Space and time evolution of electron distributions in gases with large inelastic-collision cross sections

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The perturbative solution of the integral form of the kinetic equation for electrons in weakly ionized plasmas is extended to nonuniform and time-dependent situations, allowing the possibility of large energy, time, and space gradients of particle distributions. The small expansion parameter in the theory is $\delta=\min(\Delta\varepsilon/\mathscr{E},\lambda/L,1/\nu T)$, where $\Delta\varepsilon=eE\lambda$ is the electron-energy gain in the electric field E on a mean free path λ, ν is the total collision frequency, and $\mathscr{E}$, L, and T are the characteristic electron energy, distance, and time, respectively, for which the distribution function is required. Unlike the conventional two-term spherical-harmonic expansion method, the theory is not limited to a weakly anisotropic case and thus allows applications to situations where the inelastic-collision cross sections are relatively large. The problem of relaxation of the electron-energy distribution function to a new steady state, after a drop in the electric field, is considered as an example. The analytic solution of this kinetic problem is similar to that encountered in the theory of shock waves. The predictions of the theory are tested via Monte Carlo computer simulations.

I. INTRODUCTION

Distribution functions in plasmas are frequently characterized by strong time, space, and energy dependences. The self-consistent calculation of particle distributions in such cases is very difficult due to the nonlocal character of the electron transport in steep-gradient situations. For example, in laser-produced-plasma experiments very large temperature gradients may be obtained [1]. The electron velocity distribution then becomes highly anisotropic, and the conventional (Lorentz [2]) two-term spherical-harmonic expansion of the distribution function in solving the kinetic equation is inapplicable in describing the heat transfer in the plasma [3].

In the present work a different situation characterized by highly anisotropic electron distributions with steep spatial gradients and/or rapid time variations is considered, i.e., a weakly ionized gas case with large inelastic-collision cross sections in the presence of a small, space- and/or time-varying electric field. The corresponding stationary case with a uniform field was considered recently [4,5]. These studies showed that electron-energy regions in which inelastic losses are large are characterized by steep *energy* gradients in their electron-energy distributions. This, in turn, leads to a high anisotropy of the velocity distributions and thus, similarly to the above-mentioned laser-produced-plasma case, the two-term Lorentz expansion approach in solving the Boltzmann equation becomes inapplicable. For the same reason, approaches based on hydrodynamic (moments) equations in weakly ionized gases [6] cannot be used in describing the effects associated with the energy regions characterized by large inelastic electron-atom collision cross sections. The problem was resolved in Refs. [4] and [5] by using a different, integral approach to the kinetic equation. In the present work, we shall extend this approach to the case of large spatial and time gradients. We shall also allow the possibility of space and/or time-varying electric fields. The method is based on an unconventional first-order perturbation expansion in terms of a small parameter $\delta=\min(\Delta\varepsilon/\mathscr{E},\lambda/L,1/\nu T)$, where $\Delta\varepsilon=eE\lambda$ is the electron-energy gain in the electric field E on a mean free path λ; ν is the total collision frequency; and $\mathscr{E}$, L, and T are the characteristic electron energy, distance, and time, respectively, for which the distribution function is required.

There exists a similarity between the present approach to the electron kinetics and the multidimensional WKB theory used in studying waves in slowly space- and time-varying plasmas [7]. In the wave theory case, one seeks wave solutions of the form $A(\mathbf{r},t)e^{iS(\mathbf{r},t)}$ with a slowly varying amplitude A and a rapidly varying eikonal function S. Similarly, we shall represent the electron-energy distribution as $F=a(\varepsilon,\mathbf{r},t)e^{\psi(\varepsilon,\mathbf{r},t)}$, where a and ψ are slowly and rapidly varying functions of their arguments, respectively. The theory will thus involve the counterparts of the space-time components of the wave vector, i.e., $\mathbf{k}=\partial S/\partial\mathbf{r}$ and $\omega=-\partial S/\partial t$, which in the electron kinetics case will be denoted by $\boldsymbol{\beta}=\partial\psi/\partial\mathbf{r}$, $\gamma=\partial\psi/\partial t$ and the energy-space counterpart $\alpha=\partial\psi/\partial\varepsilon$. These functions are slowly varying, but may be large, thus allowing the possibility of large gradients of the distribution. For instance, in the uniform and time-independent case $\beta=\gamma=0$ and [4,5] $\alpha\simeq 1/\delta$, so that the energy gradient of the distribution function is of $O(1/\delta)$. The similarity of our approach with the WKB theory of waves goes even further when the multidimensional case (energy-space-time) is considered. We shall calculate the electron distribution problem by solving for functions a and ψ along the characteristics (the counterparts of the optical rays in

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space-time). In Sec. II we shall develop this multidimensional perturbation expansion formalism. As an application, the time-relaxation problem of the distribution function form a steady state with a uniform electric field to another steady state after an abrupt decrease in the field will be considered in Sec. III. The characteristic equation in this case is nonlinear and thus when solving for F by the method of characteristics, one may encounter the crossing of characteristics phenomenon. The problem is similar to that of a shock wave in the hydrodynamics [8]. In our case, the shock phenomenon will be seen as an abrupt change in the slope α (see above) in a small region in the energy-time space, the location of which propagates in time from lower to higher energies. These theoretical predictions will be compared with the results of Monte Carlo computer simulations in Sec. IV.

II. MULTIDIMENSIONAL NONSINGULAR PERTURBATION EXPANSION

Consider electrons in a space- and/or time-dependent, weakly ionized plasma. Define $N^-(\varepsilon,\mathbf{r},t)d\varepsilon\, d\mathbf{r}\, dt$ as the number of collisions of all types between the electrons and the gas molecules in the infinitesimal volume $d\mathbf{r}$, during the time interval dt and in the energy range $d\varepsilon$. Also, let $N^+(\varepsilon,\mathbf{r},t)d\varepsilon\, d\mathbf{r}\, dt$ represent the number of those collisions in $d\mathbf{r}$ and during dt in which the electron energy *becomes* ε *just after* a collision. The function N^- is simply related to the conventional electron-energy distribution function $F(\varepsilon,\mathbf{r},t)$:

$$N^-(\varepsilon,\mathbf{r},t)=n_e\nu(\varepsilon)F(\varepsilon,\mathbf{r},t)\ , \tag{1}$$

where n_e is the electron density, $\nu(\varepsilon)$ is the total electron collision frequency (assumed to be space and time independent), and $\int F\, d\varepsilon=1$.

