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Quasi-neutral particle simulation model with application to ion wave propagation

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A new class of particle simulation models has been developed which eliminates the high-frequency space charge oscillations while keeping the low-frequency ion-density fluctuations unmodified. Physically, the quasi-neutrality is maintained as the adiabatic electrons follow the ion-density fluctuations so as to establish the Debye shielding. It is, therefore, possible to use an integration time step comparable to the characteristic time scale of the low-frequency oscillations so that realistic plasma parameters can be used in the present simulation model. Applications to ion sound wave propagation, ion-ion two-stream instability, and the low-frequency fluctuation spectrum in a magnetic field are given. The way in which to include the nonadiabatic electrons in the model is also discussed.

I. INTRODUCTION

Particle code simulation of plasmas has become a well-established branch of plasma physics and controlled fusion research during the recent years. Various nonlinear processes inherent to plasma dynamics associated with plasma heating and confinement have been studied successfully using the particle models. In the area of fusion research, neoclassical diffusion and the heating associated with the neutral beam injection are such examples. Needless to say, there are many more simulation models being developed as the demand for numerical simulations in plasma physics and controlled fusion research increases rapidly, along with the construction of large confinement devices.

It is the purpose of this paper to describe a new class of particle simulation models in which the quasi-neutral condition is approximately satisfied so that the high-frequency oscillations associated with electron inertia are eliminated. Examples of such oscillations are ion sound waves, electrostatic ion-cyclotron waves, low-frequency drift waves, trapped particle modes in a toroidal system, and magnetohydrodynamic oscillations. Several examples are shown to test the model. They are the propagation of ion sound waves, ion-ion two-stream instabilities, and the low-frequency electrostatic fluctuations in a magnetic field including the drift waves in an inhomogeneous plasma. Discussions are given as to how to include the nonadiabatic electrons.

II. MODEL

In order to develop a particle simulation model which eliminates the high-frequency oscillations, let us consider the simplest example first, namely, the one-dimensional ion sound wave in a thermal plasma. Assume a low-frequency ion-density fluctuation n_i' from its equilibrium state n_0,

$$n_i = n_0 + n_i' \ .$$

Associated with this density fluctuation is the low-frequency electrostatic potential ϕ in which the electrons quickly reach the well-known Boltzmann law

$$n_e = n_0 \exp(e\phi/T_e) \ . \tag{1}$$

The resultant potential is then determined from the Poisson equation

$$\partial^2\phi/\partial x^2 = -4\pi e(n_i - n_e) \ . \tag{2}$$

Ion-density fluctuations may be determined from the cold fluid equations

$$\begin{aligned} &\frac{\partial n_i}{\partial t} + \frac{\partial}{\partial x}(n_i v_i) = 0 \ , \\ &\frac{\partial v_i}{\partial t} + v_i \frac{\partial v_i}{\partial x} = -\frac{e}{m_i}\frac{\partial \phi}{\partial x} \ . \end{aligned} \tag{3}$$

Linearizing Eqs. (1) and (3) and assuming a phaser $\exp(i\omega t - ikx)$ for the linear quantities, density fluctuations for the electrons, the ions, and the dispersion relation are

$$n_e'/n_0 = e\phi/T_e \ , \tag{4}$$

$$n_i'/n_0 = (k^2/\omega^2)(e/m_i)\phi \ , \tag{5}$$

and

$$(k^2 + k_e^2)\phi = 4\pi e n_i' = (k^2\omega_{pi}^2/\omega^2)\phi \ , \tag{6}$$

where k_e is the electron Debye wavenumber, $k_e^2 = 4\pi n_0 e^2/T_e$. Equation (6) gives the well-known dispersion relation for the ion wave

$$\omega^2 = k^2 c_s^2 = k^2 T_e/m_i \ ,$$

for $k^2 \ll k_e^2$. When the dispersion relation is used in Eqs. (4) and (5), it is easy to show that the quasi-neutrality $n_e' = n_i'$ is satisfied automatically.

It is clear in the preceding argument that the key assumption for the charge neutrality is given by Eq. (1) or Eq. (4) where the massless electrons follow the ions adiabatically so as to screen the resultant potential. Note that the quasi-neutrality $n_i' = n_e'$ is the consequence of Eq. (4). The effect of electrons can be seen more clearly from Eq. (6) where the potential due to ion-den-

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sity fluctuation is shielded by the electrons and this is the physical interpretation of the quasi-neutrality.

In the usual particle simulation model, both ions and electrons are pushed according to the equation of motion together with the Poisson equation to determine the potential. In such a model, it is clear that the charge neutrality, Eq. (4), is not satisfied in general, since the electrons do not always follow the ions because of their inertia. In fact, it is well known that the electron and ion density fluctuations are predominantly out-of-phase, which generate very strong electrostatic space charge oscillations at the plasma frequency. This high-frequency oscillation is so strong in numerical simulations that it can easily mask the weak ion sound wave for many cases.

