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Dispersion Relation for Computer-Simulated Plasmas

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ABSTRACT

A dispersion relation for a computer-simulated plasma in which the effects of discreteness in space and time are treated exactly is derived. In the limit that the mesh spacing and the time step go to zero independently, the well-known results associated with a collisionless plasma are obtained. Nonphysical Landau damping of a wave by particles traveling at phase velocities associated with frequency "aliases" and numerical dispersion associated with a finite time step are easily avoided with small enough time steps. Discreteness in space plus interpolation between mesh points leads to modes which can be represented as sums of backward and forward traveling sinusoidal waves. The total resonant interaction of the particles with a mode is the sum of their interactions with each of the components. For a Maxwellian distribution the forward traveling components lead to damping, but the backward traveling components lead to growth. Consequently, numerically unstable modes can occur in a Maxwellian plasma.

I. INTRODUCTION

The simulation of a plasma by integrating the equations of motion of a large number of particles has been made practical with the modern advances in computer technology. One-dimensional problems can be handled quite adequately using these techniques, [1] and useful results are being obtained from 2- and 3-dimensional codes [2, 3].

In solving the equations of motion numerically, certain difficulties arise which must be dealt with. One of these problems is that of "enhanced noise," which arises because one is trying to simulate a system of 10^{20} particles with 10^4. The fluctuations generated by correlations are thus greatly magnified over the situation in a real plasma. This aspect of the situation has been treated elsewhere [2] and no further discussion will be directed towards it.

There are, however, further difficulties which must be analyzed, those associated with discreteness in space and time. The differential equations which describe the plasma must be replaced with difference equations. The process of going from

differential equations to finite differences is not unique, and a variety of methods for numerically "integrating" equations have been given. In general the systems described by these finite difference equations are very similar to the real systems they approximate, i.e., generally the various modes of the computer system can be placed into one-to-one correspondence with those of the real system, but certain properties of the mode may be different. The conversion of a weakly damped mode to a growing mode is a not-uncommon occurrence, and is referred to as numerical instability [4]. Such difficulties are usually easy to recognize, and are quickly corrected by changing the finite difference scheme. Other modifications also may occur, and, although they are not as spectacular, they may affect the accuracy of the simulation substantially. A small change in frequency is usually of little consequence as is a small amount of "numerical damping." There are, however, cases where added "numerical damping" must be avoided, or, at the very least, the deviations need be known in order to properly interpret the results.

This information is, of course, contained in the linear dispersion relation for waves in the system. Since equivalent dispersion relations for genuine plasmas are available for comparison, analysis of the dispersion relation of the computer system is currently the most effective approach to evaluating the accuracy of the simulation.

For concreteness and simplicity the derivation of the dispersion relation for a particular one-dimensional electrostatic code will be given. The method, however, is quite general and the extension to more complex systems is straightforward. The code we choose to analyze is a PIC code (Particle-In-Cell) developed by Morse and Nielson [1]. The results may, also, be applied almost immediately to the CIC codes (Cloud-In-Cell) developed by C. K. Birdsall [2].

II. A Typical Finite Difference Scheme

A set of one-dimensional macro-particles (infinite sheets having a given charge per unit area and mass per unit area) are allowed to move within a region of length L. An equal amount of charge per unit area is assumed uniformly distributed throughout the region and does not move. Assume at time t, the position and velocities of all macro-particles are known. To find the positions and velocities one time-step, τ, later, the following procedure is used.

A set of N mesh points are defined in the region $0 \leqslant x \leqslant L$. Thus, if D is the spacing between the mesh points, we have $L = ND$. At these points a surface charge density is defined

$$\sigma(n) = (q/A)\, CN(n), \qquad n = 1, 2, \ldots, N. \tag{1}$$

The q is the charge within an area A on one of the sheets, and $CN(n)$ is the effective number of charge sheets at the mesh point n.

The number $CN(n)$ for each of the mesh points is arrived at by going through the list of particle positions, $x_i(t)$, and by distributing the charge number "1" that it carries between the two mesh points that it currently lies between. Suppose for a particular particle the mesh point index, n', is determined such that $n'D \leqslant x \leqslant (n'+1)D$. The amount of charge attributed to mesh point n' is then

$$\Delta\sigma(n') = (q/A)(n' + 1 - x/D), \tag{2}$$

while the amount given to the mesh point $(n'+1)$ is

$$\Delta\sigma(n'+1) = (q/A)(-n' + x/D). \tag{3}$$

The sum of these contributions is "1" times q/A, but, as the sheet moves from $x = n'D$ to $x = (n'+1)D$, the charge density at $n'D$ decreases uniformly while the charge density at $(n'+1)D$ increases uniformly. The charge density $\sigma(n)$ is thus the sum of all the contributions of the sheets near enough to contribute. A constant background charge is also distributed uniformly over the mesh points.

