Electric field dependence of transient electron transport properties in rare-gas moderators

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A discrete-ordinate method of solution of the time-dependent Boltzmann-Fokker-Planck equation for electron swarms in rare-gas moderators is employed in the study of the time dependence of the average electron energy, mobility, and transverse diffusion coefficient versus the strength of an externally applied electric field. The solution of the Fokker-Planck equation is based on the expansion of the solution in the eigenfunctions of the Lorentz-Fokker-Planck operator. With the transformation to an equivalent Schrödinger eigenvalue problem, the eigenvalue spectrum is shown to be entirely discrete, thereby validating the eigenfunction-expansion approach. The effects studied include the effect of an electric field on the thermalization times, a comparison of the effects of moderators with and without Ramsauer minima in the momentum-transfer cross sections, and the effect of an external electric field on the transient negative-mobility phenomena predicted in an earlier paper. A comparison with experimental results for Xe shows good agreement with the calculations.

I. INTRODUCTION

The study of the transient behavior of a nonequilibrium ensemble of electrons in different moderators has important applications in many different fields, and the theoretical description of the approach to equilibrium is an important endeavor. Examples of important applications include the interpretation of electron-swarm experiments,[1–3] delayed luminescence in gases,[4] radiation chemistry and biology,[5] laser physics,[6,7] discharge devices,[8] and many other applications.

The present paper is a continuation of the authors' recent works[9,10] on the thermalization of low-energy electrons in rare-gas moderators. The earlier work was concerned with the transient behavior of the transport properties of the electron population in the limit of zero external electric field. The present paper extends the earlier work to include a study of the effect of finite external electric field on the transient behavior of the distribution function, the average electron energy, the mobility, the transverse diffusion coefficient, and the corresponding thermalization times. The determination of the electron-distribution function and the transient behavior involves the solution of the appropriate Boltzmann or Fokker-Planck (FP) equation.

This electron-thermalization problem has been considered by several authors with different methods of analysis. Olaussen and Hemmer[11] have carried out an analytical study of the asymptotic short-time transient mobility of a hard-sphere cross section. Mozumder[12] and Tembe and Mozumder[13] have assumed that the electron-distribution function is a pseudo-Maxwellian characterized by a time-dependent temperature. A discussion and critique of this approach has been presented in the earlier papers.[9,10] Knierem *et al.*[14] have employed traditional moment methods of solution of the FP equation. This approach is based on the expansion of the distribution function about a Maxwellian characterized with the time-dependent electron temperature. With this expansion, differential equations for the lower-order moments are derived from the FP equation. Although the FP equation is linear, the resulting moment equations are characterized by nonconstant coefficients, due to the collision operator being parameterized with a time-dependent temperature. Consequently, a numerical integration of the moment equations is required. Monte Carlo simulations of the thermalization of electrons have also been carried out by Koura.[15] Pitchford and Green[16] have studied the zero-field thermalization and the effect of an electric field for model systems characterized by constant cross sections and constant collision frequency.

The present paper employs the discrete-ordinate (DO) method introduced in earlier papers by Shizgal,[17] and Shizgal and Blackmore,[18] and employed in the earlier study of electron thermalization.[9,10] The solution of the FP equation appropriate to the present problem is solved with a standard eigenfunction expansion of the distribution function. This is a useful approach, since the reciprocals of the eigenvalues are the characteristic relaxation times of the system. The DO method provides an extremely efficient numerical procedure for the evaluation of the eigenvalues and the corresponding eigenfunctions, as well as the transport coefficients. The transport coefficients are given as integrals over the distribution function. Their evaluation is facilitated due to the fact that the distribution function is determined at the set of quadrature points for which rapid convergence of the integrations involved is obtained.

The connection is made between the eigenvalue problem associated with the FP equation that occurs for the electron-thermalization problem, and an equivalent eigenvalue problem based on a Schrödinger equation as described by Garrett,[19] Braglia *et al.*,[20] and in a recent paper on FP equations for bistable systems by Blackmore and Shizgal.[21] The equivalence with a Schrödinger problem is important, as it provides useful information with regard to the nature of the eigenvalue spectrum and, in particular, whether it has a continuum portion. We

demonstrate that there is no continuum to the eigenvalue spectrum for the rare-gas moderators by demonstrating that the potential in the Schrödinger equation equivalent to the FP equation is bounded. Consequently, the expansion of the distribution function in the discrete eigenfunctions is appropriate. We also show that the description based on a Schrödinger equation with some effective potential function provides a useful interpretation of the results presented later in the paper.

The effects examined in the present work are the effects of the electric field on the transient behavior of the average energy, mobility, and diffusion coefficient. In particular, we are interested in a comparison of the thermalization behavior in He and Ne as compared with the behavior in the heavier gases, Ar, Kr, and Xe, whose cross sections are characterized by deep Ramsauer-Townsend minima. Section II of the paper outlines the theoretical formulation for the time development of the electron-velocity distribution function. The DO method of solution is discussed in Sec. III. The transformation of the FP eigenvalue equation to the equivalent Schrödinger problem is presented in Sec. IV, together with results of the nature of the eigenvalue spectrum. The results for the transient behavior are presented and discussed in Sec. V. A summary of the results and conclusions appears in Sec. VI.

II. TIME EVOLUTION OF THE ELECTRON DISTRIBUTION

The basic methodology of the present paper follows closely the formalism in earlier papers[9,10,18] and overlaps the discussion in standard references on electron-transport theory.[22–24] The point of departure is the connection with the general FP equation and the equivalent Schrödinger equation within the context of the DO method of solution. The time evolution of the anisotropic, spatially homogeneous, electron velocity distribution function (VDF) is based on the expansion in Legendre polynomials,[9,10,14,24] that is,

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

where θ is the angle between $\mathbf{v}$ and the polar axis chosen in the direction of the electric field. For the rare-gas moderators at low electron energies, for which only elastic collisions need be included, only the terms in $l=0$ and $l=1$ need be retained. The coupled equations for the first two terms f_0 and f_1 are given by

$$\frac{\partial f_0}{\partial t}+\frac{eE}{3m}\left[\frac{\partial}{\partial v}+\frac{2}{v}\right]f_1 = \frac{m}{Mv^2}\frac{\partial}{\partial v}\left[v^3\nu\left[1+\frac{k_BT_b}{mv}\frac{\partial}{\partial v}\right]\right]f_0 , \tag{2a}$$

$$\frac{\partial f_1}{\partial t}+\frac{eE}{m}\frac{\partial f_0}{\partial v}=-\nu f_1 , \tag{2b}$$