It is clear, from the preceding argument, that one way to guarantee the quasi-neutrality in the simulation is to assume that the electrons form a Debye-shielding cloud around the ion-density fluctuations. The Poisson equation is then modified to

$$(k^2 + k_e^2)\,\phi = 4\pi e(n_i - n_0) \tag{7}$$

together with the equation of motion for the ions

$$dv_i/dt = (e/m_i)\,E\ ,$$

$$dx_i/dt = v_i\ ,$$

to determine the ion density. Note that in this formalism, the contribution from the electrons is given totally by $k_e^2\phi$, which is valid as long as they are adiabatic. When the contribution of the nonadiabatic electrons becomes important, then Eq. (7) should be modified accordingly. This is a more difficult problem and the solution appears to depend on the problems considered. Some considerations are given in Sec. IV.

Note also that there is no approximation made for the ion dynamics in the model so that the model should be very useful in studying the nonlinear behavior of plasmas associated with ion dynamics.

The linearization of the electron Boltzmann distribution used in Eq. (7) is valid as long as the density fluctuation n_i'/n_0 is a few percent. When n_i'/n_0 becomes larger, then the linearization is not appropriate and one has to use the nonlinear Poisson equation given by

$$\nabla^2\phi = 4\pi e n_i - 4\pi e n_0 \exp(e\phi/T_e)\ .$$

It is possible to solve this by iteration for this case. First, the solution for the potential ϕ_0, using the linearized density fluctuations, is found from Eq. (7). Then, the corrected potential ϕ is found by using ϕ_0 in the electron Boltzmann distribution to solve for ϕ. One can iterate this procedure a few times until the solution converges.

So far, we have only considered the one-dimensional ion sound wave. It is clear that the model can be extended to many different cases in multi-dimensional simulations as long as the electron contribution is primarily adiabatic, which is the characteristic property for low-frequency oscillations.

The electron density fluctuation for the electrostatic waves in a magnetic field may in general,[1] be written as

$$4\pi e n_e' = k_e^2 \sum_{n=-\infty}^{\infty} \exp(-k_y^2 v_e^2/\Omega_e^2)\, I_n(k_y^2 v_e^2/\Omega_e^2) \times\left[1 + \frac{\omega - \omega_e^*}{\sqrt{2}k_z v_e}\, Z\left(\frac{\omega - n\Omega_e}{\sqrt{2}k_z v_e}\right)\right]\phi \tag{8}$$

where the magnetic field is in the z direction, $\omega^* = (cT_e k_y/eB)\,(d\ln n/dx)$ is the diamagnetic drift frequency due to plasma inhomogeneity in the x direction, Z is the plasma dispersion function,[2] and the electron distribution function is assumed to be an isotropic Maxwellian.

For low-frequency $\omega \ll \omega_{ce}$, long-wavelength $k_y^2 v_e^2/\Omega_e^2 \ll 1$ oscillations and $k_z \neq 0$, Eq (8) is reduced to

$$4\pi e n_e' = \left[1 + \frac{\omega - \omega^*}{\sqrt{2}k_z v_e}\, Z\left(\frac{\omega}{\sqrt{2}k_z v_e}\right)\right] k_e^2\phi\ . \tag{9}$$

For a small phase velocity $\omega/\sqrt{2}\,k_z v_e \ll 1$, Eq. (9) reduces to Eq. (4), and therefore, Eq. (7) should be valid as long as the nonadiabatic effect is ignored.

Needless to say, there are many cases where the small nonadiabatic effect arising from Landau or collisional damping can cause instabilities, in which case, those nonadiabatic electrons should be included in the simulation. Note also, that nowhere have we assumed $n_e = n_i$ explicitly in the model, and this is very important, since n_e is not equal to n_i for the unstable plasmas when ϕ grows to large amplitude. Such an example is the case of anomalous diffusion due to drift instabilities.

III. APPLICATION OF THE MODEL

A. Propagation of the ion sound wave

In this first example, we have considered the propagation of ion sound waves in a thermal plasma and confirmed that the model correctly produces the expected ion sound fluctuations. The simulation is carried out in one dimension using an electrostatic dipole code. As described in the previous section, only the ions are pushed and the modified Poisson equation (7) is used.

