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Conservative Finite-Difference Schemes for the Fokker–Planck Equation Not Violating the Law of an Increasing Entropy

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Two finite-difference schemes for the Fokker–Planck equation in the case of an isotropic function of the charge particles are constructed. These schemes are first-order accurate with respect to time and second-order accurate with respect to $\varepsilon \equiv v^2$. The schemes conserve the number of particles and energy, and the entropy change is nonnegative. A relation between the incresing entropy law and the stability of the finite-difference schemes is established.

A fully conservative principle for finite-difference schemes is developed by Samarski and Popov [1]. The principle means that finite-difference equations approximating differential ones must have all conservative laws inherent in the starting differential problem. The first of the fully conservative schemes approximating isotropic Fokker–Planck equation was published in [2].

As shown in [3] the nonconservative difference schemes for calculating plasma magnetic traps were not sufficiently accurate, and the fully conservative schemes approximating the Fokker–Planck equation for both axis-symmetrical [4, 5] and full three-dimensional [6] cases were constructed. These schemes are especially good for problems in which such plasma parameters as temperature and density are determined by the tails of distribution functions. With the help of the scheme [5, 7] the parameters of a centrifugal trap were calculated [8]. However, stability and convergence of difference schemes for the Fokker–Planck equation have not been investigated because of their complexity.

In this paper we construct two fully conservative schemes for the isotropic Fokker–Planck equation not violating the law of increasing entropy and having a Maxwellian as an exact steady-state solution. We consider also the relationship between the stability of the schemes and increasing entropy. One of the schemes is a gradient method maximizing entropy under the condition that both the number of particles and the energy are constant. The time step τ which gives the increasing entropy is obtained in explicit form. The other scheme, being simpler, is suitable for constructing an implicit scheme.

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A three-dimensional Fokker–Planck equation for a closed system of charge particles[1] in Cartesian coordinates can be written in the following form [9]:

$$\frac{\partial f}{\partial t}=\sum_{\alpha,\beta}\frac{\partial}{\partial v_\alpha}\int\left(f'\frac{\partial f}{\partial v_\beta}-f\frac{\partial f'}{\partial v'_\beta}\right)G_{\alpha\beta}(\mathbf{v},\mathbf{v}')\,d\mathbf{v}',$$

where

$$G_{\alpha\beta}(\mathbf{v},\mathbf{v}')=\frac{1}{|\mathbf{v}-\mathbf{v}'|}\left(\delta_{\alpha\beta}-\frac{(v_\alpha-v'_\alpha)(v_\beta-v'_\beta)}{|\mathbf{v}-\mathbf{v}'|^2}\right),$$

$f\equiv f(\mathbf{v},t)$, $f'\equiv f(\mathbf{v}',t)$, $\delta_{\alpha\beta}$ is the Kronecker delta.

For the case of an isotropic distribution function the Fokker–Planck equation in spherical coordinates is

$$\frac{\partial f}{\partial t}=\frac{1}{v^2}\frac{\partial}{\partial v}\int_0^\infty\left(f'\frac{1}{v}\frac{\partial f}{\partial v}-f\frac{1}{v'}\frac{\partial f'}{\partial v'}\right)G(v,v')\,vv'^2\,dv', \tag{1}$$

where

$$G(v,v')=\frac{4\pi}{3}\left(\frac{v^2}{v'}+\frac{v'^2}{v}-\left|\frac{v^2}{v'}-\frac{v'^2}{v}\right|\right),$$

$$f\equiv f(v,t),\qquad f'\equiv f(v',t).$$

In papers [2–5] the variables v, t are independent. It is more convenient to use $\varepsilon=v^2$ as the independent variable; then Eq. (1) can be rewritten in the form

$$\frac{\partial f}{\partial t}=\frac{1}{\sqrt{\varepsilon}}\frac{\partial}{\partial\varepsilon}\int_0^\infty\left(f'\frac{\partial f}{\partial\varepsilon}-f\frac{\partial f'}{\partial\varepsilon'}\right)g(\varepsilon,\varepsilon')\,d\varepsilon', \tag{2}$$

where

$$g(\varepsilon,\varepsilon')=\tfrac{1}{2}(\varepsilon^{3/2}+\varepsilon'^{3/2}-|\varepsilon^{3/2}-\varepsilon'^{3/2}|),$$

$$f\equiv f(\varepsilon,t),\qquad f'\equiv f(\varepsilon',t).$$

For the sake of convenience, we define the number of particles N, energy E, and entropy S by the following formulas

$$N=\int_0^\infty f\varepsilon^{1/2}\,d\varepsilon,\qquad E=\int_0^\infty f\varepsilon^{3/2}\,d\varepsilon,\qquad S=-\int_0^\infty f\ln f\varepsilon^{1/2}\,d\varepsilon.$$

During the system evolution the values of N and E are constants, and entropy S can only increase (Boltzmann's H-theorem). A Maxwellian is an exact steady-state

[1] For simplicity, we shall consider the particles with the same charge.

solution of Eq. (2); it maximizes the entropy S at N, E given [10]. Conservation laws and the principle of increasing entropy are not connected with a concrete form of the function $g(\varepsilon, \varepsilon')$. This function is symmetric with respect to ε, ε' and non-negative ($g(\varepsilon, \varepsilon') \geqslant 0$).

