

## Hot-electron zero-field mobility and diffusion in rare-gas moderators

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An efficient discrete-ordinate method of solution of the time-dependent Boltzmann equation is employed in the calculation of the zero-field electron mobility and diffusion coefficients for hot-electron thermalization in rare-gas moderators. The discrete-ordinate method is modified to permit a rescaling of the quadrature points. This procedure is somewhat analogous to the two-temperature-moment methods employed in the theoretical analysis of electron swarms. The time-dependent transport coefficients are given as a sum of exponential decay terms characterized by the discrete eigenvalues of the Lorentz-Fokker-Planck operator for elastic electron-atom collisions. For argon, krypton, and xenon, the time dependence is strongly influenced by the Ramsauer-Townsend minimum and leads to maxima in the transient mobility and diffusion coefficient. Helium and neon with hard-sphere-like cross sections exhibit transient mobilities which initially are below the thermal zero-field mobility and then increase to the thermal mobilities as the electron distribution approaches equilibrium. The transient mobility for cross sections with Ramsauer minima are sufficiently sensitive to the details of the cross sections such that it may be feasible to distinguish between different cross sections experimentally. The calculations also indicate that the transient mobility is insensitive to the initial distribution function. A nonequilibrium phenomenon not previously recognized is the possibility of a negative transient mobility which occurs provided that the momentum-transfer cross section increases sufficiently rapidly with energy.

### I. INTRODUCTION

There are a variety of physical phenomena which involve a knowledge of the time evolution of the velocity distribution function (VDF) of strongly epithermal electrons. Some examples include the calculation of electron thermalization times in the analysis of swarm experiments,<sup>1-3</sup> studies of electron scavenging or attachment,<sup>3</sup> delayed luminescence in gases,<sup>4</sup> pulsed transient conductivity experiments,<sup>5</sup> thermalization of photoelectrons in the ionosphere,<sup>6,7</sup> and the VDF of solar-wind electrons.<sup>8</sup> The need to develop a computationally efficient and accurate method of solution of the Boltzmann equation<sup>9</sup> (BE) which yields the time-dependent VDF is clear.

The present paper employs a modified version of the discrete-ordinate (DO) method introduced in previous papers.<sup>10-13</sup> The DO method is a familiar method of solution of integral equations and has been employed in this way in the solution of the integral BE for the relaxation of test particles in a heat bath<sup>14</sup> and for the reaction of hot atoms.<sup>15</sup> In these applications, the DO method is based on a Gaussian quadrature rule for numerical integration. For the electron thermalization problem, the integral Boltzmann collision operator is well approximated by the differential Lorentz-Fokker-Planck (LFP) operator,<sup>9</sup> owing to the small electron-atom mass ratio. Shizgal and Blackmore<sup>13</sup> have recently developed a DO method applicable to differential equations analogous to its use in the solution of integral equations. In the present work, as in the earlier calculation of electron thermalization times,<sup>12</sup> the DO method is based on the Gaussian quadrature rule associated with speed polynomials.<sup>16</sup> The previous paper<sup>12</sup> demonstrated the efficiency of the DO method in

the calculation of the VDF, the energy thermalization times and the influence of Ramsauer minima in the cross sections. The present paper extends the earlier work to include a calculation of the (zero-field) electron mobility and diffusion coefficients.

The DO formalism is here extended to permit a rescaling of the quadrature points while retaining the self-adjoint form of the LFP operator. The rescaling of the quadrature points is an important procedure, since it extends the energy range spanned by the quadrature points without an increase in their total number. The procedure can be compared with the two-temperature electron transport theory<sup>17-19</sup> where one uses a weight function characterized by an effective temperature which differs from the temperature of the moderator. It is anticipated that the present method will be computationally more efficient than the traditional moment methods.<sup>17-20</sup> The DO method is certainly more efficient than the numerical integrations by Braglia *et al.*<sup>21</sup> in the determination of the eigenvalues and eigenfunctions of the LFP operator.

The basic objective of the present work is to determine the time dependence of the mobility and diffusion coefficients of electrons in inert gas moderators. The initial VDF of electrons is chosen to be either a  $\delta$  function or a Gaussian distribution in speed and unidirectional consistent with the work by Mozumder,<sup>22-24</sup> and Knierim *et al.*<sup>20</sup> It is important to mention that our calculations show that the relaxation times are not very sensitive to the details of the initial distribution provided that the initial energy is above the Ramsauer minimum. Mozumder assumed that the VDF can be taken to be a pseudo-Maxwellian throughout the thermalization process. The relaxation is then followed with a numerical integration of

moment equations for the temperature and bulk velocity. As discussed in the previous papers,<sup>11,12</sup> there is no justification for this procedure. The work by Knierim *et al.*<sup>20</sup> is an extension of Mozumder's work in that additional moments are retained. However, since the moment equations have to be integrated numerically this approach is not as efficient as the present DO method. It is useful to point out that the moment method transforms a linear operator equation into an infinite set of coupled differential equations with nonconstant coefficients. This does not appear to be a useful approach.

In Sec. II, the Gaussian quadrature procedure based on speed points is applied to the calculation of the thermal mobility and diffusion, and the rescaling procedure is introduced. Section III contains a brief development of the electron transport theory with numerical procedures and results presented in Sec. IV.

## II. GAUSSIAN QUADRATURE EVALUATION OF THERMAL TRANSPORT COEFFICIENTS

The standard expressions for the thermal electron mobility  $\mu_{th}$  and diffusion coefficient  $D_{th}$  are<sup>9,25</sup>

$$n\mu_{th} = \frac{4\pi e}{3kT_b} \left[ \frac{2\pi kT_b}{m} \right]^{-3/2} \int_0^\infty e^{-mv^2/2kT_b} \frac{v^3}{\sigma_m(v)} dv$$

and (1)

$$D_{th} = \frac{kT_b}{e} \mu_{th},$$

where  $m$  and  $e$  are the electron mass and charge, respectively,  $T_b$  and  $n$  are the temperature and number density of the moderator, respectively, and  $\sigma_m(v)$  is the momentum-transfer cross section for electron-atom collisions. With the substitution of the reduced speed

$x = (m/2kT)^{1/2}v$ , characterized by a temperature  $T$  not necessarily equal to the moderator temperature  $T_b$ , we get

$$n\mu_{th} = \frac{4e}{3} \left[ \frac{\pi mkT_b}{2} \right]^{-1/2} s^4 \times \int_0^\infty e^{-x^2} x^3 \frac{e^{-x^2(s^2-1)}}{\sigma_m((2kT_b/m)^{1/2}sx)} dx, \quad (2)$$

where  $s = (T/T_b)^{1/2}$ . The integration in Eq. (2) is done numerically with an  $N$ th-order Gaussian quadrature procedure defined by

$$\int_0^\infty e^{-x^2} x^2 f(x) dx \approx \sum_{i=1}^N w_i f(x_i), \quad (3)$$

where  $w_i$  and  $x_i$  are the weights and points, respectively. This quadrature is based on speed polynomials orthogonal on  $(0, \infty)$  with weight function  $w(x) = e^{-x^2} x^2$ .<sup>16</sup> The variable  $s$  in the integrand in Eq. (2) is the rescaling parameter and the integral is independent of  $s$ . However, for a given set of quadrature points, increasing  $s$  permits extension of the speed range so as to ensure convergence of the integral. It is important to note that there is a dependence on  $T_b$  and  $s$  in the momentum-transfer cross section. To simplify the notation we will henceforth write  $\sigma_m(x) \equiv \sigma_m((2kT_b/m)^{1/2}sx)$ .

The momentum-transfer cross sections employed are the cross sections reported by Nesbet,<sup>26</sup> O'Malley and Crompton,<sup>27</sup> and Haddad and O'Malley<sup>28</sup> for helium, neon, and argon, respectively. In addition, the cross sections tabulated by Mozumder<sup>23</sup> for argon, xenon, and krypton were used in the form

$$\sigma_m(v) = \sigma_m(0) \exp \left[ \sum_{k=1}^{12} a_k (v/v_{th})^k \right].$$

TABLE I. Convergence of  $nD_{th}$  ( $10^{22} \text{ cm}^{-1} \text{ sec}^{-1}$ ) with  $N$  and comparison with experiment ( $T_b = 300 \text{ K}$ ).