We can now write the following *nonlocal* relation between N^+ and N^-:

$$N^-(\varepsilon,\mathbf{r},t)=\int N^+(\varepsilon_0,\mathbf{r}_0,t_0)\rho(\varepsilon_0,\mathbf{r}_0,t_0\rightarrow\varepsilon,\mathbf{r},t)d\mathbf{r}_0 d\varepsilon_0 dt_0\ . \tag{2}$$

where ρ is the transition probability from the electron state $(\varepsilon_0,\mathbf{r}_0,t_0)$ *just after* a collision to a new state $(\varepsilon,\mathbf{r},t)$ *just before* the next collision. On the other hand, there exists an additional *local* relation between N^+ and N^-, i.e.,

$$N^+(\varepsilon,\mathbf{r},t)=N^-(\varepsilon,\mathbf{r},t)-\frac{\nu_r(\varepsilon)}{\nu(\varepsilon)}N^-(\varepsilon,\mathbf{r},t)+\frac{\nu_r(\varepsilon+\xi)}{\nu(\varepsilon+\xi)}N^-(\varepsilon+\xi,\mathbf{r},t)\ , \tag{3}$$

where ν_r is the total inelastic-collision rate, ξ is the energy loss in inelastic collisions, and we assumed, for simplicity, that only a *single* type of inelastic collisions is present [otherwise, the last two terms in (3) become sums over different inelastic-collision processes]. Equation (3) represents the conservation of the number of particles in collisions (a possible multiplication of electrons in ionizations is neglected). Equations (2) and (3) comprise a complete set of equations for N^+ and N^-, provided the probability function ρ is known.

We proceed now to the case of weakly space-time-varying electric fields $\mathbf{E}(\mathbf{r},t)$, such that the field variation as seen by an electron between two successive collisions is small, i.e.,

$$\frac{1}{\nu}\left|\frac{d\ln E}{dt}\right|\simeq O(\delta),\quad \lambda\left|\frac{d}{d\mathbf{r}}\ln E\right|\simeq O(\delta)\ , \tag{4}$$

where $\delta\ll 1$ is the small parameter defined in Sec. I. We shall also assume, for simplicity, that $\nu=$const. The case when $\Delta\varepsilon\,|d(\ln\nu)/d\varepsilon|\sim O(\delta)$ can be dealt with similarly to Ref. [4]. Furthermore, again for simplicity, we shall limit the theory to one spatial coordinate and direction, i.e., assume that $\mathbf{E}=E(x,t)\hat{\mathbf{e}}_x$. Finally, the electromagnetic effects, associated with the time variation of E, will be neglected.

The distribution function N^- decreases rapidly with energy in energy regions characterized by large inelastic losses (see below) so that the ratio $N^-(\varepsilon+\xi)/N^-(\varepsilon)$ in these regions is small. Then the third term in the right-hand side of Eq. (3) can be neglected. The resulting equation combined with Eq. (2) then yields a single integral equation for N^+ describing the distribution function in large inelastic loss energy regions:

$$\int_0^\infty d\tau\int_{-\infty}^{\varepsilon}dz\int dr\, N^+(\varepsilon-z,x-r,t-\tau)\times\rho(\varepsilon-z,x-r,t-\tau\rightarrow\varepsilon,x,\tau)=\frac{N^+(\varepsilon,x,t)}{1-A}\ , \tag{5}$$

where $A=\nu_r/\nu$ and new variables $z=\varepsilon-\varepsilon_0$, $\tau=t-t_0$, and $r=x-x_0$ were introduced instead of ε_0, t_0, and x_0, respectively. More exact conditions for the validity of neglecting the third term in Eq. (3) can be found by using the final results of our theory. For instance, in the example considered later in Sec. III, we show that N^+ in large inelastic loss energy regions is proportional to $\exp(-v\sqrt{\varepsilon/B}\,)$ with $v=$const, $B=e^2E^2/2m\nu^2$, and E being the electric field in the problem. Thus the approximation is justified for sufficiently weak electric fields. The smallness of E does not contradict the large anisotropy of the velocity distributions in this case. Indeed, in stationary and time-independent situations we showed [4,5] that the anistropy in large inelastic loss regions is *independent of* E for small values of E. The decrease of E results only in fewer electrons penetrating these energy regions.

Observe now that the probability function ρ depends only on the electron trajectory dynamics strictly *between* two successive collisions and, therefore, does not depend on the value of the inelastic energy loss in collisions. Furthermore, since the probability of gaining the values of z, τ, and r in excess of the average values of these quantities (i.e., $\Delta\varepsilon$, $1/\nu$, and λ, respectively) is exponentially small, the transition probability density ρ in (5) is a sharply peaked function of z, τ, and r [its width is of $O(\delta)$ with respect to all the three variables]. Linear integral equations with kernels obeying this property can be

found in solving a short-wavelength electromagnetic wave propagation problem characterized by a weakly nonlocal conductivity (the generalized WKB problem) [7]. We are now using the mathematical similarity of the problems and as for the waves seek solutions of Eq. (5) in the form

$$N^{+}(\varepsilon,x,t)=a(\varepsilon,x,t)\exp[\psi(\varepsilon,x,t)] , \tag{6}$$

where if one defines

$$\alpha=\frac{\partial\psi}{\partial\varepsilon},\quad \beta=\frac{\partial\psi}{\partial x},\quad \gamma=\frac{\partial\psi}{\partial t} , \tag{7}$$

then a, α, β, and γ are assumed to be slowly varying functions of ε, x, and t in the sense that if G is one of these functions, then

$$\frac{1}{\alpha}\left|\frac{\partial \ln G}{\partial\varepsilon}\right|,\quad \frac{1}{\beta}\left|\frac{\partial \ln G}{\partial x}\right|,\quad \frac{1}{\gamma}\left|\frac{\partial \ln G}{\partial t}\right|\simeq O(\delta) . \tag{8}$$

Nevertheless, we still allow the functions $\langle |z| \rangle\alpha$, $\lambda\beta$, and γ/ν to be of $O(1)$, i.e., include the possibility of having steep gradients of the distribution function. Such singular behavior of the exponent ψ in (6) is already known in uniform and time-independent situations [see, for example, Eq. (49) in Ref. [4]). The important difference between the assumed form (6) and that used in the WKB theory [7] is in the assumption that ψ in Eq. (6) is real, while the exponent is a purely imaginary function in the WKB case. This difference, however, does not affect the above-mentioned scaling properties of various functions, so that the solution in both cases can proceed similarly.

