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Numerical Integration Methods of the Vlasov Equation*

GLENN JOYCE AND GEORG KNORR†

University of Iowa, Iowa City, Iowa 52240

AND

HOMER K. MEIER

Oak Ridge National Laboratory, Oak Ridge, Tennessee

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The methods of integrating the nonlinear Vlasov equation are reviewed, compared and interrelations are investigated. Another method is given which allows a truncation of the resulting infinite matrix without causing numerical instabilities. Its application to the linear and nonlinear Vlasov equation is discussed. It is shown that the cause for numerical instability is based on approximating a continuous eigenvalue spectrum by a discrete spectrum.

1. INTRODUCTION

One possibility of investigating nonlinear effects in plasma physics is the numerical simulation of plasmas [1]. Numerical methods have been used to an ever increasing extent recently. One numerical approach is, following the trajectories of particles directly [2, 3]. Another approach produces solutions of the Vlasov equation,

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \frac{e}{m} \mathbf{E}(\mathbf{x}, t) \cdot \frac{\partial f}{\partial \mathbf{v}} = 0, \tag{1}$$

supplemented by Poisson's equation,

$$\frac{\partial \mathbf{E}}{\partial \mathbf{x}} = 4\pi n q \left(1 - \int f dv\right).$$

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It is sometimes advantageous to transform these equations from the representation in $x - v$ space.

There are essentially two transformation methods with which solutions of the Vlasov equation have been obtained: The Hermite expansion [4] and the Characteristic Function method [5]. Both methods have advantages and shortcomings and the relation between them has not been investigated previously.

It is the purpose of this paper to clarify the close connection between them and to report several new methods which resulted in increased numerical stability and in an appreciable savings of computer time. In Section 2 and 3 we describe the Hermite expansion and the characteristic function method. In Section 4 we describe a new transform method, the power transform. In Section 5 a new method of truncating the resulting infinite system is described and in Section 6 the truncation is analyzed in terms of the eigenvalue spectrum of a simplified system. In Section 7 the method of damping the coefficients of the matrix is presented, which can also be used for numerical stabilization.

2. The Hermite Expansion

In the Hermite Expansion the velocity dependence of the distribution function is represented by Hermite polynomials

$$f(x, v, t) = \sum_{\nu=0}^{\infty} b_\nu(x, t)\, He_\nu(v) \exp(-\tfrac{1}{2}v^2)$$

$$= \sum_{n=-\infty}^{+\infty} \sum_{\nu=0}^{\infty} Z_{n,\nu}(t) \exp(ik_0 nx) \frac{1}{N_\nu} He_\nu(v) \exp(-\tfrac{1}{2}v^2), \tag{2}$$

where

$$Z_{-n,\nu} = Z^*_{n,\nu}\,.$$

$Z^*_{n,\nu}$ is the complex conjugate of $Z_{n,\nu}$.

We are using here the notation of Ref. [6] N_ν is a normalization factor which is arbitrary in principle. The orthogonality relation is

$$\int_{-\infty}^{+\infty} He_\nu(v)\, He_\mu(v) \exp(-\tfrac{1}{2}v^2)\, dv = \sqrt{2\pi}\,\nu!\,\delta_{\mu\nu}\,. \tag{3}$$

It is seen from Eq. (2) that $Z_{n,\mu}$ is a linear combination of the first μ moments of the distribution function for mode number n. Thus, only distribution functions for which all moments exist can be represented by Eq. (2). Even if all moments of f

exist, expansion (2) may not exist. It follows from the theory of orthogonal functions that the expansion (2) converges in the mean only if

$$\int_{-\infty}^{+\infty} [f(x, v, t) \exp(\tfrac{1}{4}v^2)]^2 < \infty.$$

It is evident that this condition is much more stringent than the existence of all moments.

When the series (2) is inserted into the Vlasov equation and the coefficients for each mode and Hermite function are collected, one obtains the following infinite system of differential equations:

$$\dot{Z}_{n,\nu} + ik_0 n \left[\frac{N_\nu}{N_{\nu-1}} Z_{n,\nu-1} + (\nu + 1) \frac{N_\nu}{N_{\nu+1}} Z_{n,\nu+1}\right]$$

$$+ \frac{N_\nu}{N_{\nu-1}} \sum_{m=-\infty}^{+\infty} E_{n-m} Z_{m,\nu-1} = 0, \qquad m \neq n \tag{4}$$

and Poisson's equation becomes

$$ik_0 n E_n(t) = -Z_{n,0} \frac{\sqrt{2\pi}}{N_0}.$$

The system (4) excels by its ease of computation. It is a system of ordinary differential equations of first order and has been used by several investigators [1]. As computers handle only finite systems it has to be truncated in the index n and ν. However, truncation in n does not cause any difficulties.