$N$	He <sup>a</sup>	Ne <sup>b</sup>	Ar <sup>c</sup>	Ar <sup>d</sup>	Xe <sup>e</sup>	Kr <sup>e</sup>
2	0.6390	7.5539	2.1895	2.6068	0.0826	0.239
4	0.6389	7.5038	2.3556	3.1747	0.0881	0.251
6	0.6389	7.5029	2.3607	3.0789	0.0880	0.251
8		7.5029	2.3604	3.0631	0.0880	
10			2.3604	3.0676		
20				3.0754		
30				3.0751		
40				3.0751		
Experiment	0.641 <sup>e</sup> 0.635* <sup>e</sup>	7.48 <sup>f</sup> 7.16* <sup>f</sup>	2.85 <sup>g</sup>	2.85 <sup>g</sup>	0.103 <sup>h</sup>	0.324 <sup>h</sup>

<sup>a</sup>Cross section of Nesbet (Ref. 26).

<sup>b</sup>Cross sections of O'Malley and Crompton (Ref. 27).

<sup>c</sup>Cross sections compiled by Mozumder (Ref. 22).

<sup>d</sup>Cross sections of Haddad and O'Malley (Ref. 28).

<sup>e</sup>Reference 25, p. 600; asterisk denotes  $T_b = 295 \text{ K}$ .

<sup>f</sup>Reference 25, p. 605; asterisk denotes  $T_b = 293 \text{ K}$ .

<sup>g</sup>Reference 25, p. 608.

<sup>h</sup>Reference 31.

TABLE II. Convergence of  $nD_{th}$  ( $10^{22}$  cm $^{-1}$  sec $^{-1}$ ) vs  $N$  and  $s$  for neon;  $T_b = 290.1$  K.

$s/N$	10	20	30	40
0.5	7.2877	7.4591	7.4638	7.4640
0.8	7.4638	7.4640	7.4640	7.4640
1.0	7.4640	7.4640	7.4640	
1.2	7.4640			
1.5	7.4637			
2.0	7.4557			

Table I demonstrates the extremely rapid convergence of the quadrature rule with  $s=1$ , in the calculation of  $nD_{th}$ . The convergence is marginally slower for argon owing to the deep Ramsauer minimum at 0.25 eV and a cross section which varies rapidly with energy.

Table II shows the convergence of  $nD_{th}$  for neon as a function of the number  $N$  of quadrature points and the re-scaling parameter  $s$ . For  $s < 1.0$  the quadrature points are scaled to lower energies and the contribution to the integral in Eq. (2) from the high-energy portion of the electron distribution function is too small, and  $nD_{th}$  decreases with decreasing  $s$ . For  $s > 1.0$  the points are scaled to higher energies and are spread out in the thermal energy range and the accuracy of the integration at the lowest energies is diminished, and  $nD_{th}$  decreases with increasing  $s$ .

### III. TIME EVOLUTION OF THE ELECTRON DISTRIBUTION

Since the formalism of electron transport theory appears in standard references,<sup>9,25</sup> only a brief outline is presented here. The time evolution of the anisotropic, spatially homogeneous, electron VDF is based on the expansion in Legendre polynomials,<sup>17</sup> that is,

$$f(\vec{v}, t) = \sum_{l=0}^{\infty} f_l(v, t) P_l(\cos\theta), \quad (4)$$

where  $\theta$  is the angle between  $\vec{v}$  and the polar axis chosen in the direction of the external electric field which is considered in the present case to be vanishingly small. The coupled equations for the first two terms  $f_0$  and  $f_1$  are<sup>17,25</sup>

$$\begin{aligned} \frac{\partial f_0}{\partial t} + \frac{eE}{3m} \left[ \frac{\partial}{\partial v} + \frac{2}{v} \right] f_1 \\ = \frac{m}{Mv^2} \frac{\partial}{\partial v} \left[ v^3 v_1 \left[ f_0 + \frac{kT_b}{mv} \frac{\partial f_0}{\partial v} \right] \right], \quad (5a) \end{aligned}$$

$$\mu(t) = -\frac{e}{3m} \int_0^t \left[ \int_0^{\infty} e^{-v_1 t'} v^3 \frac{\partial f_0(v, t-t')}{\partial v} dv \right] dt' / \int_0^{\infty} f_0 v^2 dv, \quad (8)$$

where it is understood that  $f_0$  is evaluated in the limit  $E \rightarrow 0$ .

The mobility for time domain (i) should be the mobility for free electrons plus corrections to take account of collisions with atoms. The velocity  $\vec{v}$  after a time interval  $t$  is related to the initial velocity  $\vec{v}_0$  by  $\vec{v} = \vec{v}_0 + e\vec{E}t/m$  ow-

$$\frac{\partial f_1}{\partial t} + \frac{eE}{m} \frac{\partial f_0}{\partial v} = -v_1 f_1, \quad (5b)$$

where  $M$  is the mass of the moderator atoms,  $E$  is the electric field strength, and  $v_1(v) = nv\sigma_m(v)$  is the collision frequency. An equivalent approach to Eq. (5) is based on linear-response theory.<sup>29,30</sup>

The relaxation of the VDF can be divided into two broad time domains defined by (i)  $v_1 t \lesssim 1$  and (ii)  $v_1 t \gg 1$ . This epochal relaxation of the VDF arises from the small mass ratio  $m/M$  in Eq. (5a). Anisotropies of the VDF, i.e.,  $f_l(v, t)$ ,  $l \geq 1$ , decay quickly to zero in time domain (i), while the isotropic portion of the VDF,  $f_0(v, t)$ , which involves energy exchange, approaches the thermal distribution slowly in time domain (ii).<sup>10,11,14</sup> The directed velocity decays to zero in time domain (i), whereas the mobility and diffusion coefficients exhibit some initial transient behavior followed by a much slower approach in time domain (ii). We present the formalism for the analysis of the time evolution over both time domains in comparison to the work of Mozumder<sup>22-24</sup> and Knierim *et al.*<sup>17</sup> Detailed numerical calculations presented in Sec. IV are restricted to the long-time dependence. Although field-dependent terms appear in Eq. (5), we are here interested in the behavior in the limit  $E \rightarrow 0$ . We also take all electrons to have an initial speed of  $v_0$  in the  $z$  direction.<sup>17,22-24</sup>

Equation (5b) can be integrated for  $f_1$  and is given by

$$f_1(v, t) = f_1(v, 0) e^{-v_1 t} - \frac{eE}{m} \int_0^t e^{-v_1 t'} \frac{\partial f_0(v, t-t')}{\partial v} dt', \quad (6)$$

where  $f_1(v, 0)$  is the initial value. With Eq. (6), Eq. (5a) gives a single equation for  $f_0(v, t)$ . The net directed velocity is given by<sup>18,30</sup>

$$w(t) = \frac{\frac{1}{3} \int_0^{\infty} f_1(v, t) v^3 dv}{\int_0^{\infty} f_0(v, t) v^2 dv}, \quad (7)$$

which consists of a field-independent transient contribution that arises from the term  $f_1(v, 0) e^{-v_1 t}$  in Eq. (6), and a field-dependent part  $\Delta w(t)$  that arises from the integral term in Eq. (6). The field-dependent part defines a mobility which is defined by  $\mu(t) = \Delta w(t)/E$  and given by

ing to the field acceleration. The free-electron mobility is therefore

$$\mu_{\text{free}}(t) = |\vec{v} - \vec{v}_0| / E = \frac{e}{m} t.$$

The initial transient mobility in domain (i) can be calcu-

lated by replacing  $f_0(v, t - t')$  with  $f_0(v, 0) \sim \delta(v - v_0)/v^2$  in Eq. (8), since in this time domain  $f_0$  is little altered from its initial value. This procedure yields

$$\mu(t) = \frac{e}{m} \frac{1 - e^{-v_1^0 t}}{v_1^0} \left[ 1 - \frac{1}{3} \frac{v_0}{v_1^0} \frac{dv_1}{dv} \Big|_{v=v_0} \right] + \frac{ev_0 t}{3m v_1^0} \frac{dv_1}{dv} \Big|_{v=v_0} e^{-v_1^0 t}, \quad (9)$$

which for very short times  $v_1^0 t \ll 1$ , is given by

$$\mu(t) = \frac{et}{m} \left[ 1 - \frac{1}{2} nv_0 \sigma_m(v_0) t \times \left[ 1 + \frac{1}{3} \frac{d \ln v \sigma_m(v)}{d \ln v} \Big|_{v=v_0} \right] + O(t^2) \right], \quad (10)$$

where an expansion in  $t$  has been used and  $v_1^0 = v_1(v_0)$ . The mobility given by Eq. (10) gives the free particle mobility  $et/m$  as  $t \rightarrow 0$ . For long times in domain (i)  $v_1(v_0)t > 1$ , though short with respect to domain (ii), the exponential terms in Eq. (9) vanish and we obtain

$$\mu^{(0)} = \frac{2}{3} \frac{e}{m} \frac{1}{nv_0 \sigma_m(v_0)} \left[ 1 - \frac{1}{2} \left[ \frac{v}{\sigma_m(v)} \frac{d \sigma_m(v)}{dv} \right]_{v=v_0} \right]. \quad (11)$$

$\mu^{(0)}$  is the effective "initial" mobility for the relaxation in time domain (ii) and can be negative if  $\sigma_m(v)$  at  $v = v_0$  increases sufficiently rapidly with  $v$ . The significance of negative contributions to the mobility are discussed in Sec. V.

