Statistical Approach to the Solution of Fokker-Plank Kinetic Equation

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1. INTRODUCTION

The behaviour of fast minority ions in tokamak (alpha-particles, NB ions, ICRH minority etc.) in the vast majority of applications can be described by linear drift kinetic equation with Fokker-Plank (FP) collisional operator. It is a second order linear partial differential equation. The difficulties in solving it arise from the large number of phase variables. This is typical for the modelling of real experimental conditions. In some important applications the number of variables can be reduced by averaging the FP equation over the particle bounce period [1]. The reduced "banana averaged" FP equation for fast particles in axisymmetrical tokamak has four essential variables (particle energy, magnetic moment, "minor radius" and time). In the presence of small perturbations of the magnetic field (TF ripple, MHD) it is still possible to reduce full equation to a 3D one but with additional diffusive terms [2].

The JET experiment with reduced number of TF coils [3] highlighted the need for the development of effective numerical codes for the treatment of fast particle ripple loss. A significant number of discharges must be analysed, time dependent, and for different classes of fast particles. The present paper is devoted to the development of Monte-Carlo technique for the solution of FP equation.

2. LANGEVIN EQUATIONS FOR SINGLE PARTICLE RANDOM MOTION

It is well known [4] that differential equations can be solved by statistical or Monte-Carlo methods, which are particularly useful for multi dimensional problems. In these methods the solution of the equation is obtained by calculations of large number of test particle random orbits.

We shall follow the procedure used in [3] and derive the equations for single particle random motion corresponding to a generalised FP equation

$$\frac{\partial f_0}{\partial t} + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x_i} \sqrt{g} \ J^i = S, \tag{1}$$

where particle fluxes have the form:

$$J^i = U^i f - D^{ik} \ \partial f / \partial x_k, \tag{2}$$

where U^i is convective velocity, D^{ik} - matrix of diffusion coefficients. In the last equations and below the usual convention on summation over the repeating indexes is assumed. Using Eq. (1) we can express the mean value of a variable x_i,

$$\langle x_i \rangle = \int x_i f \sqrt{g} d^n x,$$

in terms of U^i and D^{ik} as follows:

$$\frac{d}{dt} \langle x_i \rangle = \int x_i \frac{df}{dt} \sqrt{g} d^n x = \int J^i \sqrt{g} d^n x$$

For J^i given by Eq. (2) last expression takes form

$$V_i = \frac{d}{dt} \langle x_i \rangle = U^i + \int \left\{ \frac{\partial}{\partial x_k} D^{ik} \sqrt{g} \right\} f d^n x. \tag{3}$$

The test particle thus has an average velocity, V_i, which is the sum of convective velocity, U^i, and the corrections due to an inhomogeneity of the diffusion rates.

The same procedure can be used for evaluation of the second central moments,

$$\sigma_{ij} = \left\langle \left(x_i - <x_i> \right) \left(x_j - <x_j> \right) \right\rangle.$$

After some algebra one obtains:

$$\frac{d}{dt} \sigma_{ij} = \int \left\{ D^{ij} + D^{ji} \right\} f \sqrt{g} d^n x. \tag{4}$$

If the test particles have the same initial conditions at $t = 0$, or $f = \delta(x - x_0)$, then after small time step Δt they will have Gaussian distribution function

$$f(\Delta t) = \frac{\left(\det C_{ij} \right)^{\frac{1}{2}}}{\pi^{n/2}} \exp\left\{ -\Sigma C_{ij}(x_i - \Delta x_i)(x_j - \Delta x_j) \right\}, \tag{5}$$

where $C_{ij}^{-1} = 2\sigma_{ij}$. The matrix σ_{ij} and the shift of the Gaussian function, Δx_i, can be found from Eq. (3) and Eq. (4) as follows:

$$\Delta x_i = V_i \Delta t + O\left(\Delta t^2\right) = \left(U^i + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x_k} D^{ik} \sqrt{g}\right)_{x=x_o} \Delta t + O\left(\Delta t^2\right), \qquad (6)$$

$$\sigma_{ij} = \Delta t \left\{D^{ij} + D^{ji}\right\}_{x=x_o} + O\left(\Delta t^2\right). \qquad (7)$$

The new distribution function can be generated by Monte-Carlo methods, calculating sufficiently large number of random orbits of test particles starting with the same initial conditions. The simplest way to generate (5) in 1D case is to use the finite difference equation [4]:

$$x^{m+1} = x^m + V\Delta t \pm \{2D\Delta t\}^{\frac{1}{2}}, \qquad (8)$$

with random sign $\pm$ at the last term. Here $x^m = x(t)$ and $x^{m+1} = x(t + \Delta t)$.

Another approach to generate (5) is to use a random numbers ξ_n with Gaussian distribution

$$x^{(m+1)} = x^{(m)} + V\Delta t + \{2D\Delta t\}^{\frac{1}{2}} \xi^{(m)}, \qquad (9)$$

where $\left\langle \xi^{(1)} \xi^{(m)} \right\rangle = 0$ for $m \neq 1$ and

$$f(\xi) = \frac{1}{(2\pi)^{\frac{1}{2}}} \exp\left\{-\xi^2 / 2\right\}. \qquad (10)$$

The advantage of the last method is that it generates a Gaussian distribution in one time step which allows the use of much larger time step $\Delta t < L^2 / 2D$, where $L = \left(\frac{1 \partial D}{D \partial x}\right)^{-1}$ is spatial scale length, in compare with the first method, Eq. (8).