These surface-charge densities are then used to calculate a value for the electric field at the points $x = (n + \frac{1}{2})D$, which are located in between the points at which the charge is located. The difference equation used is Gauss's Law for surfaces:

$$E_{n+1/2} - E_{n-1/2} = 4\pi\,\sigma(n). \tag{4}$$

Periodic boundary conditions are used, and the overall charge-neutrality of the system gives $E_{N+1/2} = E_{1/2}$.

Values of the electric field at the mesh points $x = nD$ are now obtained as the simple averages of the values at the neighboring half steps

$$E_n = \tfrac{1}{2}(E_{n+1/2} + E_{n-1/2}). \tag{5}$$

The actual electric field that accelerates a macro-particle located at the point x is now obtained from the values E_n by linear interpolation between neighboring mesh points. For a particle at the point x such that

$$n'D \leqslant x \leqslant (n'+1)D,$$

the electric field is:

$$E(x) = E_{n'}(n' + 1 - x/D) + E_{n'+1}(-n' + x/D). \tag{6}$$

In order to handle the largest number of particles, a simple time integration scheme is usually used. The following method, which is obviously time-centered, is common:

$$\text{Let } t = j\tau, \qquad j = \text{integer}$$

$$v(j\tau + \tfrac{1}{2}\tau) - v(j\tau - \tfrac{1}{2}\tau) = (q\tau/m)\,E[x(j\tau)] \tag{7'}$$

$$x(j\tau + \tau) - x(j\tau) = \tau v(j\tau + \tfrac{1}{2}\tau). \tag{8'}$$

This particular form of the equations is, however, inconvenient for analysis. In order to avoid the conceptual difficulties involved in following a particle's motion in phase space when its x- and v-coordinates are never defined at the same time, an equivalent set of equations is introduced.

$$v(j\tau + \tau) - v(j\tau) = (q\tau/m)\, E[x(j\tau)] \tag{7}$$

$$x(j\tau + \tau) - x(j\tau) = \tau v(j\tau + \tau). \tag{8}$$

This alternate method of writing the equations is, in fact, the way they appear in the actual listing of a code when they are used. Thus after evaluating $E(x)$ for a given particle, Eq. (7) is used to update the velocity. Then, using the new velocity Eq. (8) gives the new position. At this point the cycle or time step is completed and the current values of position and velocity are stored for use as input parameters for the next step.

III. Derivation of the Dispersion Relation

Assume a solution for the $E_{n+1/2}(t)$ of the form

$$\begin{aligned} E_{n+1/2}(t) &= E_0 e^{i\omega t} e^{ikx} \\ &= E_0 \exp[i\omega j\tau_e + ik(n + \tfrac{1}{2})\, D], \end{aligned} \tag{9}$$

where $t = j\tau$ and $x = (n + \frac{1}{2})\, D$ as before. In a region of length L with periodic boundary conditions, k is restricted to $k = 2\pi\kappa/L$ where $\kappa = \pm 1, \pm 2, \ldots$, and $L = ND$.

Following the procedure outlined in the previous section, the E_n's are obtained

$$E_n = E_0 \cos(\tfrac{1}{2}kD)\, e^{i\omega t} e^{iknD}. \tag{10}$$

To obtain $E(x)$ assume

$$E(x) = \sum_{p=-\infty}^{\infty} C_p(k)\, e^{i2\pi px/L}. \tag{11}$$

The $C_p(k)$ is then given by:

$$C_p(k) = L^{-1} \sum_{n=0}^{N-1} \int_{nD}^{(n+1)D} e^{-i2\pi px/L} E(x)\, dx. \tag{12}$$

