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Simulation of Dust-Acoustic Waves

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Abstract. We use molecular dynamics (MD) and particle-in-cell (PIC) simulation methods to investigate the dispersion relation of dust-acoustic waves in a one-dimensional, strongly coupled (Coulomb coupling parameter = Γ = ratio of the Coulomb energy to the thermal energy = 120) dusty plasma. We study both cases where the dust is represented by a small number of simulation particles that form into a regular array structure (crystal limit) as well as where the dust is represented by a much larger number of particles (fluid limit).

Introduction

Plasmas are generally characterized by a large number of collective modes of oscillation. The addition of dust grains to a plasma can modify existing modes or excite new waves (1-3). High frequency modes (>> frequencies associated with the dust) can be altered, because the dust is charged and can modify the number of unattached electrons in the system or the relative drift between the plasma electrons and ions. More interesting effects occur at lower frequencies, where the dust dynamics enters directly. Since the dust charge q_d can be large, typically 10^3 - 10^5 electron charges, and the dust mass m_d is also large (~ 10^{12} proton masses for a one micron radius spherical grain), the charge to mass ratio of dust grains is very small, $q_d/m_d << 1$; however, the dust plasma frequency, ~ $q_d/m_d^{1/2}$, can be significant. Both electrostatic and electromagnetic modes involving dust exist, and many have been studied analytically. One of the most interesting wave modes is the dust-acoustic mode (4-5), which results from the oscillatory motion in a plasma with two species of widely differing masses, in this case dust and plasma ions, rather than electrons and ions. Dust-acoustic waves have been studied in a number of laboratory experiments

(6-8), in which the basic dispersion properties of the waves have been measured. Dust-acoustic waves are also though to occur in space, such as in the E-ring in the inner magnetosphere of Saturn (9-10).

While one thinks of plasma as being in a gaseous state, it has been shown experimentally in the last few years that dust grains in a plasma can form into a regular crystalline lattice (11-13). By adjusting the parameters of the plasma discharge, the "plasma crystal" can melt, i.e., be changed into a liquid or a gas. The plasma crystal is thought to be analogous to other Coulomb systems that can exist in a solid state when the coupling parameter, Γ, the ratio of the Coulomb energy to the thermal energy, exceeds ~ 170. Since the charge on a dust grain can be very large, it is possible achieve dusty plasmas with $\Gamma \sim 10^3$ - 10^5. The plasma crystal is easily observed with a scanning laser and a video camera, and forms in a few seconds. Dust-acoustic waves can be excited in these plasmas by applying a small voltage pulse to a probe in the discharge. The characteristics of the waves can be used to determine properties of the dust grains, such as their charge and screening length (7). Like ordinary solids, low-frequency waves in a plasma crystal may exhibit dispersion properties that depend on the lattice (14,15). However, the measured wave properties in these systems seem to correspond to those obtained from simple fluid theory (7). Enhanced fluctuations are also associated with the melting of the crystal (11,16,17). In addition, strongly coupled plasma effects may occur in these systems (18,19), although they do not appear to be significant in present experiments.

In this paper we discuss properties of dust-acoustic waves generated by computer simulation. As described previously, there is general interest in the properties of the waves in both the fluid limit when the dust is continuously distributed, which is how most theoretical treatments of wave properties in a dusty plasma are formulated, as well as in the crystalline phase, when the dust consists of a few large grains collected into a regular lattice. The possible existence of lattice vibrations and strongly coupled effects in such systems is also of interest. Simulations allow the properties of the waves to be studied in the absence of complicated effects, such as variable grain charge, collisions with the background neutral gas, spatial inhomogeneities, boundary effects, etc., although such effects could be addressed by calculations in the future.

Since the background plasma primarily provides shielding, the most straightforward simulation model is molecular dynamics (MD) that calculates directly the interaction of N_d dust grains with fixed charge and mass (20-22). Each grain is characterized by a screened Coulomb (Yukawa) potential, which takes into account the effects of the background plasma. The MD approach allows the grains to interact at distances shorter than a Debye length. Hence, strongly coupled plasma and lattice effects at short wavelength are also included directly. An alternative approach is to again treat the grains as discrete particles, but use a grid to compute the fields that the particles experience. In this particle-in-cell (PIC) method, the plasma electrons and ions are treated as a Boltzmann fluid at constant temperature (23). One simulates this system in the usual manner, using PIC methods for the grain dynamics and solving Poisson's equation to obtain the electric field (24). While our eventual goal is the study of dust-acoustic-like fluctuations in laboratory experiments, we realize the need to start at a fairly elementary level and address some of the most fundamental issues first. Thus, we concentrate on one-dimensional systems in which the dust is considered either as very fine grains, which can be modeled as a fluid, or as massive grains, as one finds in a plasma crystal. A more complete report of this work has been submitted elsewhere (25).