Figure 1 shows the results from such run. We use $T_e/T_i = 10$, $\omega_{pi}\,\Delta t = 0.2$ (Δt is the integration time step), $\lambda_e = \Delta = a$ (Δ is the grid size and a is the particle size), and 6400 ions. Figure 1(a) shows the time correlation function of the fourth Fourier mode and Fig. 1(b) is the power spectrum of the same mode.[3] We see a coherent wave at the expected frequency of the ion sound wave. Note that there is no electron plasma oscillation in the model and the electric field energy is less than 10^{-4} of the particle energy, which is smaller than that in a conventional particle code. This is because the low-frequency ion sound waves are quasi-neutral so that the electric field energy associated with them is very small. In thermal equilibrium, the fluctuation field energy per mode associated with the sound wave, is $L(E^2)_k/8\pi = k^2\lambda_e^2 T_e/2$ for $k^2\lambda_e^2 \ll 1$ while the energy at the plasma oscillation is $L(E^2)_k/8\pi = T_e/2$. Here, L and λ_e are the length of the system and the electron Debye length, respectively, therefore, the noise level is much lower for the present model especially for the long-wavelength modes.

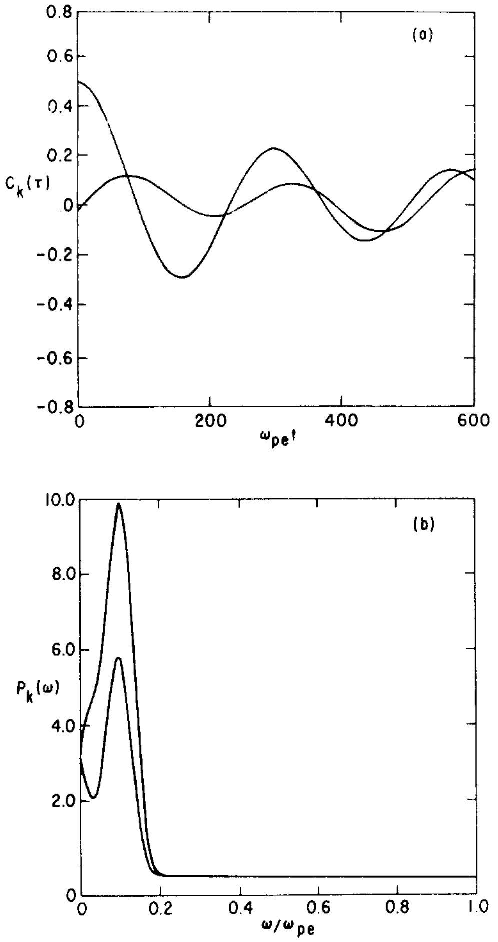

FIG. 1. Correlation function of the electric field for the fourth mode (a) and its frequency spectrum (b).

Note also that the time step used here is much larger than the conventional particle code which typically employs $\omega_{pe}\Delta t = 0.2 \sim 0.4$[3] while $\omega_s \Delta t = 0.2 \sim 0.4$ for the present model so that $\omega_{pe}\Delta t$ can be as large as $(m_i/m_e)^{1/2}$ in the present model.

Figure 2(a) shows the numerically determined dispersion relation. Note that the agreement with the theory

$$\omega_s = \frac{kc_s(1 + 3\,T_i/2T_e)}{[1 + k^2\lambda_e^2 \exp(k^2 a^2)]^{1/2}} \tag{10}$$

is excellent. Figure 2(b) indicates similar results from the second run using $\omega_{pi}\,\Delta t = 1$ and $\lambda_e = 0.2\Delta$ with the other parameters unchanged. This run is to confirm that the large time step, such as $\omega_s \Delta t \approx 0.2$ and small Debye length $\lambda_e < \Delta$, may be used in the model since there is no plasma oscillation in the model.

It is clear from these runs that the plasma oscillations are complely eliminated and that one should be able to use Δt several orders of magnitude greater than that employed in a conventional code when realistic parameters are used. Note that there was no grid instability[4] observed due to the small Debye length.

B. Ion-ion two stream instability

As the second example, let us consider an ion-ion two-stream instability excited by counterstreaming ions in a warm electron background.[5] The instability takes place only for the short-wavelength mode, $k \gtrsim k_e$, since the electrons are not able to neutralize the ion-density fluctuations completely.

The dispersion relation is given by

$$1 + \frac{1}{k^2\lambda_e^2} = \frac{1}{4k^2\lambda_i^2}\, Z'\left(\frac{\omega - kv_0}{\sqrt{2}\,kv_i}\right) + \frac{1}{4k^2\lambda_i^2}\, Z'\left(\frac{\omega + kv_0}{\sqrt{2}\,kv_i}\right) \tag{11}$$

for two equal counterstreaming ion beams. Growth rate is a fraction of ion plasma frequency, and the most unstable wavelength corresponds to $k \sim v_0/\omega_{pi}$.