The one dimensional Eq. (9) can be easily generalised for multi dimensional case (nD):

$$x_i^{m+1} = x_i^m + V_i \Delta t + A_{ik} \xi_k^m; \quad (i,k = 1,...n), \qquad (11)$$

where ξ - random vector with noncorrelated components, $\langle \xi_k \xi_l \rangle = \delta_{kl}$ and $f(\xi_k)$ defined by Eq. (10). Matrix A_{ik} can be found from algebraic equation

$$A_{ik} A_{jk} = \sigma_{ij} \qquad (12)$$

which follows from comparison second central moments Eq. (9) and Eq. (11).

For solving Eq. (12) we have to remind the following features of the matrix σ_{ij}. One can always find local basis in which σ_{ij} is a diagonal matrix with diagonal elements equal to diffusion rates along the new main axis multiplied by time. Therefore, the determinant of the matrix σ_{ij} could not be negative. If $\det \sigma_{ij} = 0$ it means that diffusion rates along some directions are zero and the particle cloud can spread in time only along a phase volume which has smaller dimension than the dimension of the phase volume n (1D in 2D problem, or 1D or 2D in 3D case). The number of non zero diagonal elements is equal to the matrix rank $m \leq n$.

To find an appropriate solution for A_{jk} we introduce the following notations:

$$d_1 = \sigma_{11}; \quad d_2 = \begin{vmatrix} \sigma_{11} \sigma_{12} \\ \sigma_{12} \sigma_{22} \end{vmatrix}; \quad d_3 = \begin{vmatrix} \sigma_{11} \sigma_{12} \sigma_{13} \\ \sigma_{21} \sigma_{22} \sigma_{23} \\ \sigma_{31} \sigma_{32} \sigma_{33} \end{vmatrix}; \quad \cdots$$

We shall assume that the first m terms of this row not equal to zero $(d_i \geq 0)$. If it is not true it is possible to rename variables. Because the matrix σ_{ij} is symmetric one we have freedom in choosing elements A_{ij} and therefore we can assume A_{ij} to be a triangular matrix, i.e. $A_{ij} = 0$ for $j > i$. This makes it possible to write the following recurrent formulas for matrix elements A_{ij}:

$$A_{11} = (d_1)^{\frac{1}{2}},$$
$$A_{11} = \sigma_{1i} / A_{11}; \quad i = 2, n,$$

$$\left. \begin{aligned} A_{ik} &= 0. \quad ; \quad i = 1, \ k - 1 \\ A_{kk} &= (d_k / d_{k-1})^{\frac{1}{2}}, \\ A_{ik} &= \sigma_{ki} / A_{kk} \quad ; \quad i = k + 1, n \end{aligned} \right\} \quad 1 < k \leq m \qquad (13)$$

$$A_{ik} = 0. \quad k > m.$$

Therefore Eq. (6), (7), (11), (13) are equivalent to the FP equation given by Eq. (1).

3. THE RESULTS OF NUMERICAL TESTS

The statistical approach described above has been tested by simple numerical tests. The tests were aimed to compare numerical schemes given by Eq. (8) and Eq. (9) and find limitations on the time step Δt.

3.1. TESTS WITH 1D EQUATION

The first test was made on the basis of 1D FP equation:

$$\frac{\partial f}{\partial t} = \frac{1}{\sqrt{g}}\frac{\partial}{\partial x}\sqrt{g}\ D(x)\frac{\partial f}{\partial x}.$$

(14)

with boundary conditions $\partial f/\partial x = 0$ at $x = 0$ and $x = 1$ (conservation of number of particles). Eq. (14) was solved numerically by calculating random orbits of 1000 particles. Two methods of generating random orbits Eq. (8), Eq. (9) has been compared using a constant time step dt for the all particles. The distribution function $f(t,x)$ has been calculated at a given time t by counting number of particles in 20 spatial sells distributed uniformly over $x \subset [0,1]$.

The first test was a comparison of numerical solution of Eq. (14) $\left(D = 0.25,\ \sqrt{g} = 1\right)$ with analytical solution:

$$f(t,x) = \frac{1}{(4\pi Dt)^{1/2}}\sum_k\left\{\exp\left(-(x-x_0+2k)^2\ /\ 4Dt\right) + \exp\left(-(x+x_0+2k)^2\ /\ 4Dt\right)\right\}.$$

(15)

Fig. 1 and Fig. 2 show the evolution of the distribution function calculated by Gaussian (Eq. (9)) and constant step (Eq. 8) schemes with a small time step dt = 0.001 (spatial step <dx> $\cong$ 0.02). Both methods show good agreement with the analytical solution. As was expected the Gaussian approach is not sensitive to the time step, which is illustrated by Fig. 3. On the contrary the constant step method fails when the random spatial step becomes larger than box size, as in Fig. 4.

The sensitivity of MC solution to the time step has been checked for a nonuniform diffusion rate $D = x(1-x)$ $\left(\sqrt{g} = 1\right)$. It was found that the numerical

solution is not sensitive to the time step up to 0.064 (illustrated in Fig. 5) which corresponds to the spatial step of 0.18. At larger time step a visible systematic error appears in the MC solution which is connected with nonuniformity of the diffusion rate. For chosen size of the boxes the constant-step scheme failed at dt = 0.005. Both methods provide MC solutions close to each other at small time step dt = 0.001.

The next two tests were devoted to the MC solution of Eq. (1) with a non constant Jacobian. The steady state solution of Eq. (1) is f = 1 for any arbitrary function $\sqrt{g}(x)$. On the other hand number of particles in each box which is actually calculated in MC solution, dN = $f\sqrt{g}dx$, is not constant at $t-\infty$ but is expected to form the particular distribution dN ~ $\sqrt{g}(x)$.

The establishment of a steady state solution was checked for two Jacobians. Fig.6 shows evolution of distribution function calculated for $\sqrt{g} = 0.1 + 1.8x$. At large time t ≥ 1 the distribution function reaches the correct steady state solution f = 1.