where M is the mass of the moderator atoms, E is the electric field strength, and $\nu(v)=nv\sigma$, where σ is the momentum-transfer cross section and n is the number density of the moderator. Owing to the small electron to moderator mass ratio, initial anisotropies of the distribution function (f_l, $l>0$) decay very quickly before appreciable energy relaxation.[9,10] The energy relaxation occurs on a much longer timescale and the present work is concerned with this time domain. This was referred to as time domain (ii) in the earlier paper.[9] With a nonzero electric field there will be an initial anisotropy at the beginning of this time domain and the distribution function will be somewhat different than the value at $t=0$. We ignore these effects and set $\partial f_1/\partial t=0$ and substitute the result for f_1 from Eq. (2b) in Eq. (2a). In addition, reduced units $x=(m/2k_BT)^{1/2}v$ and $t'=t/\tau$, where

$$\tau=\left[\frac{nm}{2M}\sigma_0\left[\frac{2k_BT_b}{m}\right]^{1/2}\right]^{-1} \tag{3}$$

are employed, with $\hat{\sigma}(x)=\sigma(x)/\sigma_0$, and σ_0 is some convenient hard-sphere cross section. In Eq. (3), T_b is the temperature of the moderator which can differ from the temperature T used to define the reduced speed x. The quantity $s^2=T/T_b$ is the parameter used to scale the points in the DO method as discussed in the previous paper[10] and in Sec. III of this paper. With these definitions, and f_1 from Eq. (2b), the equation for f_0 is given by

$$\frac{\partial f_0}{\partial t'}=\frac{s}{x^2}\frac{\partial}{\partial x}\left[2x^4\hat{\sigma}f_0+\frac{x^2}{s^2}B(x)\frac{\partial f_0}{\partial x}\right] , \tag{4}$$

where

$$B(x)=x\hat{\sigma}+\frac{(\alpha/s)^2}{x\hat{\sigma}} . \tag{5}$$

The quantity α is a field-strength parameter given by

$$\alpha^2=\frac{M}{6m}\left[\frac{eE}{n\sigma_0k_BT_b}\right]^2 . \tag{6}$$

With Eq. (4), the steady solution attained at $t=\infty$ is easily shown to be given by

$$f_0(x,\infty)=D(x)=C\exp\left[-2s^2\int_0^x\frac{(x')^2\hat{\sigma}}{B(x')}dx'\right] , \tag{7}$$

where C is a normalization constant. The function $D(x)$ is the well-known Davydov distribution for electrons in an applied electric field.[22,23] In the absence of an electric field ($\alpha=0$), $D(x)$ is the Maxwellian at T_b.

Equation (4) can be written in the form of a general FP equation by setting

$$f_0=\exp[-d(x)]g_0 , \tag{8}$$

where $d(x)$ is the argument of the exponential in the Davydov distribution in Eq. (7), that is,

$$d(x)=2s^2\int_0^x\frac{(x')^2\hat{\sigma}}{B(x')}dx' . \tag{9}$$

With Eq. (8) in Eq. (4), one finds that

$$\frac{\partial g_0}{\partial t'}=\frac{1}{s}\left[-A(x)\frac{\partial g_0}{\partial x}+B(x)\frac{\partial^2 g_0}{\partial x^2}\right]=-Lg_0 , \tag{10}$$

where $B(x)$ is given by Eq. (5) and

$$A(x)=2s^2x^2\hat{\sigma}-\frac{2B(x)}{x}-\frac{dB(x)}{dx} . \tag{11}$$

Equation (10) is the desired form for the differential equation for g_0. This form is particularly useful as there has been considerable discussion of the solution of this type of FP equation.[25–28] In particular, Blackmore and Shizgal[21] have recently provided a general DO method of solution of this general form for arbitrary coefficients $A(x)$ and $B(x)$. A discussion of this method of solution is presented in Sec. III.

The method of solution employed in the present paper is based on the eigenfunction expansion of the solution and parallels the work in earlier papers.[9,10] The formal solution of Eq. (10) is

$$g_0(x,t')=e^{-Lt'}g_0(x,0) , \tag{12}$$

where $g_0(x,0)$ is the initial value. If g_0 is expanded in the eigenfunctions ϕ_k of the Lorentz-FP operator L, then

$$g_0(x,t')=\sum_{k=0}^{\infty} a_k\phi_k(x)\exp(-\lambda_k t') , \tag{13}$$

where

$$L\phi_k=\lambda_k\phi_k . \tag{14}$$

The eigenfunctions ϕ_k are orthogonal with the steady distribution $x^2D(x)$ as a weight function. The expansion coefficients in Eq. (13) are determined by the initial distribution function, that is,

$$a_k=\int_0^{\infty} x^2D(x)\phi_k(x)g_0(x,0)dx .$$

With the distribution given by Eq. (13), the transient behavior of the average energy $E(t')$, mobility $\mu(t')$, and the transverse diffusion coefficient $D_T(t')$ can be shown to be given by summations of the form

$$E(t')=\sum_{k=0}^{\infty} e_k\exp(-\lambda_k t') , \tag{15}$$

$$\mu(t')=\sum_{k=0}^{\infty} \mu_k\exp(-\lambda_k t') , \tag{16}$$

$$nD_T(t')=\sum_{k=0}^{\infty} d_k\exp(-\lambda_k t') . \tag{17}$$

The explicit form of the coefficients in Eqs. (15)–(17) is presented in Sec. III, where the application of the DO method is discussed. In this way the problem is reduced to one of determining the eigenvalues λ_k and eigenfunctions ϕ_k of the FP operator L. A comparison of the transient behavior of the longitudinal and transverse diffusion coefficients is presented in a separate paper. The expression for the longitudinal diffusion coefficient differs somewhat from the formalism presented here.

III. DISCRETE-ORDINATE METHOD OF SOLUTION OF THE EIGENVALUE PROBLEM

The eigenfunctions and eigenvalues of the FP equation can be determined by expanding the eigenfunctions in a suitable basis set and diagonalizing the (approximate) matrix representative of the FP operator in this basis set. This is essentially a Rayleigh-Ritz variational calculation of the eigenfunctions. As discussed in a previous paper, an optimum choice of basis set for the solution of Eq. (10) might be the one based on functions orthonormal with the steady solution $x^2D(x)$ as the weight function. However, the generation of such a basis set is difficult due to the well-known numerical instability inherent in this problem. Alternate basis sets can be chosen that are based on a weight function that approximate the steady solution.