Ordering assumptions (8) allow us to expand the integrand in Eq. (5) to $O(\delta)$, neglecting higher than first-order derivatives of the slowly varying quantities:

$$\begin{aligned}\int_0^\infty d\tau\int_{-\infty}^{\varepsilon} dz\int dr\left[a(\varepsilon,x,\tau)-z\frac{\partial a}{\partial\varepsilon}-r\frac{\partial a}{\partial x}-\tau\frac{\partial a}{\partial t}\right]\\ \times\exp\left[\psi(\varepsilon,x,t)-\alpha z-\beta r-\gamma\tau+\tfrac{1}{2}\left[z^2\frac{\partial\alpha}{\partial\varepsilon}+r^2\frac{\partial\beta}{\partial x}+\tau^2\frac{\partial\gamma}{\partial\tau}+2zr\frac{\partial\alpha}{\partial x}+2z\tau\frac{\partial\alpha}{\partial\tau}+2r\tau\frac{\partial\beta}{\partial t}\right]\right]\\ \times\rho(\varepsilon-z,x-r,t-\tau\to\varepsilon,x,t)=\frac{a(\varepsilon,x,t)\exp[\psi(\varepsilon,x,t)]}{1-A} .\end{aligned} \tag{9}$$

If one further expands the exponent in the integrand in Eq. (9) to first order in δ and defines

$$\begin{aligned}R(\alpha,\beta,\gamma)&=\int_0^\infty d\tau\int_{-\infty}^{\varepsilon} dz\int dr\, e^{-\alpha z-\beta r-\gamma\tau}\\ &\quad\times\rho(\varepsilon-z,x-r,t-\tau\to\varepsilon,x,t) ,\end{aligned} \tag{10}$$

then to $O(\delta)$ one obtains

$$\begin{aligned}&a_\varepsilon R_\alpha+a_x R_\beta+a_t R_\gamma\\ &+\frac{a}{2}(\alpha_\varepsilon R_{\alpha\alpha}+\beta_x R_{\beta\beta}+\gamma_t R_{\beta\gamma}\\ &+2\alpha_x R_{\alpha\beta}+2\alpha_t R_{\alpha\gamma}+2\beta_t R_{\beta\gamma})=a\left[\frac{1}{1-A}-R\right] ,\end{aligned} \tag{11}$$

where the notation $(\cdots)_\mu=\partial(\cdots)/\partial\mu$ is used. Note that the $O(1)$ term aR in the left-hand side of Eq. (9) was transferred to the right-hand side in Eq. (11) so that the left-hand side in Eq. (11) is of $O(\delta)$. This fact allows us to solve this equation by the perturbation method. For this, we must separate different order contributions in R first. We write

$$R=S+Q+O(\delta^2) , \tag{12}$$

where $S\simeq O(1)$ and $Q\simeq O(\delta)$. We shall evaluate functions S and Q for a uniform, but time-dependent problem in the Appendix.

The zero-order part of Eq. (11) yields

$$D(\alpha,\beta,\gamma;\varepsilon,x,t)\equiv S-\frac{1}{1-A}=0 . \tag{13}$$

This equation is the kinetic counterpart of the commonly used dispersion relation in the multidimensional WKB theory of waves in weakly varying plasmas [7]. As in the WKB theory (the geometric optics), Eq. (13) comprises a first-order nonlinear partial differential equation for ψ, which can be solved by the method of characteristics (the counterpart of the rays of the geometric optics). The characteristics are the curves in the ε-x-t space defined via

$$\begin{aligned}\frac{d\varepsilon}{ds}&=D_\alpha ,\\ \frac{dx}{ds}&=D_\beta ,\\ \frac{dt}{ds}&=D_\gamma ,\end{aligned} \tag{14}$$

where s is the parameter along the characteristics. The

rest of the unknown functions in D, i.e., α, β, γ, and ψ, can be found along the characteristics by solving equations

$$\begin{aligned}\frac{d\alpha}{ds}&=-D_\varepsilon\ ,\\ \frac{d\beta}{ds}&=-D_x\ ,\\ \frac{d\gamma}{ds}&=-D_t\ ,\\ \frac{d\psi}{ds}&=-\alpha D_\alpha-\beta D_\beta-\gamma D_\gamma\ .\end{aligned}\tag{15}$$

Note that $dD/ds\equiv 0$ along the characteristics. In order to solve Eqs. (14) and (15), one must specify the initial conditions. Those are the initial values of ψ and *two* of the derivatives $\psi_\varepsilon=\alpha$, $\psi_x=\beta$, and $\psi_t=\gamma$. The third derivative can then be found at the initial integration point from Eq. (13).

We return now to the $O(\delta)$ part of Eq. (11) and observe that it describes evolution of function a along the same characteristics (14), i.e.,

$$\frac{da}{ds}+a\,[Q+\tfrac{1}{2}(\alpha_\varepsilon S_{\alpha\alpha}+\beta_x S_{\beta\beta}+2\alpha_x S_{\alpha\beta}+2\alpha_t S_{\alpha\gamma}+2\beta_t S_{\beta\gamma})]=0\ .\tag{16}$$

In order to complete our theory and fully reduce the kinetic problem to the solution of a system (14), (15), and (16) of first-order ordinary differential equations, we still need equations for the symmetric dyadic $\partial^2\psi/\partial\mu\partial\upsilon$ $(\mu,\upsilon=\varepsilon,x,t)$ along the characteristics. The required equations are readily obtained. For example,

$$\begin{aligned}\frac{d}{ds}\left[\frac{\partial^2\psi}{\partial\varepsilon\partial x}\right]&=\frac{d}{ds}(\alpha_x)\\ &=\left[D_\alpha\frac{\partial}{\partial\varepsilon}+D_\beta\frac{\partial}{\partial x}+D_\gamma\frac{\partial}{\partial t}\right]\alpha_x\\ &=\frac{\partial}{\partial x}\left[\frac{d\alpha}{ds}\right]-\alpha_\varepsilon D_{\alpha x}-\alpha_x D_{\beta x}-\alpha_t D_{\gamma x}\\ &=-D_{\varepsilon x}-\frac{\partial^2\psi}{\partial\varepsilon^2}D_{\alpha x}-\frac{\partial^2\psi}{\partial\varepsilon\partial x}D_{\beta x}-\frac{\partial^2\psi}{\partial\varepsilon\partial t}D_{\gamma x}\ .\end{aligned}\tag{17}$$

More generally, one has

$$\frac{d}{ds}\left[\frac{\partial^2\psi}{\partial\mu\partial\upsilon}\right]=-D_{\mu\upsilon}-\frac{\partial^2\psi}{\partial\mu\partial\varepsilon}D_{\alpha\upsilon}-\frac{\partial^2\psi}{\partial\mu\partial x}D_{\beta\upsilon}-\frac{\partial^2\psi}{\partial\mu\partial t}D_{\gamma\upsilon}\ ,\tag{18}$$

which completes the system of ordinary differential equations for the kinetic problem. These equations [Eqs. (14), (15), (16), and (18)] can now be easily solved numerically, subject to whatever boundary conditions characterize a given physical situation. A case, that yields analytic solutions will be considered in Sec. III.