Figure 3 shows the electric field energy associated with the instability, frequency spectrum, and the ion velocity distribution. The parameters of the simulation are 64 grid points, 12 800 ions, $T_e/T_i = 25$, $\lambda_e = 4\Delta$, $v_0/c_s = 0.4$, and $\omega_{pi}\Delta t = 0.2$.

After the exponential growth, the field energy saturates

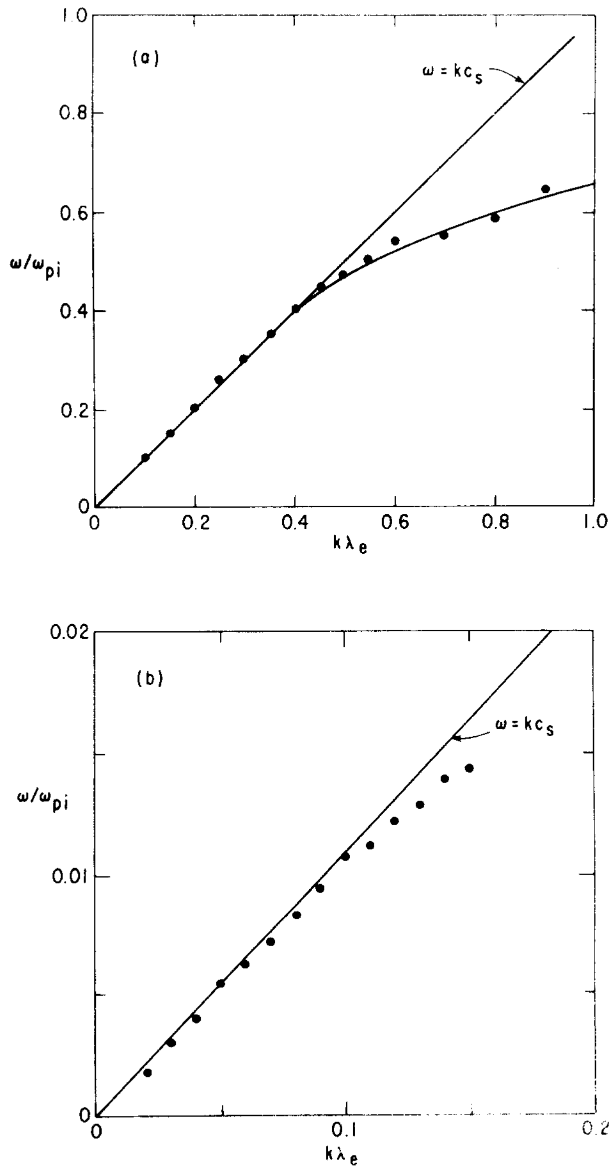

FIG. 2. Dispersion relation from the measured frequency and the comparison with linear theory.