The present work employs the DO method introduced in previous papers.[10,21] The explicit expansion of the eigenfunctions in the basis set is not employed. Rather, the eigenfunctions are determined at a discrete set of points which coincide with the points of a quadrature procedure based on a set of polynomials. This representation of the eigenfunctions is entirely equivalent to the representation in terms of the coefficients in the polynomial expansion, as there exists a unitary transformation between the two representations. In the present work, the quadrature procedure based on speed polynomials $B_n(x)$ orthogonal with respect to the weight function $w(x)=x^2\exp(-x^2)$ is employed, that is,

$$\int_0^{\infty} w(x)G(x)dx=\sum_{i=1}^{N} w_iG(x_i) , \tag{18}$$

where w_i and x_i are the weights and points, respectively.[17,18] However, the operator L is self-adjoint with respect to the steady solution $x^2D(x)$ and not with respect to weight function $w(x)$. As discussed at length in the paper by Blackmore and Shizgal,[21] the symmetric representative of L can be constructed by evaluating the matrix representative in the basis set of functions orthonormal with respect to $x^2D(x)$, and transforming to the DO representation with the appropriate unitary transformations. The result is that the eigenvalues λ_k and corresponding eigenfunctions

$$\psi_k=[x^2D(x)/w(x)]^{1/2}\phi_k(x)$$

are determined by diagonalizing the (symmetric) matrix L_{ij} in the DO basis set, given by

$$L_{ij}=\frac{1}{s}\sum_{k=1}^{N} B(x_k)[D_{ki}+h(x_k)\delta_{ik}][D_{kj}+h(x_k)\delta_{jk}] , \tag{19}$$

where

$$h(x)=\frac{w'(x)}{2w(x)}-\frac{[x^2D(x)]'}{2x^2D(x)} \tag{20a}$$

$$=\frac{d'(x)}{2}-x \tag{20b}$$

and D_{ki} is the derivative operator.[21] In the absence of an electric field ($\alpha=0$), Eq. (20b) reduces to $h(x)=x(s^2-1)$ and Eq. (19) coincides with Eq. (33) of the previous paper.[10] As discussed there, the parameter s is chosen so as to be able to scale the quadrature points appropriately. This scale factor (and the temperature T used to define the reduced speed) increases with increasing electric field. This is analogous to the use of an effective temperature in the moment method. [In Ref. 10, Eq. (25b) should have

read $t'=t/s\tau$, which differs from the dimensionless time in the present paper by the factor $1/s$.]

An important advantage of the DO method of solution is that the eigenfunctions are determined at the set of quadrature points appropriate for the integral evaluation of the coefficients in Eqs. (15)–(17) for the transient transport coefficients. It is important to note that the eigenfunctions determined with the diagonalization of Eq. (19) are proportional to the zeroth eigenfunction

$$\psi_0(x)=[x^2D(x)/w(x)]^{1/2}$$

with eigenvalue $\lambda_0=0$. The steady solution is thus determined without explicit evaluation of the integral in Eq. (7).

The calculation of the time dependence of the average energy and the transverse diffusion coefficient involve integrals of the form

$$P(t')=\int_0^\infty f(v,t')p(v)v^2dv = s^3\int_0^\infty D(x)g_0(x,t')p(x)x^2dx \ , \tag{21}$$

where $p(x)$ equals $k_BT_bs^2x^2$ and

$$\frac{1}{3}\left[\frac{2k_BT_b}{m}\right]^{1/2}\frac{sx}{\sigma(x)}$$

for the average energy $E(t')$ and the diffusion coefficient $D_T(t')$, respectively. With the expansion of $g_0(x,t')$ given by Eq. (13), we find that the coefficients in Eqs. (15) and (17) are of the form

$$p_k=a_ks^3\int_0^\infty D(x)\phi_k(x)p(x)x^2dx \ .$$

In terms of the eigenfunctions $\psi_k(x)$, this integral can be written in a form appropriate for the Gaussian quadrature of Eq. (18), that is,

$$p_k=a_ks^3\int_0^\infty w(x)\left[\frac{x^2D(x)}{w(x)}\right]^{1/2}\psi_k(x)p(x)dx = a_ks^3\sum_{i=1}^N w_i\left[\frac{x_iD(x_i)}{w(x_i)}\right]^{1/2}\psi_k(x_i)p(x_i) \ .$$

The calculation of the time-dependent mobility $\mu(t')=W(t')/E$, where $W(t')$ is the drift velocity, involves $f_1(v,t')$ of Eq. (2b). With the neglect of the time derivative of f_1, we calculate f_1 in terms of f_0 and its velocity derivative as discussed in the previous paper.[9] The result for the mobility after an integration by parts is

$$\mu(t')=-\frac{e}{6ns}\left[\frac{2}{mk_BT_b}\right]^{1/2}\int_0^\infty w(x)\left[\frac{x^2D(x)}{w(x)}\right]\left[\frac{2}{x}-\left[\frac{d\sigma}{dx}\right]\right]\frac{1}{\sigma(x)}g_0(x,t')dx \ .$$

The coefficients in Eq. (16) are given by

$$\mu_k=-\frac{ea_k}{6ns}\left[\frac{2}{mk_BT_b}\right]^{1/2}\sum_{i=1}^N w_i\left[\frac{x_i^2D(x_i)}{w(x_i)}\right]^{1/2}\left[\frac{2}{x_i}-\left[\frac{d\sigma}{dx}\right]_{x=x_i}\right]\frac{1}{\sigma(x_i)}\psi_k(x_i) \ .$$

IV. EIGENVALUE SPECTRUM OF FP OPERATOR: EQUIVALENT SCHRÖDINGER EIGENVALUE PROBLEM

The transient behavior of the electron swarm is determined with the expansion of the distribution function in the eigenfunctions of the FP operator. The nature of the eigenvalue spectrum of the collision operator determines the details of the time evolution of the distribution function and there have been many general discussions of this in the literature, particularly with regard to neutron-transport theory,[29] hot-atom chemistry,[30] and kinetic-theory problems for which the test-particle moderator mass ratio is closer to unity.[31] Much of the interest is with respect to the presence or absence of a continuous portion to the eigenvalue spectrum. It has generally been thought that the eigenfunction method of solution will not be valid or converge slowly if the continuous portion of the spectrum is not included. However, it has been demonstrated recently[32] that expansions with finite basis sets which do not include the continuum eigenfunctions in a rigorous fashion can yield converged solutions. In the present case, we show that the potential in the Schrödinger equation corresponding to the eigenvalue problem tends to infinity as $x\to0$ and $x\to\infty$, and the eigenvalue spectrum of the FP operator is entirely discrete.

If the change of variable

$$y=\int_0^x[B(x')]^{-1/2}dx'$$

and the definition $\phi_k(x)=e^{C(x)}\psi_k(x)$ are made, then it can be shown that[19–21]

$$\frac{d^2\psi_k}{dy^2}-[V(y)-\lambda_k]\psi_k=0 \ , \tag{22}$$

where

$$V(y)=\left[\frac{dC}{dy}\right]^2-\frac{d^2C}{dy^2}$$

and

$$C(y(x))=\int_0^x\frac{A(x')}{2B(x')}dx'+\tfrac{1}{4}\ln B(x) \ .$$

TABLE I. Convergence of eigenvalues λ_n (in units of τ^{-1}); $T_b=290.1$ K.