In order to compute $Z_{n,\nu}$ for the next time step, $Z_{n,\nu+1}$ has to be known. Choosing $Z_{n,\nu} \equiv 0$, for $\nu > \nu_m$ results in what appears to be a kind of numerical instability after some time. One is thus forced to use a large number of coefficients ($\nu_m \sim 0(1000)$) in order to obtain the correct macroscopic quantities for times of the order $t \sim 100\omega_{pe}^{-1}$. We will return to this point later and discuss now the method of the characteristic function.

3. The Characteristic Function Method

In this method, we employ for reasons described elsewhere [1], a Fourier transform in velocity space and write

$$f(x, v, t) = \sum_{n=-\infty}^{+\infty} f_n(v, t) \exp(ik_0 n x)$$

$$= \sum_{n=-\infty}^{+\infty} \int_{-\infty}^{+\infty} F_n(y, t) \exp(-ivy) \frac{dy}{2\pi} \exp(ik_0 n x). \tag{5}$$

The Fourier transformation of a distribution function is well known in statistics and is called the characteristic function. Inserting Eq. (5) into the Vlasov and Poisson equations we obtain the system

$$\frac{\partial F_n(y,t)}{\partial t} + nk_0 \frac{\partial F_n(y,t)}{\partial y} + \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} iyiE_m yFn_{-m}(y,t) = 0,$$
$$iE_n(t) = -k_0^{-1}n^{-1}F_n(0,t), \qquad n \neq 0, \tag{6}$$

where

$$F_{-n}(y,t) = F_n(-y,t)^*.$$

The formal solution can be written as

$$F_n(y,t) = F_n(y - nk_0t, 0) + \sum_{m=-\infty}^{+\infty} m^{-1} \int_0^t d\tau [y + nk_0(\tau - t)]$$
$$\cdot F_m(0,t) F_{n-m}(y + nk_0(t-\tau), \tau). \tag{7}$$

Equation (7) can easily be written as a finite difference scheme, if n is small, i.e., if we are interested in cases where only a few modes suffice for an adequate description. If one wants to keep many modes, it is advantageous not to decompose the distribution function into Fourier modes but to stay in configuration space. This approach will be treated in a forthcoming paper by J. Nuehrenberg.

Similar to the truncation of the Hermite system at ν_m, we can follow the solution of Eqs. (6) and (7) only in a finite interval in the transformed velocity variable y. But contrary to the Hermite transformation this causes no difficulties or numerical instabilities, if one assumes $F(y)$ to vanish outside $-y_m < y < +y_m$.

The two methods described appear to be two very different approaches. Yet there is a very intimate connection.

4. The Power Transform

As is well known, the m-th derivative of a characteristic function $F_n(y,t)$ with respect to y for $y = 0$ is proportional to the m-th moment of the distribution function

$$\int_{-\infty}^{+\infty} v^m f_n(v,t)\, dv = (-i)^m \frac{\partial^m}{\partial y^m} F_n(y,t)\Big|_{y=0}. \tag{8}$$

We are interested in the first few moments and so we write $F_n(y, t)$ as an expansion in powers of y,

$$F_n(y, t) = \sum_{\nu=0}^{\infty} a_{n\nu}(t)\, g_\nu y^\nu \exp(-\tfrac{1}{2}y^2). \tag{9}$$

The coefficient g_ν is still arbitrary. For the actual computations it has been chosen $g_\nu = 2^{\nu/2}\Gamma(\nu/2 + 1)/\Gamma(\nu + 1)$. With this choice the a_ν tend to be of the same order of magnitude. The exponential factor has been added to enforce convergence of the series if it is truncated.