The second example was calculation of the evolution for the Jacobian and diffusion rate shown at Fig. 7c. Fig. 7a shows the evolution of initially peaked distribution function with time. At t = 1 f(t,x) reaches the steady state solution f = 1, Fig. 7b. At the same time number of particle in the boxes has a spatial distribution with a peak which corresponds to the peak in $\sqrt{g}$, Fig. 7c.

Therefore the 1D tests show that the Gaussian randomisation scheme seems to be preferable because it allows larger time/spatial step (natural limit of $\Delta x < \left(\dfrac{1 \partial D}{D \partial x}\right)^{-1}$) in compare with constant step randomisation.

3.2 TEST WITH 2D EQUATION

The aim of 2D tests was to check the scheme given by Eq. (11)-(13) and find limitations on the time step in Eq. (11). We used 2D FP equation with a constant diffusion rate in vertical direction as a simplest model of ripple diffusion and pitch angle scattering:

$$\frac{\partial f}{\partial t} = \frac{1}{a}\frac{\partial}{\partial a} a \ D \ \sin^2(\vartheta)\frac{\partial f}{\partial a} + \frac{1}{a}\frac{\partial}{\partial a} a \ D\frac{\sin\vartheta\cos\vartheta}{a}\frac{\partial f}{\partial \vartheta} +$$

$$\frac{1}{a}\frac{\partial}{\partial \vartheta} a \ D\frac{\sin\vartheta\cos\vartheta}{a}\frac{\partial f}{\partial a} + \frac{1}{a}\frac{\partial}{\partial \vartheta} a \left(D\frac{\cos^2(\vartheta)}{a^2} + D_o \right)\frac{\partial f}{\partial \vartheta}.$$

(15)

Here, a and ϑ are co-ordinates in the polar co-ordinate system: $R = a\cos\vartheta$, $z = a\sin\vartheta$. The diffusion rate D_0 describes particle scattering over the surface a = const, i.e. represent pitch angle scattering, and other terms in the right hand side of Eq. (15) represent a ripple diffusion operator, $\partial/\partial z(D\partial f/\partial z)$, written in the polar co-ordinates. Therefore, at D = 0 one may expect spreading of an initial cloud of test particles over ϑ at a fixed initial a, and at D_0 = 0 spreading over 1D curve, $R = a\cos\vartheta = const$. Because in the new variables the diffusion tensor is not a constant the test particle has a mean velocity defined by Eq. (3),

$$V_a = \frac{D\cos^2\vartheta}{a} \ ; \quad V_\vartheta = -\frac{2D\cos\vartheta\sin\vartheta}{a^2};$$

(16)

Fig. 8 shows that in the two limiting cases D = 0 and D_0 = 0 the particle cloud stays on the 1D lines a = const and R = const. The transversal spreading of the cloud in the latter case is connected with combined effect of the finite time step and "wrong" boundary condition - mirror reflection from the boundaries.

Fig. 9 show the effect of the finite time step in the case D_0 = 0. It can be seen that in order to reach a reasonably accuracy one needs to use a small time step Ddt < 0.001 ($\cong 10^3$ time steps for relaxation of distribution function). It should be mentioned that the contribution which arises from average velocity produces the necessary compensation of a "centrifugal" particle drift from the curve. Because D_0 = const relaxation over ϑ is not sensitive to the time step.

Finally Fig. 10 shows 2D spreading of the initial test particle cloud in the case D = D_0 = 0.25.

Therefore in the multi dimensional case with anisotropic diffusion tensor the maximum time step can be increased significantly if one choose the co-ordinate system with one of the axes directed along the principal axis of the diffusion tensor with the maximum rate. In the example presented above it means that if

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$D \gg D_0$ then it is better to use Cartesian co-ordinates R,z, but in the opposite case, $D \ll D_0$, polar co-ordinates are preferable.

SUMMARY

The numerical tests show that the Monte-Carlo scheme described by Eq. (11) and Eq. (13) reproduces solutions of the FP equation. The Gaussian scheme, Eq. (9), seems to be preferable because it allows larger time step then the constant step scheme, given by Eq. (8). In the multi dimensional case the "right" choice of the co-ordinate system can help to increase the time step.