Theory and Simulations

We consider low-frequency electrostatic waves in a dusty plasma. The plasma is characterized by ions of number density n_i, charge $Z_i e$, mass m_i, and temperature $T_i = 1/2 m_i v_i^2$, and electrons of density n_e, mass m_e, charge $-e$, and temperature $T_e = 1/2 m_e v_e^2$. The dust grains are all assumed to be the same size (spherical with radius a), with mass m_d, charge $q_d = Z_d e$ (<0), and temperature T_d. The dust charge density n_d then relates the electron and ion densities through the condition of charge neutrality. We define the dust plasma frequency $\omega_d = (4\pi n_d Z_d^2 e^2/m_d)^{1/2}$ and $k_D = \lambda_D^{-1} = (\lambda_{De}^{-2} + \lambda_{Di}^{-2})^{1/2}$, where $\lambda_{D\alpha} = (T_\alpha/4\pi n_\alpha Z_\alpha^2 e^2)^{1/2}$ is the Debye length for the α–th species. When $T_e \sim T_i$, and ($n_e \sim n_i$), $\lambda_D \sim \lambda_{De}$, while for $T_e >> T_i$, which will be valid for most of the results presented in this paper, $\lambda_D \sim \lambda_{Di}$.

The dispersion relation relating the frequency of the waves ω to the wavenumber k for dust-acoustic waves [e.g., Eq. (11) of Ref (9)] is readily obtained by linearizing and combining the continuity and momentum equations for all three species in standard fashion (4,5,9). This dispersion relation is modified by several effects that are important in various applications of dust-acoustic waves. First, dust-acoustic waves are often observed in dusty plasma crystals. The presence of dust-acoustic fluctuations can be related to the periodicity of the lattice and seem to be associated with the melting of the crystal (11,16). Dust-acoustic-like lattice waves have been analyzed using well known techniques from solid state physics (15,26). A simple expression involving nearest neighbor interactions is given in Ref. (15) [Eq. (20)]. Strongly coupled plasma effects may also occur in dusty plasmas, which are characterized by the Coulomb coupling parameter Γ. Strongly coupling ($\Gamma > 1$) can occur when the grains are fairly big (> few micron in radius), since the dust charge can be very large. For large Γ (> 170 for 3-D systems, > 120 for 2-D systems) strong coupling effects are manifested in the formation of crystalline-like structures in the dust. However, such effects can also be considered in the limit of smaller grains, where fluid theory applies. In this regime, strong coupling effects have recently been considered theoretically by Rosenberg and Kalman (18) and Murillo (19). The analysis in Ref. (18) gives expressions that are valid in the long wavelength limit. Equation (xx) of Ref. (19) is a more approximate expression in which the strong coupling correction is an average over a range of Γ's.

To show how these effects modify the dispersion relation in a quantitative manner, we consider a set of specific parameters, which are roughly based on typical experimental conditions in rf discharges, that will be used throughout the study. Using ion quantities as normalization, with $Z_i = 1$, we assume $n_d/n_i = 10^{-4}$, $Z_d = -2000$, $T_d/T_i = 1$ and $m_d/m_i = 10^{12}$. This further implies, $n_e/n_i = 0.8$, and assuming $T_e/T_i = 40$, $k_D \sim \lambda_{Di}^{-1} = k_i$. Using $n_d d^3 = 1$, implies a particle spacing d of $k_i d = 5.3$. For the above parameters, one finds the coupling parameter $\Gamma \sim 120$ for $T_d/T_i = 1$.With these parameters, the dispersion relation including the various additional effects can be plotted. The fluid dispersion relation for these parameters is plotted in Fig. 1 as a solid line. The real frequency ω is linear at small k, and bends over as k/k_i approaches unity. Superimposed on the figure is the dispersion relation modified by the lattice (dashed line) and strongly coupled effects (dotted line). At short wavelengths, the strongly coupled effects (19) lead to a reduction of the frequency. Lattice effects (15) lead to an even larger reduction of the frequency compared to the fluid case. For short wavelengths where $kd > \pi$ ($k/k_i = 0.6$), the wave dispersion becomes negative; for $kd = 2\pi$, the frequency is roughly zero.