When series (9) is inserted into Eq. (6) and equal powers of y are collected, one obtains a system which is very similar to Eq. (4):

$$\dot{a}_{n,\nu} - nk_0 \left[\frac{g_{\nu-1}}{g_\nu} a_{n,\nu-1} - (\nu + 1)\frac{g_{\nu+1}}{g_\nu} a_{n,\nu+1}\right]$$

$$- k_0^{-1} \frac{g_{\nu-1}}{g_\nu} \sum_{m=-\infty}^{+\infty} m^{-1} a_{m,0} a_{n-m,\nu-1} = 0. \tag{10}$$

We show now that the $a_{n,\nu}$ are equal to the $Z_{n,\nu}$ in Eq. (4) except for a complex factor: According to Eqs. (2), (5), and (9) we can write $f_n(v, t)$ in two different ways

$$\sum_{\nu=0}^{\infty} Z_{n,\nu} N_\nu^{-1} He_\nu(v)\, e^{-1/2v^2} = \sum_{\nu=0}^{\infty} a_{n,\nu} g_\nu \int_{-\infty}^{+\infty} \frac{dy}{2\pi}\, y^\nu e^{-1/2y^2 - iyv}.$$

The integral can be written as

$$i^\nu \frac{d^\nu}{dv^\nu} \int_{-\infty}^{+\infty} \frac{dy}{2\pi} \exp(-\tfrac{1}{2}y^2 - iyv),$$

and the integration can easily be performed. Using the Rodriguez formula for Hermite polynomials we find

$$Z_{n,\nu} = \sqrt{2\pi}\,(-i)^\nu\,(N_\nu g_\nu)\, a_{n,\nu}\,. \tag{11}$$

The establishes the close relation between the Hermite transform and the characteristic function.

For symmetric initial conditions, as mostly used by Armstrong [4] the $a_{-,\nu}$ are all real whereas the $Z_{n,\nu}$ are alternately real and imaginary.

5. Cut-Off Procedure

When we integrate system (10) numerically, we meet the same difficulty of truncating the system with respect to the discrete v-coordinate. This remark applies to both nonlinear and linear cases. There is no reason to assume any kind of regularity between subsequent $a_{n,v}$. However if the linear Vlasov equation is represented in the form (10) and integrated, we obtain a very regular pattern for the amplitudes $a_{n,v}$ ($v = 0, 1, 2,...$) for large v. An example is given in Fig. 1. The coefficients appear to be a discrete plot of an otherwise continuous function in v.

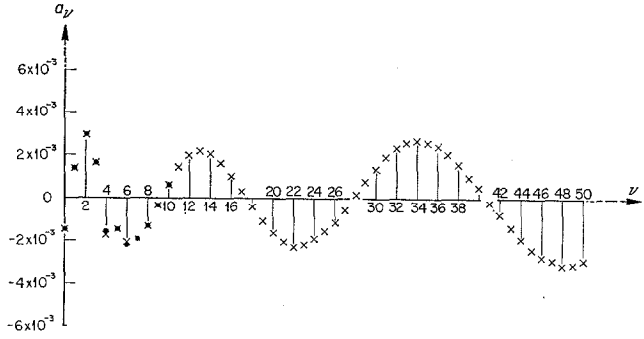

FIG. 1. Plot of the real amplitudes a_v of system (10) for time $t = 20\ \omega_{pe}^{-1}$ for the following initial condition: $f(x, v, t = 0) = 1/\sqrt{2\pi}\exp(-\frac{1}{2}v^2)[1 + 0.1\cos\frac{1}{2}x]$. This corresponds to a stable standing wave with wave length $\lambda = 4\pi\lambda_d$ (λ_d = Debye length). The system (10) has been changed so that it represents the linearized Vlasov equation. The amplitudes for $v > 8$ form a very regular pattern. · represents results when the maximum v was 10. x represents results when the maximum v was 20, 50, and 100. The extrapolation used was of fourth order.

It is therefore natural to guess the $(v_m + 1)$ coefficient by a polynomial extrapolation and thus close the system (10). This method worked very well for the linear Vlasov equation. Polynomials of order 0, 1, 2, 3, and 4 were used, and the system (10) was truncated for v_m equal to 200, 100, 50, down to $v_m = 10$. We checked the real and imaginary part of ω for the case of a stable standing wave, f_0 being a Maxwellian. The real part of ω was strictly invariant for all conditions. The imaginary part of ω, representing Landau damping showed a relative deviation of $\Delta\gamma/\gamma = 0.8\,\%$ when v_m was as low as 10. For $t = 100\omega_{pe}^{-1}$, this is equivalent to a deviation of $12\,\%$ of the amplitude of the electric field. Thus we have shown that contrary to the belief of Grant and Feix [7] the difficulty of cutoff can be avoided for the linear Vlasov equation.