N	λ_0	λ_1	λ_3	λ_5	λ_{10}	λ_{15}	λ_{20}
			He, $E/n=1.0$ Td[a]				
10	0.0041	298.35	1129.5	3362.8			
20	2×10^{-8}	298.24	1090.6	1998.1	5938.1	51 306	
30	1×10^{-9}	298.24	1090.6	1998.0	4475.4	7599.6	24 487
40					4475.3	7022.7	9956.9
50						7022.7	9499.7
60							9499.7
			Ar, $E/n=0.05$ Td				
10	0.0042	94.032	442.22	1548.0			
20	1×10^{-4}	91.210	360.03	715.43	2604.6	9164.0	
30	1×10^{-5}	91.157	358.06	693.71	1940.3	4026.3	9599.0
40	5×10^{-6}	91.156	358.01	692.64	1847.1	3245.5	6344.9
50	3×10^{-7}			692.59	1835.3	3103.9	4922.0
60	6×10^{-11}			692.58	1833.5	3068.5	4253.8
70					1833.4	3062.2	4462.0
80						3061.0	4447.3

[a]1 Td$=10^{-17}$ V cm^2.

V. RESULTS AND DISCUSSION

The eigenvalues and eigenfunctions were determined by diagonalizing the DO-matrix representative of the FP operator, that is, the matrix L_{ij} given by Eq. (19). Table I illustrates the rate of convergence of the lowest eigenvalues for two typical cases. Similar results were obtained for other gases for different field strengths and temperatures. The lowest eigenvalue λ_0 should be zero as a consequence of particle conservation. The corresponding eigenfunction is related to the steady Davydov distribution as mentioned previously. The approach of λ_0 to zero with an increase in the number of quadrature points is an indication of the efficiency of the speed polynomials in approximating the steady solution. The rate of convergence is more than adequate for the present work and for the comparison with available experimental data that is made. The rate of convergence is rapid for a moderator with a momentum-transfer cross section which varies slowly with energy such as helium. The cross sections employed are those reported by Nesbet[33] for He, by O'Malley and Crompton[34] for Ne, by Mozumder[12] for Ar, Kr, and Xe, and by Haddad and O'Malley[35] for Ar when explicitly mentioned.

In Fig. 1, we show, for krypton as moderator, the stationary (normalized) Davydov distribution determined with a Simpson's-rule integration of the integral in Eq. (7) (solid curve), as well as the same distribution calculated

TABLE II. Dependence of eigenvalues and steady transport parameters with scaling parameter s; $T_b=290.1$ K, $N=50$.

s	T	λ_0	λ_1	λ_3	$\langle E\rangle$[a]	W	nD_T
			He, $E/n=5.0$ Td[b]				
1.064	328.4	317.3	2413	6202	1.304	15.45	3.123
1.333	515.2	90.73	1210	3175	1.965	12.88	3.856
1.869	1013	3.0754	580.7	1376	2.786	11.57	4.730
2.392	1660	0.0763	502.7	971.0	2.884	11.52	4.842
2.721	2149	−0.122(−3)	495.8	906.6	2.889	11.52	4.847
3.447	3447	−0.685(−7)	495.8	906.0	2.889	11.52	4.847
4.552	5932	−0.109(−6)	495.8	906.2	2.889	11.52	4.847
			Kr, $E/n=0.5$ Td				
1.064	328.4	9.246	1217	3304	1.620	1.677	11.73
1.333	515.2	0.110(−2)	1085	2588	1.659	1.584	11.52
1.869	1013	0.2444(−3)	1085	2588	1.659	1.584	11.52
2.392	1660	0.517(−3)	1085	2588	1.659	1.584	11.52
2.893	2427	0.379(−3)	1085	2588	1.659	1.584	11.52
4.049	4756	0.301(−2)	1086	2592	1.659	1.584	11.52
5.307	8170	0.2226	1087	2586	1.658	1.587	11.53

[a]$\langle E\rangle$, W, and nD_T in units of eV, 10^5 cm sec^{-1} and 10^{22} cm^{-1} sec^{-1}, respectively.
[b]1 Td$=10^{-17}$ V cm^2.

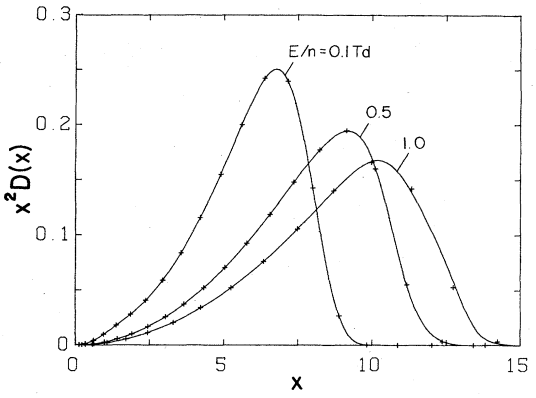

FIG. 1. Davydov distribution $x^2D(x)$ for several electric field strengths E/n: ——, Simpson's-rule integration, Eq. (7); + + +, discrete-ordinate result determined from eigenfunctions $x_i^2D(x_i)=\psi_0^2(x_i)/[w(x_i)w_i]$; krypton gas is the moderator, $T_b=290.1$ K, $N=20$.

from the eigenfunction $\psi_0(x_i)$ determined with the DO method, that is, by diagonalization of L_{ij} given by Eq. (19). The points (+) in Fig. 1 are the values of the Davydov distribution determined with the DO method with $N=20$. The efficiency of the DO method should be clear, particularly when the points are scaled appropriately as is done in Fig. 1 so as to place as many points as possible in the energy region where the distribution function is largest. Consequently, the scaling becomes important with an increase in E/n. For a particular cross section and E/n, the optimum value of s can be determined by trial and error in an effort to set λ_0 as close to zero as possible as shown in Table II. The results in Table II show the way in which the lowest eigenvalues and the average energy, drift velocity, and transverse diffusion coefficient vary with a change in the scaling parameter s. The effective temperature T corresponding to this optimum scaling parameter is considerably less than $\langle E\rangle/k$. It is useful to note that the other quantities are for the most part independent of s near this optimum value. We also show in Table III the convergence versus the number of quadrature points N of the average energy, drift velocity, and transverse diffusion coefficient.

TABLE III. Convergence of the steady average energy, drift velocity, and transverse diffusion coefficient ($T_b=290.1$ K).