III. TIME RELAXATION OF THE ELECTRON-ENERGY DISTRIBUTION

Consider a situation where for $t<0$ the plasma is in a spatially uniform steady state with a constant electric field E_1. Such a stationary case in gases characterized by large inelastic-collision cross sections (a highly anisotropic situation) was investigated previously, [4,5]. At $t=0$, we abruptly (on the time scale shorter than the mean-free-path time) decrease the electric field to a new value E_2. The distribution function will then relax to a new stationary state corresponding to the value E_2 of the electric field. As in Sec. II, we shall consider the case $\nu=$const and assume that $\nu_r=$const for energies above the inelastic-collision energy threshold ξ (ν_r vanishes, of course, for $\varepsilon<\xi$). Furthermore, as in Ref. [4], we shall use the isotropic electron angular scattering model. Then we can use the probability ρ as given in Eqs. (26) and (27) in Ref. [4] (see the Appendix).

Let us apply the theory of Sec. II to the above-mentioned problem of relaxation of the electron-energy distribution function, assuming the independence of N^+ on x (i.e., $\beta=0$). It is shown in the Appendix that the function R [see Eq. (12)] in the case of interest is given by

$$R=S+Q=S+\frac{\alpha}{4\varepsilon}S_{\alpha\alpha}\ ,\tag{19}$$

where

$$S=\frac{1}{4\alpha\sqrt{\varepsilon B}}\ln\left|\frac{1+\gamma/\nu+2\sqrt{\varepsilon B}\,\alpha}{1+\gamma/\nu-2\sqrt{\varepsilon B}\,\alpha}\right|\tag{20}$$

and $B=e^2E^2/2m\nu^2$. Then to zero order in δ [see Eq. (13)]

$$D(\alpha,\gamma,\varepsilon)=\frac{1}{2\sqrt{\varepsilon B_2}\alpha}\ln\left|\frac{1+\gamma/\nu+2\sqrt{\varepsilon B_2}\alpha}{1+\gamma/\nu-2\sqrt{\varepsilon B_2}\alpha}\right|-\frac{1}{1-A}=0\ ,\tag{21}$$

which is our nonlinear, first-order partial differential equation for ψ. It is advantageous now to transform to new dimensionless variables $x'=\sqrt{\varepsilon/B_2}$ and $t'=\nu t$ in order to eliminate one of the variables in D and simplify the equations, respectively. We shall denote the partial derivatives of ψ with respect to the new variables as $\upsilon=\partial\psi/\partial x'$ and $\gamma'=\partial\psi/\partial t'$. Their relations to the derivatives of ψ with respect to the old variables are $\upsilon=2\alpha\sqrt{\varepsilon B_2}$ and $\gamma'=\gamma/\nu$. With these definitions, Eq. (21) becomes

$$D=\frac{1}{2\upsilon}\ln\left|\frac{1+\gamma'+\upsilon}{1+\gamma'-\upsilon}\right|-\frac{1}{1-A}=0\ .\tag{22}$$

Thus, the set of ordinary differential equations [Eqs. (14), (15), and (16)] describing the problem of interest can be written as

$$\begin{aligned}&\frac{dx'}{dt'}=\frac{D_\upsilon}{D_{\gamma'}},\quad \frac{d\upsilon}{dt'}=D_x=0,\quad \frac{d\gamma'}{dt'}=D_t=0\ ,\\ &\frac{d\psi}{dt'}=\upsilon\frac{D_\upsilon}{D_{\gamma'}}-\gamma'\ ,\end{aligned}\tag{23}$$

and

$$\frac{da}{dt'}=-\frac{a}{D\gamma}\left[\frac{\alpha}{4\varepsilon}S_{\alpha\alpha}+\tfrac{1}{2}(\alpha_\varepsilon S_{\alpha\alpha}+2\alpha_t S_{\alpha\gamma}+\gamma_t S_{\gamma\gamma})\right]$$
$$=-\frac{a}{D_{\gamma'}}(\tfrac{1}{2}v_{x'}S_{vv}+v_{t'}S_{v\gamma'}+\tfrac{1}{2}\gamma_{t'}S_{\gamma'\gamma'})\ . \tag{24}$$

Here we replaced the parameter s along the characteristics by normalized time t'. We see from Eqs. (23) that v and γ' are constants along the characteristics, and thus are equal to their values at the boundaries in the region of interest in the x'-t' plane. Furthermore, it follows from Eq. (23) that the characteristic curve in our case is

$$x'=\frac{D_v}{D_{\gamma'}}t'+x_0'\ . \tag{25}$$

Due to the nonlinearity of the characteristic equation (22), the slope $D_v/D_{\gamma'}$ of the characteristic curve (25) (a straight line) is still a function of v and γ' and therefore the characteristics originating at different boundary points may cross. The problem of the crossing of characteristics is well known in the theory of shock phenomena. In order to demonstrate the similarity, we shall rearrange the terms in the characteristic equation (22) and write it in the form

$$\gamma'+1-v\coth[v/(1-A)]=0\ . \tag{26}$$

Then, after differentiating Eq. (26) with respect to x' and using the relation $\gamma_{x'}=v_{t'}$, we obtain

$$v_{t'}+[\phi(v)]_{x'}=v_{t'}+\phi_v v_{x'}=0\ , \tag{27}$$

where

$$\phi(v)=-v\coth\frac{v}{1-A}\ . \tag{28}$$

An equation of form (27) occurs in the theory of shocks. It may yield shock or rarefaction solutions depending on the sign of the second derivative ϕ_{vv} and the boundary conditions [8]. In our case, where the electric field is decreased abruptly, the boundary conditions correspond to the shock-type solution, as will be shown below. Since these results are known consequences of Eq. (27), we shall complete the solution for ψ by using this equation, although one can also proceed via Eqs. (23).