The question arises how this cutoff procedure works in the nonlinear case.

We found that it depends very much on the case treated. If the amplitudes of the electric fields are quite small the results will be similar to the linear limit. If the electric fields become so large that the homogeneous velocity distribution is changed appreciably, the truncation by extrapolation still stabilizes the system. The coefficients $a_{n,\nu}$ do however no longer lie on a continuous curve but show some scattering which increases with increasing nonlinearity. Thus some inaccuracy is introduced by the truncation. We have found [9] however, that up to times $t = 60\omega_{pe}^{-1}$ the inaccuracies thus introduced are small when $\nu_m = 80$ or larger.

We now consider the nature of the truncation instability and its stabilization.

6. Eigenvalue Theory

It is evidently the second term in Eq. (1) which prohibits the closure of system (10). Therefore the simplest equation in which we can study the problem of closure is given by

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = 0$$

or in terms of the characteristic function, confining ourselves to one mode only,

$$\frac{\partial F}{\partial t} + nk_0\frac{\partial F}{\partial y} = 0. \tag{12}$$

The solution is clearly

$$F(y, t) = F(y - nk_0 t, 0).$$

When we write

$$F(y, t) = \sum_{\nu=0}^{\infty} b_\nu(t)\, h_\nu y^\nu e^{-1/2y^2}, \tag{13}$$

the b_ν are proportional to the $a_{n,\nu}$ in the expansion (9) and the system resulting from Eqs. (12) and (13) is

$$h_\nu \dot{b}_\nu + nk_0[h_{\nu+1}(\nu + 1)\, b_{\nu+1} - h_{\nu-1}b_{\nu-1}] = 0. \tag{14}$$

We want to determine the eigenvalue spectrum and eigensolutions of this system and try the ansatz:

$$b_\nu(t) = \xi_\nu \exp(i\omega t)$$

which results in

$$\frac{i\omega}{nk_0}\xi_\nu + \left[\frac{\nu+1}{h_\nu/h_{\nu+1}}\xi_{\nu+1} - \frac{h_{\nu-1}}{h_\nu}\xi_{\nu-1}\right] = 0. \tag{15}$$

If we now choose

$$h_\nu/h_{\nu+1} = i(\nu+1) \qquad \text{or}$$
$$h_\nu = h_0/i^\nu \nu!,$$

we find that

$$\xi_{\nu+1} = \frac{\omega}{nk_0}\xi_\nu - \nu\xi_{\nu-1}\,. \tag{16}$$

This is just the recurrence relation for the Hermite polynomials and so we can write

$$\xi_\nu = He_\nu\left(\frac{\omega}{nk_0}\right).$$

For the infinite system (14) the eigenvalue spectrum is continuous and we may write the solution of Eq. (14) as

$$b_\nu(t) = \int_{-\infty}^{+\infty} g\left(\frac{\omega}{nk_0}\right)\psi_\nu\left(\frac{\omega}{nk_0}\right)\exp(i\omega t)\,d\omega, \tag{17}$$

where the cylinder function ψ_ν is given by

$$\psi_\nu = He_\nu(v)\exp(-\tfrac{1}{2}v^2),$$

b_ν is thus the Fourier transform of the function $g\psi_\nu$ and under quite weak conditions on g, we have

$$\lim_{t\to\infty} b_\nu(t) = 0$$

If the system (14) is truncated by the condition

$$b_{N+\mu}(t) = 0, \qquad \mu = 0, 1, 2,..., \tag{18}$$

we find

$$He_N\left(\frac{\omega}{nk_0}\right) = 0.$$

The truncated system has now a discrete spectrum of eigenvalues. There are N

eigenvalues and they are given by the zeros of the N-th Hermite polynomial, $\omega = nk_0\alpha_\mu{}^N; \mu = 1, 2, 3,..., N$. The solution of the truncated system is now given by

$$b_\nu(t) = \sum_{\mu=1}^{N} g(\omega_\mu)\, \psi\left(\frac{\omega_\mu}{nk_0}\right) e^{i\omega_\mu t} \tag{19}$$

and the N values $g(\omega_\mu)$ specify exactly the N values $b_\nu(0)$; it is evident that $b_\nu(t)$ in Eq. (19) is an almost periodic function of time, contrary to the $b_\nu(t)$ in Eq. (17). We realize that the apparent numerical instabilities which Armstrong and other investigators have seen, are not so much numerical instabilities in the usual sense, but due to the attempt of representing a continuous eigenspectrum by a discrete finite spectrum.