A function $f(\varepsilon, t)$ is defined on a semifinite interval $[0, \infty)$. However, to make the numerical calculations, it is necessary to use a finite interval $[0, \varepsilon_0]$, and the conservation laws will be valid if we neglect the exponential small fluxes of particles and energy through the domain boundaries. Hence, we change the function $g(\varepsilon, \varepsilon')$ as follows:

$$g(\varepsilon, \varepsilon') = \tfrac{1}{2}(\varepsilon^{3/2} + \varepsilon'^{3/2} - |\varepsilon^{3/2} - \varepsilon'^{3/2}|)\, \varphi(\varepsilon)\, \varphi(\varepsilon'),$$

where $\varphi(\varepsilon) = 1 - \eta(\varepsilon - \varepsilon_0)$ is a step function ($\eta(x) = 0$ at $x \leqslant 0$, $\eta(x) = 1$ at $x > 0$). Then we can rewrite Eq. (2) for the finite interval $[0, \varepsilon_0]$,

$$\frac{\partial f}{\partial t} = (1/\sqrt{\varepsilon})\frac{\partial}{\partial \varepsilon}\int_0^{\varepsilon_0}\left(f'\frac{\partial f}{\partial \varepsilon} - f\frac{\partial f'}{\partial \varepsilon'}\right) g(\varepsilon, \varepsilon')\, d\varepsilon' \tag{3}$$

with the following boundary condition

$$\int_0^{\varepsilon_0}\left(f'\frac{\partial f}{\partial \varepsilon} - f\frac{\partial f'}{\partial \varepsilon'}\right) g(\varepsilon, \varepsilon')\, d\varepsilon'|_{\varepsilon = \varepsilon_0} = 0.$$

Equation (3) is considered as a basis for constructing our fully conservative finite-difference schemes. Let $\{\varepsilon_{i-1/2} = (i - 1/2)h,\ i = 1, 2, \ldots, I,\ Ih = \varepsilon_0;\ t^n = n\tau,\ n = 0, 1, \ldots\}$ be a mesh and $f^n_{i\pm 1/2} = f(\varepsilon_{i\pm 1/2}, t^n)$, $f^n_i = \tfrac{1}{2}(f^n_{i-1/2} + f^n_{i+1/2})$, $i = 1, \ldots, I-1$, $g_{ii'} = \tfrac{1}{2}h^{3/2}(i^{3/2} + i'^{3/2} - |i^{3/2} - i'^{3/2}|)(1 - \delta_{i,I})(1 - \delta_{i',I})$, $i, i' = 0, 1, \ldots, I$. We approximate Eq. (3) by the following finite-difference scheme

$$\begin{aligned}
&\frac{f^{n+1}_{i-1/2} - f^n_{i-1/2}}{\tau} = (\bar{\varepsilon}_{i-1/2})^{-1/2}\,\frac{P^n_i - P^n_{i-1}}{h},\\
&P^n_i = \sum_{i'=1}^{I-1}\left(f^n_{i'}\,\frac{f^n_{i+1/2} - f^n_{i-1/2}}{h} - f^n_i\,\frac{f^n_{i'+1/2} - f^n_{i'-1/2}}{h}\right) g_{ii'}h\\
&\qquad = \sum_{i'=1}^{I-1}(f^n_{i'-1/2}f^n_{i+1/2} - f^n_{i'+1/2}f^n_{i-1/2})\, g_{ii'},\\
&(\bar{\varepsilon}_{i-1/2})^{1/2} = \frac{1}{h}\int_{\varepsilon_{i-1}}^{\varepsilon_i}\varepsilon^{1/2}d\varepsilon = \frac{2}{3h}\cdot(\varepsilon_i^{3/2} - \varepsilon_{i-1}^{3/2}).
\end{aligned} \tag{4}$$

The auxiliary function P^n_i is proportional to a flux of particles and equal to zero at $i = 0$, $i = I$. The mesh function $(\bar{\varepsilon}_{i-1/2})^{1/2}$ is required such that the finite-difference equation at a fixed i and $h \to 0$ approximates Eq. (3) at $\varepsilon = 0$.

Eq. (3) can be transformed to the form

$$\frac{\partial f}{\partial t} = \frac{1}{\sqrt{\varepsilon}}\frac{\partial}{\partial \varepsilon}\int_0^{\varepsilon_0}\left(\frac{\partial}{\partial \varepsilon}\ln f - \frac{\partial}{\partial \varepsilon'}\ln f'\right) ff' g(\varepsilon, \varepsilon')\, d\varepsilon'. \tag{5}$$

We approximate Eq. (5) by the finite-difference scheme (4) with another particle flux P, that is,

$$\frac{f^{n+1}_{i-1/2} - f^n_{i-1/2}}{\tau} = (\bar{\varepsilon}_{i-1/2})^{-1/2} \frac{P^n_i - P^n_{i-1}}{h},$$
$$P^n_i = \sum_{i'=1}^{I-1} \left(\frac{\ln f^n_{i-1/2} - \ln f^n_{i'-1/2}}{h} - \frac{\ln f^n_{i'+1/2} - \ln f^n_{i'+1/2}}{h} \right) f^n_i f^n_{i'} g_{ii'} h. \tag{6}$$