The longitudinal diffusion coefficient  $D_L(t)$  and the transverse diffusion coefficient  $D_T(t)$  are velocity moments of the functions  $f^{(L)}(\vec{v}, t)$  and  $f^{(T)}(\vec{v}, t)$ , respectively, where these are the coefficients in the expansion of the spatially inhomogeneous distribution in powers of the spatial gradient of the electron number density.<sup>17,29,30</sup> Symmetry considerations show that  $f^{(L)}$  and  $f^{(T)}$  have Legendre polynomial expansions of the form<sup>18,29</sup>

$$f^{(L)}(\vec{v}, t) = \sum_{l=0}^{\infty} f_l^{(L)}(v, t) P_l(\cos \theta),$$

$$f^{(T)}(\vec{v}, t) = \sum_{l=0}^{\infty} f_l^{(T)}(v, t) P_l^{(1)}(\cos \theta),$$

where  $\theta$  is the angle between  $\vec{v}$  and the average directed velocity, and  $P_l^{(1)}$  is the associated Legendre polynomial of order 1. The diffusion coefficients are given by

$$D_K(t) = \frac{\frac{1}{3} \int_0^{\infty} f_1^{(K)}(v, t) v^3 dv}{\int_0^{\infty} f_0(v, t) v^2 dv}, \quad (12)$$

where  $K$  denotes either  $L$  or  $T$ . The coefficients  $f_1^{(K)}$  are evaluated in terms of  $f_0$ ,  $f_1$ , and  $f_2$  and are given by<sup>29</sup>

$$\frac{\partial f_1^{(L)}}{\partial t} + w(t) f_1 - v(f_0 + \frac{2}{5} f_2) = -v_1 f_1^{(L)} \quad (13a)$$

and

$$\frac{\partial f_1^{(T)}}{\partial t} + v(\frac{1}{5} f_2 - f_0) = -v_1 f_1^{(T)}. \quad (13b)$$

The time dependence of  $f_0$  is given by Eq. (5a) and of  $f_l$ ,  $l > 0$ , is given by<sup>17</sup>

$$f_l(v, t) = f_l(v, 0) e^{-v_l t}, \quad (14)$$

where

$$v_l = nv(\sigma_0 - \sigma_l),$$

and

$$\sigma_l = 2\pi \int_0^{\pi} P_l(\cos \theta) \sigma(v, \theta) \sin \theta d\theta.$$

The initial values  $f_l(v, 0)$  are related to  $f_0(v, 0)$  with  $f_1(v, 0) = 3f_0(v, 0)$  and  $f_2(v, 0) = 5f_0(v, 0)$ . For an initial  $\delta$ -function distribution and with Eqs. (7) and (14) we have that

$$w(t) = v_0 e^{-v_1^0 t}.$$

The solutions to Eqs. (13a) and (13b) can now be obtained and are

$$f_1^{(L)}(v, t) = f_1^{(L)}(v, 0) e^{-v_1 t} - \frac{v}{v_1} f_1(v, 0) (e^{-v_1 t} - e^{-2v_1 t}) + \frac{2}{5} v f_2(v, 0) \frac{e^{-v_1 t} - e^{-v_2 t}}{v_2 - v_1} + v \int_0^t e^{-v_1 t'} f_0(v, t - t') dt' \quad (15)$$

and

$$f_1^{(T)}(v, t) = f_1^{(T)}(v, 0) e^{-v_1 t} - \frac{1}{5} v f_2(v, 0) \frac{e^{-v_2 t} - e^{-v_1 t}}{v_1 - v_2} + v \int_0^t e^{-v_1 t'} f_0(v, t - t') dt'. \quad (16)$$

With Eqs. (15) and (16) in Eq. (12), the diffusion coefficients are given by

$$D_L(t) = D_I(t) + e^{-v_1^0 t} \left[ D_L(0) + \frac{2}{3} v_0^2 \frac{1 - e^{-(v_2^0 - v_1^0)t}}{v_2^0 - v_1^0} - v_0^2 \frac{1 - e^{-v_1^0 t}}{v_1^0} \right], \quad (17)$$

and

$$D_T(t) = D_I(t) + e^{-v_1^0 t} \left[ D_T(0) - \frac{1}{3} v_0^2 \frac{1 - e^{-(v_2^0 - v_1^0)t}}{v_2^0 - v_1^0} \right], \quad (18)$$

where

$$D_I(t) = \frac{1}{3} \int_0^{\infty} \int_0^t e^{-v_1 t'} f_0(v, t - t') \times v^4 dt' dv / \int_0^{\infty} f_0 v^2 dv. \quad (19)$$

In the long-time limit  $v_1^0 t \gg 1$ , the initial transients of  $D_L$ ,  $D_T$ , and  $D_I$  decay and the diffusion becomes isotropic, that is,

$$\left. \begin{array}{l} D_L(t) \\ D_T(t) \end{array} \right\} \rightarrow D_I(t) \approx D(t) \text{ for } t \gg 1/v_1^0$$

where

$$D(t) = \frac{\frac{1}{3n} \int_0^\infty f_0(v,t) \frac{v^3}{\sigma_m(v)} dv}{\int_0^\infty f_0(v,t) v^2 dv}. \quad (20)$$

For an initial  $\delta$ -function distribution  $D_L(0) = D_T(0) = 0$  in Eqs. (17) and (18), and from Eqs. (17)–(19) for time domain (i), we have that

$$D_L(t) \approx D^{(0)} \left[ (1 - e^{-v_1^0 t})(1 - 3e^{-v_2^0 t}) + 2v_1^0 \left[ \frac{1 - e^{-(v_2^0 - v_1^0)t}}{v_2^0 - v_1^0} \right] e^{-v_1^0 t} \right], \quad (21)$$

and

$$D_T(t) \approx D^{(0)} \left[ 1 - e^{-v_1^0 t} - v_1^0 \left[ \frac{1 - e^{-(v_2^0 - v_1^0)t}}{v_2^0 - v_1^0} \right] e^{-v_1^0 t} \right], \quad (22)$$

where  $D^{(0)}$  is determined from Eq. (20) with the  $\delta$ -function speed distribution, that is,

$$D^{(0)} = \frac{1}{3n} \left\langle \frac{v}{\sigma_m(v)} \right\rangle \quad (23a)$$

$$= \frac{1}{3n} \frac{v_0}{\sigma_m(v_0)}. \quad (23b)$$

The quantity  $D^{(0)}$  is the isotropic diffusion coefficient at the start of domain (ii), analogous to  $\mu^{(0)}$  given by Eq. (11). It is important to point out that Mozumder<sup>23</sup> employed the definition Eq. (23a) with a pseudo-Maxwellian distribution over the domain (i) for which the definition is not rigorously correct and diffusion is anisotropic. Also, Eqs. (21) and (22) differ from the corresponding results derived by Knierim *et al.*<sup>18</sup> who defined quantities independent of the initial number-density gradient which is equivalent to a neglect of the time derivatives of  $f_1^{(L)}$  and  $f_1^{(T)}$  in Eq. (13). We have employed the general time-dependent definition<sup>29,30</sup> of the diffusion coefficient for the special case of an initial localized and unidirectional

beam of monoenergetic electrons. This has no effect on the asymptotic approach to  $D^{(0)}$  and the relaxation in domain (ii).