To study dust acoustic waves numerically, we employ both particle-in-cell (PIC) and molecular dynamics (MD) methods. MD methods are conceptually simpler, in that one computes directly the 2-body interactions between N_d charged dust grains. By including all the interactions, one treats both short range and long range interactions

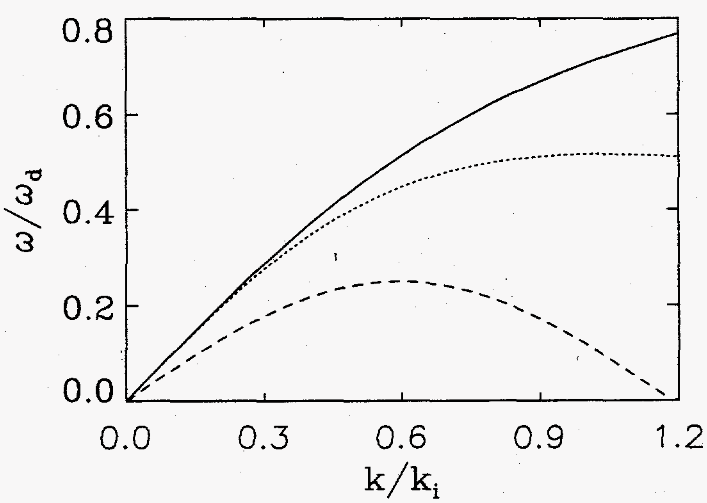

FIGURE 1. Real frequency ω, normalized to the dust plasma frequency ω_d, versus wavenumber k, normalized to the inverse ion Debye length k_i, as computed from: fluid theory (solid curve), fluid theory with strongly coupled correction (dotted curve), and lattice dynamics (dashed curve).

identically. The effect of the background plasma is included as the shielding around each of the grains, with the potential surrounding each particle assumed to be a shielded Coulomb (Yukawa) potential. MD simulations generally are characterized by rather high noise levels, due to the short-range interactions. And because of the need to resolve each grain-grain interaction, the time step is relatively small. Increasing the particle number decreases the intergrain particle spacing and thus leads to small time steps and longer computer runs. This is offset by the ability to model short-range interactions self-consistently and the simplicity of extending the calculations to three dimensions. For doing complex problems, there are sophisticated methods available to make MD more efficient (20), but for the one-dimensional calculations to be presented here, they are not necessary.

While direct, MD-like methods were used in the early days of numerical simulation of collisionless plasmas, PIC methods replaced them in the early 70's. In the PIC method, the electromagnetic fields that the particles experience are stored on a grid (24). The field information at the grid points located on either side of each particle is interpolated to the particle position to determine the instantaneous force by which the particle is advanced to the next time level. After the particles are moved, their charges and currents are interpolated back onto the grid. The electromagnetic fields are then solved on the grid. This method of interpolation between particles and grid has the advantage that short-range interactions are smeared out, reducing the level of fluctuations considerably. Further smearing of the short-range forces occurs because of additional smoothing that can be applied to the source terms when the solving the field equations. Long range interactions are essentially similar to the MD approach. In the case of PIC, one can use only a few simulation particles to represent the large grains in a dusty plasma crystal (23,27), or many simulation particles to represent a quasi-continuum of dust grains as would be described by fluid theory (28). PIC methods are more efficient when many particles are employed. One can show that PIC methods require only $N_d \log N_d$ interactions per time step, compared to N_d^2 for MD. However, PIC calculations in more than one spatial dimension require some effort to solve the field equations. In the calculations to follow, we consider only electrostatic interactions and hence just solve Poisson's equation. We assume that all the dust grains have an identical, fixed charge, but one could also imagine allowing the grain charge to vary in time or having a distribution of charges/sizes.

The PIC and MD simulations carried out in this study have been initialized in the same manner. Particles are placed in the simulation domain at equally spaced positions and given random thermal velocities. Periodic boundary conditions are used for both particle motion and the electric field. Due to the development of fluctuations, the particles acquire random displacements from these positions. After some time interval (usually $\omega_d t = 50$), a collision operator is turned on to cool off the particles to a prescribed temperature. In all of the simulations, we use a similar time-step, $\omega_d \Delta t = 0.05$. The simulations are run (after the initial randomization and cooling period of

$100\omega_d^{-1}$) for $410\omega_d^{-1}$, during which time (8192 time steps) we collect the electrostatic potential on the grid. The grid consists of 128 equally spaced positions for a system length of $Lk_i = 85$. In the case of the MD simulations, where no potential profile or even a grid is needed, we calculate the potential on a fictitious grid in the same manner as for the PIC simulations. We then Fourier transform the data in space and time. For each wavenumber, we obtain a spectrum of frequencies. The spread of frequencies about the mean is about 5-10%. From suitable wave-power averaged frequencies, we compute a mean frequency ω for each wavenumber, k. We will show plots of the dispersion relation, ω versus k, for the various runs we discuss.