Equations (4) and (6) are first-order accurate with respect to time t and second-order accurate with respect to the energy variable ε, except in the neighborhood of $\varepsilon = 0$, where it is first-order accurate with respect to ε. The number of particles N, system energy E and entropy S for our schemes are defined by the formulas

$$N = \sum_{i=1}^{I} f^n_{i-1/2} (\bar{\varepsilon}_{i-1/2})^{1/2} h, \qquad E = \sum_{i=1}^{I} f^n_{i-1/2} \varepsilon_{i-1/2} (\bar{\varepsilon}_{i-1/2})^{1/2} h,$$
$$S = -\sum_{i=1}^{I} f^n_{i-1/2} \ln f^n_{i-1/2} (\bar{\varepsilon}_{i-1/2})^{1/2} h.$$

It is easily to show that Eqs. (4) and (6) are fully conservative. We can verify it for Eq. (6) as follows:

$$\frac{\Delta N}{\tau} = \sum_{i=1}^{I} (P^n_i - P^n_{i-1}) = P_I - P_0 \equiv 0,$$
$$\frac{\Delta E}{\tau} = \sum_{i=1}^{I} (P^n_i - P^n_{i-1}) \varepsilon_{i-1/2} = -\sum_{i=1}^{I-1} P^n_i h$$
$$= \sum_{i=1}^{I-1} \sum_{i'=1}^{I-1} \left(\frac{\ln f^n_{i+1/2} - \ln f^n_{i-1/2}}{h} - \frac{\ln f^n_{i'+1/2} - \ln f^n_{i'-1/2}}{h} \right) f^n_i f^n_{i'} g_{ii'} h^2 = 0.$$

The last equality is valid due to the antisymmetrical dependence of the expression in the brackets on indices i, i'. The Maxwellian $(f_{i-1/2})_M = a \exp(-b\varepsilon_{i-1/2})$, where a, b are constants, is an exact steady-state solution of the finite-difference equations (4) and (6). The coefficients a, b are determined by the number of particles and energy

$$N = a \sum_{i=1}^{I} \exp(-b\varepsilon_{i-1/2}) (\bar{\varepsilon}_{i-1/2})^{1/2} h, \qquad E = a \sum_{i=1}^{I} \exp(-b\varepsilon_{i-1/2}) \varepsilon_{i-1/2} (\bar{\varepsilon}_{i-1/2})^{1/2} h.$$

From the physical point of view it is clear that the values ε_0 and h must be chosen such a way that inequalities $Nh \ll E \ll N\varepsilon_0$ are satisfied. In this case $a \simeq 2\pi^{-1/2} N (3N/(2E))^{3/2}$, $b \simeq 3N/(2E)$.

Equation (6) can be considered as a gradient method maximizing entropy S at the number of particles N and energy E constant. Noting that

$$(\text{grad } S^n)_i = -(\ln f^n_{i-1/2} + 1)(\bar{\varepsilon}_{i-1/2})^{1/2} h,$$

$$\ln f^n_{i+1/2} - \ln f^n_{i-1/2} = -h^{-1}[(\bar{\varepsilon}_{i+1/2})^{-1/2}(\text{grad } S^n)_{i+1} - (\bar{\varepsilon}_{i-1/2})^{-1/2}(\text{grad } S^n)_i]$$

we can write Eq. (6) as follows:

$$\mathbf{F}^{n+1} = \mathbf{F}^n + \tau L^n \text{ grad } S^n, \tag{7}$$

where $F^n_i \equiv f^n_{i-1/2}$, $i = 1,..., I$, and L^n is a matrix with the elements

$$L^n_{ii'} = (\bar{\varepsilon}_{i-1/2}\bar{\varepsilon}_{i'-1/2})^{-1/2} h^{-1}\left(\frac{Q^n_{i,i'} - Q^n_{i-1,i'}}{h} - \frac{Q^n_{i,i'-1} - Q^n_{i-1,i'-1}}{h}\right), \qquad i, i' = 1,..., I,$$

$$Q^n_{i,i'} = h^{-1}\delta_{ii'} \sum_{k=1}^{I-1} f^n_i f^n_k g_{ik} h - f^n_i f^n_{i'} g_{ii'}, \qquad i, i' = 0, 1,..., I.$$

To reduce Eq. (6) to the form (7) note that the integrodifferential equation (2) can be transformed to a "gradient" form

$$\frac{\partial f}{\partial t} = \int_0^\infty d\varepsilon' \frac{\delta S}{\delta f'} L(\varepsilon, f; \varepsilon', f'),$$

where $\delta S/\delta f' = -(\ln f' + 1)(\varepsilon')^{1/2}$ is a variational derivative of an entropy and

$$L(\varepsilon, f; \varepsilon', f') = (\varepsilon\varepsilon')^{-1/2} \frac{\partial^2}{\partial\varepsilon\, \partial\varepsilon'}\left[\delta(\varepsilon - \varepsilon') \int_0^\infty ff'' g(\varepsilon, \varepsilon'')\, d\varepsilon'' - ff' g(\varepsilon, \varepsilon')\right].$$