Since we seek a physically meaningful solution for the *single* function

$$N^+(x',t')=a\exp(\psi)\ ,$$

the boundary conditions on a and ψ are not independent. Let us discuss these boundary conditions. The region of interest in the x'-t' plane in which the solution is required is shown in Fig. 1(a). The point x_0 in the figure denotes the threshold value $\sqrt{\xi B_2}$, for inelastic collisions. Consider first the boundary $x'=x_0$, $t'>0$. The bulk of the electron-energy distribution is confined to the region below the threshold ($\varepsilon<\xi$) and only a small fraction of electrons penetrates the region $\varepsilon>\xi$, regardless of the values (E_1, or E_2) of the electric field, provided the field in sufficiently small. Thus, we can assume that

$$N^+(\xi,t)=N^+(x_0,t')=\text{const}(t').$$

Then on the boundary $x'=x_0$, $t'>0$ [see Fig. 1(a)] a and ψ can be set constant, e.g., $a=a_1$ and $\psi=0$. Then $\gamma=\psi_t=0$ on this boundary, while $v=v_1=\text{const}$ is determined from the characteristic equation (22) with $\gamma'=0$, i.e.,

$$\frac{1}{2v_1}\ln\left|\frac{1+v_1}{1-v_1}\right|=\frac{1}{1-A}\ . \tag{29}$$

This equation yields two solutions for v_1. Both are equal in magnitude, but have opposite signs and $|v_1|<1$. Only the negative solution is physical, since for the positive solution $dx/dt'=D_v/D\gamma'$ is negative, thus yielding the characteristic direction leading away from the region of interest ($x>x_0$).

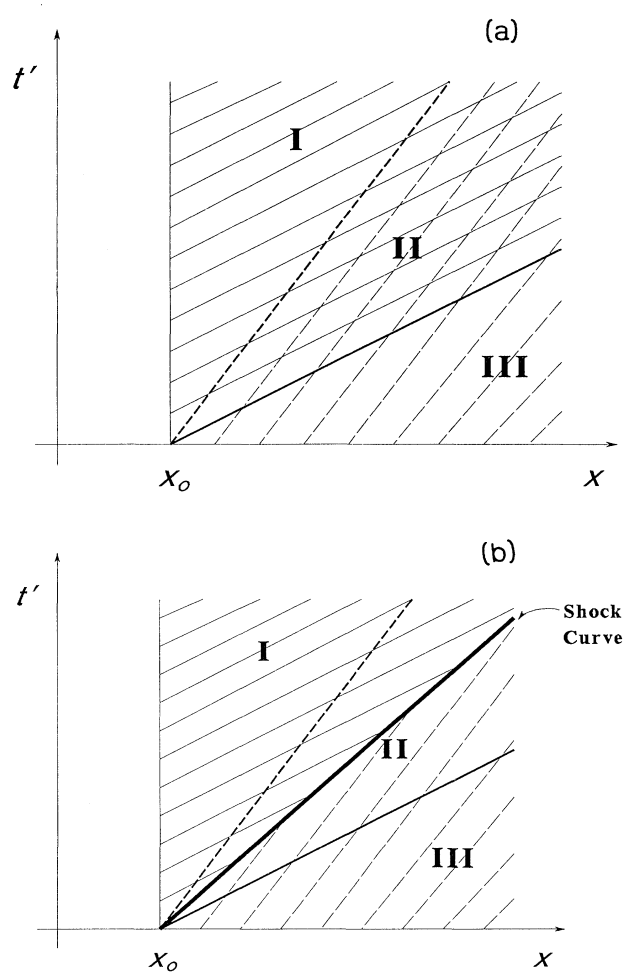

FIG. 1. The solution plane and the region of interest. (a) The characteristics for the $E_2<E_1$ case. The two types of characteristics, originating at different boundaries, cross each other in region II. (b) The shock curve in the vicinity of which the slope of the distribution changes rapidly is created in region II. The shock curve separates regions characterized by different characteristic directions.

Consider now the second boundary, i.e., the semiaxis $t'=0$, $x'\geq x_0$ [see Fig. 1(a)]. Here the distribution function corresponds to the initial steady-state distribution corresponding to the equilibrium at the higher value E_1 of the electric field. This initial distribution is characterized by function $\alpha=\psi_\varepsilon=v_1/(2\sqrt{\varepsilon B_1})$ where again v_1 is the solution of the characteristic equation (29) with $\gamma'=0$. Since at $t'=+0$ (i.e., immediately after the electric field assumes its new lower value E_2) the distribution function N^+ is still characterized by the same function ψ (and, thus, the same ψ_ε), the value of v on the semiaxis $t'=0$, $x'\geq x_0$ [and therefore also along the characteristics (25) originating on this boundary] is

$$v_r=2\psi_\varepsilon\sqrt{\varepsilon B_2}=v_1\sqrt{B_2/B_1}=v_1\frac{E_2}{E_1}\ . \tag{30}$$

The function γ' on this boundary is then determined by Eq. (26), with $v=v_r$, i.e.,

$$\gamma'_r=v_r\coth\frac{v_r}{1-A}-1<0\ . \tag{31}$$

(The value of γ'_r would be positive if instead of decreasing the electric field, one would increase its value at $t'=0$.) The set of boundary conditions is completed by recalling the results of Ref. [4], showing that for constant field E_1,

$$N^+(\varepsilon>\xi)=N^+(x'>x_0,t'=0)=a_r e^{v_1 x_1}=a_r e^{v_r x}\ , \tag{32}$$

where $x_1=\sqrt{\varepsilon/B_1}$ and a_r is a constant. Since at the crossing point of the time and the energy boundaries ($t'=0$, $x=x_0$), the distribution function is single valued, we have

$$a_r=a_1 e^{-v_r x_0} \tag{33}$$

and thus, finally,

$$\begin{aligned} N^+(x'>x_0,t'=0)&=a_1 e^{v_r(x-x_0)}\ ,\\ \psi(x'>x_0,t'=0)&=v_r(x-x_0)\ . \end{aligned} \tag{34}$$