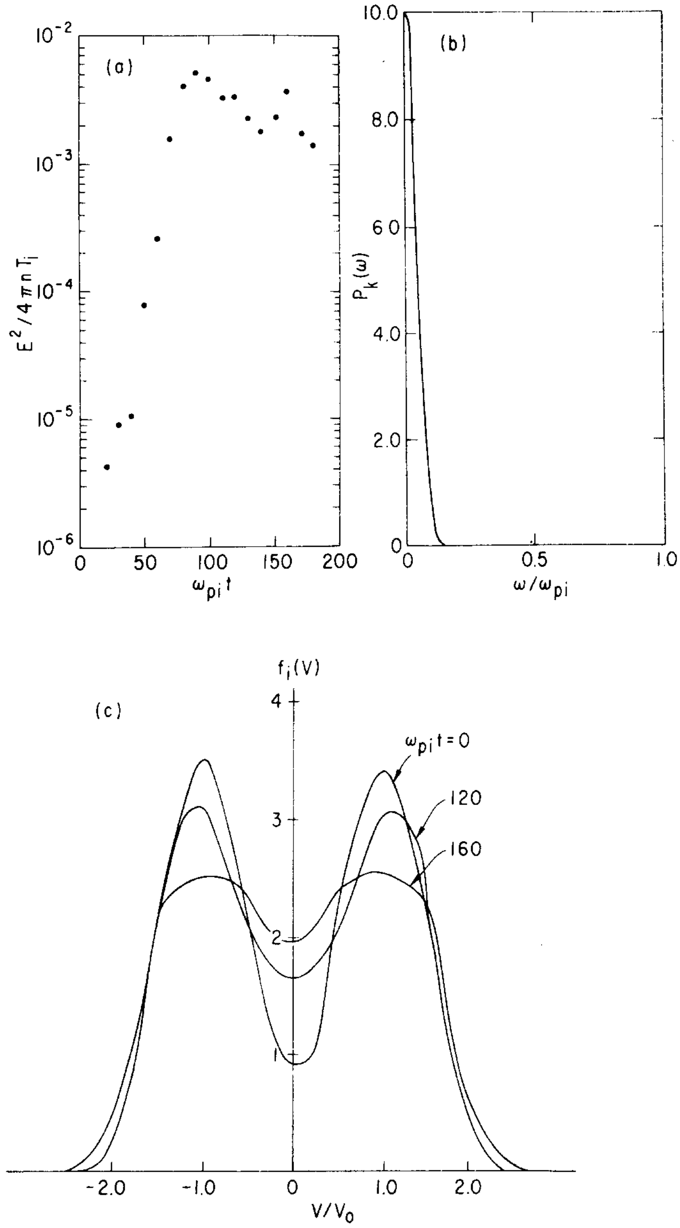

FIG. 3. Ion-ion two-stream instability. The development of the electric field energy (a), frequency spectrum (b), and the ion velocity distribution (c).

at $E^2/4\pi n T_i \sim 10^{-3}$ and the initial well-defined two-ion beams are partially thermalized by this time. Note that the initial noise is very low without using a quiet start. The frequency spectrum indicates that the instability is of the purely growing type as predicted by the linear theory. It is worth mentioning that this calculation took only a few minutes on an IBM 360/91 using a FORETRAN code. It would be very difficult to simulate this instability using a conventional particle code because of noise and computing time.

C. Fluctuations in a magnetic field

Let us consider the propagation of low-frequency ion fluctuations in a magnetic field. When an external magnetic field is imposed on a plasma, motion across the magnetic field is prohibited and quasi-neutrality is maintained as the electrons follow the ions *along* the field lines. It is clear then that the flute-type mode, $k_z = 0$, for example, may not be quasi-neutral. Furthermore, whether or not the plasma is quasi-neutral in a magnetic field is not a trivial question in an inhomogeneous plasma where the low-frequency turbulence generated by the drift-type instabilities causes the anomalous diffusion of ions and electrons which, in general, are not the same and, therefore, large charge separations are built up.[6]

The electrostatic dispersion relation for small amplitude ion oscillations in a magnetic field is given by

$$1 + \frac{1}{k^2\lambda_e^2} + \frac{1}{k^2\lambda_i^2} \times \sum_{n=-\infty}^{\infty}\left[1 + \exp(-\lambda)\, I_n(\lambda)\, \frac{\omega - \omega_i^*}{\sqrt{2}\,kv_i}\, Z\!\left(\frac{\omega - n\Omega_i}{\sqrt{2}\,kv_i}\right)\right] = 0 \qquad (12)$$

for $k_y^2\rho_e^2 \ll 1$ and $\omega/k_z v_e \ll 1$, where $\lambda = k_y^2 v_i^2/\Omega_i^2$. The interesting case is for $k_z/k_y \ll 1$ and the solutions of Eq. (12) are well-known electrostatic ion-cyclotron waves (ion Bernstein modes)

$$\omega = n\Omega_i(1 + I_n(\lambda)\, e^{-\lambda}) \ , \quad n = 1, 2, \ldots ,$$

the low-frequency ion acoustic mode,

$$\omega = k_z c_s$$

and the drift mode

$$\omega = \omega_e^*$$

in an inhomogeneous plasma. Note that lower hybrid oscillations $\omega \approx \omega_{pi}$ and oblique electron plasma oscillations $\omega = \omega_{pe} k_z/k_y$ are not the solutions of Eq. (12) since they are shielded by the electrons.

To test the dispersion relation, a frequency spectrum for the fluctuations is measured using a two and one-half dimensional model[7] with the modified Poisson equation (7). The parameters for the simulations are 64 $\times$64 grid, 128$\times$128 ions, $\omega_{pi}/\Omega_i = 10$, $T_e/T_i = 4$, $\lambda_e/\Delta = 1$, $\omega_{pi}\Delta t = 1$, and $k_z/k_y = 0.02$. Note that the choice of the time step gives $\Omega_i \Delta t = 0.1$, which is small enough to resolve cyclotron harmonics.