The matrix L^n is symmetric and nonnegative. A set of vectors ξ, for which the quadratic form $(\xi, L^n\xi)$ is equal to zero, is a two-dimensional linear subset with the basis $\mathbf{e}_1$, $\mathbf{e}_2$. The components $e_{1i} = h(\bar{\varepsilon}_{i-1/2})^{1/2}$, $e_{2i} = h\varepsilon_{i-1/2}(\bar{\varepsilon}_{i-1/2})^{1/2}$ are independent of time t^n. A projection of the vector $\mathbf{F}^n$ to the vector $\mathbf{e}_1$ determines the number of particles $N = \sum_{i=1}^I f^n_{i-1/2}(\bar{\varepsilon}_{i-1/2})^{1/2} h$, and a projection of the vector $\mathbf{F}^n$ to the vector $\mathbf{e}_2$ determines the system energy $E = \sum_{i=1}^I f^n_{i-1/2}\varepsilon_{i-1/2}(\bar{\varepsilon}_{i-1/2})^{1/2} h$.

An entropy change is nonnegative if time step τ is small enough. Indeed, $S^{n+1} = S(\mathbf{F}^{n+1}) = S^n + \tau(\text{grad } S^n, L^n \text{ grad } S^n) + O(\tau^2) \equiv S^n + \tau A + O(\tau^2)$. Using properties of the matrix L^n, it can be shown that A is strong positive for the non-Maxwellians (if $A = 0$ then grad $S^n = \alpha\mathbf{e}_1 + \beta\mathbf{e}_2$ hence $f^n \equiv f_M$). Therefore $S^{n+1} \geqslant S^n$ at small time step τ. If the inequality

$$\kappa^n \equiv \max_i |(f^n_{i+1/2} - f^n_{i-1/2})/f^n_i| \ll 1$$

holds, the time step τ guaranteeing incresing entropy for Eq. (6) can be obtained in the following explicit form (see the Appendix):

$$\tau < \tau_0 = \tfrac{1}{2} b^n h^2 / \max_i \left[(\bar{\varepsilon}_{i-1/2})^{-1/2} \sum_{i'=1}^{I} \tfrac{1}{2} (g_{i,i'} + g_{i-1,i'}) f_{i'}^n h \right]. \tag{8}$$

The value $b^n \approx 1$ at κ^n small.[2] Numerical calculations show that inequality (8) is necessary also for stability. The right side of (8), $R \geqslant h^2/(4NE)^{1/2}$, is independent of the values f_i^n, therefore the incresing entropy on every time step is nonnegative at $\tau < h^2/(4NE)^{1/2}$. To prove that condition (8) is sufficient for stability is not a simple task, we will publish a proof at a later date.

Analysis of Eq. (7) is easier when the system state is near equilibria. In this case $\mathbf{F}^n = \mathbf{F}_M + \delta\mathbf{F}^n$, $F_{Mi} = a \exp(-b\varepsilon_{i-1/2})$, and only the linear terms with respect to $\delta\mathbf{F}^n$ remain in (7):

$$\delta\mathbf{F}^{n+1} = \delta\mathbf{F}^n - \tau L_M C^2 \, \delta\mathbf{F}^n. \tag{9}$$

Here L_M is L^n matrix calculated for $\mathbf{F}^n = \mathbf{F}_M$, C is the diagonal matrix with the main diagonal elements $c_{ii} = [h(\bar{\varepsilon}_{i-1/2})^{1/2}(F_{Mi})^{-1}]^{1/2}$. The deviation from an equilibrium state at t^n with the initial deviation $\delta\mathbf{F}^0$ is defined as

$$\delta\mathbf{F}^n = C^{-1}(I - \tau\tilde{L}_M)^n C \, \delta\mathbf{F}^0,$$
$$\tilde{L}_M = C L_M C,$$

here I denotes a unit matrix. At $\tau < \tau_0 = 2/\lambda_{\max}$ ($\lambda_{\max}$ is the maximal eigenvalue of the nonnegative matrix $\tilde{L}_M$) the deviation from an equilibrium state $\delta\mathbf{F}^n$ obviously approaches zero as $n \to \infty$. This time step limitation is a stability condition for the explicit scheme (7) when the system is near equilibria. It can be shown easily that this condition coincides with the increasing entropy condition (8) for $\mathbf{F}^n = \mathbf{F}_M$. Consider the reasons that make it possible to calculate simply the maximal allowable time step, with the system approaching equilibria. When τ exceeds τ_0 instability appears mainly due to the fast oscillation part of the mesh function $\delta f_{i-1/2}^n$. Hence, only the term containing the second finite-difference derivative with respect to ε should be left in (9). Therefore, for the first approximation the time step limitation is the same as in the case of the explicit scheme approximating equation

$$\frac{\partial}{\partial t} \delta f = D(\varepsilon) \frac{\partial^2}{\partial \varepsilon^2} \delta f, \qquad D(\varepsilon) = \varepsilon^{-1/2} \int_0^{\varepsilon_0} f_M(\varepsilon') \, g(\varepsilon, \varepsilon') \, d\varepsilon'.$$