At this point, we proceed to the solution of Eqs. (24) and (27) for a and ψ. Equation (27) yields

$$v(x',t')=v(x'-\phi_v t')\ . \tag{35}$$

This result reflects the fact that $v(x,t)$ is a constant along the characteristics (25) with the value determined by boundary conditions, i.e., v_1 for characteristics originating on the boundary $x'=x_0$, $t'>0$, or v_r if the characteristics start on the semiaxis $t'=0$, $x'>x_0$. The slope of the characteristics, $\phi_v=D_v/D_{\gamma'}$, also depends on its origin and is either $\phi_v(v_1)$, or $\phi_v(v_r)$. In our case, $|v_1|>|v_r|$ (since $E_2>E_1$) and therefore we have $\phi_v(v_1)<\phi_v(v_r)$, so that the characteristics originating on different boundaries cross each other in the t'-x' plane [region II in Fig. 1(a)]. Formally, in the crossing region one obtains an unphysical, double-valued solution for v. The shock theory [8] suggests the way for resolving this difficulty. According to this theory, the characteristics do not cross in a region but rather on a curve (the shock curve) which separates the characteristics of different types [see Fig. 1(b)]. The slope of the shock curve (the shock speed) is given by

$$\begin{aligned} \frac{dx'_{\rm sh}}{dt'}&=\frac{v_1\coth[v_1/(1-A)]-v_r\coth[v_r/(1-A)]}{v_1-v_r}\\ &\equiv\frac{[\phi(v)]}{[v]}\ . \end{aligned} \tag{36}$$

The shock curve is thus a straight line passing the point $x'=x_0$, $t'=0$, separating the boundary regions, with different values of v. We shall compare these predictions of the shock theory with the results of computer simulations in Sec. IV. Here, assuming the validity of the shock-type solution, we shall construct the solution for the distribution function above and below (to the right of) the shock curve, ignoring meanwhile the immediate vicinity of the shock. First, consider the region below the shock line. Here $v=v_r=$const and $\gamma'=\gamma_r=$const and thus, by definition,

$$v_r=\frac{\partial\psi}{\partial x'},\quad \gamma'_r=-1+v_r\coth\frac{v_r}{1-A}=\frac{\partial\psi}{\partial t'}\ . \tag{37}$$

By integrating these equations for ψ subject to the boundary condition (34), we obtain

$$\psi_r=v_r(x'-x_0)-\left[v_r\coth\frac{v_r}{1-A}-1\right]t'\ . \tag{38}$$

Similarly, above the shock line, where $v=v_1$ and $\gamma'=0$, we have

$$\psi_1=v_1(x-x_0)\ . \tag{39}$$

Finally, we solve Eq. (24) for a. This equation describes the variation of a along the characteristics. We observe that the right-hand side of Eq. (24) involves derivatives of γ and v with respect to x and t. Since the values of γ and v are constants above and below the shock line, the right-hand side of Eq. (24) vanishes and therefore a remains constant in both regions. But, in our case, $a=a_1=a_r$ on the boundaries and thus it preserves this value through all the region of interest. Therefore, below the shock line the full solution for the distribution function is

$$\begin{aligned} N_r^+(x',t')&=a_1\exp[v_r(x'-x_0)-\gamma' t']\\ &=a_1\exp[v_r(\sqrt{\varepsilon/B}-\sqrt{\xi/B})-\gamma\nu t]\ , \end{aligned} \tag{40}$$

while above the shock line

$$\begin{aligned} N_1^+(x',t')&=a_1\exp[v_1(x'-x_0)]\\ &=a_1\exp[v_1(\sqrt{\varepsilon/B}-\sqrt{\xi/B})]\ , \end{aligned} \tag{41}$$

where the values of constants v_1, v_r, and $\gamma'=\gamma'_r$ are found from Eqs. (29), (30), and (31), respectively.

It is interesting to observe that one can approach the shock phenomenon described above from a different point of view. By equating expressions (40) and (41), we find a curve in the x'-t' plane on which the distributions, given by two different formulas, are the same, i.e., the straight line

$$x' = \frac{\gamma'}{v_1 - v_r} t' + x_0 \ . \tag{42}$$

This is actually the shock line. Indeed, it passes through $x' = x_0$, $t' = 0$, and its slope is the same as given by Eq. (36). This can be seen if one substitutes $1+\gamma$ for $v_r \coth v_r / 1 - A$, and 1 for $v_1 \coth[v_1/(1-A)]$ in Eq. (36), as follows from Eq. (26). Thus, the shock line, separating the regions of two different types of characteristics according to the shock theory, physically, is the line on which the two solutions obtained from our first-order perturbation scheme are matched continuously.

Finally, we discuss the vicinity of the shock line. Here, as mentioned above, our solution for N^+ is continuous, but, nevertheless, the first-order perturbation expansion yields discontinuous derivatives (slopes) of the distribution function with respect to x' (and t'). In reality, this discontinuity does not exist in the vicinity of the shock and our result indicates the braking of the first-order expansion approach in this region. The exact solution, of course, has continuous but rapidly varying derivatives in the shock region. On the other hand, the width of this rapid variation region is not larger than of $O(\delta)$, since otherwise the first-order expansion would be valid. Mathematically, this narrowness of the shock region means that higher-order derivatives, neglected in expansion (9), become important and the first-order expansion is inapplicable. The way to approach the problem in the shock region is to consider it separately as a thin boundary layer in which the exact integral equation (5) is solved directly, rather than via an expansion of the integrand in this equation in powers of δ. One possible approach, yielding a *smooth*, but rapidly varying solution in the vicinity of the shock line, is to use the solution (40) and (41) (we shall denote this distribution by N^+_{old}) as an initial guess in the left-hand side of Eq. (5), thus yielding an improved, smooth distribution N^+_{new} in the shock region as [see Eq. (5)]

$$N^+_{\text{new}}(\varepsilon,t) = (1-A)\int_0^\infty d\tau \int_{-\infty}^{\varepsilon} dz\, N^+_{\text{old}}(\varepsilon - z, t-\tau) \times \rho(\varepsilon - z, t-\tau \to \varepsilon, t) \ . \tag{43}$$

This result can be further improved by repeating the iterative procedure.