Now in the range $nD \leqslant x \leqslant (n + 1)\, D$, $E(x)$ is given by Eq. (6) with $n = n'$. Performing the above operations and using the fact that $k = 2\pi\kappa/(ND)$, one obtains the result

$$E(x) = E_0 e^{i\omega t} \cos(\tfrac{1}{2}kD) \sum_{l=-\infty}^{\infty} R_l{}^2 e^{ik_l x}, \tag{13}$$

where

$$R_l = \sin(\tfrac{1}{2}kD)/(\tfrac{1}{2}k_lD) \tag{14}$$

$$k_l = k + 2\pi l/D. \tag{15}$$

Regarding $E(x)$ as a first-order quantity and linearizing the equations of motion, one obtains to zero order

$$v_0(j\tau + \tau) - v_0(j\tau) = 0 \tag{16}$$

$$x_0(j\tau + \tau) - x_0(j\tau) = \tau v_0(j\tau + \tau). \tag{17}$$

The zero-order motion is thus

$$v_0(j\tau) = v_0 = \text{constant} \tag{18}$$

$$x_0(j\tau) = j\tau v_0 + x_0(0). \tag{19}$$

To first order in $E(x)$ the difference equations for v_1 and x_1 are

$$v_1(j\tau + \tau) - v_1(j\tau) = (q\tau E_0/m)\cos(\tfrac{1}{2}kD)\sum_{l=-\infty}^{\infty} R_l^2 \exp[i\omega j\tau + ik_lx_0(0) + ik_lv_0j\tau]. \tag{20}$$

$$x_1(j\tau + \tau) - x_1(j\tau) = \tau v_1(j\tau + \tau). \tag{21}$$

The usual method of solving the orbit equations involves the use of Laplace transforms. The arguments leading to Landau damping then arise from certain mathematical requirements which must be satisfied while inverting the transform [5].

A different approach will be introduced here. In it Landau damping arises from an infinitesimal resistivity. The "resonant" particles differ from the "bulk" particles in that their orbits are dominated by the resistivity rather than inertia. The effect remains in the limit of zero resistivity since, although the number of particles which are "resonant" goes to zero, the amplitude of their orbits goes to infinity.

The equations with which we are dealing constitute an idealization of a computer-simulated plasma (and a real plasma when appropriate limits are taken) in which there exists a small but finite amount of collisional damping. The case of interest is the one in which this damping is negligible. Thus a small amount of damping will be introduced into the above equations, and the dispersion relation obtained in the limit that this damping goes to zero will thus correspond to the case of interest. It is convenient to write the damping term in the form: $(1 - e^{-\nu\tau})/\tau$.

The first-order equations are now

$$v_1(j\tau + \tau) - v_1(j\tau) + (1 - e^{-\gamma\tau})\, v_1(j\tau)$$
$$= (q\tau E_0/m)\cos(\tfrac{1}{2}kD) \sum_{l=-\infty}^{\infty} R_l^2 \exp[i\omega j\tau + ik_l x_0(0) + ik_l v_0 j\tau] \tag{22}$$

$$x_1(j\tau + \tau) - x_1(j\tau) = \tau v_1(j\tau + \tau). \tag{23}$$

Using difference-equation analogues of the methods for handling similar differential equations these equations can be "summed" from $t = -\infty$ to $j\tau$ to give:

$$v_1(j\tau) = (q\tau E_0/m)\cos(\tfrac{1}{2}kD) \sum_{l=-\infty}^{\infty} R_l^2 \frac{\exp(i\omega j\tau + \gamma\tau + ik_l x)}{\exp\{i\tau(\omega - i\gamma + k_l v_0)\} - 1} \tag{24}$$

$$x_1(j\tau) = (q\tau^2 E_0/m)\cos(\tfrac{1}{2}kD)$$
$$\cdot \sum_{l=-\infty}^{\infty} R_l^2 \frac{\exp(i\omega j\tau + ik_l x)\exp\{i\tau(\omega - i\gamma + k_l v_0)\}}{[\exp\{i\tau(\omega - i\gamma + k_l v_0)\} - 1][\exp\{i\tau(\omega + k_l v_0)\} - 1]}. \tag{25}$$

A first-order distribution function must now be constructed using these expressions for the trajectories. To do this, one makes use of the fact that any function of the constants of the motion is itself a constant of the motion. The constants of the motion in this case are

$$x_0(0) = x(j\tau) - x_1(j\tau) - j\tau\{v(j\tau) - v_1(j\tau)\} \tag{26}$$

$$v_0(0) = v(j\tau) - v_1(j\tau). \tag{27}$$

If $F[x_0(0), v_0(0)]$ is the distribution of $x_0(0)$ and $v_0(0)$ at $t = j\tau = 0$, then $F[x - x_1 - j\tau(v - v_1),\ v - v_1]$ is the corresponding distribution of x and v at $t = j\tau$. Furthermore, if x_1 and v_1 are small

$$F = F(x - j\tau v, v) - (x_1 - j\tau v_1)\,\partial F/\partial x - v_1 \partial F/\partial v. \tag{28}$$