The explicit scheme is known to be stable at $\tau < \tau_0 = h^2[2 \max_\varepsilon D(\varepsilon)]^{-1}$. A small increase in τ_0 causes the local instability (in the vicinity of the point of maximum $D(\varepsilon)$) to increase exponentially:

$$\delta f_{i-1/2}^n \sim (1 - 2\tau/\tau_0)^n (-1)^i \exp[-(\varepsilon_{i-1/2} - \varepsilon^*)^2/l^2],$$
$$l = h^{1/2}[2D(\varepsilon^*)/|D''(\varepsilon^*)|]^{1/4}, \tag{10}$$

[2] More accurately, the value $b^n = (1 - 0.5\kappa^n)(1 + 4\kappa^n)^{-1}$ at $\kappa^n \leqslant 1$.

here ε^* is the point of maximum $D(\varepsilon)$. To calculate our case: $\tau_0 = 0.77h^2/(NE)^{1/2}$, $\varepsilon^* = 2.26/b$, $l = 1.1(h/b)^{1/2}$; constant b is defined by the Maxwellian, $f_M = a\exp(-b\varepsilon)$.

It is possible to write Eq. (4) in the form similar to (7); that is, $\mathbf{F}^{n+1} = \mathbf{F}^n + \tau L^n \mathbf{U}^n$, where

$$U_1^n = -\gamma(\bar{\varepsilon}_{1/2})^{1/2}h,$$

$$U_i^n = -\left[\gamma + \sum_{i'=1}^{i-1}(f_{i'+1/2}^n - f_{i'-1/2}^n)/f_{i'}^n\right](\bar{\varepsilon}_{i-1/2})^{1/2}h;$$

γ is a constant. For the non-Maxwellians $(\mathbf{U}^n, L^n\mathbf{U}^n) > 0$. As in the case of Eq. (6),

$$S^{n+1} = S^n + \tau(\text{grad } S^n, L^n\mathbf{U}^n) + O(\tau^2).$$

The inequality $(\text{grad } S^n, L^n\mathbf{U}^n) \geqslant (\mathbf{U}^n, L^n\mathbf{U}^n)$ holds always, therefore $S^{n+1} \geqslant S^n$ at small time step τ. The value of τ_0 for Eq. (4) is defined by Eq. (8). On the basis of Eq. (4) it is easily to construct an implicit scheme convenient for numerical calculations.

Numerical experiments illustrate a relationship between the law of an increasing entropy and stability of Eqs. (4) and (6). The qualitative considerations of the initiation of the scheme instability near a Maxwellian are valid in the case of any smooth distribution function. The time of scheme instability (10) development near the maximum of the diffusion coefficient

$$D(\varepsilon, t) = (1/\sqrt{\varepsilon})\int_0^{\varepsilon_0} f(\varepsilon', t)\, g(\varepsilon, \varepsilon')\, d\varepsilon'$$

is significantly smaller than the characteristic time of the coefficient change. Using the principle of "frozen" coefficients and the von Neumann spectral method [11] one can obtain the following restriction on a time step

$$\tau < \tau_\Omega = \frac{h^2}{2\max D(\varepsilon, t)}.$$

This coincides with Eq. (8) which guarantees incresing entropy.

For the calculations we make use of Eq. (6) in the interval $[0, \varepsilon_0]$, $\varepsilon_0 = 5$ with the mesh size $h = 0.025$ and the time step $0.7h^2/(NE)^{1/2} \leqslant \tau \leqslant 0.8h^2/(NE)^{1/2}$. The initial function is

$$f_0(\varepsilon) = 0.716(1+\varepsilon)/(1+\varepsilon^5). \tag{11}$$

Initially

$$\max D(\varepsilon, 0) \equiv D(\varepsilon^*, 0) = 0.71(NE)^{1/2}.$$

at $\varepsilon^* = 1.21$, and $\tau_\Omega = 0.7h^2/(NE)^{1/2}$. Calculations are made with $\tau = 0.75h^2/(NE)^{1/2}$ that is 7% more than τ_Ω. Note that the numerical instability development described