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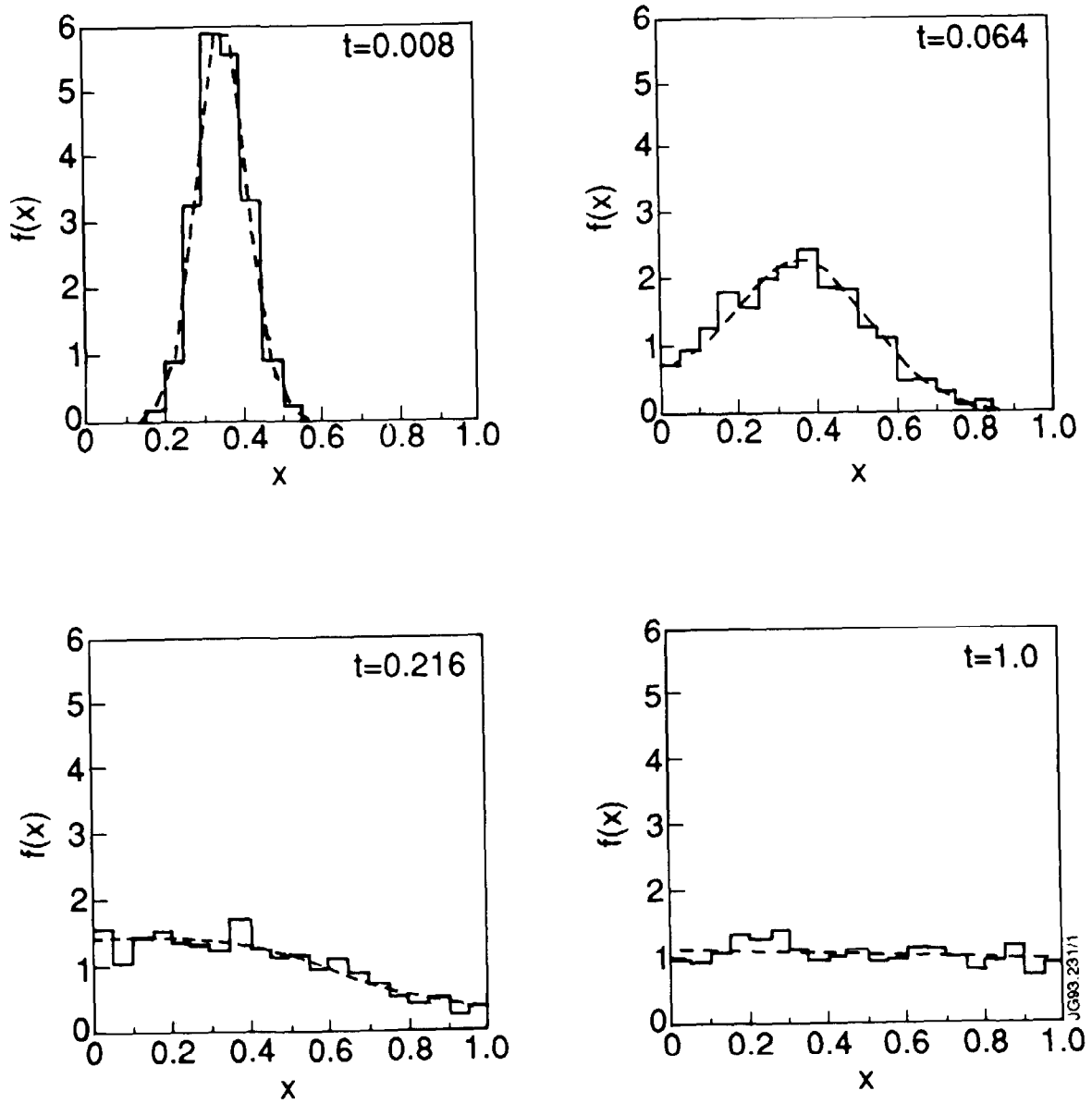
Fig. 1   Comparison of numerical solution of Eq. (14) with exact analytic one. Gaussian scheme. 1000 particles, dt = 0.001.