If the ω_μ in Eq. (19) are densely spaced, it is to be expected that they form a good approximation to Eq. (17) for small times. For arbitrarily large times the approximation is bound to fail.

One can remedy the situation by adding a small imaginary part to the eigenvalues ω_μ. Then the solution (17) is well approximated by Eq. (19) for small times by the truncated system. For large times the imaginary part of ω_μ damps the solution sufficiently to avoid recurrence. One way of achieving this goal is to replace the truncation condition (18) by something else, e.g. an extrapolation. We then obtain

$$b_{N+1} = \sum_{\mu=0}^{N} (-)^\mu\, \alpha_\mu b_{N-\mu} \tag{20}$$

It has been reported above, that this method works very well for the linearized Vlasov equation. The explicit calculation of the resulting eigenvalues becomes quite involved, however, even for the simplest extrapolation formula. We therefore give only the result for a zero order extrapolation

$$a_{n,N+1} = a_{n,N}$$

for the truncated system (10) without the sum term. If the number N of coefficients a_ν is large, we find

$$\begin{aligned} &\operatorname{Re}\omega = \pi(\mu + \tfrac{1}{2})\, N^{-1/2}, \\ &\operatorname{Im}\omega = \ln\sqrt{N}/\sqrt{N}, \qquad \mu = 0, \pm 1, \pm 2,\ldots . \end{aligned} \tag{21}$$

We have restricted ourselves to small μ, such that $|\mu| \ll \sqrt{N}$.

We can also prescribe explicitly the imaginary part by writing

$$He_{N+1}\left(\frac{\omega - i\lambda}{nk_0}\right) = 0. \tag{22}$$

Expanding this into a Taylor series and using the differential relation for Hermite polynomials, we obtain

$$He_{N+1}\left(\frac{\omega}{nk_0}\right) = -\sum_{l=1}^{N+1}\left(\frac{i\lambda}{nk_0}\right)^l \binom{N+1}{l} He_{N+1-l}\left(\frac{\omega}{nk_0}\right). \tag{23}$$

This is exactly equivalent to Eq. (22) because the Taylor series is finite. From Eq. (23), we conclude that

$$h_{N+1}b_{N+1}(t) = -\sum_{l=1}^{N+1}\frac{(-)^l}{l!}\left(\frac{\lambda}{nk_0}\right)^l b_{N+1-l}(t)\, h_{N+1-l}\,. \tag{24}$$

This formula shows the same structure as Eq. (20): b_{N+1} is a linear function of the $b_{N-\nu}$ and the sign of the coefficients is alternating. Computer calculations using Eq. (24) with $1.5 < \lambda < 2.5$ also showed satisfactory results without any numerical instabilities.

7. Damped Matrix

The methods of truncation discussed so far did not change the system of differential equations (10). If we change it in such a way that the $a_{n,\nu}$ with ν close to N are heavily damped, their amplitude can never become large and a truncation is equivalent to a reasonable guess of $a_{n,N}$. This corresponds to a smoothing of the distribution function if the ripples in v exceed a certain steepness. The coefficients $a_{n,\nu}$ which have small ν are only indirectly affected by the damping of the $a_{n,\nu}$ which have large ν. The selective damping can, for example, accomplished by adding a term

$$-\epsilon\nu^{2r}a_{n,\nu} \tag{25}$$

to the right side of Eq. (10). ϵ is of the order N^{-2r} and $r = 1, 2, 3$.

The same approach has been chosen independently by Armstrong [8]. He has shown that the term (25) corresponds to the collision operator

$$C(v)^{2r}f = \epsilon\left[\frac{\partial}{\partial v}\left(\frac{\partial}{\partial v} + v\right)\right]^{2r} f,$$

on the right side of the Vlasov equation (1). It is clearly seen that it smoothes preferentially the steep ripples of the distribution function f in velocity space.

ACKNOWLEDGMENTS

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