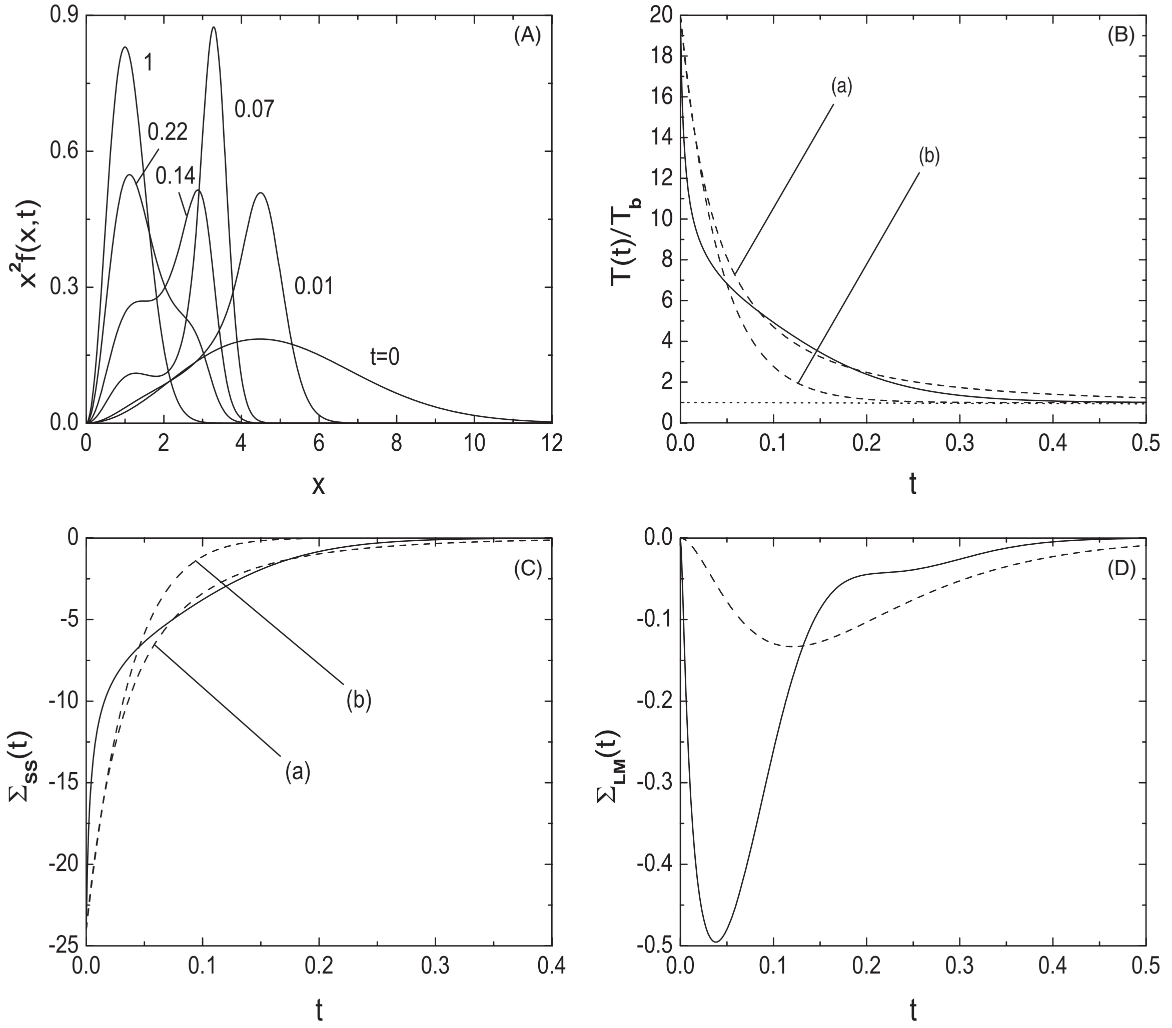

FIG. 6. Relaxation of electrons in Ar with an initial Maxwellian distribution at $T(0) = 20T_b$; see caption to Fig. 5; $t_0 = 6752$ in units of 10^{11}cm^{-3} s; $T_b = 290.1$ K; (a) hard sphere ($\sigma_0 = 0.23$ Å^2); (b) Maxwell molecules ($a = 6$, $\sigma_0 = 13.57$ Å^2).