N	E (eV)	W (10^5 cm sec^{-1})	nD_T (10^{22} cm^{-1} sec^{-1})
		He, $E/n=1.0$ Td	
10	0.3161	6.566	1.650
20	0.4861	5.179	1.988
30	0.5590	4.841	2.109
40	0.5592	4.841	2.110
50	0.5592	4.841	2.110
FEM[a]	0.5582	4.829	2.108
		Ar, $E/n=0.05$ Td	
10	0.3579	4.745	40.15
15	0.6428	1.524	31.74
20	0.6025	1.714	32.83
30	0.6552	1.480	31.44
40	0.6552	1.480	31.44
FEM	0.6552	1.480	31.43

[a]Results with a Simpson's-rule finite-element method.

The nature of the convergence of the smallest eigenvalues shown in Table I suggests that the eigenvalue spectrum is discrete. In this regard, it is useful to illustrate the potential functions $V[y(x)]$ that occur in the Schrödinger equation, Eq. (22). Figure 2 compares the (dimensionless) potential functions for helium and xenon for several electric field strengths. We have chosen to show these potentials versus the reduced velocity variable $v/v_{\rm th}=x[T/(435.15\ {\rm K})]^{1/2}$. For low E/n, the potentials vary approximately as $1/y^2$ as $y\to 0$ and a deep narrow well occurs near the origin $v/v_{\rm th}=0$. The point $y=0$ corresponds to a node for all the eigenfunctions. For He and Ne, for which the cross sections are monotonic functions of the relative energy (see Fig. 3 of Ref. 9), the potential has a single broad minimum at larger $v/v_{\rm th}$, as shown in Fig. 2(a) for helium. For the smallest eigenvalues and low E/n, it is possible to approximate the potential well by an harmonic potential and to obtain approximate analytic eigenvalues which qualitatively agree with the exact numerical results. For the heavier moderators (Ar, Kr, and Xe), which are characterized by momentum-transfer cross

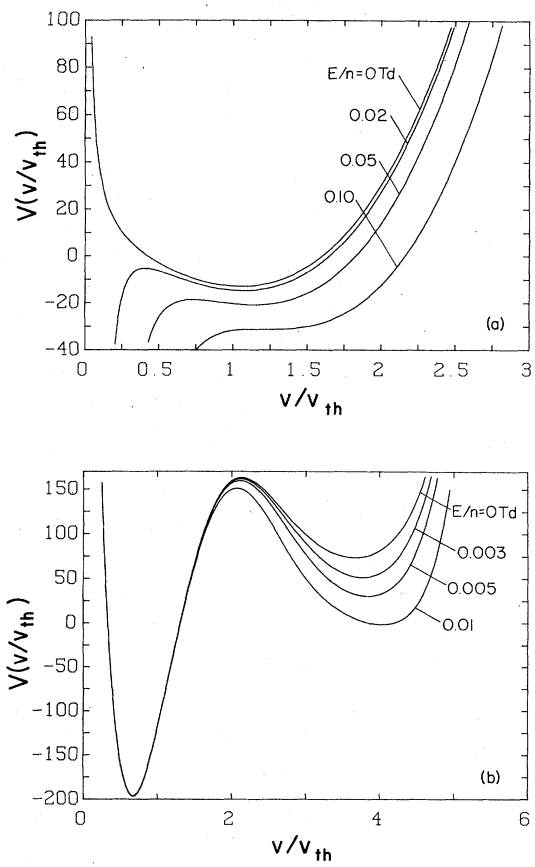

FIG. 2. Potential functions in the Schrödinger equation equivalent to the Fokker-Planck equation. (a) Helium and (b) xenon.

sections with Ramsauer minima, the potentials possess two minima, the second occurring close to the energy of the Ramsauer minima, as seen in Fig. 2(b) for xenon. We later show that this feature can be employed to appreciate some details in the transient behavior of the distribution function. In particular, $V\rightarrow\infty$ as $v/v_{\rm th}\rightarrow 0$ and $v/v_{\rm th}\rightarrow\infty$, and no continuum exists in the eigenvalue spectrum.

An interesting result is obtained for the cross section $x\sigma(x)=a$, where a is constant independent of energy, that is, $\sigma(x)$ is the Maxwell cross section. It is easily shown with Eqs. (5), (11), and (22) that the potential corresponding to this cross section is given by $V(y)=a^2y^2-3a$ and is independent of the electric field strength. This property is a useful check of the DO method since the eigenvalues are the well-known harmonic-oscillator eigenvalues given by $\lambda_k=4ak$. In addition, the dependence of the eigenvalues on E/n for realistic cross sections can be understood in relation to this particular model for which there is no field dependence.

The dependence of the smallest eigenvalues on E/n is shown in Fig. 3 for He and Xe, which illustrate the behavior typical of moderators whose cross sections do and do not exhibit a Ramsauer minimum. As can be seen, the lowest eigenvalues for Xe exhibit a minimum in their variation versus E/n. For cross sections decreasing faster than $1/x$, the eigenvalues can decrease with increasing E/n, whereas for cross sections decreasing slower than $1/x$ or increasing with energy the eigenvalues will increase with increasing E/n. The result for He gives increasing eigenvalues with increasing E/n. The smaller eigenvalues are determined by the lower energy, decreasing portion of the cross sections (for Ar, Kr, and Xe), whereas the larger eigenvalues are determined by the higher-energy portion of the cross sections. Since the relaxation times are related to the reciprocal of these eigenvalues, the E/n dependence of the thermalization times is given qualitatively by the reciprocal of the eigenvalues.

The transient behavior of the average energy, diffusion coefficient, and mobility is shown in Figs. 4–6, respectively. The initial distribution function is a delta function with an initial energy given by the value of $u_0=v/v_{\rm th}$, where $v_{\rm th}$ is the rms speed at $T_b=290.1$ K.[10,12] Although the choice of an initial delta-function distribution may be considered as unrealistic, previous calculations[9] have shown that the relaxation times are not very sensitive to

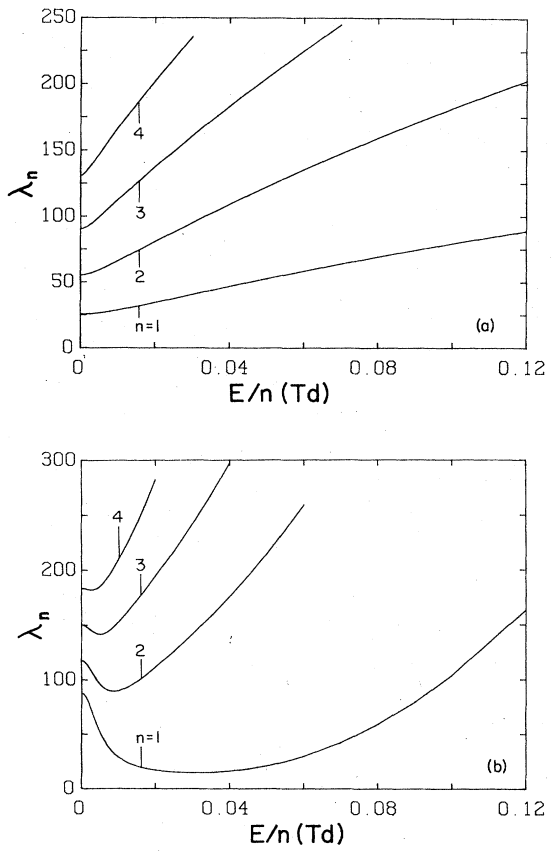

FIG. 3. Variation of eigenvalues with E/n; λ_n in units of τ^{-1}. (a) Helium and (b) xenon.