#### IV. DISCRETE-ORDINATE EVALUATION OF TIME-DEPENDENT MOBILITY AND DIFFUSION COEFFICIENTS

In this section, the time evolution of  $\mu(t)/\mu_{th}$  and  $D(t)/D_{th}$  as given by Eqs. (8) and (19) are determined with the solution of Eq. (5a) for  $f_0(v,t)$  in the limit  $E \rightarrow 0$ . This corresponds to time domain (ii) with initial values calculated with Eqs. (11) and (23) representing an initial  $\delta$ -function speed distribution. As in previous papers,<sup>10–12</sup>  $f_0(v,t)$  is determined in terms of the eigenfunctions and corresponding eigenvalues of the Lorentz-Fokker-Planck operator, defined by the right-hand side of Eq. (5a), that is,

$$\begin{aligned} Lf_0 &= -\frac{m}{Mv^2} \frac{\partial}{\partial v} \left[ v^3 v_1 \left[ f_0 + \frac{kT_b}{mv} \frac{\partial f_0}{\partial v} \right] \right] \\ &= \frac{nkT_b}{M} \left[ \frac{\partial}{\partial v} + \frac{2}{v} \right] v \sigma_m(v) \left[ \frac{\partial}{\partial v} + \frac{mv}{kT_b} \right] f_0, \quad (24) \end{aligned}$$

where the definition of  $v_1$  has been used. With the replacement of  $v$  with the dimensionless speed  $x$ , and the definitions

$$g_0(x, t') = e^{-\gamma x^2} f_0(x, t') \quad (25a)$$

and

$$t' = t \left[ \frac{T}{T_b} \right]^{1/2} \left[ \frac{1}{2} \frac{nm \bar{\sigma}_m}{M} \left[ \frac{2kT_b}{m} \right]^{1/2} \right], \quad (25b)$$

Eq. (5a) is transformed to

$$\frac{\partial g_0}{\partial t'} = \left[ \frac{\partial}{\partial x} + 2\gamma x + \frac{2}{x} \right] x \hat{\sigma}_m(x) \left[ \frac{\partial}{\partial x} + 2x(\gamma + s^2) \right] g_0 \quad (26a)$$

$$= -L'g_0, \quad (26b)$$

where  $\gamma$  is a constant to be specified later. In Eq. (25b)  $\bar{\sigma}_m$  is some convenient hard-sphere cross section<sup>12</sup> and  $\hat{\sigma}_m(x) = \sigma_m(x)/\bar{\sigma}_m$  in Eq. (26). The quantity  $s = (T/T_b)^{1/2}$  is the scaling parameter introduced in Sec. II. In terms of these new variables, the mobility and diffusion coefficients are given by

$$n\mu(t') = -\frac{1}{3} \left[ \frac{M}{m} \right] \frac{1}{\bar{\sigma}_m} \left[ \frac{2e^2}{mkT_b} \right]^{1/2} s^4 \int_0^{t'} \int_0^\infty w(x) x e^{-\eta_1 t''} e^{(1+\gamma)x^2} \left[ \frac{d}{dx} + 2\gamma x \right] g_0(x, t' - t'') dx dt'', \quad (27)$$

$$nD(t') = \frac{1}{3} \left[ \frac{2kT_b}{m} \right]^{1/2} s^4 \frac{\eta_1(x_0)}{x_0 \sigma_m(x_0)} \int_0^{t'} \int_0^\infty w(x) x^2 e^{-\eta_1 t''} e^{(1+\gamma)x^2} g_0(x, t' - t'') dx dt'', \quad (28)$$

where  $\eta_1(x) = nv\sigma_m(x)t/t'$ . It is useful to note that  $g_0$  is normalized according to

$$s^3 \int_0^\infty w(x) e^{(1+\gamma)x^2} g_0(x, t') dx = 1. \quad (29)$$

The formal solution to Eq. (26) is

$$g_0(x, t') = e^{-L't'} g_0(x, 0), \quad (30)$$

where  $g_0(x, 0)$  is the initial value. If  $g_0(x, 0)$  is expanded

in the eigenfunctions  $\phi_k(x)$  of the Lorentz-Fokker-Planck operator  $L'$ , then

$$g_0(x, t') = \sum_k \left[ \int_0^\infty w(x') \phi_k(x') g_0(x', 0) dx' \right] \phi_k(x) e^{-\lambda_k t'}, \quad (31)$$

where  $L' \phi_k = \lambda_k \phi_k$ . The eigenvalues and corresponding eigenfunctions of  $L'$  are determined with the discrete-ordinate method.<sup>13</sup> The method is based on the discrete-ordinate representation  $\underline{D}$  of the derivative operator defined such that the derivative of some arbitrary function at a quadrature point is given by

$$g'(x_i) = \sum_{k=1}^N D_{ik} \sqrt{w_k/w_i} g(x_k).$$

The construction of the matrix  $\underline{D}$  for the quadrature based on speed polynomials<sup>16</sup> is described in detail in an earlier paper.<sup>13</sup> The eigenvalues and eigenfunctions are determined with a numerical diagonalization of the discrete-ordinate representation of  $L'$ , that is, the matrix with elements

$$L'_{ij} = \sum_{k=1}^N [D_{ki} + 2\delta_{ik} x_k (1 + \gamma)] x_k \hat{\sigma}_m(x_k) \times [D_{kj} + 2\delta_{jk} x_k (\gamma + s^2)]. \quad (32)$$

Although  $\gamma$  in Eq. (25a) is independent of the scaling parameters, the choice  $\gamma = -\frac{1}{2}(s^2 + 1)$  yields a symmetric matrix

$$L'_{ij} = \sum_{k=1}^N [D_{ki} + \delta_{ik} x_k (s^2 - 1)] x_k \hat{\sigma}_m(x_k) \times [D_{kj} + \delta_{kj} x_k (s^2 - 1)] \quad (33)$$

which for  $s = 1$  (no scaling), reduces to Eq. (19) of Ref. 12. The eigenvalues of  $\underline{L}'$  are real and the corresponding eigenfunctions satisfy

$$\int_0^\infty w(x) \phi_k(x) \phi_l(x) dx = \delta_{kl}.$$

With the approximation  $\eta_1(x) \gg \lambda_k$  in Eqs. (27) and (28), the expressions for the relaxation of the mobility and diffusion coefficients can be written as a sum of exponential terms, that is,

$$\mu(t') = \sum_{k=1}^N \mu_k e^{-\lambda_k t'}, \quad (34)$$

and

$$D(t') = \sum_{k=1}^N D_k e^{-\lambda_k t'}, \quad (35)$$

where the coefficients depend on the expansion of the initial distribution in the eigenfunctions  $\phi_k$ . These coefficients are given by

$$\mu_k = -\frac{M}{3nm\bar{\sigma}_m} \left[ \frac{2e^2}{mkT_b} \right]^{1/2} a_k s^4 \times \int_0^\infty \frac{w(x)x}{\eta_1(x)} e^{(1+\gamma)x^2} \left[ \frac{d}{dx} + 2\gamma x \right] \phi_k(x) dx, \quad (36)$$

and

$$D_k = \frac{1}{3n} \left[ \frac{2kT_b}{m} \right]^{1/2} a_k s^4 \frac{\eta_1(x_0)}{x_0 \bar{\sigma}_m(x_0)} \times \int_0^\infty \frac{w(x)x^2}{\eta_1(x)} e^{(1+\gamma)x^2} \phi_k(x) dx, \quad (37)$$

where

$$a_k = \int_0^\infty w(x) \phi_k(x) g_0(x, 0) dx.$$

For the initial  $\delta$ -function distribution, that is,

$$g_0(x, 0) = \frac{e^{-(1+\gamma)x^2} \delta(x - x_0)}{w(x)s^3},$$

we have that

$$a_k = s^{-3} e^{-(1+\gamma)x_0^2} \phi_k(x_0). \quad (38)$$

The present study of the thermalization of hot electrons is based on Eqs. (34)–(38), with the discrete-ordinate determination of the eigenvalues  $\lambda_k$  and eigenfunctions  $\phi_k$ . The integrations in Eqs. (36) and (37) are performed with the quadrature rule [Eq. (3)] and the eigenfunctions determined at the quadrature points.