IV. COMPUTER SIMULATION AND COMPARISON WITH THE THEORY

This section describes the computer simulation for testing the time-relaxation theory presented in Sec. III. The simulation scheme is basically a Monte Carlo-type procedure which differs from that described in Ref. [4] by the addition of the time dependence. For simplicity, we also omitted the use of the advanced splitting and Russian roulette methods [4] in the present simulations. The time dependence was included as follows. We start the simulation with a single electron, experiencing a random walk in the energy space due to collisions with a constant collision frequency ν in a uniform electric field. The time of flight between the collisions and the probability of the collision channel (elastic or inelastic scattering) are evaluated as usual by using pseudorandom numbers distributed uniformly in the interval [0,1] (see details in Ref. [4]). In order to include the time, we register not only the energy but also the time *just before* each collision. Since we are interested in starting from the steady-state distribution characterized by the initial value E_1 of the electric field, we successively used a *single* random free path by the test electron in the field E_1. After each such step, the energy of the test electron was memorized, the time was set to zero, and we continued the time-dependent simulation with this electron in a new (lower) electric field E_2. The simulation in the field E_2 is continued for as many collisions as are required to reach the final time of the simulation. In the course of this random walk, according to the energy and time *after* each collision, an integer 1 is added to a two-dimensional array, representing the time-dependent distribution function N^+ with each energy-time box having resolution of $\Delta t = 1/\nu$ and $\Delta\varepsilon = 0.1$ eV. After reaching the final time in the field E_2, we return to the initial field E_1 and make a new *single* random step of the test electron with the initial energy memorized from the previous step in the field E_1. The new energy after this step (the energy just after the collision) is memorized again, the time is set to zero, and a new sequence of time-dependent simulations is performed in field E_2. This process is repeated many times, until the necessary statistics is reached. The important parameter of the simulation is $A = \nu_r/\nu$, measuring the relative number of inelastic collisions. The inelastic-collision threshold energy $\xi = 4$ eV and the value of $A = 0.4$ (for $\varepsilon > \xi$, while $A = 0$ for $\varepsilon < \xi$) were used in the simulations. With the above-mentioned energy-time box size, this choice of pa-

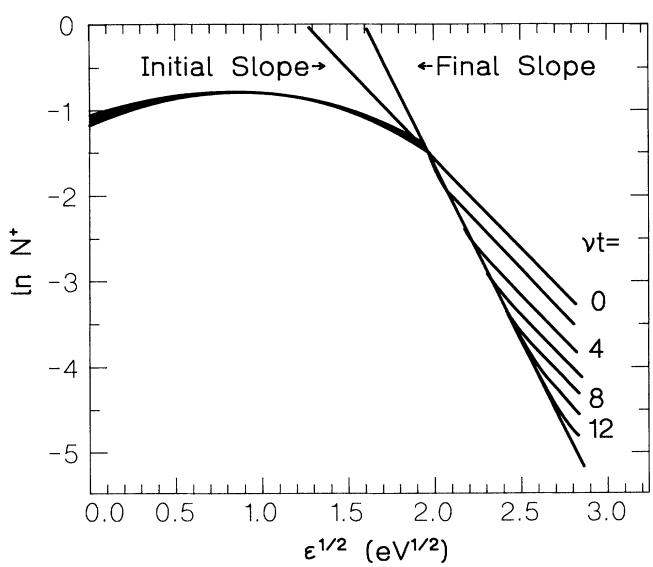

FIG. 2. The time relaxation of the distribution function to a new steady state with the time steps $2/\nu$. The parameters are $A = 0.4$, $\xi = 4$ eV, $B_1 = 0.04$ eV, and $B_2 = 0.01$ eV. The higher energies relax later than the low energies although the collision frequency is energy independent.

rameters yields a sufficient statistics in the tail if 1.5×10^7 electrons are sampled from the initial distribution.

The results of the simulations are shown in Fig. 2 for $B_1=0.04$ eV and $B_2=0.01$ eV. The statistical errors in these simulations were less than the width of the lines shown in the Figure (note that we use a semilogarithmic display of the results). The distributions in the figure correspond to different times with the time step $2/\nu$. As assumed in Sec. III, the distribution is indeed almost constant of time below the threshold ($\varepsilon<4$ eV). Furthermore, we see that at each time the distribution tail is comprised of two regions, each characterized by a different, but constant slope in the $\ln N^+-\sqrt{\varepsilon}$ plane and that each slope corresponds to either the initial or the final values $v_1=0.91$ and $v_r=0.46$, as predicted by the theory in this case. Note also that, as expected, the lower energies relax first to the new steady state and, as the time progresses, the particles at higher energies join the distribution with the final slope v_r. At each time, in Fig. 2, there exists a narrow transition region of width $\Delta\varepsilon\simeq0.1$ eV where the slope is neither v_1 nor v_r. This is the shock region. This region is seen in more detail in Fig. 3(a), where we show only the tail portion of the distributions of Fig. 2. The points of the shock front are constructed in Fig. 3(a) as crossings between the initial and the final slopes at each time. The energies at these points are then shown in Fig. 3(b) as functions of the normalized time $t'=\nu t$. This is the shock curve discussed in Sec. III. The slope of this line (the velocity of the shock) is 0.64, as predicted by the theory [see Eq. (36)] in this case.