The solution of Eq. (27) is given by Eq. (15) with $a = 1$. Thus, for the MM model the Fokker-Planck equation reduces to the time rate of change of the temperature. The flux in speed space, $J(x)$, as given by the right-hand side of Eq. (26) alters the speed distribution function in the same way as does the change in $T(t)$. This is not the case for other cross sections, where the corresponding flux in speed space changes the shape of the initial Maxwellian distribution function.

The relaxation of electrons in Ar for $E/n = 0$ and with an initial Maxwellian distribution at $T(0) = 20T_b$ is shown in Fig. 6. The main characteristic that results from this change of initial condition with respect to the Gaussian is the rapid and more pronounced deformation of the initial Maxwellian into bimodal distributions at intermediate times, as shown in Fig. 6(A). The evolution of the temperature and the Kullback-Leibler entropy $\Sigma_{\mathrm{SS}}(t)$ is similar to those in Figs. 2(B) and 2(C), respectively. The evolution of $\Sigma_{\mathrm{LM}}(t)$ is shown in Fig. 6(D). It is initially zero and has a minimum at approximately $t = 0.04$, where the departure of distribution function from a local Maxwellian is a maximum. For larger times, this function presents several changes in concavity, which is a consequence of the bimodal nature of the intermediate distribution functions. This is in turn a consequence of the deep Ramsauer-Townsend minimum of the e-Ar momentum-transfer cross section. As for the e-Ne system, the relaxation to a local Maxwellian for e-Ar requires about the same time as for the distribution function to relax to the equilibrium Maxwellian; see Table I(b).

V. RELAXATION TIME FOR A MULTI-EXPONENTIAL RELAXATION

There are numerous physical situations such as in the present study where the time evolution of some quantity is given by a sum of exponentials. As shown in Sec. II, each term in the sum for the distribution function, Eq. (10), and the temperature, Eq. (11), is characterized by an eigenvalue of the linear Fokker-Planck operator. The aim of this section is to characterize the relaxation process for both the distribution function and the temperature in terms of a single relaxation time indicative of the time scale of the processes. As mentioned earlier, the fitting of data to multi-exponential functions

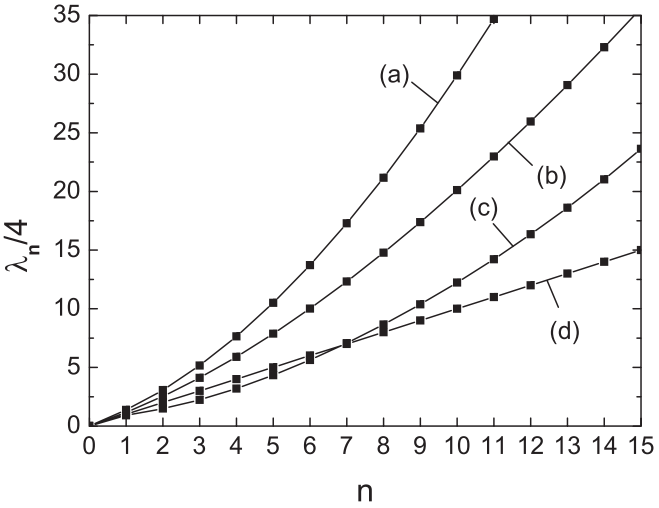

FIG. 7. Lower-order eigenvalues of the discretized Fokker-Planck operator; $\alpha = 0$; λ_n in units of t_0^{-1}. (a) Ne ($\sigma_0 = 0.37\,\text{Å}^2$), (b) hard spheres ($\sigma_0 = 0.37\,\text{Å}^2$), (c) Ar ($\sigma_0 = 1.19\,\text{Å}^2$), and (d) Maxwell molecules ($a = 1, \sigma_0 = 40\,\text{Å}^2$).

has been studied extensively and is an ill-defined problem [40,48–50,56]. In the event that the eigenvalue spectrum has a separation for a pair of eigenvalues by more than an order of magnitude, the relaxation would be characterized by more than one time scale, and a single relaxation time might not be an adequate description. For the systems studied here, there is no evidence for such a behavior. In Fig. 7 we show the variation of the lowest eigenvalues of the Fokker-Planck operator versus n for the e-Ne and e-Ar cross sections, curves (a) and (c), respectively. The convergence of the eigenvalues versus the number of quadrature points was obtained to four significant figures. Also shown are the lowest eigenvalues for the MM [curve (b)] and hard-spheres cross sections [curve (d)]. For the MM cross section, λ_n varies linearly with n as discussed previously [28,45]. For the other cross sections, the separation between successive eigenvalues does increase, although it is not pronounced. Therefore, we expect that for the e-Ne and e-Ar systems the thermalization can be characterized by single average relaxation times.