## V. CALCULATIONS AND RESULTS

The time variation of the diffusion coefficient and the mobility were determined with Eqs. (34)–(38) with the eigenvalues  $\lambda_k$ , determined by diagonalizing the DO representative of the Lorentz-Fokker-Planck operator [Eq. (33)]. The reduced time  $t' = t/\tau$  [Eq. (25b)] is employed, and the time scales are listed in Table III together with the hard-sphere cross sections  $\bar{\sigma}_m$ . The hard-sphere cross sections are defined so that  $\lambda_1$  is the same for each case. The convergence of the eigenvalues was reported in the earlier paper.<sup>12</sup> In the present work, the invariance of the product  $\lambda_k t'$  with the scaling parameter was studied. Detailed calculations demonstrated that if the number of quadrature points is moderately large ( $N > 30$ ) then  $\lambda_k t'$ , for many of the lower-order eigenvalues, is independent of the scaling parameter  $s$  for  $s$  in the range 0.5–3. This permits rescaling the quadrature points so that a particular point coincides with the initial speed as required to represent a  $\delta$ -function in the DO basis.

TABLE III. Definition of time scales.

Moderator	$T$ (K)	$\bar{\sigma}_m$ ( $\text{\AA}^2$ )	$\tau$ ( $10^{11}$ sec/cm <sup>3</sup> )
He	290.1	5.457	28.52
Ne	290.1	0.366	2143
Kr <sup>a</sup>	290.1	10.53	309.0
Xe <sup>a</sup>	290.1	18.71	273.0
Ar <sup>a</sup>	290.1	1.191	1303
Ar <sup>a</sup>	450.0	0.713	1748
Ar <sup>a</sup>	700.0	0.473	2113
Ar <sup>b</sup>	290.1	0.702	2213

<sup>a</sup>Polynomial fit to the tabulated cross section data given by Mozumder (Ref. 12).

<sup>b</sup>Cross section given by Haddad and O'Malley (Ref. 28).

Figure 1 shows the time variation of  $D(t')/D_{th}$  for four moderators and different initial speeds for an initial  $\delta$ -function distribution. The initial speed  $u_0$  is in units of the thermal speed  $v_{th}=1.148 \times 10^7$  cm/sec defined by Mozumder<sup>22</sup> corresponding to  $kT_b$  equal to 0.025 eV at 290.1 K. For  $u_0=2, 3, 4,$  and  $4.8$ , the initial energy is 0.150, 0.338, 0.600, and 0.864 eV. For the heavier moderators, an important consideration is the initial speed  $u_0$  relative to the position of the Ramsauer minima in the cross sections. These occur at approximately  $v/v_{th}=2.6, 3.6,$  and  $4.0$  for Ar, Kr, and Xe, respectively (see Fig. 3 of Ref. 12). It is important to notice that  $D(t)/D_{th}$  can be extremely large due to the Ramsauer minima. The behavior shown in Fig. 1 is similar to the results for energy relaxation in the earlier paper.<sup>12</sup> For helium, with a cross section that is almost constant, the diffusion coefficient decays monotonically from the initial value, whereas for the other moderators shown, there is a maximum attained owing to the Ramsauer minima in the cross sections for these moderators. Note that for Kr and Xe, the maxima are attained only for  $u_0=4.8$  which is sufficiently above the Ramsauer minimum, such that a maximum in  $D(t')/D_{th}$  occurs for both moderators.

Figure 2 illustrates the corresponding variation of  $\mu(t')/\mu_{th}$ . The behavior for He is monotonically increasing whereas for the other moderators shown, there are extremum values owing to the Ramsauer minima. The occurrence of negative mobilities at short times for initial values of  $u_0$  above the Ramsauer minima can be understood by considering the thermal mobility which with Eq. (4) can be written as

$$\mu_{th} = -\frac{e}{3m} \int_0^\infty \frac{v^3}{v_1} \frac{df_0^M}{dv} dv / \int_0^\infty f_0^M v^2 dv, \quad (39)$$

where  $f_0^M$  is the Maxwellian. If an integration by parts is performed then

$$\mu_{th} = \frac{e}{m} \int_0^\infty \frac{v^2}{v_1} \left[ 1 - \frac{v}{3v_1} \frac{dv_1}{dv} \right] f_0^M dv / \int_0^\infty f_0^M v^2 dv \quad (40)$$

provided that for  $v \rightarrow 0$ ,  $v_1$  is more slowly varying than  $v^3$ . The term in large parentheses in the integrand above can be negative for speeds such that  $(v/3v_1)(dv_1/dv) > 1$ . Although  $\mu_{th} > 0$ , there are negative contributions to the in-

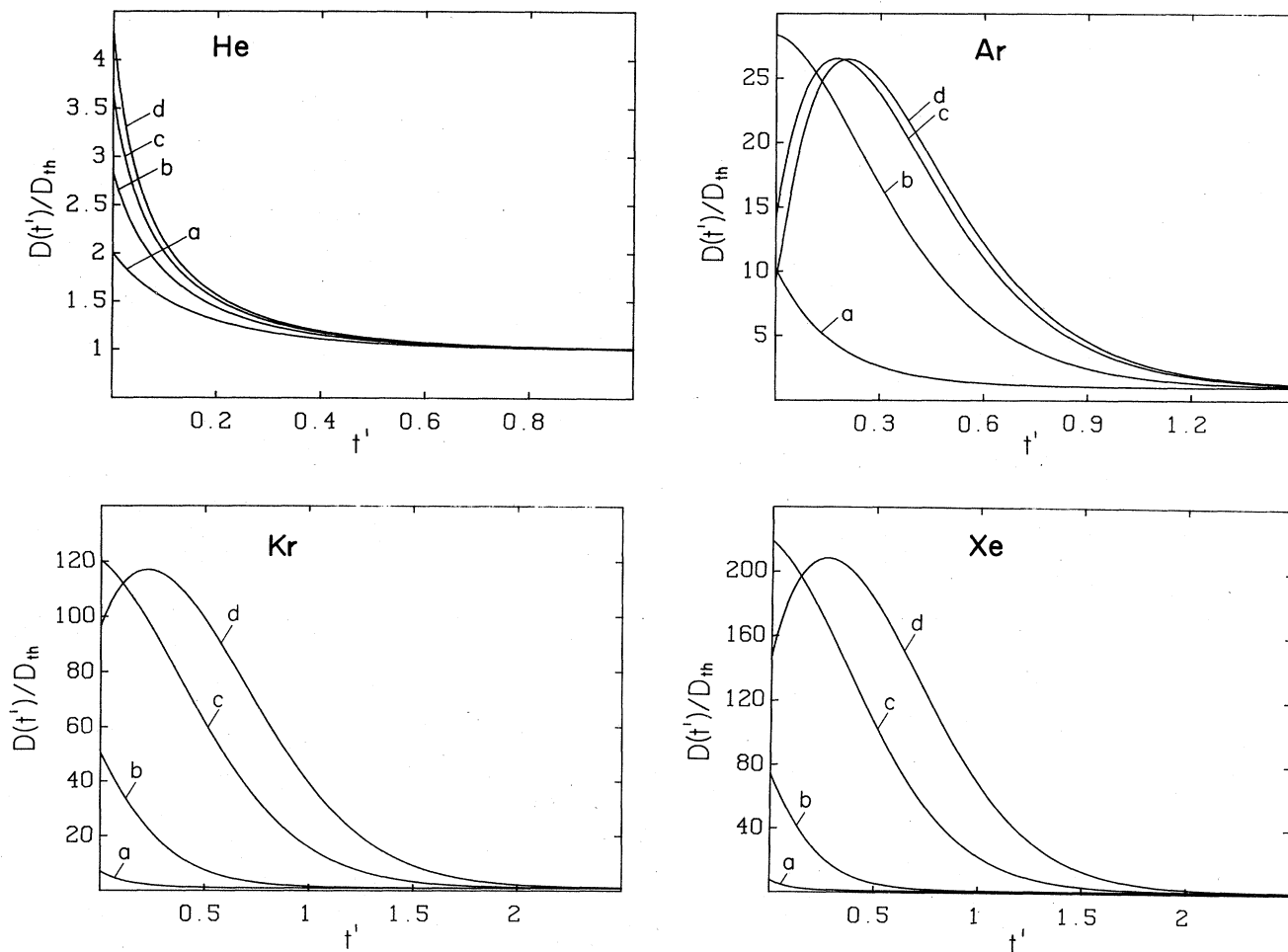


FIG. 1. Time variation of the diffusion coefficient. Initial  $\delta$ -function distribution with  $u_0$  equal to curves (a) 2.0, (b) 3.0, (c) 4.0, and (d) 4.8;  $T_b=290.1$  K.