Thus one identifies the usual zero and first-order distribution functions:

$$f_0(x, v, t) = F(x - j\tau v, v). \tag{29}$$

$$f_1(x, v, t) = -(x_1 - j\tau v_1)\,\partial F/\partial x - v_1 \partial F/\partial v. \tag{30}$$

In making the coordinate transformation in phase space from $(x_0(0), v_0(0))$ to (x, v), one must also transform the volume element: $dx_0(0)\, dv_0(0) \to J\, dx\, dv$, where J is the Jacobian of the transformation. Since f_0 and f_1 are usually defined such that no Jacobian appears in the expressions for the moments, the function

$J \cdot F$ should be used in place of F in Eqs. (29) and (30). In this case as in most, however, $J = 1 + 0(\gamma)$, and it is convenient to neglect these terms immediately.

Using (x, v) and (x_0, v_0) interchangeably in the first-order terms, and confining the discussion to a uniform zero-order distribution, ($f_0(x, v, t) = f_0(v)$ only) the following expression is obtained for f_1

$$f_1 = -(q\tau E_0/m)\cos(\tfrac{1}{2}kD)\, e^{i\omega j\tau} \sum_{l=-\infty}^{\infty} \frac{R_l^2 \exp(ik_l x + \gamma\tau)}{\exp\{i\tau(\omega - i\gamma + k_l v)\} - 1} \cdot \frac{\partial f_0}{\partial v}. \quad (31)$$

From this quantity the $CN(n)$ can be obtained

$$CN(n) = \int_{-\infty}^{\infty} dv \int_{(n-1)D}^{nD} (1 - n + x/D) f_1\, dx + \int_{-\infty}^{\infty} dv \int_{nD}^{(n+1)D} (n + 1 - x/D) f_1\, dx. \quad (32)$$

And finally combining the results of this operation with Eq. (4) the dispersion relation is obtained.

$$1 - \frac{4\pi q^2}{mA}\cos(\tfrac{1}{2}kD) \sum_{l=-\infty}^{\infty} R_l^3 k_l^{-1} \int_{-\infty}^{\infty} \frac{i\tau e^{\gamma\tau}\, \partial f_0/\partial v}{\exp\{i\tau(\omega - i\gamma + k_l v)\} - 1}\, dv = 0. \quad (33)$$

IV. Properties of a Single Wave in a Maxwellian Plasma

Consider the special case

$$f_0(v) = (N_p/L)(\pi v_T)^{-1/2} \exp(-v^2/v_T^2), \quad (34)$$

where N_p is the total number of "macro-particles" in length L. The dispersion relation in this case reduces to

$$1 + 2\cos(\tfrac{1}{2}kD) \sum_{l=-\infty}^{\infty} R_l^3 \{\omega_p^2/(k_l v_T)^2\}\, W(\omega, k_l) = 0, \quad (35)$$

where

$$\omega_p^2 = 4\pi q^2 N_p/(mAL), \qquad v_T^2 = 2T/m$$

$$W = \lim_{\gamma \to +0} \pi^{-1/2} \int_{-\infty}^{\infty} \tfrac{1}{2}k_l v_T \tau e^{\gamma\tau} \cot\{\tfrac{1}{2}\tau(\omega - i\gamma + k_l v_T u)\}\, u \exp(-u^2)\, du \quad (36)$$

The terms R_l and k_l are defined in Eqs. (14) and (15) and m and q are the amount of charge and mass associated with area A on a macro-particle or sheet.

For real ω and k_l the function $W(\omega, k_l)$ has both real and imaginary parts. The real part is

$$\mathrm{Re}(W) = \sum_{l=-\infty}^{\infty} \pi^{-1/2} \int_{-b}^{b} \tfrac{1}{2}k_l v_T \tau \cot\{\tfrac{1}{2}\tau(\omega + k_l v_T u)\}(u + 2jb) \exp\{-(u + 2jb)^2\}\, du, \quad (37)$$

where $b = \pi/(k_l v_T \tau)$, and where principal values are taken at the poles. The corresponding imaginary part of W is:

$$\mathrm{Im}(W) = -\sum_{j=-\infty}^{\infty} \pi^{-1/2} \left(\frac{\omega\tau + 2\pi j}{\tau \mid k_l \mid v_T}\right) \exp\left[-\left(\frac{\omega\tau + 2\pi j}{\tau \mid k_l \mid v_T}\right)^2\right]. \tag{38}$$