From an inspection of the relaxations of $T(t)/T_b$, $\Sigma_{\rm SS}(t)$ and $\Sigma_{\rm LM}(t)$ reported in the previous section, we can qualitatively conclude that for each system studied the approach to equilibrium is approximately on the same time scale for all these quantities, and therefore the distribution functions approach equilibrium on about the same time scale as does the temperature. We are interested in characterizing these relaxations with a single relaxation time and thus quantifying this conclusion. However, the assignment of a single relaxation time to the various time-dependent quantities is not a uniquely well defined procedure. The times $\tau_{1.01}$ and $\tau_{1.1}$ employed in many comparisons of theory and experiment for electron relaxation [4,5,16,23,46,47] appear not be appropriate for this objective as they are representative of the long-time behavior, especially $\tau_{1.01}$. We are interested in a definition that represents an average over the time history of the process.

We consider two definitions of a relaxation time both based on a single exponential relaxation. If the quantity of interest is denoted by $F(t)$, we define

$$\tau_1 = \frac{1}{F(0)}\int_0^\infty F(t)\,dt \tag{28}$$

and

$$\tau_2 = \frac{\int_0^\infty tF(t)\,dt}{\int_0^\infty F(t)\,dt}. \tag{29}$$

These definitions have been used in the study of other relaxation processes, which include ferromagnetic relaxation [57], Brownian motion in double-well potentials [58], and fluorescence [59]. In the particular case in which $F(t)$ is a multi-exponential function of N terms,

$$F(t) = \sum_{n=1}^{N} c_n e^{-\lambda_n t}, \tag{30}$$

the values of τ_1 and τ_2 give, respectively, the relaxation times of pure exponentials $C_1 e^{-t/\tau_1}$ and $C_2 e^{-t/\tau_2}$ whose area are the same as the area under $F(t)$, with C_1 and C_2 such that

$$\tau_1 = \sum_{n=1}^{N}\frac{c_n}{\lambda_n}\bigg/\sum_{n=1}^{N} c_n \tag{31}$$

and

$$\tau_2 = \sum_{n=1}^{N}\frac{c_n}{\lambda_n^2}\bigg/\sum_{n=1}^{N}\frac{c_n}{\lambda_n}. \tag{32}$$

In particular, $C_1 = F(0)$. Therefore, τ_1 and τ_2 are just the weighted mean of the relaxation times λ_n^{-1} for the terms in the sum of Eq. (30), where the weights are given by the coefficients c_n and c_n/λ_n, respectively. If $F(t)$ is a pure exponential, then τ_1 and τ_2 are equal and coincide with the single relaxation time that parametrizes $F(t)$.

In Table II we provide the values of τ_1 and τ_2 for the quantities $T(t)/T_b$, $\Sigma_{\rm SS}(t)$ and $\Sigma_{\rm LM}(t)$ for the e-Ne and e-Ar

TABLE II. Relaxation times in units of 10^{11}cm^{-3} s for $T(t)/T_b$, $\Sigma_{\rm SS}(t)$ and $\Sigma_{\rm LM}(t)$; $E/n = 0$; (a) $f(x,0) = A\exp[-\beta(x - x_0)^2]$ with $\beta = 20$ and $x_0 = 5.5$, (b) initial Maxwellian with $T(0) = 20T_b$; for Ne, HS, and MM see Figs. 1–5, for Ar see Figs. 2–6; bold numbers denote the ratio of rows for $T(t)/T_b$ and $\Sigma_{\rm SS}(t)$; according to the definition of τ_1, missing entries are the result of $\Sigma_{\rm LM}(0) = 0$ for the initial Maxwellian.