Figure 4 shows the power spectrum for the propagation of different values of k_z/k_y and k_y in a homogeneous plasma. It is clearly seen that several ion-cyclotron harmonics are generated slightly above the cyclotron frequency and its harmonics. For $k_\perp \rho_i \lesssim 1$, the maximum peak of the spectrum is at the cyclotron frequency, and it shifts to higher harmonics for $k_\perp\rho_i > 1$. There is also one low-frequency oscillation well below the ion-cyclotron frequency representing the low-frequency ion sound branch. These frequencies agree well with the linear theory. The field energy was only 0.1% of the ion kinetic energy in spite of the use of only four particles per cell. Since the electrostatic ion-cyclotron harmonics are correctly simulated in this model, one can use the model, for example, to study the ion beam-induced cyclotron instabilities associated with neutral injection into a tokamak.[8]

Figure 5 shows the power spectrum of the fluctuations in an inhomogeneous plasma using the two and one-half

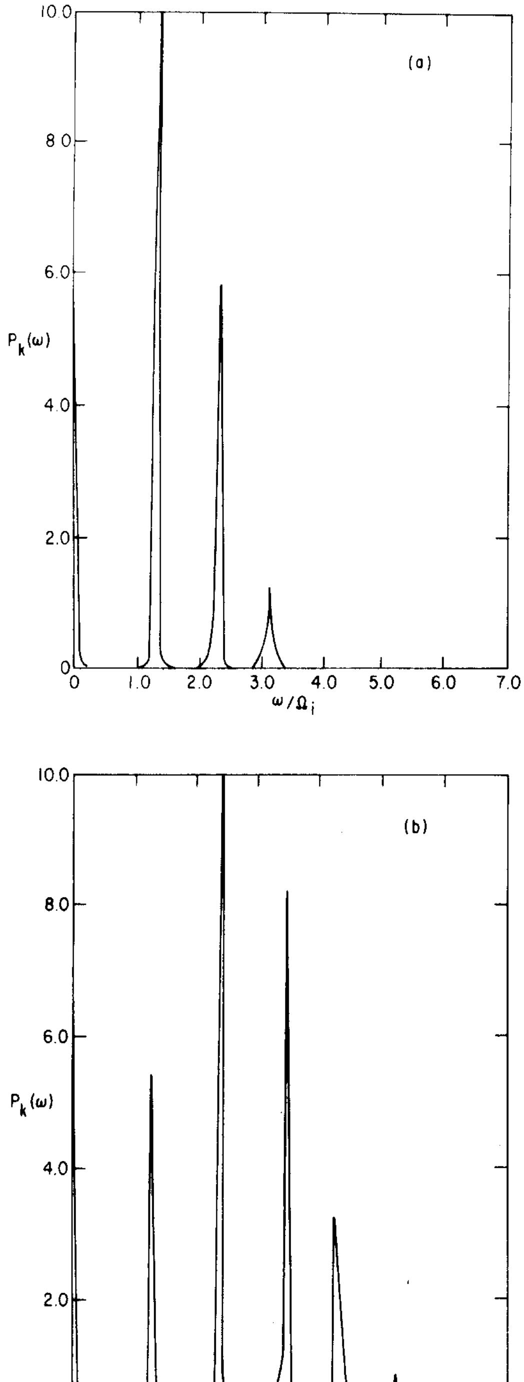

FIG. 4. Frequency spectrum for the ion fluctuations in a homogeneous plasma in a magnetic field. $k_z/k_y = 0.02$ and $k_y\rho_i = 1$ (a) and $k_y\rho_i = 1.5$ (b).

dimensional model. In addition to the ion-cyclotron harmonics, low-frequency drift oscillations can be clear ly seen in the figure. The observed frequency is larger than the ion sound frequency in homogeneous plasma shown in Fig. 4 and is close to $\omega = \omega_e^* \beta/(2-\beta)$ as predicted from the linear theory where $\beta = e^{-\lambda} I_0(\lambda)$ with $\lambda = k_\perp^2 \rho_i^2$. The parameters of the simulation are the same as before except for the inhomogeneous density profile in the x direction, which is taken as a hyperbolic tangent.[7] The observation of low-frequency drift oscillations $\omega \ll \Omega_i$ using realistic plasma parameters is quite encouraging and the model may serve as an important tool for the study of nonlinear development and anomalous diffusion due to drift instabilities in three-dimensional cylindrical and toroidal simulations.[9] These calculations using the two and one-half dimensional model took 0.5 h or so on an IBM 360/91 for each case.