In the cold plasma or hydrodynamic limit, $\pi/(\tau k_l v_T) > \omega/(k_l v_T) \gg 1$, the following approximate expressions are obtained

$$\mathrm{Re}(W) \cong -\frac{(\frac{1}{2}k_l v_T \tau)^2}{2\sin^2(\frac{1}{2}\omega\tau)} - \frac{(\frac{1}{2}k_l v_T \tau)^4}{2\sin^4(\frac{1}{2}\omega\tau)}\left(\tfrac{3}{2} - \sin^2(\tfrac{1}{2}\omega\tau)\right) \tag{39}$$

$$\mathrm{Im}(W) \cong -\pi^{1/2} \frac{\omega}{\mid k_l \mid v_T} \exp\left[-\left(\frac{\omega}{\mid k_l \mid v_T}\right)^2\right]. \tag{40}$$

V. Summary and Conclusions

A dispersion relation for a computer-simulated plasma has been derived in which the effects of discreteness in time and space are included exactly. The method is quite general and may be applied to simulation models which contain the effects of the complete electromagnetic field, more than one species, higher dimensions and different spatial interpolation and time "integration" methods. In the limit that the mesh spacing, D, and the time step, τ, go to zero independently, the well-known results associated with the Vlasov description of a collisionless plasma are obtained.

A finite time step leads to a dispersion relation which has an infinite set of solution frequencies for a given k:

$$\omega_j = \omega_0(k) + 2\pi j/\tau, \qquad \text{for} \quad j = 0, \pm 1, \pm 2, \pm 3, \ldots .$$

These frequency aliases arise in the following way. The computational procedure requires that all functions of time be evaluated at the discrete points, $t = j\tau$. What happens in between is ignored. Obviously a number of interpolation schemes could be applied to define the quantities at intermediate times. If the interpolation schemes are restricted to those involving sine and cosine curves only, an infinite set of frequencies can still be used. These frequencies are the frequency "aliases," and all of them except the principal mode ($j = 0$), lead to interpolation schemes which are physically "unreasonable."

Numerical difficulties associated with these aliases are easily avoided in practice by making the time step short. The condition is

$$\begin{aligned} \tau &< 2\pi/(\mid \omega \mid + \mid k_{\max} v_{\max} \mid) \\ &\lesssim 2\pi/(\omega_p + \pi v_T/D), \end{aligned} \tag{41}$$

where v_{max} is the speed of the fastest particle. In practice τ must be smaller than the above restrictions since substantial numerical dispersion is introduced for $\tau \cong \pi/\omega$, or $\tau \cong \pi/(k_{max}v_{max})$. Thus to minimize numerical dispersion, one must have

$$\tau \ll \pi/(\omega_p + \pi v_T/D). \tag{42}$$

The effect of discreteness in space is quite different from that in time. As in the time a density at a discrete set of points, $x = nD$, is defined and a difference equation is used to solve for the electric field at another set of points, $x = (n + \frac{1}{2})D$. At this point, however, the similarities cease, since an interpolation procedure between the discrete set of mesh points is introduced. Thus, one is not dealing with a principal mode and its aliases, but is, instead, dealing with a very complicated mode which can be expressed as a sum over the principal mode and its aliases.

In a given system the lowest modes are best described. If the number of mesh points ($N = L/D$) is large, both the numerical dispersion and the contributions of the "aliases" to the properties of the mode can be made negligible. If one wishes a good description of the lowest l modes, then

$$D \ll L/(2l). \tag{43}$$

$$N \gg 2l. \tag{44}$$

Of interest, in addition to the above criteria on D and τ, is the question of numerical instability of any of the modes. An examination of the dispersion relation, Eq. (35), and the expression for the imaginary part of W, Eq. (40), shows that the total Landau damping of a mode is the sum of the contributions from its sinusoidal components. Moreover, the resonant interaction associated with those components having a phase velocity in the same direction as the principal component lead to damping, while those having a phase velocity in the opposite direction lead to growth. For the lower modes, the principal component dominates and Landau damping is well described. For higher modes relatively equal contribution can come from the backward components, and the possibility of instability exists. It is easy to verify that in the case $\omega D/(\pi v_\tau) \cong 3.5$, modes in the neighborhood of $k = \frac{2}{3}k_{max} = 2\pi/(3D)$ are unstable. Thus instability can occur in parameter ranges of interest. Extensive numerical work is required to delineate more completely the unstable parameter ranges.

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