	(a)				(b)			
Process	Ne	Ar	HS	MM	Ne	Ar	HS	MM
				τ_1				
$T(t)/T_b$	67	454	51	4.98	60	363	47	4.98
$\Sigma_{\rm SS}(t)$	46	352	38	4	41	278	34	4.08
$\Sigma_{\rm LM}(t)$	72	398	41	2.96	—	—	—	—
	1.5	**1.3**	**1.3**	**1.3**	**1.5**	**1.3**	**1.4**	**1.2**
				τ_2				
$T(t)/T_b$	167	608	81	4.90	170	590	80	4.90
$\Sigma_{\rm SS}(t)$	93	470	49	3.67	93	452	47	3.69
$\Sigma_{\rm LM}(t)$	162	455	69	3.34	238	600	133	10.7
	1.8	**1.3**	**1.7**	**1.3**	**1.8**	**1.3**	**1.7**	**1.3**

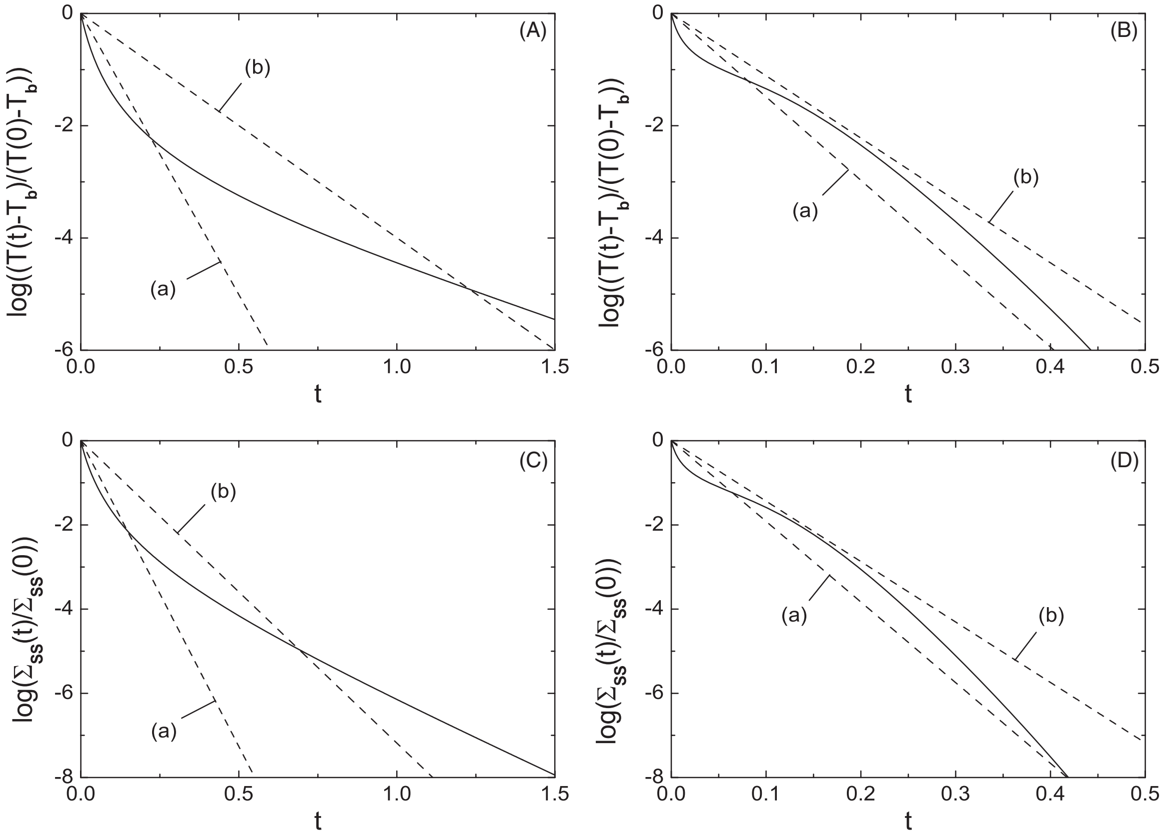

FIG. 8. Time variation of $\log[(T(t)-T_b)/(T(0)-T_b)]$ and $\log[\Sigma_{\rm SS}(t)/\Sigma_{\rm SS}(0)]$ (solid curves) for electrons in Ne (left) and Ar (right); $E/n=0$; see caption to Figs. 1(B) and 1(C) and Figs. 2(B) and 2(C). Dashed curves are straight lines through the origin with slopes (a) $-1/\tau_1$ and (b) $-1/\tau_2$.