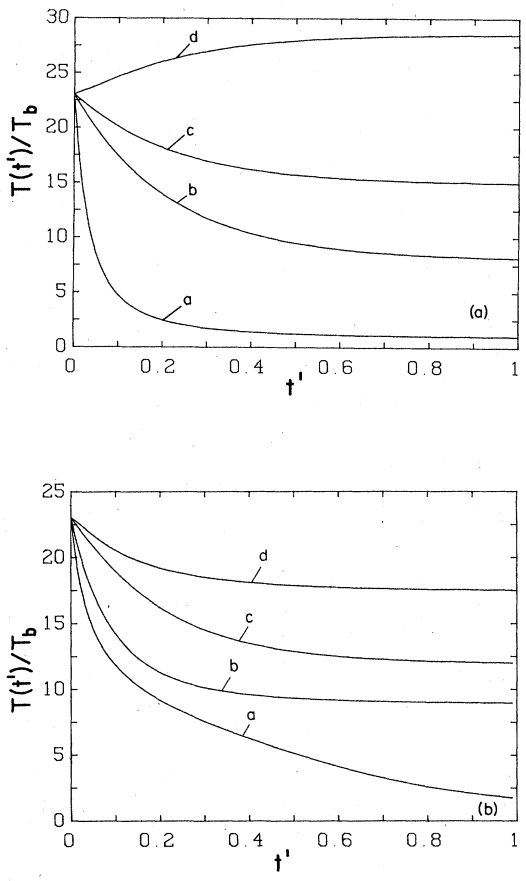

FIG. 4. Variation of $T(t')/T_b$ vs E/n. Initial delta-function distribution with $u_0=4.8$ or initial energy is 0.864 eV. $T_b=290.1$ K, E/n in Td, and τ in 10^{11} sec cm^{-3} for (a) helium are equal to *a*, 0, 28.51; *b*, 0.5, 3.54; *c*, 1.0, 2.44; *d*, 2.0, 1.75. For (b) argon, they are equal to *a*, 0, 1304; *b*, 0.01, 603.2; *c*, 0.02, 171.4; *d*, 0.05, 79.79.

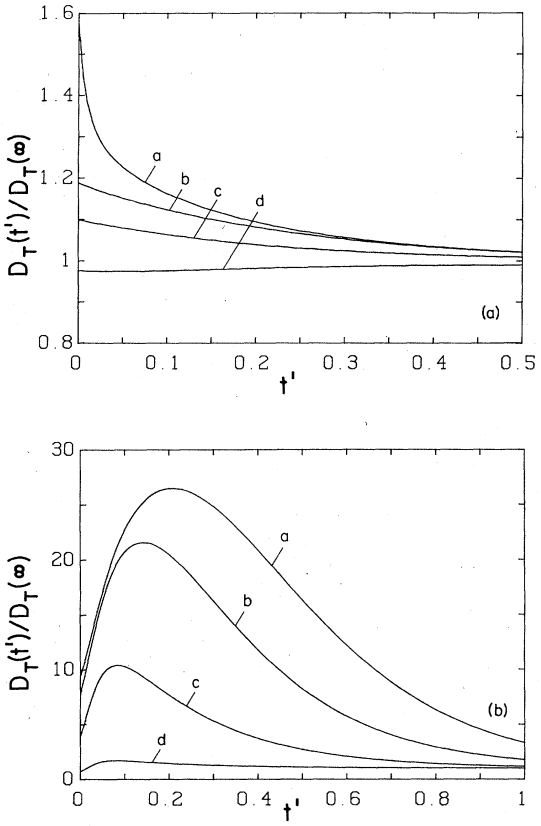

FIG. 5. Variation of $D_T(t')/D_T(\infty)$ vs E/n. Initial delta-function distribution with $u_0=4.8$ or initial energy is 0.864 eV. $T_b=290.1$ K, E/n in Td, and τ in 10^{11} sec cm^{-3} for (a) neon are equal to *a*, 0, 2135; *b*, 0.05, 68.45; *c*, 1.0, 46.05; *d*, 0.2, 32.56. For (b) argon, they are equal to *a*, 0, 1304; *b*, 0.001, 1811; *c*, 0.002, 2756; *d*, 0.005, 2139.

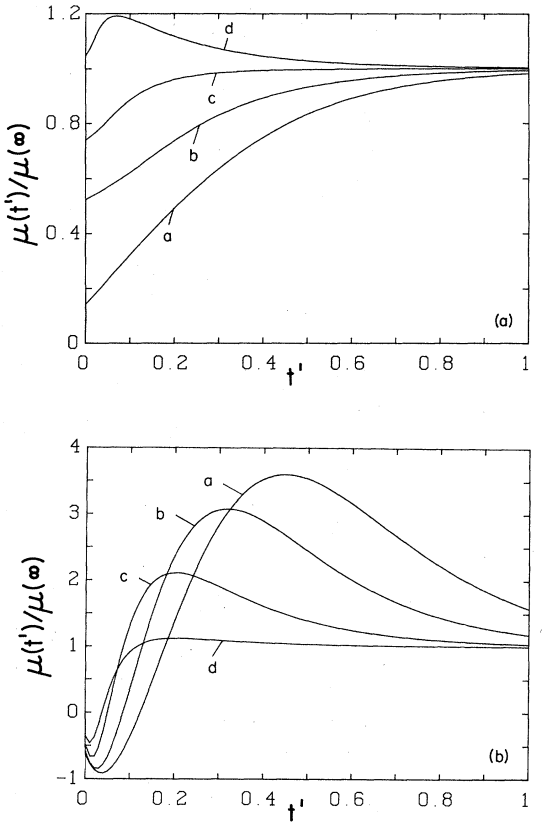

FIG. 6. Variation of $\mu(t')/\mu(\infty)$ vs E/n. Initial delta-function distribution with $u_0=4.0$ or initial energy is 0.600 eV. $T_b=290.1$ K, E/n in Td, and τ in 10^{11} sec cm^{-3} for (a) helium are equal to *a*, 0, 28.51; *b*, 0.5, 3.54; *c*, 1.0, 2.44; *d*, 2.0, 1.75. For (b) argon, they are equal to *a*, 0, 1304; *b*, 0.001, 1811; *c*, 0.002, 2756; *d*, 0.005, 2139.