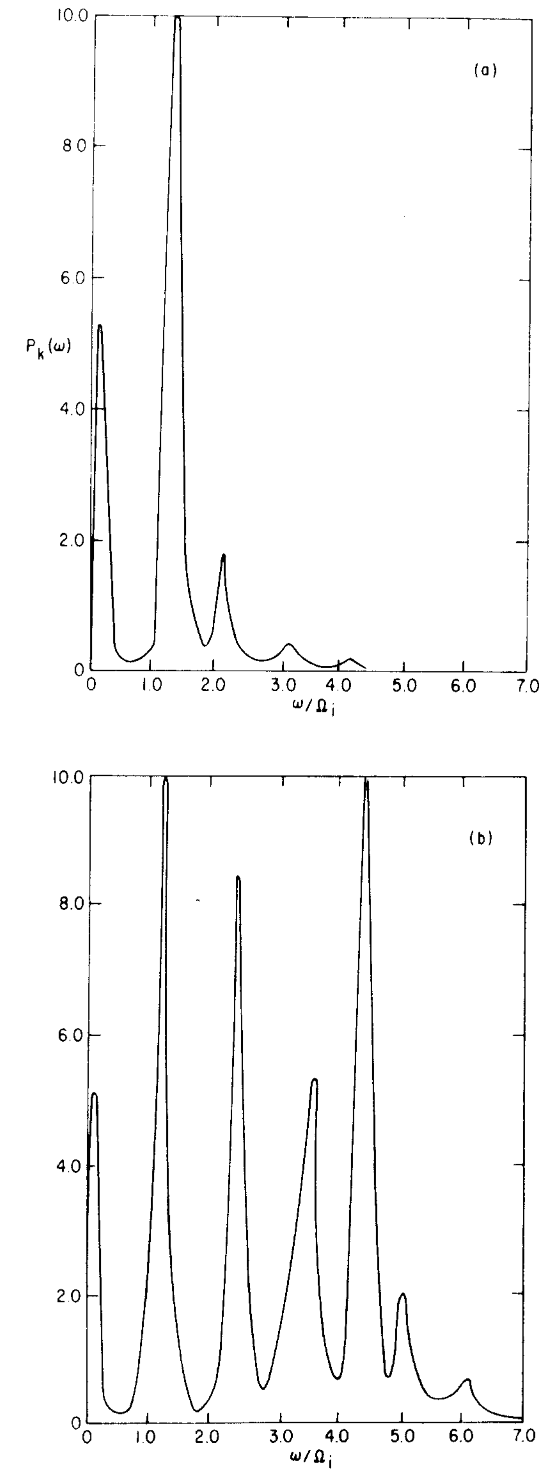

FIG. 5. Frequency spectrum in an inhomogeneous plasma. $k_z/k_y = 0.02$ and $k_y\rho_i = 0.5$ (a) and $k_y\rho_i = 1.5$ (b).

IV. DISCUSSIONS ON THE NONADIABATIC ELECTRONS

We have shown that the quasi-neutral simulation model discussed previously is very useful for the low-frequency oscillations associated with ion dynamics and makes it possible to use realistic parameters in the simulation. In this section let us consider the possibilities of including nonadiabatic electrons in order to model the Landau or collisional damping in the simulation. While we have not solved this problem completely, two different methods have been tried.

The first model, which may be called a quasi-linear model, is to include linear Landau damping in the Poisson equation. For the case of a one-dimensional ion sound wave, the electron Landau damping may be given by

$$\frac{\gamma}{\omega}=\left(\frac{\pi}{2}\right)^{1/2}\frac{c_s}{v_e}\exp\left(-\frac{c_s^2}{2v_e^2}\right) \tag{13}$$

for a Maxwellian velocity distribution where $\omega = kc_s$. The Poisson equation (7) is now modified to

$$[k^2+k_e^2+i(\pi/2)^{1/2}k_e^2(c_s/v_e)\exp(-c_s^2/2v_e^2)]\,\phi = 4\pi e(n_i-n_0) \tag{14}$$

which gives the correct electron-Landau damping when the linear response for the ion-density fluctuation Eq. (5) is used. The Landau damping given by Eq. (13) must be determined from the instantaneous electron velocity distribution. Therefore, in this model, electrons must be pushed in the simulation only to determine the Landau damping rate. Furthermore, only the quasi-linear diffusion is included for electron nonlinearity. This method may be used for collisional plasmas.

The second model is more general and can be fully nonlinear. In this model, the resonant electrons are separated from the adiabatic electrons and are followed as the discrete particles in the simulation. The phase velocity of the ion sound or drift waves is, in general, much smaller than the electron thermal velocity, $\omega/k_z \ll v_e$, and therefore, resonant electrons are low-energy particles. The fraction of the resonant electrons is small as long as $e\phi/T_e$ is small.