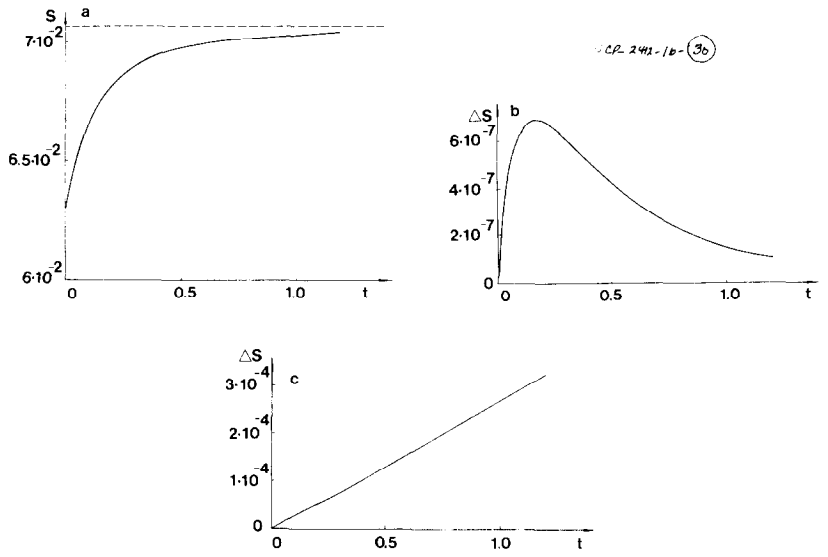

FIG. 1. (a) Time dependence of the entropy obtained by the scheme (6). (b) Entropy difference as a function of time obtained by schemes (6) and (4). (c) Entropy difference as a function of time obtained by the scheme (6) and the nonconservative scheme.

above takes place in the limit $h \to 0$. At a finite mesh size h the picture has a more complex character. When the ripples on the interval of the distribution function decrease monotonicaly, the value τ_Ω increases from $0.7h^2/(NE)^{1/2}$ to $0.72h^2/(NE)^{1/2}$, and the point of diffusion coefficient maximum changes from $\varepsilon^* = 1.21$ to 1.36. The location domain differs from the theoretical value (10) and equals $l = 0.21$. After 288 iterations, decreasing entropy begins. The ripple amplitudes equal about one third of the value of the phone distribution function. At $\tau = 0.7h^2/(NE)^{1/2}$ the calculations are stable, and the entropy grows monotonically (Fig. 1a). Similar results were obtained by Eq. (4) at $\tau \leqslant 0.7h^2/(NE)^{1/2}$: the entropy grows monotonically, but slower than in the case of Eq. (6). In Fig. 1b the time dependence of the difference $\Delta S = S_1 - S_2$ for the initial distribution function (11) given above is depicted. Here S_1 is an entropy calculated by Eq. (6) and S_2, by Eq. (4). At large time this difference goes to zero because these schemes have a Maxwellian as a steady-state solution. Using a nonconservative scheme (e.g., the scheme not conserving an energy) the behavior of entropy is qualitatively different. In Fig. 1c the time dependence of the difference $\Delta S = S_1 - S_3$ for the same initial distribution function $f_0(\varepsilon)$ is depicted. Here S_3 is the entropy calculated by the nonconservative scheme similar to [12].[3] Numerical dissipation of energy [2, 3] results in lower growth of entropy. After time $t > 1.17$, entropy decreases, and the system goes off the sought steady state. This indicates that application of nonconservative schemes is inadequate.

[3] The scheme was written in the variables ε, t; it conserves the number of particles in the finite interval $[0, \varepsilon_0]$.

APPENDIX

(1) At $\tau < \tau_0$ (Eq. (8)) it can be shown that

$$\delta^n \equiv \max_i |(f^{n+1}_{i-1/2} - f^n_{i-1/2})/f^n_{i-1/2}| \leqslant 2\kappa^n(1+2\kappa^n)^{-1}, \tag{A1}$$

where

$$\kappa^n \equiv \max_i |(f^n_{i+1/2} - f^n_{i-1/2})/f^n_i|.$$

Indeed, using Eq. (6) produces

$$|f^{n+1}_{i-1/2} - f^n_{i-1/2}|(f^n_{i-1/2})^{-1}$$
$$= \tau(f^n_{i-1/2})^{-1}(\bar{\varepsilon}_{i-1/2})^{-1/2}\frac{|P^n_i - P^n_{i-1}|}{h} \leqslant \frac{2\tau}{h^2}\max_k \left|\ln\frac{f^n_{k+1/2}}{f^n_{k-1/2}}\right|$$
$$\max_k\left[(f^n_{k-1/2})^{-1}(\bar{\varepsilon}_{k-1/2})^{-1/2}\sum_{i'=1}^{i-1}(f^n_k g_{k,i'} + f^n_{k-1} g_{k-1,i'})f^n_{i'}h\right].$$

Since

$$f^n_k \leqslant f^n_{k-1/2}(1-\tfrac{1}{2}\kappa^n)^{-1}, \qquad f^n_{k-1} \leqslant f^n_{k-1/2}(1-\tfrac{1}{2}\kappa^n)^{-1}$$

and

$$\max_k\left|\ln\frac{f^n_{k+1/2}}{f^n_{k-1/2}}\right| \leqslant \kappa^n(1+\tfrac{1}{9}(\kappa^n)^2) \quad \text{at} \quad \kappa^n \leqslant 1$$

therefore

$$\delta^n < 4\frac{\tau}{h^2}\frac{\kappa^n(1+\frac{1}{9}(\kappa^n)^2)}{1-\frac{1}{2}\kappa^n}\max_k\left[(\bar{\varepsilon}_{k-1/2})^{1/2}\sum_{i'=1}^{i-1}\tfrac{1}{2}(g_{k,i'} + g_{k-1,i'})f^n_{i'}h\right]$$
$$< \frac{2\kappa^n(1+\frac{1}{9}(\kappa^n)^2)}{1+4\kappa^n} < \frac{2\kappa^n}{1+2\kappa^n}.$$