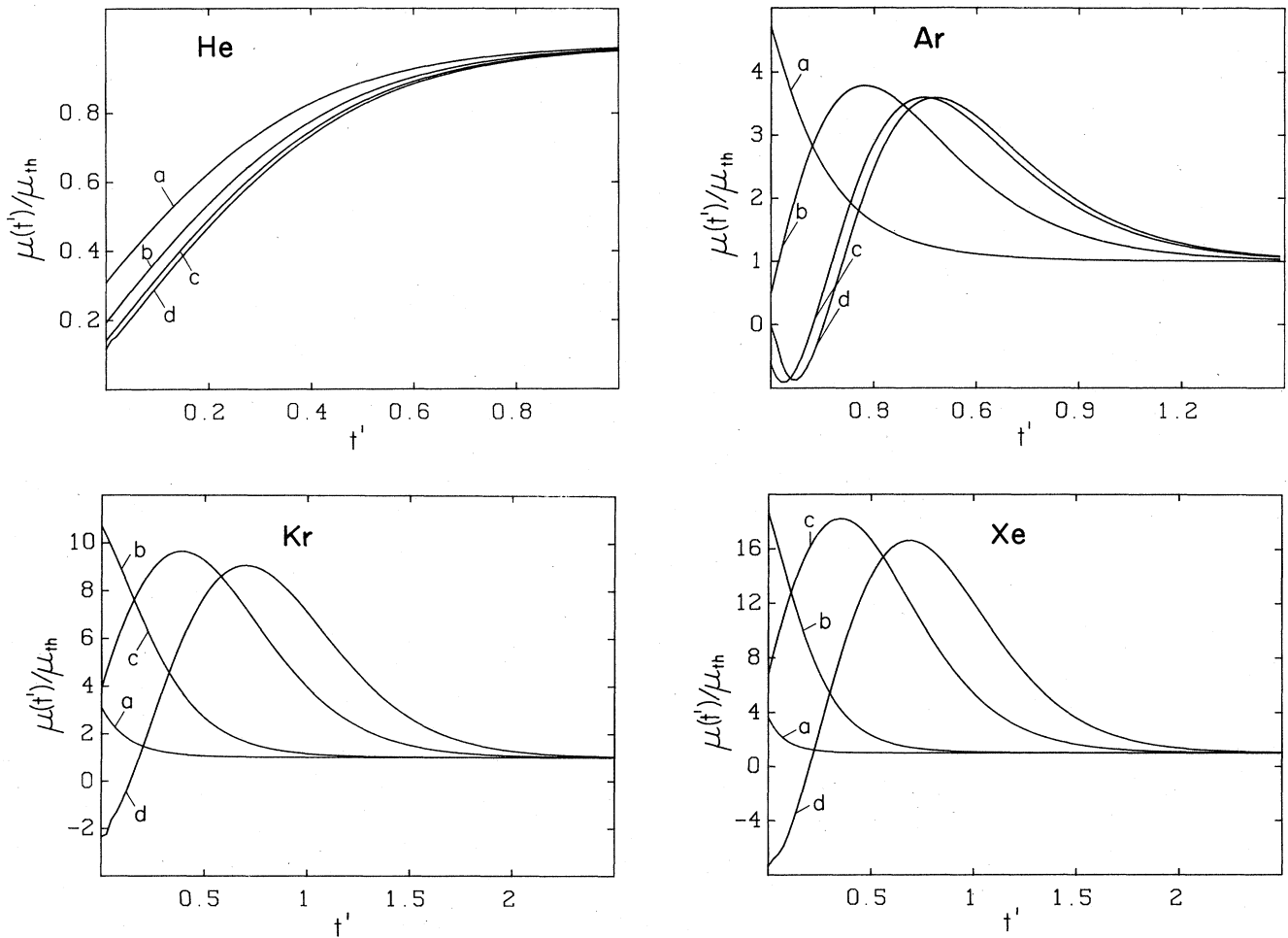


FIG. 2. Time variation of the mobility (see caption, Fig. 1).

tegration in Eq. (40). For an initial nonequilibrium anisotropic distribution, where  $f_0^M$  is replaced by  $f_0(v, t)$  as shown by Eq. (8) for  $\nu_1 t \gg 1$ , these negative contributions may dominate such that initially and for short times the average motion of the electrons can be opposite to the direction of force owing to the electric force (in the  $E \rightarrow 0$  limit). This can be understood physically as follows. In the limit  $E \rightarrow 0$  and for short times in domain (ii), the velocity distribution is almost isotropic. Electrons with velocity components in the electric force direction gain energy, whereas other electrons with velocity components opposite to the force direction lose energy. Hence the forward-moving electrons have shorter free-flight paths than backward-moving electrons when the cross section increases rapidly with energy. Hence the average displacement is slightly in favor of backward-moving electrons and the net mobility is negative. These ideas are implicit in the standard free-path method of transport theory.<sup>25</sup> The extent of the negative mobility depends on the details of the momentum-transfer cross section and its variation with energy. Table IV lists the initial values  $\mu(0)/\mu_{th}$  for argon with two different cross sections and several temperatures. The sensitivity of the initial mobility on the cross section is evident. Figure 3 shows the en-

ergy variation of the two momentum cross sections, one reported by Mozumder<sup>22</sup> and the other by Haddad and O'Malley.<sup>28</sup>

The behavior in Fig. 2 demonstrates that for  $u_0$  above the Ramsauer minima, the mobility can decrease below the initial value to a minimum, then increase to a maximum followed by a slower monotonic approach to the thermal value. The behavior for Kr and Xe is qualitatively similar whereas the results for Ar differ owing to the Ramsauer minimum occurring at a lower energy than for the other moderators. As might be expected there is a close similarity in the time-dependent relaxation of the mobility and diffusion coefficient. We can write

TABLE IV. Initial mobilities  $\mu^{(0)}/\mu_{th}$  for argon.

$u_0$	$T_b = 290.1 \text{ K}^a$	$290.1 \text{ K}^b$	$450 \text{ K}^a$	$700 \text{ K}^b$
2.0	4.702	7.296	3.101	2.196
3.0	0.4999	-2.740	0.3300	0.234
4.0	-0.6354	-0.1824	-0.419	-0.297
4.8	-0.03627	0.0021	-0.0239	-0.0169

<sup>a</sup>Cross section by Mozumder, Ref. 23.

<sup>b</sup>Cross section of Haddad and O'Malley, Ref. 28.



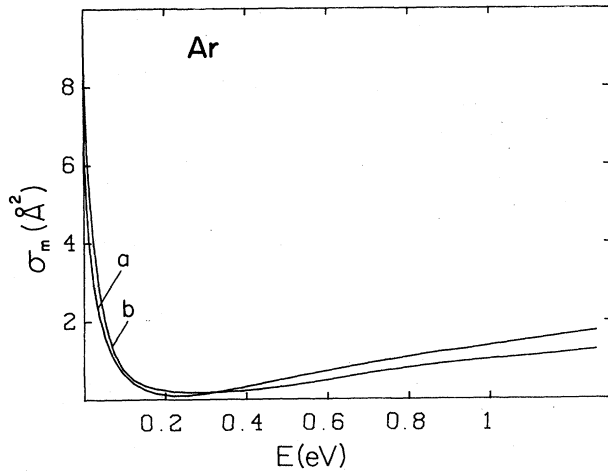


FIG. 3. Momentum-transfer cross sections for argon: curve (a) Haddad and O'Malley cross section, Ref. 28; curve (b) Mozumder cross section, Ref. 22.

$$\mu(t') = \mu_1(t') + \mu_2(t'),$$

where

$$\mu_1(t') = \frac{e}{kT_b} D(t')$$

and

$$\begin{aligned} n\mu_2(t') = & -\frac{1}{6} \left[ \frac{2e^2}{mkT_b} \right]^{1/2} \frac{\eta(x_0)s^2}{x_0\sigma_m(x_0)} \\ & \times \int_0^{t'} \int_0^\infty xw(x)xe^{-\eta_1 t''} e^{(1+\gamma)x^2} \\ & \times \left[ \frac{d}{dx} + 2x(\gamma + s^2) \right] \\ & \times g_0(x, t' - t'') dx dt'' . \end{aligned}$$

For  $t' \rightarrow \infty$ ,  $\mu_2(t') \rightarrow 0$  as required by the Einstein relation. At short times,  $\mu_2(t')$  can be negative and if  $|\mu_2| > \mu_1$  then  $\mu(t')$  is negative whereas  $D(t')$  and  $\mu_1(t')$  are always positive.