We will consider two limiting cases. To model dusty crystal-like structures in both MD and PIC simulations, we use 32 particles in the simulation. For the parameters given above, this corresponds to a particle spacing of about one electron Debye length (5 ion Debye lengths), with $d = n_d^{-1/3}$. In the PIC simulations, this corresponds to about one particle every four computational cells. For the PIC calculations, we will also consider the fluid limit, where the dust is presented by roughly 100 particles per cell. In this case, the particle number is so large and the interparticle spacing is so small that MD methods are impractical. In these calculations we show only results with Γ = 120. Other simulations (25) consider a range of Γ's, include collisional effects and plasma flow, and address numerical issues associated with the different simulation techniques.

We begin with MD simulations for a plasma crystal containing 32 dust grains. The results are shown in Fig. 2, in a format used in subsequent plots. Plotted in the top panel as curves are the dispersion relations from Fig. 1 (solid curve, fluid theory; dotted curve, fluid theory with the strongly coupled correction; dashed curve, lattice theory). Superimposed on the figure are closed circles that represent the real frequency ω measured in the simulation as a function of wavenumber. In these calculations one finds that a regular crystal structure forms. The points on the graph correspond rather closely to the dispersion relation predicted by the lattice theory (15), with the frequency dropping to near zero at $k/k_i = 1.2$, corresponding to $kd = 2\pi$. The bottom panel shows the wave intensity in each wavenumber P(k) in arbitrary units. Out to about $k/k_i = 0.9$, the spectrum is relatively flat, but the wave levels increase at shorter wavelengths due to the large interparticle fluctuations.

Results of PIC simulations using the same number of particles are shown in Fig. 3. One sees in comparing with Fig. 2 that the results are very similar, showing wave dispersion characteristic of a solid lattice. In the PIC simulations, the frequency for the lattice waves is slightly larger than the theoretical value (and the value obtained in the MD calculations). Because of the sharing of charge between gird points used in the PIC method, this suggests that the average particle spacing is slightly smaller than d, so that ω is slightly larger (15). This conjecture has been confirmed by redoing the simulations using a nearest grid point method of charge accumulation instead of distributing the charge between the two neighboring grid points (24). Moreover,

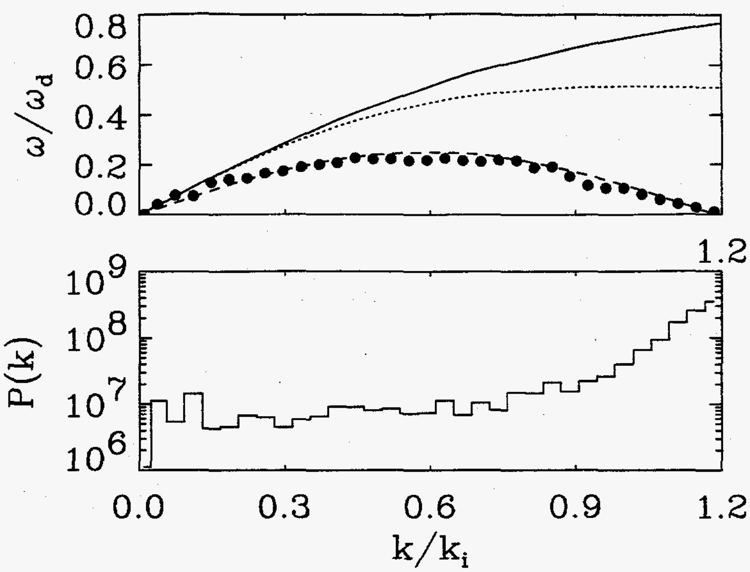

FIGURE 2. (top panel) ω versus k from MD simulations with N_d=32; (bottom panel) corresponding wave intensity P(k). Curves in this and subsequent figures are the theoretical results from Figure 1.