the form of the initial distribution function. This is probably due to the rapid broadening of the distribution functions. In each case, we compare the results for two moderators to illustrate the particular effect of the Ramsauer minima in the cross sections. Figure 4 shows the transient electron temperature and illustrates the heating of the electrons with increasing E/n; the final steady value of $T(\infty)/T_b$ is greater than unity and increases with an increase in E/n. The results are shown in the reduced timescale and it is important to take into account the values of τ for each curve as given in the figure caption. The effect of an increase in the electric field is to move the distribution function out to much higher energies relative to the zero-field situation and the relaxation is determined by the higher-energy portion of the cross sections. For the heavier moderators, an increase in the field results in a disappearance of the effects [maximum in $D_T(t')/D_T(\infty)$, and negative mobilities] attributable to the Ramsauer minima in the cross sections for these moderators, as shown in Figs. 5(b) and 6(b). The initial mobility is determined by the initial delta-function distribution and is independent of E/n. However, the duration of the negative mobility transient, when it occurs, is reduced by the electric field.

For He and Ne, the relaxation times shown in Table IV decrease with an increase in E/n owing to the increase in the eigenvalues reflecting the nearly constant momentum-transfer cross sections for these moderators. Physically, the electric field speeds up the electron-atom collision rate (thereby enhancing the collisional energy-dissipation rate and shortening the relaxation times) by driving the swarm through the moderator gas. For the Maxwell cross section $x\sigma(x)=$const, the collision rate is independent of the field so that the intrinsic energy-dissipation rate is not increased, as reflected in eigenvalues which are independent of E/n.

For the heavier moderators, Ar, Kr, and Xe, the initial increase in the relaxation times with a small increase in E/n is clearly evident in Table IV. The relaxation times attain a maximum value for an E/n value near the minimum in λ_1, and then decrease with further increase in the electric field. This behavior is consistent with the results in Fig. 3 for the eigenvalues. This field dependence is attributable to the Ramsauer minima that occurs in the

TABLE IV. Relaxation times versus electric field strength E/n in units of 10^{-17} V cm^2. $T_b=290.1$ K; the initial distribution is a delta function at $u_0=4.0$ in units of $v_{th}=1.148\times10^7$ 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 stationary value) to decay to within 1.01 of the stationary value. Asterisks denote values of τ for relaxation to 1/1.01 or 1/1.1 of the stationary value. Cross sections are those reported by Mozumder (Ref. 12).

	$\tau(1.01)$			$\tau(1.1)$		
E/n	Energy	Mobility	Diffusion	Energy	Mobility	Diffusion
			He			
0.0	32.34	31.99*	28.45	18.54	18.24	24.64
0.1	4.816	10.87	10.09	3.189	6.464*	5.554
0.2	7.247	6.786*	6.245	4.294	3.895*	3.262
0.3	5.363	5.003*	4.570	3.039	2.734*	2.225
			Ne			
0.0	1986	2387	1403	985.4	1356	392.3
0.01	242.2	249.9*	149.9	144.1	154.6*	38.25
0.05	63.56	65.15*	34.62	30.17	33.09*	1.099*
0.10	7.538	15.61	2.588	1.064	6.854*	1.016*
			Ar			
0.0	2505	2487	2814	1853	1832	2170
0.003	3889	3231	4116	2352	1694	2578
0.005	2085	519.4	2120	1034	298.8	1068
0.01	453.0	475.4	421.4	172.9	219.1	88.67
0.025	74.32	108.8	23.67	14.08	56.02	1.144*
0.05	54.35	70.08	43.54	14.06*	29.91	7.144
0.10	34.62	45.30	31.75	13.89	23.76	10.36
			Xe			
0.0	636.8	663.1	748.0	496.5	524.5	611.8
0.01	1371	1395	1793	959.7	984.7	1382
0.05	1159	919.7	1188	589.9	350.8	619.5
0.06	705.6	460.5	717.9	303.9	72.72	316.2
0.10	126.1	107.8	122.6	1.402	20.68	20.24
0.20	21.80*	31.60	20.01	7.044*	15.90	6.660
1.00	7.159	9.892	7.323	3.027*	5.590	3.068
			Kr			
0.0	764.7	751.9	847.4	599.5	588.3	689.2
0.001	780.3	768.4	869.6	609.3	598.6	704.9
0.005	1170	1148	1407	848.4	826.3	1086
0.01	2040	1884	2472	1398	1242	1830
0.02	2316	1972	2432	1378	1034	1494
0.03	1004	664.3	1021	443.2	120.6	460.4
0.04	397.4	127.7	395.2	108.3	38.79	109.0
0.10	44.99*	61.16	29.59	15.21*	29.42	8.726

cross sections for these moderators. For Kr and Xe, the electric field effect is very pronounced accounting for increases by more than a factor of 2. This effect appears to be associated with the speed distribution function attaining a bimodal form during the thermalization as illustrated in Fig. 7 for krypton. The higher-energy peak of the bimodal distribution function is always close to the energy where the cross section is at a minimum. This same phenomenon also occurs for Ar and Xe. Owing to the small cross section near the Ramsauer minimum, some electrons are temporarily "trapped" in this energy range and the eventual relaxation rate to the stationary distribution is prolonged. This phenomenon may also be understood in terms of a "tunneling" in the potential function in the equivalent Schrödinger equation, see Fig. 2(b). A comparison of the field dependence of the thermalization times for two cross sections for argon is shown in Table V. Although the cross sections are rather similar (see Fig. 3 of Ref. 9), there is some difference in the thermalization times obtained with these cross sections.

Figure 8 compares theoretical calculations of the transient mobility with the recent experimental results by Warman *et al.*[36] for several E/n values. The theoretical curves assume an initial delta-function distribution with

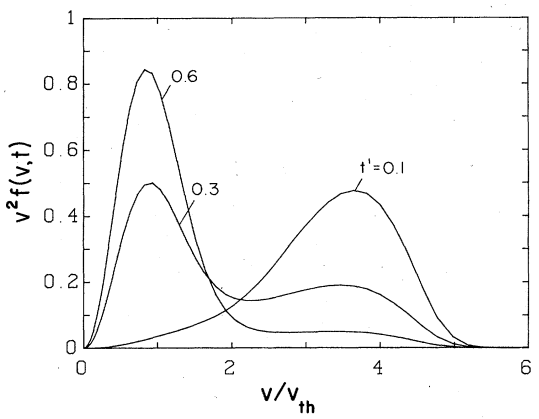

FIG. 7. Time-dependent distribution in krypton. $u_0=4.0$, $T_b=290.1$ K. Times shown are in units of $\tau=130.6\times10^{11}$ sec cm^{-3}; $E/n=0.01$ Td.