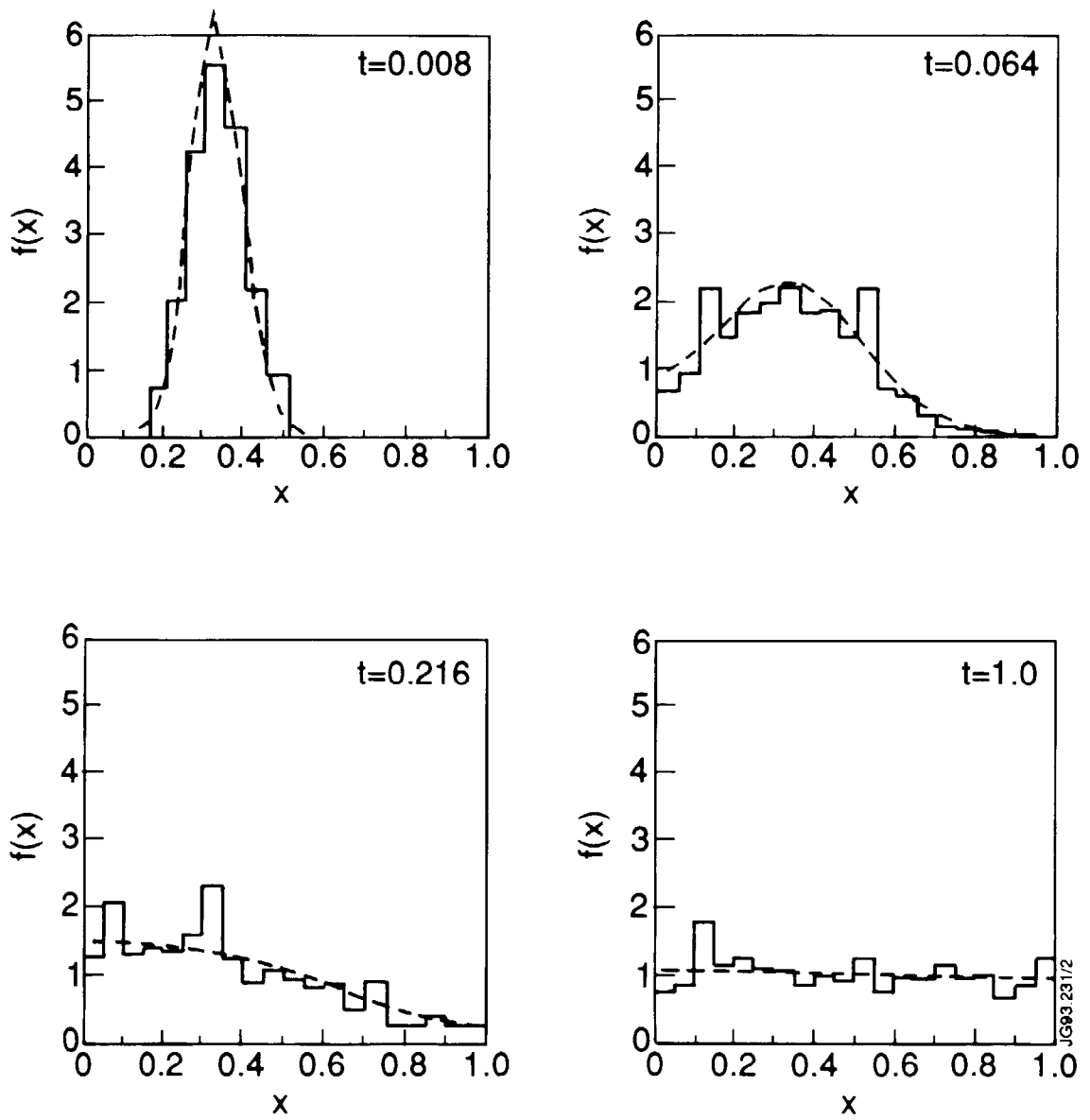
Fig. 2   The same as in Fig. 1 but for constant-step scheme.
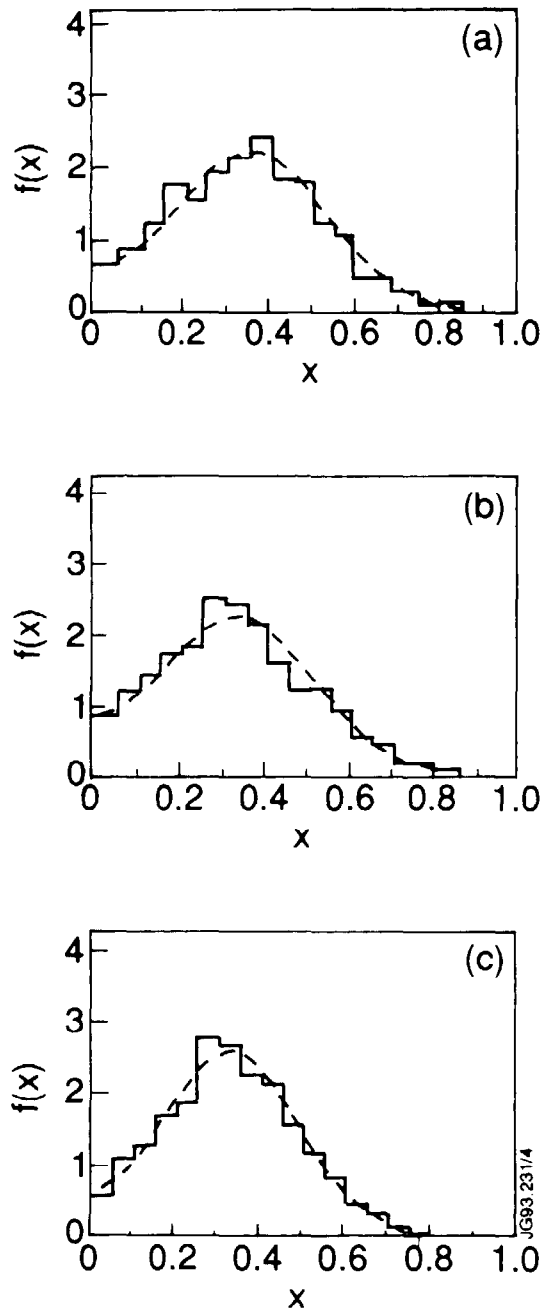
Fig. 3   Sensitivity of the Guassian scheme to the time step. Dashed line exact analytical solution.