systems with an initial (a) Gaussian and (b) Maxwellian distribution function. The relaxation times were computed with the finite difference solution of the Fokker-Planck equation and the time integrations in Eqs. (28) and (29). For e-Ne, the results correspond to Figs. 1(B)–1(D) and 5(B)–5(D), and for e-Ar the values reported correspond to Figs. 2(B)–2(D) and 6(B)–6(D). A good check is to compare the values τ_1 and τ_2 of the temperature relaxation for the MM cross section, since in this case the temperature relaxes as a pure exponential irrespective of the initial distribution, and therefore τ_1 and τ_2 must equal $1/(4a)$ in units of t_0. For $a=4$ and $t_0=78.45$ we have $\tau=4.9$ in units of $10^{11}\mathrm{cm}^{-3}$ s, which is in agreement with the four entries for MM. As shown in the table, the relaxation times for $T(t)/T_b$ and $\Sigma_{\rm SS}(t)$ are in the same order regardless of the initial distribution. Thus, the approach of $T(t)$ and $f(x,t)$ to a steady state occurs approximately on the same time scale for each system. According to τ_1, the temperature of e-Ne relaxes 1.5 times faster than the Leibler-Kullback entropy $\Sigma_{\rm SS}(t)$ does, while this value is 1.3 for the e-Ar system. A similar result is found for τ_2, which gives 1.8 for e-Ne and 1.3 for e-Ar. These values are very close to those for the hard-sphere and MM momentum-transfer cross sections, as shown in the table.

We show in Fig. 8 the time dependence of $\log[(T(t)-T_b)/(T(0)-T_b)]$ and $\log[\Sigma_{\rm SS}(t)/\Sigma_{\rm SS}(0)]$ in comparison with the linear dependencies (dashed straight lines) with relaxation times τ_1 [curve (a)] and τ_2 [curve (b)] given by the values reported in Table II(a) for an initial Gaussian distribution function. The results for e-Ne are on the left, whereas the results for e-Ar are on the right of the figure. Although the effective exponentials C_1e^{-t/τ_1} and C_2e^{-t/τ_2} are not intended to fit these quantities, the figures suggest that they are good representatives for the relaxation processes taking place in these systems. For e-Ne, curves (a) seem to provide a better description for small times while curves (b) give a better overall description. The curves (a) seem to underestimate the relaxation curves. For the e-Ar system, curves (a) and (b) are closer to each other, suggesting that the system might relax on average closer to a single exponential. Note that in this analysis only $T(t)/T_b$ is a multi-exponential function, and thus in this case τ_1 and τ_2 are given by the relations in Eqs. (31) and (32), respectively. These expressions provide a direct link between the relaxation of $T(t)/T_b$ and the eigenvalue spectrum of the Fokker-Planck operator L defined in Eq. (7). This connection is less obvious but still present for the quantities $\Sigma_{\rm SS}(t)$ and $\Sigma_{\rm LM}(t)$. The set of curves corresponding to an initial Maxwellian distribution are not shown since they are very similar to the curves for the initial Gaussian distribution, except for $\Sigma_{\rm LM}(t)$. For this quantity, the relaxation time τ_1 can not be used, since $\Sigma_{\rm LM}(0)=0$ (which explains the empty entries in Table II).

We investigate the relaxation times for electrons in Ne and Ar heated by an external electric field. In Table III we show the values of τ_1 and τ_2 for the temperature ratio $T(t)/T_{\rm SS}$ and the Kullback-Leibler entropy $\Sigma_{\rm SS}(t)$ versus E/n. The initial distribution is a Maxwellian at the bath temperature

TABLE III. Relaxation times in units of 10^{11}cm^{-3} s versus E/n in Td; 1 Td $= 10^{-17}$ V cm^2; see caption to Fig. 4; bold numbers denote the ratio of columns $T(t)/T_{\text{SS}}$ and $\Sigma_{\text{SS}}(t)$.