The change in the approach to equilibrium for different moderator temperatures is shown in Fig. 4 for argon with

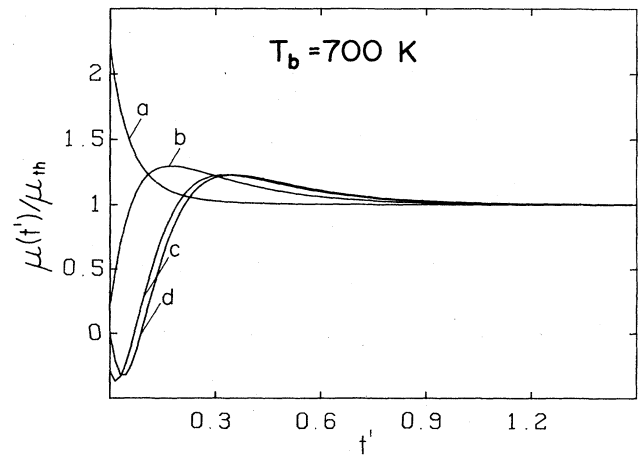
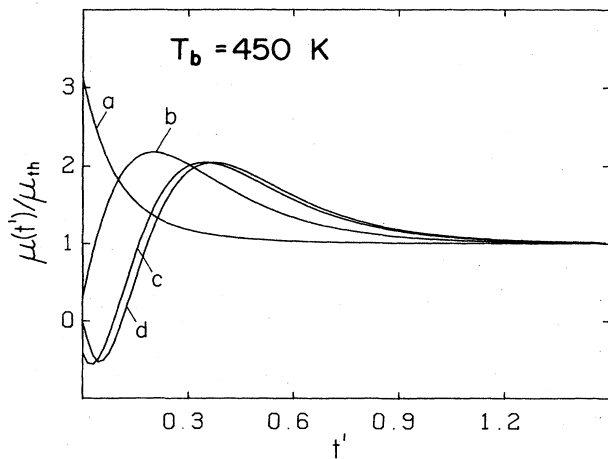
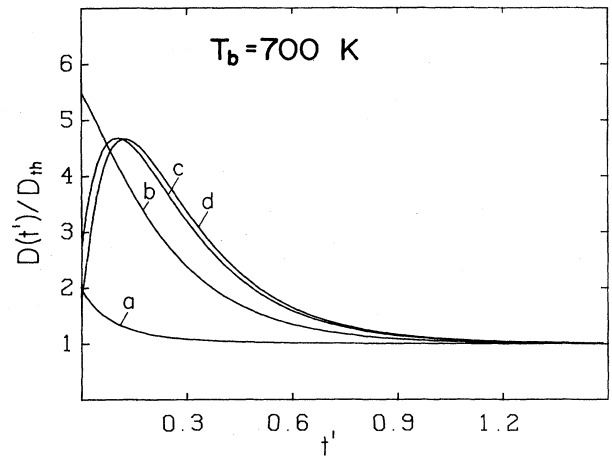
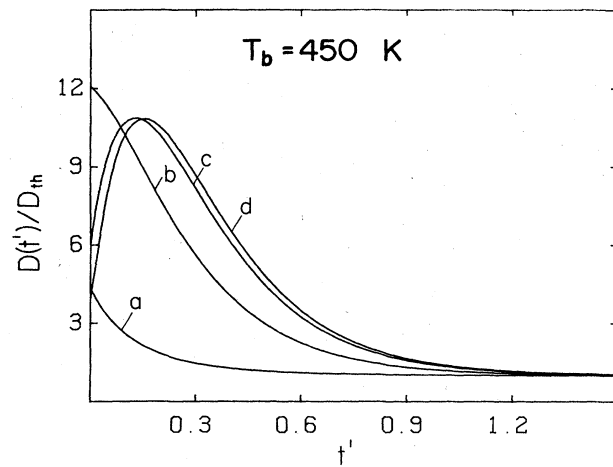


FIG. 4. Temperature dependence of the approach to thermal equilibrium: Initial  $\delta$ -function distribution; argon.  $u_0$  equal to curves (a) 2.0, (b) 3.0, (c) 4.0, and (d) 4.8.

TABLE V. Relaxation times vs initial speed.  $T=290.1$  K;  $u_0$  is the initial speed in units of  $v_{th}=1.148 \times 10^7$  cm sec $^{-1}$ .  $\tau(1.01)$  is the time, in units of  $10^{11}$  sec cm $^{-3}$ , required for each quantity (energy, mobility and/or diffusion coefficient relative to the thermal value) to decay to within 1.01 of the thermal value. Asterisks denote values of  $\tau$  for relaxation to 1/1.01 or 1/1.1 of the thermal value.

$u_0$	Energy	$\tau(1.01)$		Energy	$\tau(1.1)$	
		Mobility	Diffusion		Mobility	Diffusion
<b>Helium</b>						
2.0	29.64	29.29	25.75	15.83	15.55	11.93
3.0	31.49	31.16*	27.61	17.70	17.41*	13.80
4.0	32.34	31.99*	28.45	18.54	18.24*	14.64
4.8	32.73	32.39	28.85	18.94	18.64*	15.04
<b>Neon</b>						
2.0	1905	2306	1322	903.9	1275	310.8
3.0	1964	2366*	1382	963.6	1334*	370.6
4.0	1986	2387*	1403	985.4	1356*	392.3
4.8	1994	2396*	1412	994.0	1364*	400.8
<b>Argon</b>						
2.0	1430	1416	1727	826.6	819.5	1102
3.0	2277	2259	2586	1626	1606	1942
4.0	2505	2487	2814	1853	1832	2170
4.8	2547	2529	2856	1895	1873	2211
<b>Xenon</b>						
2.0	152.7	150.6	186.2	88.73	82.99	112.9
3.0	346.6	364.6	435.4	238.0	252.6	316.2
4.0	636.9	663.1	748.0	496.5	524.5	611.8
4.8	741.2	767.7	853.2	589.9	627.7	716.3
<b>Krypton</b>						
2.0	267.7	244.3	305.3	158.2	132.9	189.3
3.0	493.1	477.7	562.2	344.2	334.0	416.9
4.0	764.7	751.9	847.4	599.5	588.3	689.2
4.0	872.2	859.6	955.9	705.0	694.2	796.8

the cross section reported by Mozumder.<sup>22</sup> The results are understood by noting that for the higher temperatures the momentum-transfer cross sections at the higher energies are sampled and the effect of the Ramsauer minimum is reduced. The departures from the thermal values is smaller at the higher temperatures, though the time variation is qualitatively similar.

As is clear from the results shown in Figs. 1, 2, and 4, there is no unique definition of a relaxation time which is characteristic of the time required to attain thermal equilibrium. We have chosen to follow the previous work<sup>12,22</sup> and define relaxation times  $\tau(1.1)$  and  $\tau(1.01)$  as

the times to relax to within 10% and 1% of the thermal value of the average energy, mobility, and the diffusion coefficient. These relaxation times are shown versus the speed  $u_0$  for an initial  $\delta$ -function in Table V. For helium, energy and mobility relaxation times are very close whereas the diffusion relaxation times are 10–20% smaller. Neon is markedly different with larger mobility relaxation times than average energy relaxation times and considerably smaller diffusion relaxation times. For the three moderators with Ramsauer minima, the relaxation times for the average energy and mobility are similar while the diffusion relaxation times are 10–30% larger.