a - t = 0.064, dt = 0.001,

b - t = 0.064, dt = 0.002,

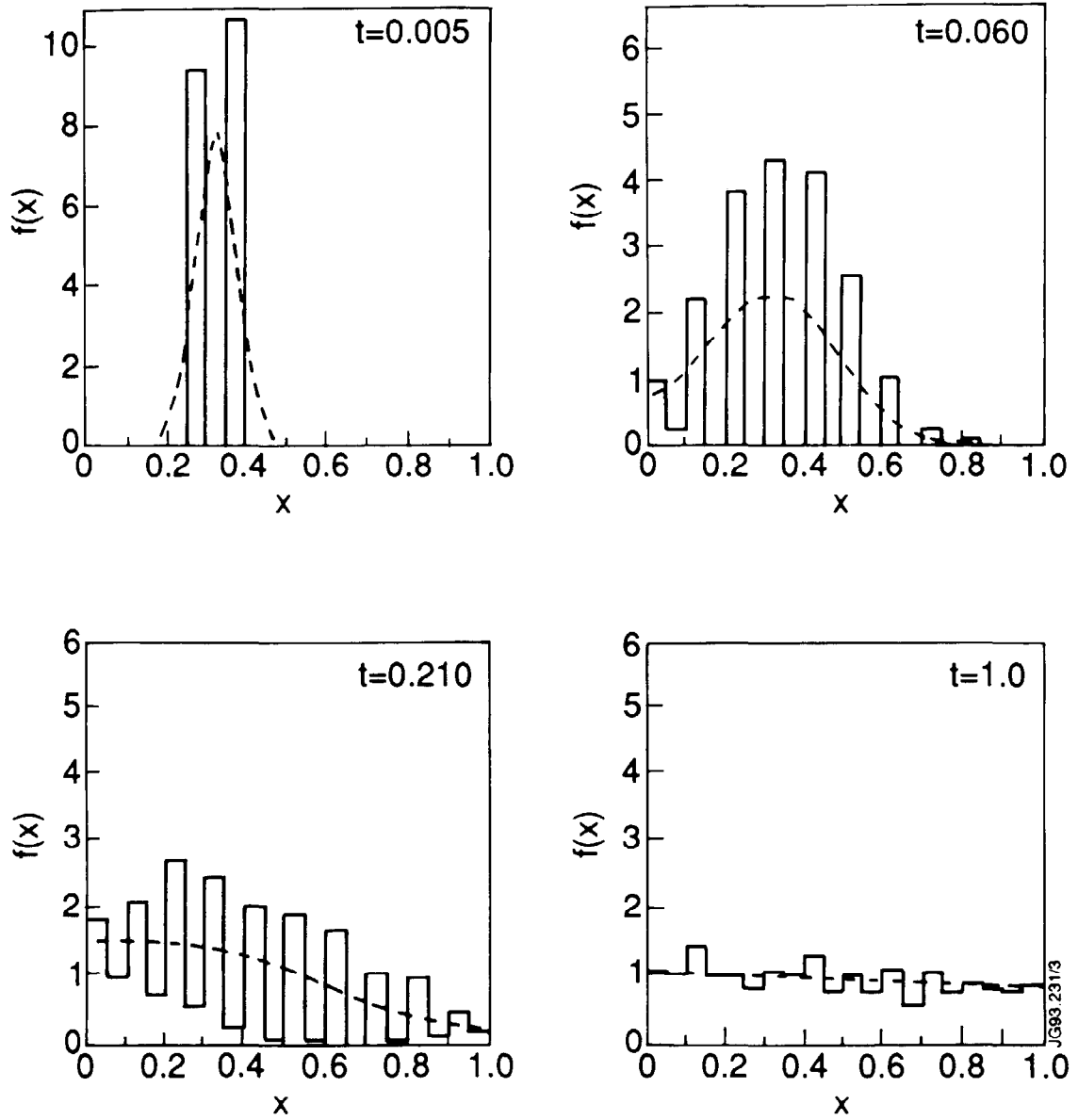c - t = 0.05,   dt = 0.05 (distribution obtained by one time step)
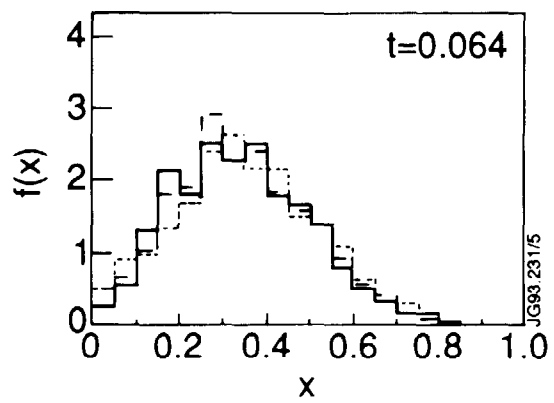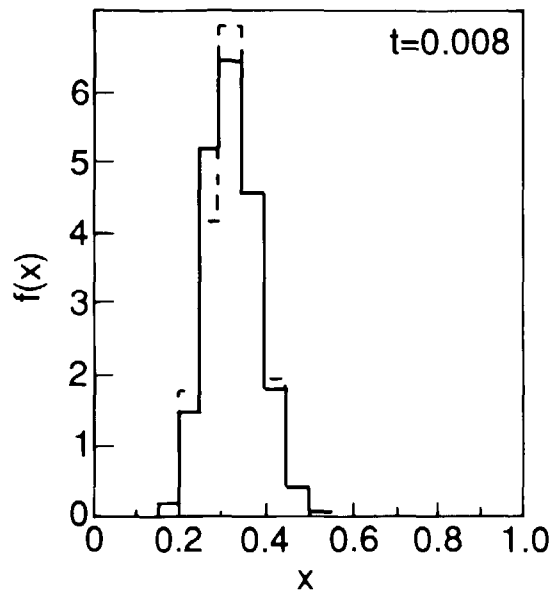
Fig 4   The time step dt = 0.005 is too big for constant-step scheme.