(2) At $\delta^n < 1$ it can be shown that

$$S^{n+1} - S^n \geqslant \tau(\operatorname{grad} S^n, L^n \operatorname{grad} S^n)(1 - 0.5(1+\delta^n)\tau\lambda^n_{\max}). \tag{A2}$$

Here $\lambda^n_{\max}$ is a maximal eigenvalue of the matrix $\tilde{L}^n = C^n L^n C^n$, where C^n is a diagonal matrix with the elements $C^n_{ii} = [h(\bar{\varepsilon}_{i-1/2})^{1/2}(f^n_{i-1/2})^{-1}]^{1/2}$. For the auxiliary function $\varphi(x) = [(1+x)\ln(1+x) - x]\cdot x^{-2}$ used below inequality $0 \leqslant \varphi(x) \leqslant \frac{1}{2}(1+\delta)$ holds at $x \geqslant -\delta$, $\delta < 1$. Let $x^n_{i-1/2} = (f^n_{i-1/2} - f^n_{i-1/2})/f^n_{i-1/2}$, then

$$S^{n+1}-S^n=-\sum_{i=1}^{I}(f_{i-1/2}^{n+1}\ln f_{i-1/2}^{n+1}-f_{i-1/2}^{n}\ln f_{i-1/2}^{n})(\bar{\varepsilon}_{i-1/2})^{1/2}h$$

$$=-\sum_{i=1}^{I}(f_{i-1/2}^{n+1}-f_{i-1/2}^{n})(\ln f_{i-1/2}^{n}+1)(\bar{\varepsilon}_{i-1/2})^{1/2}h-\sum_{i=1}^{I}f_{i-1/2}^{n}\varphi(x_{i-1/2}^{n})$$

$$\times(x_{i-1/2}^{n})^2(\bar{\varepsilon}_{i-1/2})^{1/2}h\geqslant-\sum_{i=1}^{I}(f_{i-1/2}^{n+1}-f_{i-1/2}^{n})(\ln f_{i-1/2}^{n}+1)(\bar{\varepsilon}_{i-1/2})^{1/2}h$$

$$-\tfrac{1}{2}(1+\delta^n)\sum_{i=1}^{I}(f_{i-1/2}^{n+1}-f_{i-1/2}^{n})^2(\bar{\varepsilon}_{i-1/2})^{1/2}h(f_{i-1/2}^{n})^{-1}.$$

Using (7) and expressions for grad S^n and C^n the estimate can be rewritten

$$S^{n+1}-S^n\geqslant\tau(\operatorname{grad}S^n,L^n\operatorname{grad}S^n)-\frac{\tau^2}{2}(1+\delta^n)|C^nL^n\operatorname{grad}S^n|^2.$$

Thus (A2) holds.

(3) At time $\tau<\min[\tau_0,2(1+\delta^n)^{-1}(\lambda_{\max}^n)^{-1}]$ the system entropy is not decreasing, that is $S^{n+1}\geqslant S^n$. This statement is a consequence of the formula (A2) because at such a time step τ the value of $\delta^n<1$.

(4) For the maximal eigenvalue of matrix $\tilde{L}^n$, the following estimate is obtained:

$$\lambda_{\max}^n\leqslant\frac{4}{h^2}\frac{1+2\kappa^n}{1-0.5\kappa^n}\max_k\left[(\bar{\varepsilon}_{k-1/2})^{-1/2}\sum_{i'=1}^{I}\tfrac{1}{2}(g_{k,i'}+g_{k-1,i'})f_{i'}^{n}h\right]. \tag{A3}$$

The maximal eigenvalue $\lambda_{\max}^n$ of matrix $\tilde{L}^n$ equals the maximal eigenvalue of matrix $(C^n)^2L^n$. Let $\mathbf{x}$ be the eigenvector of matrix $(C^n)^2L^n$ corresponding to the maximal eigenvalue $\lambda_{\max}^n$. Then $\lambda_{\max}^n\mathbf{x}=(C^n)^2L^n\mathbf{x}$. Using a determination of the matrix L^n for components of the vector $\mathbf{y}$ defined by the equalities $y_i=x_i(\bar{\varepsilon}_{i-1/2})^{-1/2}$ one can obtain

$$\lambda_{\max}^n y_i=-(f_{i-1/2}^{n})^{-1}(\bar{\varepsilon}_{i-1/n})^{-1/2}\frac{P_i(\mathbf{y})-P_{i-1}(\mathbf{y})}{h},$$

$$P_i(\mathbf{y})=\sum_{i'=1}^{I-1}\frac{y_{i+1}-y_i}{h}f_i^nf_{i'}^ng_{ii'}h-\sum_{i'=1}^{I-1}\frac{y_{i'+1}-y_{i'}}{h}f_i^nf_{i'}^ng_{ii'}h.$$