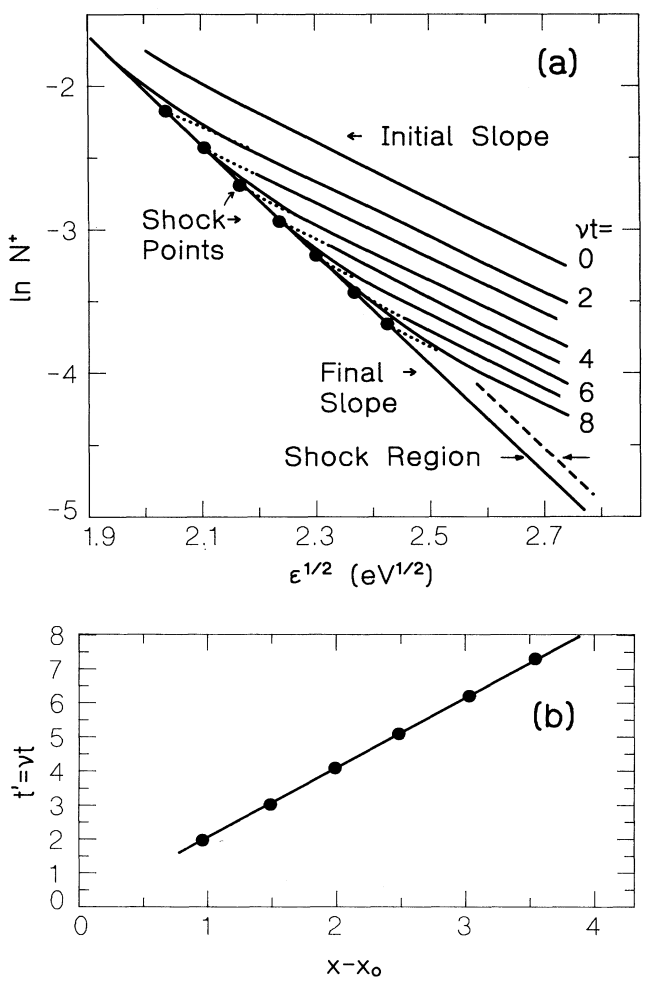

FIG. 3. The construction of the shock curve. (a) The shock points at different times are constructed as the crossings between the final slope and the continuations (the dotted line) of the part of the distribution tail characterized by the initial slope. The dotted lines represent the approximate solution, valid if the first-order approach would be applicable in the vicinity of the shock line. The width of the shock region is of $O(\delta)$. (b) The shock curve in the x'-t' plane is a straight line with the slope 0.64, as predicted by the theory.

APPENDIX: REDUCTION OF $R(\alpha,\beta,\gamma)$

By definition [see Eq. (10)]

$$R(\alpha,\beta,\gamma)=\int_0^\infty d\tau\int_{-\infty}^{\varepsilon}dz\int dr\, e^{-\alpha z-\beta r-\gamma\tau}\times\rho(\varepsilon-z,x-r,t-\tau\to\varepsilon,x,t)\ , \tag{A1}$$

where $\rho(\varepsilon_0,x_0,t_0\to\varepsilon,x,t)$ is the transition probability between the initial electron state (ε_0,x_0,t_0), i.e., its energy, coordinate, and time just after a collision and its final state (ε,x,t) just before the next collision. Denote the random time between the two successive collisions by τ. Then the electron energy and coordinate just before the second collision are

$$\begin{aligned}\tilde{\varepsilon}&=\varepsilon_0+2\sqrt{\varepsilon_0 B}\,us_0+Bu^2\ ,\\ \tilde{x}&=x_0+(2\sqrt{\varepsilon_0 B}\,us_0+Bu^2)/eE\ ,\end{aligned} \tag{A2}$$

where we limited the discussion to the constant field case, E is the electric field, $B=e^2E^2/2m\nu^2$, ν is the constant collision frequency, $s_0=\cos\Theta_0$, and Θ_0 is the initial angle (at t_0) between the electron velocity vector and the direction of the electric field. We observe now that the probability of τ being between τ and $\tau+d\tau$ is $\nu\exp(-\nu\tau)d\tau$ and denote the probability for s_0 to belong to the interval $[s_0,s_0+ds_0]$ by $\Phi(s_0)ds_0$. Then the transition probability ρ in (A1) can be expressed as

$$\rho(\varepsilon_0,x_0,t_0\to\varepsilon,x,t)=\nu e^{-\nu\tau}\int_{-1}^{+1}ds_0\Phi(s_0)\delta(x-\tilde{x})\delta(\varepsilon-\tilde{\varepsilon})\ . \tag{A3}$$

The substitution of ρ into Eq. (A1) and the use of the difference variables $z=\varepsilon-\varepsilon_0$, $r=x-x_0$ yields

$$R=\int\int\int dz\,d\tau\,dr\,e^{-\alpha z-\beta r-\gamma\tau}\times\int ds_0\nu e^{-\nu\tau}\phi(s_0)\delta(z-Z(\varepsilon-z,u,s_0))\times\delta(r-Z(\varepsilon-z,u,S_0)/eE)\ , \tag{A4}$$

where

$$Z(\varepsilon_0,u,s_0)=2\sqrt{\varepsilon_0 B}\,us_0+Bu^2 .$$

The integration with respect to r then gives

$$R=\int\int\int dz\,d\tau\exp(-\alpha z-\beta r/eE-\gamma\tau)\times\int ds_0 e^{-\nu\tau}\phi(s_0)\delta(z-Z(\varepsilon-z,u,s_0)) . \tag{A5}$$

Now we rearrange the terms in (A5) and define

$$\bar{\nu}=\gamma+\nu=\nu(1+\gamma/\nu),\quad \bar{\alpha}=\alpha+\beta/eE . \tag{A6}$$

Then (A5) becomes

$$R+\int\int dz\,d\tau\,e^{-\bar{\alpha}z}\int ds_0\nu e^{-\bar{\nu}\tau}\phi(s_0)\times\delta(z-Z(\varepsilon-z,s_0,u)) . \tag{A7}$$

At this point we assume the isotropic scattering model, i.e.,

$$\Phi(s_0)=\begin{cases}\frac{1}{2}, & |s_0|\le 1\\ 0, & |s_0|>1 ,\end{cases} \tag{A8}$$

and observe that Eq. (A7) becomes identical to that in the Appendix in Ref. [4], where one makes the substitution $\alpha\to\bar{\alpha}$ and $\nu\to\bar{\nu}$. Following the steps in that reference, we then obtain

$$R=S+\frac{\bar{\alpha}}{4\varepsilon}S_{\bar{\alpha}\bar{\alpha}} \tag{A9}$$

where

$$S=\int d\tau\,\nu e^{-\bar{\gamma}\tau}\sum_n\frac{(2\sqrt{B\varepsilon}u\bar{\alpha})^{2n}}{(2n)!}=\int d\tau\,\nu e^{-\bar{\nu}\tau}\frac{e^{\bar{\nu}u}-e^{-\bar{\nu}u}}{\sqrt{B}\,u} \tag{A10}$$

and $\bar{\nu}=2\sqrt{B\varepsilon}\bar{\alpha}$. Then, by integration,

$$S=\frac{1}{2\bar{\nu}}\ln\left|\frac{1+\bar{\nu}\nu/\bar{\gamma}}{1-\bar{\nu}\nu/\bar{\gamma}}\right|=\frac{1}{4\bar{\alpha}\sqrt{\varepsilon B}}\ln\left|\frac{1+\gamma/\nu+2\bar{\alpha}\sqrt{\varepsilon B}}{1+\gamma/\nu-2\bar{\alpha}\sqrt{\varepsilon B}}\right| . \tag{A11}$$

In the spatially uniform case ($\beta=0$), $\bar{\alpha}$ becomes α and Eq. (A11) becomes identical to Eq. (20) used in Sec. III. If, in addition, there is no time dependence, then $\gamma=0$, and we obtain the already familiar case considered in Refs. [4] and [5].

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