Fig. 5 Sensitivity of the Gaussian scheme to the time step for D = x(1-x). Solid line - dt = 0.001, dashed line - dt = 0.008, dotted line - dt = 0.064.
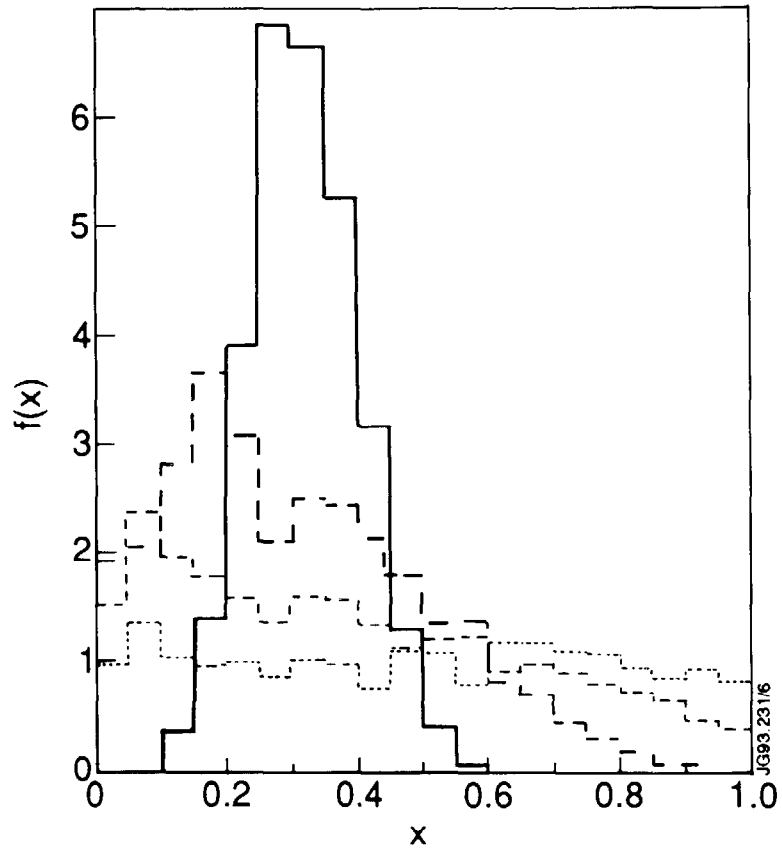
Fig. 6   Evolution of distribution function calculated for $\sqrt{g}$ = 0.1 + 1.8x.
t = 0.008, 0.064, 0.216, 1.0.
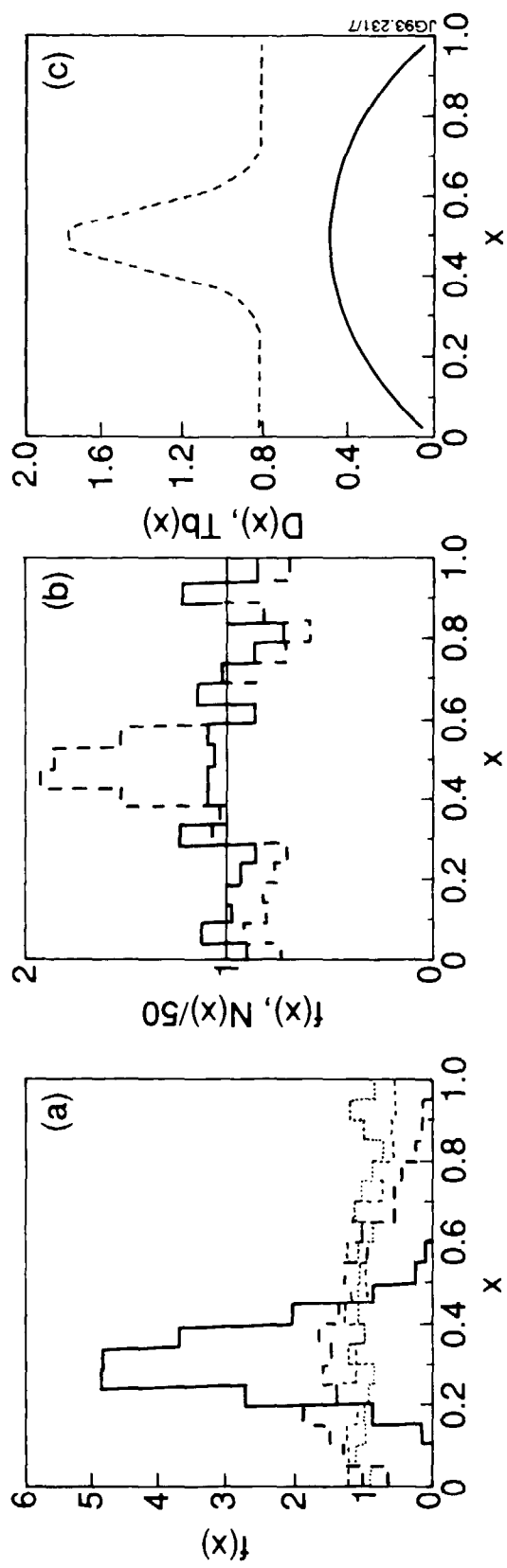
Fig. 7 Solution of Eq. (14) with D and Jacobian shown at 7c. a - evolution of distribution function, b - finite (t = 1.0) distribution function (solid line) and number of particles (dashed line).
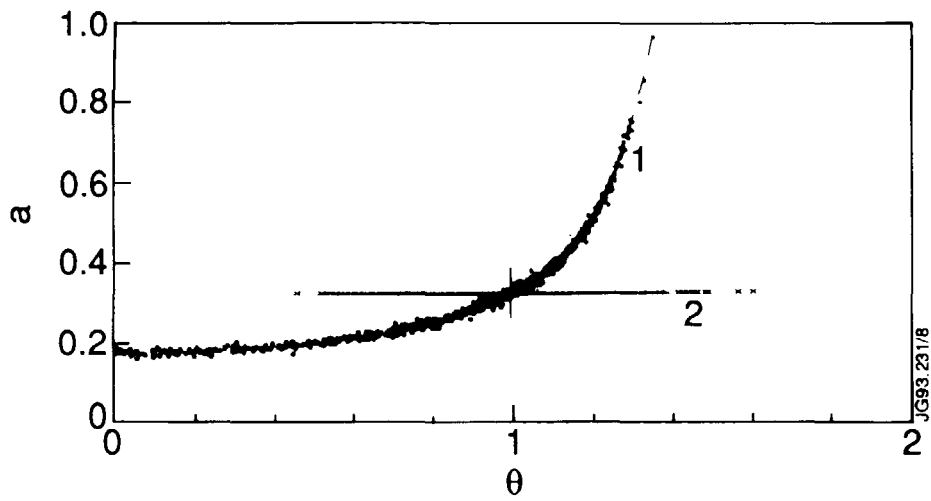
Fig. 8   Two clouds correspond to different limits,