Let us denote the first sum in $P_i(\mathbf{y})$ as $P_{1i}(\mathbf{y})$ and the second as $P_{2i}(\mathbf{y})$. It is easy to make the estimate

$$|P_{1i}-P_{1i-1}|\leqslant\frac{4}{h}\max_k|y_k|\cdot\left[\sum_{i'=1}^{I-1}\frac{1}{2}(g_{i,i'}+g_{i-1,i'})f_{i'}^{n}h\right]\frac{f_{i-1/2}^{n}}{1-0.5\kappa^n}.$$

The estimate for $|P_{2i}(\mathbf{y}) - P_{2i-1}(\mathbf{y})|$ one can derive in this way

$$
\begin{aligned}
|P_{2i} - P_{2i-1}| = \Bigg| & -(\varepsilon_i^{3/2} - \varepsilon_{i-1}^{3/2}) f_i^n \sum_{i'=i}^{I-1} (y_{i'+1} - y_{i'}) f_{i'}^n \\
& - (f_i^n - f_{i-1}^n) \sum_{i'=1}^{I-1} (y_{i'+1} - y_{i'}) f_{i'}^n g_{ii'} \Bigg| . \\
= \Bigg| & (\varepsilon_i^{3/2} - \varepsilon_{i-1}^{3/2}) f_i^n (f_i^n y_i - f_{I-1}^n y_I) \\
& + (\varepsilon_i^{3/2} - \varepsilon_{i-1}^{3/2}) f_i^n \sum_{i'=i+1}^{I-1} y_{i'} (f_{i'}^n - f_{i'-1}^n) \\
& - (f_i^n - f_{i-1}^n) \sum_{i'=1}^{I-1} (y_{i'+1} - y_{i'}) f_{i'}^n g_{i-1,i'} \Bigg| \\
\leqslant \max_k |y_k| \cdot \Bigg[& (\varepsilon_i^{3/2} - \varepsilon_{i-1}^{3/2}) f_i^n (f_i^n + f_{I-1}^n) \\
& + (\varepsilon_i^{3/2} - \varepsilon_{i-1}^{3/2}) f_i^n \sum_{i'=i+1}^{I-1} |f_{i'}^n - f_{i'-1}^n| \\
& + 2|f_i^n - f_{i-1}^n| \sum_{i'=1}^{I-1} f_{i'}^n g_{i-1,i'} \Bigg] .
\end{aligned}
$$

At $I > 2/\kappa^n$ (in reality the number of mesh points $I \gg 2/\kappa^n$) the inequality

$$
f_i^n + f_{I-1}^n < 3\kappa^n \sum_{i'=1}^{I-1} f_{i'}^n
$$

holds. Noting also that

$$
\begin{aligned}
& |f_{i'}^n - f_{i'-1}^n| \leqslant 0.5\kappa^n (f_{i'}^n + f_{i'-1}^n), \\
& |f_i^n - f_{i-1}^n| \leqslant \kappa^n (1 - 0.5\kappa^n)^{-1} f_{i-1/2}^n ,
\end{aligned}
$$

one can obtain the final estimate for $|P_{2i} - P_{2i-1}|$,

$$
\begin{aligned}
|P_{2i} - P_{2i-1}| \leqslant & \max_k |y_k| \cdot (1 - 0.5\kappa^n)^{-1} f_{i-1/2}^n \Bigg[(\varepsilon_i^{3/2} - \varepsilon_{i-1}^{3/2}) \cdot 3\kappa^n \sum_{i'=1}^{I-1} f_{i'}^n \\
& + (\varepsilon_i^{3/2} - \varepsilon_i^{3/2}) \kappa^n \sum_{i'=1}^{I-1} f_{i'}^n + 2\kappa^n \sum_{i'=1}^{I-1} f_{i'}^n g_{i-1,i'} \Bigg] \\
\leqslant & \frac{8}{h} \max_k |y_k| \cdot \sum_{i'=1}^{I-1} \frac{1}{2} (g_{i,i'} + g_{i-1,i'}) f_{i'}^n h\kappa^n \cdot \frac{f_{i-1/2}^n}{1 - 0.5\kappa^n} .
\end{aligned}
$$

Therefore, for all i,

$$\lambda^n_{\max}|y_i| \leqslant (f^n_{i-1/2})^{-1}(\bar{\varepsilon}_{i-1/2})^{-1/2}h^{-1}(|P_{1i}-P_{1i-1}|+|P_{2i}-P_{2i-1}|)$$
$$\leqslant \frac{4}{h^2}\frac{1+2\kappa^n}{1-0.5\kappa^n}\max_k|y_k|\left[(\bar{\varepsilon}_{i-1/2})^{-1/2}\sum_{i'=1}^{i-1}\frac{1}{2}(g_{i,i'}+g_{i-1,i'})f^n_{i'}h\right]$$

and the estimate (A3) holds.

(5) Using formulas (A3) and (A1) it is easy to show that $\tau_0 \leqslant 2(1+\delta^n)^{-1}(\lambda^n_{\max})^{-1}$. From this relation one obtains the following statement:

At $\tau < \tau_0$, where τ_0 is defined by formula (8), a system entropy does not decrease $S^{n+1} \geqslant S^n$ (the equality is possible if only $f^n \equiv f_M$).

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