	τ_1			τ_2		
E/n	$T(t)/T_{\text{SS}}$	$\Sigma_{\text{SS}}(t)$	Ratio	$T(t)/T_{\text{SS}}$	$\Sigma_{\text{SS}}(t)$	Ratio
			Ne			
0.01	28.22	13.19	**2.14**	25.42	14.92	**1.70**
0.15	5.580	1.284	**4.35**	6.779	2.546	**2.66**
0.35	3.740	0.723	**5.17**	4.488	1.661	**2.70**
0.55	2.906	0.529	**5.49**	3.427	1.258	**2.72**
1	1.974	0.344	**5.74**	2.267	0.816	**2.78**
			Ar			
0.001	11.98	11.59	**1.03**	7.988	7.965	**1.00**
0.005	12.34	11.52	**1.07**	8.102	7.901	**1.03**
0.01	12.72	10.97	**1.16**	8.184	7.669	**1.15**
0.03	9.562	5.527	**1.73**	6.794	4.948	**1.37**
0.15	2.263	0.588	**3.85**	3.104	1.125	**2.76**
0.25	1.592	0.347	**4.59**	2.408	0.865	**2.78**

$T_b = 290.1$ K. As the table shows, the relaxation times for e-Ne decrease with the increase of E/n. Previous studies [5] have shown that for atomic moderators such as Ne with a momentum-transfer cross section that varies slowly with energy, the eigenvalues of the Fokker-Planck operator increase with increasing field. This is in agreement with our result since the relaxation times are determined by the inverse of the eigenvalues. The relaxation times of the Kulback-Leibler entropy decreases with E/n as well. It relaxes slightly faster than the temperature but in the same order, as shown in Table III by the ratio of the relaxation times of $T(t)/T_{\text{SS}}$ and $\Sigma_{\text{SS}}(t)$ (numbers in bold). However, this ratio seems to increase with E/n.

It has also been shown [5] that for atom moderators such as Ar whose cross sections depend strongly with the energy and exhibit a Ramsauer minimum, the eigenvalues of the Fokker-Planck operator first decrease with E/n and then increase for larger values of E/n. This behavior is in agreement with the relaxation times of the temperature for the e-Ar system reported in Table III. We see that τ_1 and τ_2 increase for small values of E/n and then decrease steadily with E/n. This phenomenon seems to occur by the change in the concavity of the coefficient $B(x)$ in the Fokker-Planck equation (7), due to the action of the external field. As shown in Fig. 3(A), the position of the local extrema of $B(x)$ for $E/n = 0$ [curve (a)] are exchanged when $E/n \neq 0$ [e.g., curve (b)]. Actually, another minimum appears at x satisfying $x\widehat{\sigma}(x) = \alpha$ (not shown in the figure). This continuous transition in the shape of $B(x)$ versus E/n implies that for small values of the