1 - D = 0.25, $D_o = 0$,

2 - D = 0. $D_o = 0.25$.
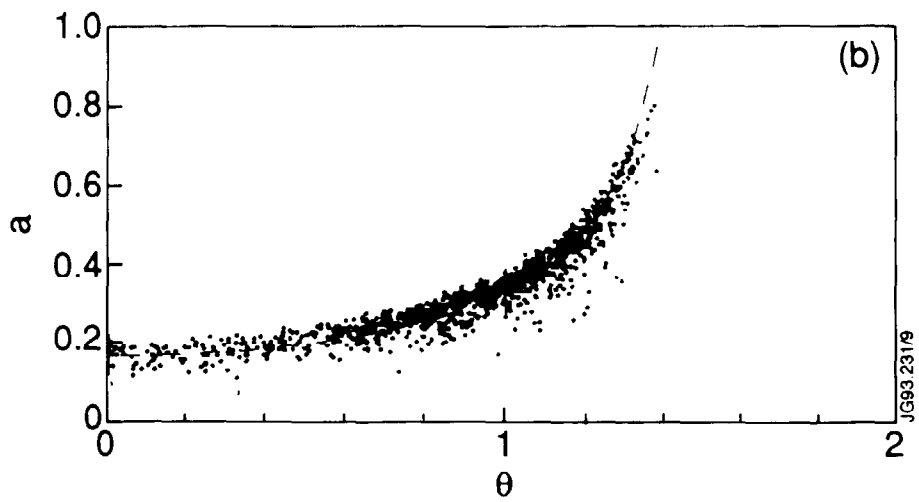
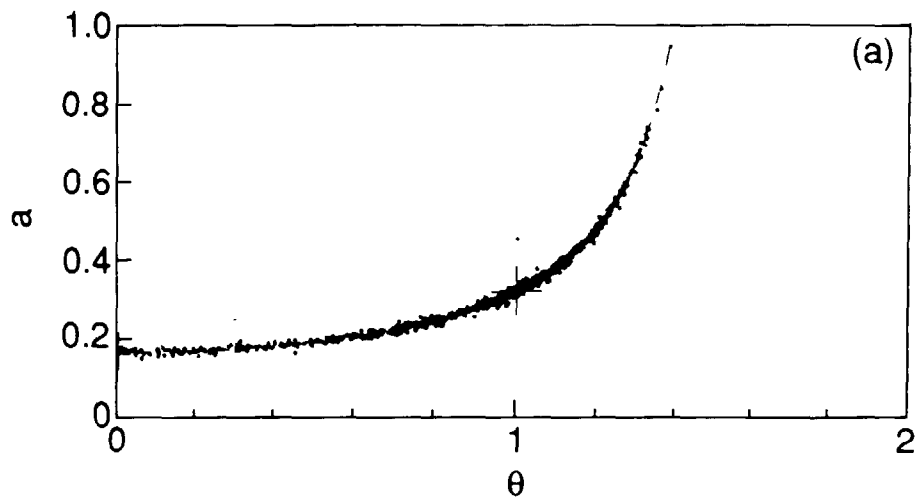t = 0.064, dt = 0.0002, dashed line - R = const.

Fig 9. Effect of finite time step. a - dt = 0.0002, b - dt = 0.005.
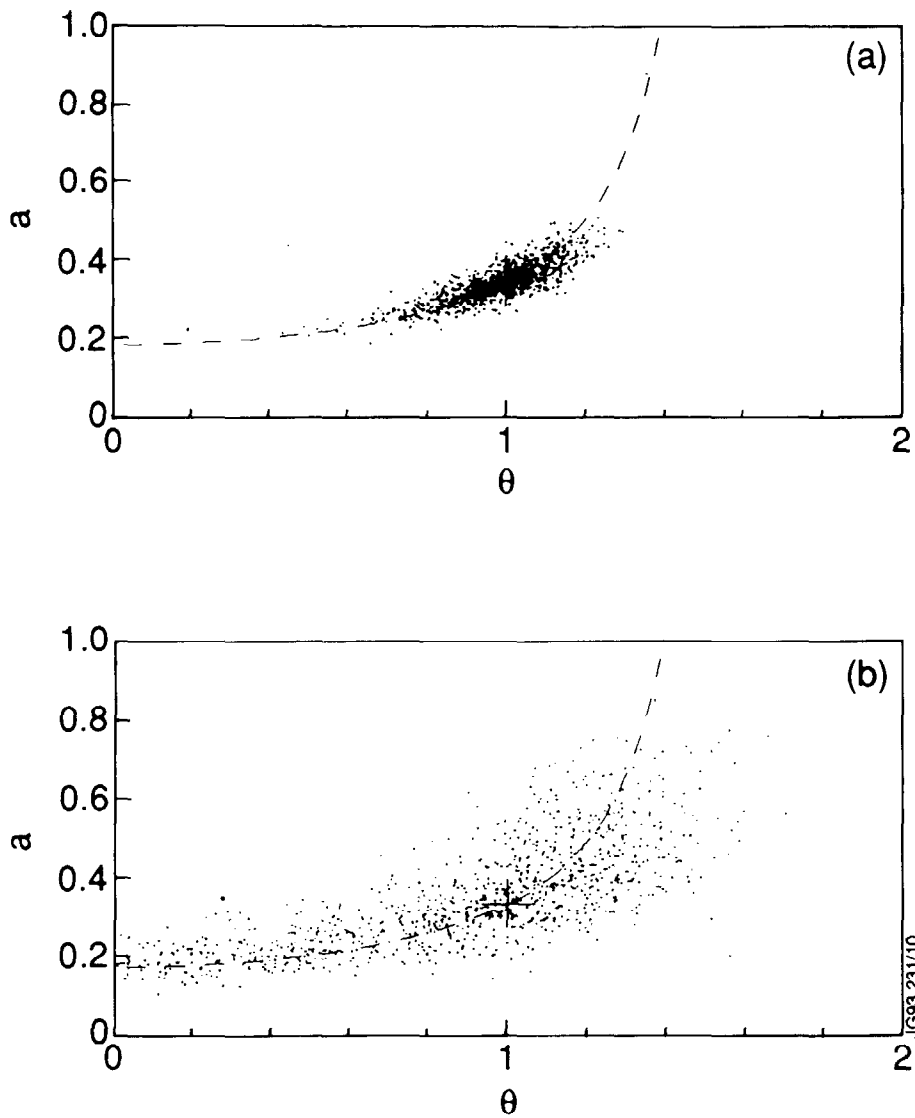
Fig. 10 Cloud spreading from initial position marked by cross.

$D = D_0 = 0.25$, $dt = 0.001$.

a - t = 0.008,

b - t = 0.064.