The Poisson equation is modified to

$$(k^2+k_e')\,\phi = 4\pi e n_i - 4\pi e n_e^r , \tag{15}$$

where $k_e'^2$ is the effective Debye wavenumber of the adiabatic electrons and n_e^r is the density of the resonant electrons, which are followed in time as discrete particles. A resonant particle may be defined as a particle whose velocity along the field line $v_{j\parallel}$ lies

$$|v_{j\parallel}-\omega/k_\parallel| \lesssim (e\phi/m_e)^{1/2} ,$$

where $\omega/k_\parallel = \pm c_s$ for the case of ion sound. In the simulation, one has to follow *all* the electrons, not just the resonant electrons, to calculate the charge density for the resonant electrons in the Poisson equation. The reason for this is that the resonant electrons are low-energy particles which have very large diffusion coefficients in velocity space. Therefore, an electron which is in the resonant region can move to the nonresonant region in a very short time. Of course, the inverse process can take place just as often. Only those particles whose velocity along the field line satisfies the resonant condition do contribute to the charge density in the Poisson equation. Note that those low-energy resonant electrons do not emit high-frequency plasma oscillations. Since the velocity of low-energy electrons is small, one can again use a large step of integration even in the presence of discrete electrons for the present case.

Simulations of the ion sound instability excited by the electron drift through the ions have been performed using a one-dimensional model. The parameters of the simulation are 64 grid, $m_i/m_e = 2500$, 12 800 ions and electrons, $\lambda_e/\Delta = 1$, $T_e/T_i = 25$, $v_0/v_e = \frac{1}{2}$, and $\omega_{pe}\Delta t = 4$. The resonant electrons are the particles whose velocities satisfy $|v-c_s| \lesssim (e\phi/m_e)^{1/2}$. Figure 6 shows the development of the total field energy due to the instability and the distribution function. There are more than 15 modes unstable in the system. The instability is found to saturate at quite a low level of $E^2/4\pi n T_e < 10^{-4}$, and we find the formation of a velocity space plateau at around the phase speed of the wave which is the sound speed in this case. The growth of each Fourier mode roughly agrees with the linear theory; however, considerable fluctuations in the energy of each Fourier mode are also found.

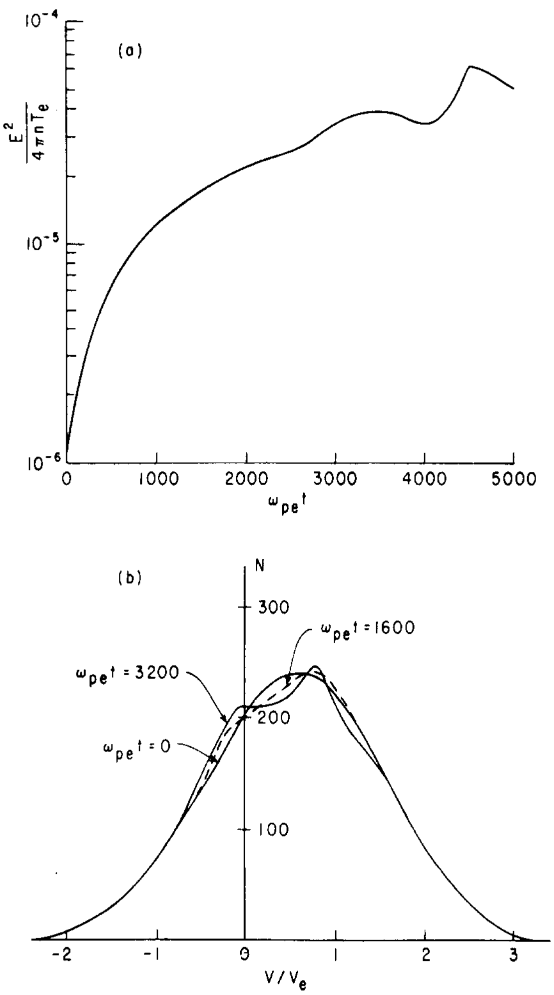

FIG. 6. Ion sound instability due to electron drift through ions. Total field energy (a), and the electron velocity distribution (b).

Whether or not one can extend this method to more complex problems such as drift wave instabilities in toroidal devices remains to be seen. The problem of separating the resonant and nonresonant electrons is rather subtle,[10] and it appears one has to try and see if this method works for the problems considered. When the amplitude of the low-frequency fluctuations becomes large approaching $e\phi/T_e \approx 1$, then it is clear the fraction of resonant electrons becomes large and the method described here will not be applied.

V. CONCLUSIONS

A quasi-neutral particle simulation model has been developed by assuming the adiabatic electrons form a Debye shielding cloud around the ion-density fluctuations. The model correctly produces the low-frequency ion oscillations while eliminating the high-frequency fluctuations. The noise level in the simulation is quite low compared with particle energy because of quasi-neutrality. Very large time steps can be taken so that the multi-dimensional simulations using realistic parameters may easily be carried out using the present model. A very important feature of the model is that $n_e = n_i$ is not assumed anywhere in the code and in fact, the model can follow $n_e \neq n_i$ whenever a strong electric field and therefore space charge separations are generated due to plasma instabilities. How to include the nonadiabatic electrons, in general, is a subtle problem and appears to depend on the case.

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