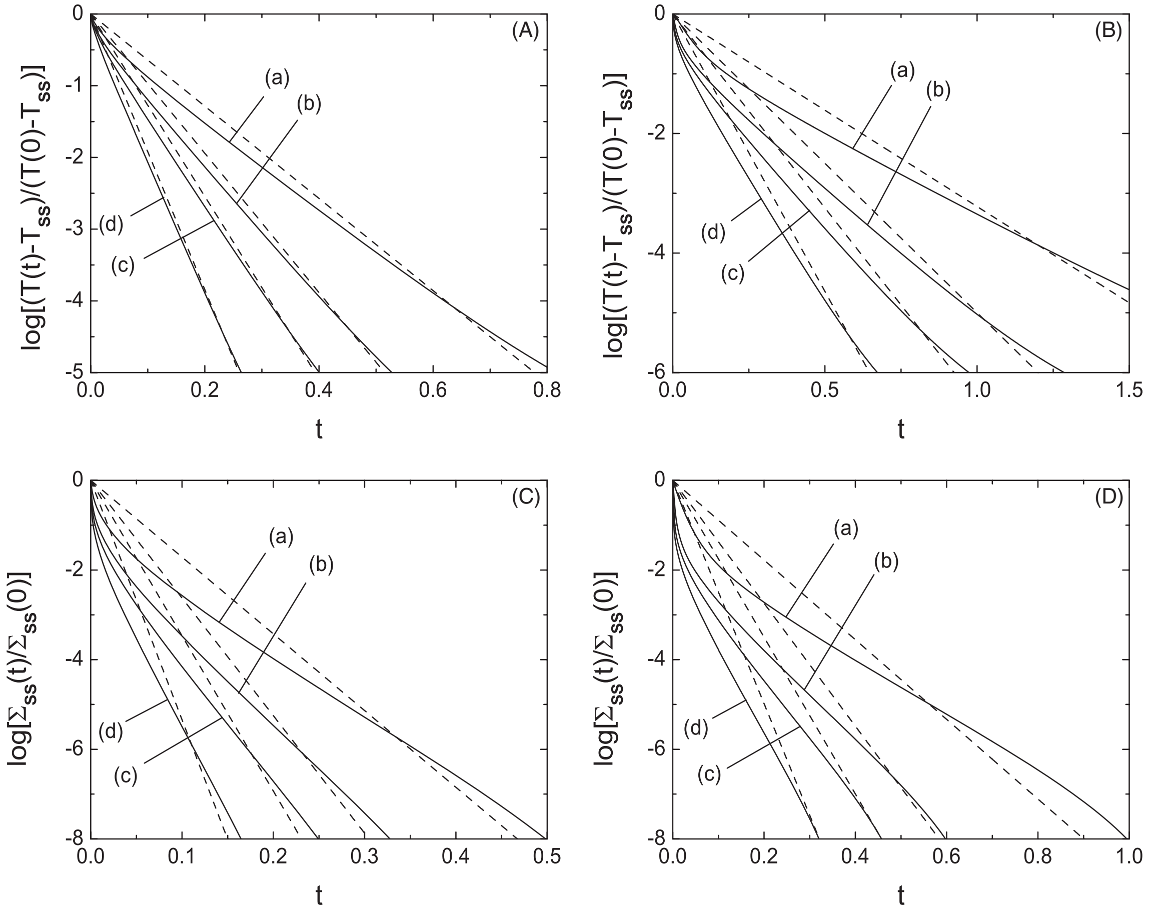

FIG. 9. The nonzero electric field time variation of $\log[(T(t) - T_{\text{SS}})/(T(0) - T_{\text{SS}})]$ and $\log[\Sigma_{\text{SS}}(t)/\Sigma_{\text{SS}}(0)]$ (solid curves) for electrons in Ne (left) and Ar (right); see caption to Fig. 4; E/n in Td is equal to (a) 0.15, (b) 0.35, (c) 0.55, and (d) 1. Dashed curves are straight lines through the origin with slope $-1/\tau_2$.

field the extrema of $B(x)$ are less pronounced and might even disappear. This means that for such external fields the Ramsauer minimum is fully compensated, the distribution function widens and the rate of change of the temperature decreases, which produces an increase in the relaxation times for $T(t)/T_b$. If the electric field increases beyond these values [which for e-Ar is between 0.01 Td and 0.03 Td according to Table III, in agreement with Fig. 3(B) in Ref. [5]], then the maximum and minimum of $B(x)$ are more pronounced, and the effect of the Ramsauer minimum is again considerable [e.g., see curve (b) in Fig. 3(A) for $E/n = 0.15$ Td). Then the intermediate bimodal distributions appear, the rate of change of the temperature increases, and therefore the relaxation times of $T(t)/T_b$ decreases. As for $\Sigma_{\mathrm{SS}}(t)$, there is no evidence that the relaxation times change monotonicity with E/n. According to Table III they decrease steadily with increasing field.

The effective exponentials associated with $T(t)/T_{\mathrm{SS}}$ and $\Sigma_{\mathrm{SS}}(t)$ with relaxation times τ_2 (dashed straight lines) reported in Table II are shown in Fig. 9 for several values of the field. They are on the average very good representatives for the evolution of these quantities, mostly for the temperature relaxation, Fig. 9(A) for e-Ne and Fig. 9(B) for e-Ar. The approximation improves with increasing field, specially for e-Ne, as shown in Figs. 9(A) and 9(C). For e-Ar, stronger deviations from linearity occur than for the e-Ne system at early values of time. This is attributed to the Ramsauer-Townsend minimum of the e-Ar momentum-transfer cross section. For the field range used, the quantities shown decrease with E/n at each time, and thus the relaxation is faster with the increase of E/n.

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