TABLE VI. Temperature dependence of relaxation times.  $\tau(1.1)$  in units of  $10^{11}$  sec cm $^{-3}$ ; cross section from Mozumder<sup>22</sup>.

$u_0$	$T$ (K)	Neon			Argon		
		Energy	Mobility	Diffusion	Energy	Mobility	Diffusion
2.0	290.1	903.9	1275	310.8	826.6	819.5	1102
	450	577.2	872.6	124.1	748.7	685.6	1044
	700	220.5	399.8	a	390.7	373.7	576.0
4.8	290.1	993.9	1364 <sup>b</sup>	400.8	1895	1873	2211
	450	671.7	966.0	219.7	1948	1805	2277
	700	447.0	673.5	116.7	1887	1314	2114

<sup>a</sup> $D(0)/D_{th}=1.058$ .

<sup>b</sup>Relaxation time to 1/1.1 of the thermal value.

TABLE VII. Energy relaxation times; different argon cross sections.  $T_b = 290.1$  K.

$u_0$	M cross section <sup>a</sup>	HO cross section <sup>b</sup>
2.0	826.6	1067
3.0	1626	2614
4.0	1853	2767
4.8	1895	2810

<sup>a</sup>Mozumder, Ref. 22;  $\bar{\sigma}_m = 1.19$  Å.

<sup>b</sup>Haddad and O'Malley, Ref. 28;  $\bar{\sigma}_m = 0.712$  Å.

Note that the relaxation times for  $u_0 = 4.0$  and  $4.8$  for argon are almost identical. Also, for  $u_0 = 4.0$  and  $4.8$ , the curves for the time-dependent mobility and diffusion coefficient for argon (Figs. 1, 2, and 4) almost coincide for all times. This confirms the suggestion by Mozumder<sup>22,23</sup> and Sowada and Warman<sup>5</sup> that the relaxation times are insensitive to the initial speed if it is well above the Ramsauer minimum.

The variation of  $\tau(1.1)$  with temperature for neon and argon is shown in Table VI. The relaxation times generally decrease with increasing temperature owing to the increase in the cross section with energy. For argon with  $u_0 = 4.8$ , the energy and diffusion relaxation times show a maximum at 450 K. In this case the initial speed is just above the Ramsauer minimum and the cross section in the vicinity of the minimum is sampled.

A comparison of energy relaxation times for two different argon cross sections is presented in Table VII. The Haddad and O'Malley cross section gives much longer relaxation times owing to the generally smaller equivalent hard-sphere cross sections  $\bar{\sigma}_m$ . The relaxation times for the Haddad and O'Malley cross section are on the average longer by a factor of 1.57, which is close to the ratio of the  $\bar{\sigma}_m$  values of 1.7 for these two cross sections.

It is of considerable interest to compare the present calculations with available experimental results. One of the difficulties of such a comparison is that the initial distribution in the experiments is largely unknown. We have

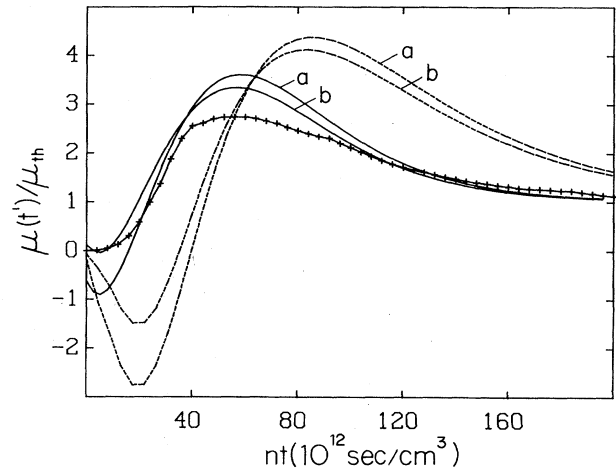


FIG. 5. Electron mobility in argon: + + +, experiment, Ref. 5; — — —, Haddad and O'Malley cross section, Ref. 28; — — —, Mozumder cross section, Ref. 22.  $T_b = 290.1$  K;  $u_0 = 4.0$ . Curves (a) initial  $\delta$ -function distribution; (b) initial Gaussian distribution,  $\alpha = 0.4$ , see text.

carried out a study of the dependence of relaxation times on the form of the initial distribution. The results shown in Table VIII are for the mobility relaxation times for an initial Gaussian distribution function of varying width. The form of the initial distribution function is given by

$$g_0(x,0) = Ax^{-1} s^{-3} \exp[-\gamma x^2 - (x^2 - x_0^2)^2 / \alpha x_0^4],$$

where  $\alpha$  determines the width and  $A$  is a normalization constant. The case  $\alpha = 0$  corresponds to the  $\delta$  function. This form of the initial distribution function is chosen to give the same average energy independent of  $\alpha$ . It is clear from the results in Table VIII that except for perhaps some initial transient at very short times, the nature of the approach to equilibrium and the relaxation times are somewhat independent of the form of the initial distribution function. In the table,  $t_{\max}$  is the time to attain the maximum in  $\mu/\mu_{th}$ . This study lends added confidence to

TABLE VIII. Mobility relaxation times for initial Gaussian distribution.  $T_b = 290.1$  K;  $u_0 = 4$ .

$\alpha$	$\mu^{(0)}/\mu_{th}$	Mozumder cross section <sup>a</sup>		
		$(\mu/\mu_{th})_{\max}$	$t_{\max}$	$\tau(1.1)$
0	-0.635	3.60	585	1832
0.10	-0.503	3.55	575	1817
0.20	-0.229	3.47	565	1805
0.30	-0.028	3.39	565	1796
0.40	0.105	3.33	565	1790
Haddad and O'Malley cross section <sup>b</sup>				
0.00	-0.182	4.36	850	2880
0.10	-0.365	4.34	840	2868
0.20	-0.315	4.26	840	2851
0.30	-0.180	4.18	840	2836
0.40	-0.065	4.14	830	2826

<sup>a</sup>Reference 22.

<sup>b</sup>Reference 28.

the significance of a comparison with experimental results where the effective initial distribution of electron speeds is unknown.

The comparison discussed above is presented in Fig. 5 where the transient mobility in argon as measured by Sowada and Warman<sup>5</sup> (curve labeled +) is compared with theoretical results for both initial  $\delta$ -function [Fig. 5(a)] and Gaussian [Fig. 5(b)] distributions, with either the Mozumder cross section or the Haddad and O'Malley cross sections. The best fit to the experimental results is the Mozumder cross section and an initial Gaussian distribution ( $\alpha=0.4$ ,  $u_0=4.0$ ).

A comparison of our calculated energy relaxation times with other theoretical calculations and the available experimental data has been presented in a previous paper.<sup>12</sup> The present paper has reported the corresponding mobility and diffusion relaxation times. At the present time, the only relevant data with which to compare are those of Sowada and Warman.<sup>5</sup> As is clear from the results in Fig. 5, we find close agreement between this experiment and our calculations with Mozumder's tabulation of the argon cross section. Table V shows almost identical energy and mobility relaxation times for argon thereby validating our original comparison with the data.<sup>12</sup>

## VI. SUMMARY

In the present paper, we have demonstrated the efficiency of the discrete-ordinate method in the calculation of the transient behavior of an electron swarm. An important advantage of the DO method is that matrix elements of the differential Fokker-Planck equation need not be

calculated. Rather, the matrix representative of the differential operator in the DO basis is determined in terms of the DO derivative operator and involves the evaluation of the cross sections at the set of discrete energies. This procedure is computationally accurate and efficient. The possibility of rescaling the quadrature points as discussed in the paper is an additional flexibility of the method.

In addition to the calculation of the relaxation times of electrons in inert-gas moderators, the present work has noted some unusual nonequilibrium phenomena with regard to the transient transport coefficients. We have shown that Ramsauer minima effects are clearly discernible in the transient mobility and diffusion coefficient. It has also been demonstrated that for certain moderators with Ramsauer minima in the cross sections and for particular initial distributions, the mobility can be negative and remain negative during an initial transient. It is interesting to speculate as to the possibility of observing this effect experimentally.

The present work has been restricted to thermalization by elastic collisions alone. The extension of the DO method to include both inelastic collisions and finite electric field effects is in progress. Although there are some important modifications to the method, preliminary calculations suggest that the method is competitive with other methods of analysis such as Monte Carlo and moment methods.

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