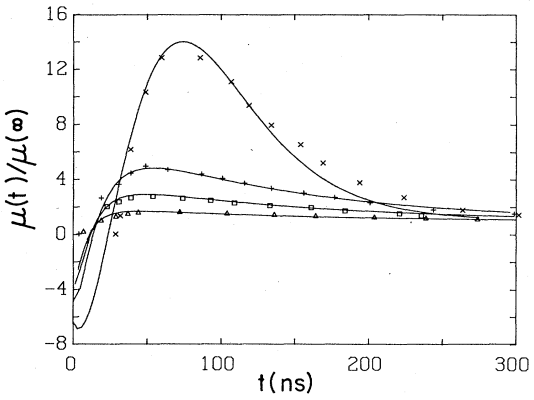

FIG. 8. Transient mobility in xenon; comparison with experiment, Ref. 34. $T_b=295$ K, $u_0=5$, and E/n in Td equal to 0.0051 ($\times$), 0.0232 ($+$), 0.0309 ($\square$), and 0.0412 ($\triangle$).

$u_0=5$ and $T_b=295$ K. The experimental transient mobilities were displayed from the start of the 20-ns x-ray pulse and have been repositioned in time in Fig. 8 so as to give the best fit to the theoretical results. The time for the experimental results were displaced by 30, 10, 13, and 5 ns for $E/n=0.0051$, 0.0232, 0.0309, and 0.0412 Td, respectively, and good agreement is obtained for all E/n. This agreement is entirely satisfactory in view of the uncertainty in the initial distribution function. For the smallest $E/n=0.0051$ Td, there are some differences in the transient mobility at the longer times shown in Fig. 8. In addition, the experimental mobilities for the longest times shown may not coincide with the stationary value $\mu(\infty)$. The fit to the theoretical results was accomplished by a slight variation of $\mu(\infty)$.

An alternate experimental arrangement for studying electron-swarm transients might be one which involves turning on an electric field in a timescale much shorter than the swarm relaxation time. If the electrons are initially in equilibrium with the moderator, the uncertainty of the form of the initial distribution function is removed. These calculations are similar to those considered by Pitchford and Green,[16] although the present work employs realistic cross sections, whereas the previous workers considered model systems. The transient mobility with krypton as moderator is shown in Fig. 9 for such a situation and the maxima shown there are attributable to the Ramsauer minimum in the cross section. For helium and neon, the transient mobility for this situation does not exhibit such features, as might have been expected. It is interesting to note that the maximum in Fig. 9 is enhanced with an increase in the electric field rather than diminished as is the case with an initial delta-function distribution. Also, the relaxation times for these field-induced effects are much shorter than the transients that ensue from nonequilibrium distributions. It was also found that whereas the cross section reported by Haddad and O'Malley[33] gives longer relaxation times than the Mozumder[12] cross section for thermalization from a nonequilibrium distribution, the reverse is the case for the field-induced transients just discussed. It is clear that either type of transient experiment can be very useful as a

TABLE V. Relaxation times versus electric field strength E/n in units of 10^{-17} V cm^2. Comparison of argon cross sections. $T_b=290.1$ K; the initial distribution is a delta function at $u_0=4.0$ in units of $v_{th}=1.148\times10^7$ cm sec^{-1}. $\tau(1.1)$ is the time, in units of 10^{11} sec cm^{-3}, required for each quantity (energy, mobility, and/or diffusion coefficient relative to the stationary value) to decay to within 1.1 of the stationary value. Asterisks denote values of $\tau(1.1)$ for relaxation to 1/1.1 of the stationary value.

	M cross section[a]			HO cross section[b]		
E/n	Energy	Mobility	Diffusion	Energy	Mobility	Diffusion
0.0	1853	1832	2170	2767	2880	3488
0.0015	2403	2173	2867	3466	2734	4109
0.0025	2570	2025	2896	2492	1337	2741
0.005	1034	298.8	1068	617.1	405.5	627.6
0.01	172.9	219.5	88.67	137.6	209.1*	55.83*
0.025	14.08	56.02	1.144*	30.27	63.70*	21.96*
0.05	14.06*	29.91	7.144	1.052*	10.71*	2.531*
0.10	13.89	23.76	10.36	12.88*	20.99	10.96

[a]Mozumder cross section, Ref. 12.
[b]Haddad and O'Malley cross section, Ref. 35.

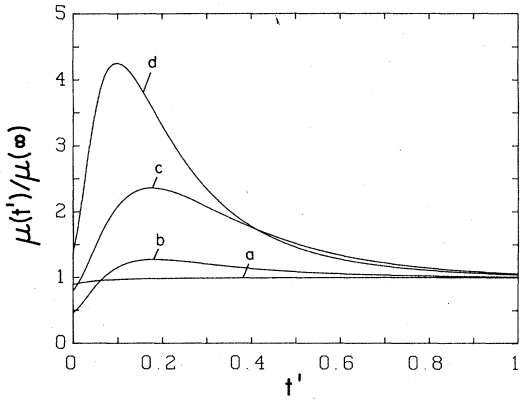

FIG. 9. Field-induced transient mobility in krypton with the electron swarm initially at equilibrium with the moderator. $T_b = 290.1$ K and E/n in Td equal to *a*, 0.01; *b*, 0.05; *c*, 0.1; *d*, 0.2.

sensitive probe of electron moderator momentum-transfer cross sections.

VI. SUMMARY

The present paper has demonstrated the efficiency and utility of the discrete-ordinate method for calculating transient electron-transport properties in the presence of an electric field. The two-term Boltzman equation is reduced to a Fokker-Planck equation with a field-dependent linear operator which is self-adjoint with a weight function $w(x)=x^2\exp(-x^2)$. This enables the calculation of transient swarm parameters in terms of the eigenvalues and eigenfunctions of the Fokker-Planck operator. The transient behavior of electrons for moderators (Ar, Kr, and Xe) with a Ramsauer minimum in the momentum-transfer cross section was contrasted with the transient behavior for moderators (He and Ne) without a minimum. The transient behavior was considered for initial nonequilibrium distributions as well as for field-induced effects in which case the initial electron swarm is in equilibrium with the moderator and the departure from equilibrium ensues by turning on the field. It was shown that the transient effects can be used as a sensitive method of distinguishing between different momentum-transfer cross sections. Also, the transient negative mobilities reported earlier for relaxation from an initial nonequilibrium distribution function were shown to be diminished with increasing electric field. A comparison with such experiments for xenon provided good agreement.

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