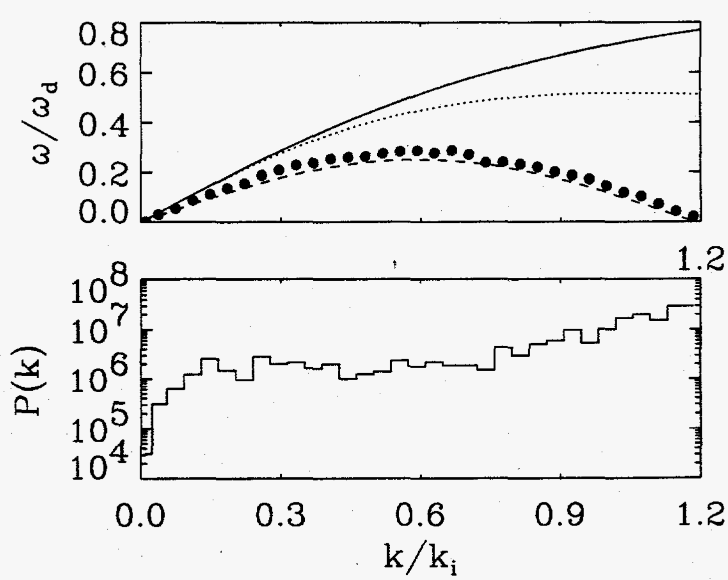

FIGURE 3. ω versus k and P(k) from PIC simulations with N_d=32.

comparing the bottom panels in these two figures, one sees that the PIC simulation is about an order of magnitude less noisy that the MD calculation, again due to the inherent smoothing associated with the accumulation of charge on a grid to solve for the electric field, rather than doing direct interactions between the grains.

We now contrast these results with a PIC simulation in the fluid regime, where the dust is represented by 100 macroparticles per computational cell (i.e., 12800 total particles). In this case, discrete effects should be negligible and one should recover the wave properties obtained from the fluid equations. As is expected, the results in Fig. 4 show a dispersion relation that resembles the fluid dispersion relation at long wavelengths, but with the strongly coupled correction (19) at short wavelengths. The corresponding wave power spectrum increases with k, and is about two orders of magnitude smaller than in the previous PIC case, The noise level is significantly reduced due to the use of many simulation particles in each cell to represent the dust. This reduces the fluctuations in the charge density and hence in the electric field.

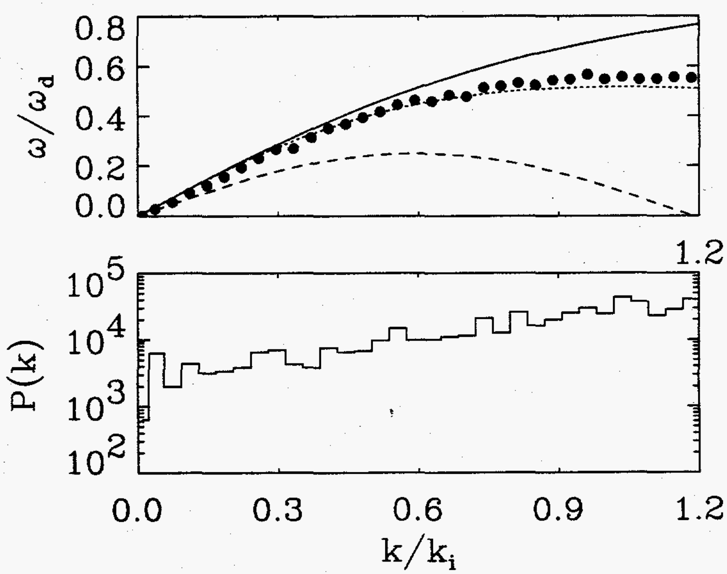

FIGURE 4. ω versus k and P(k) from PIC simulations with N_d=12800.

Summary

In this paper we have discussed the use of molecular dynamics (MD) and particle-in-cell (PIC) techniques in modeling low-frequency wave behavior in a strongly coupled dusty plasma. We have used these techniques to model dusty plasmas both in the limit where discreteness effects of the dust can be ignored and the resulting system can be described by fluid equations as well as in the limit where the dust grains are large and form into a regular, lattice-like array. In this second, so-called crystal regime, we have shown that MD methods are able to accurately simulate lattice waves when the dust is relatively cold and the coupling parameter Γ is large enough that the solid state is achieved. As one includes all the two-body interactions between grains in this method, MD simulations work best when the particle number is relatively small. On the other hand, PIC methods, which treat the grain-grain interactions indirectly through the medium of a grid on which moments are collected and the field equations are solved, have been shown to accurately model dusty plasmas in the absence of discreteness effects, i.e., the fluid regime, but modified by strongly coupled plasma effects. The crystal limit can also be modeled by PIC methods, whenever there are sufficiently few particles (e.g., about one particle every four cells) that discreteness effects appear. In this limit, with relatively few particles, PIC methods are about as computationally efficient, have lower overall noise levels, but are somewhat less accurate for doing short range interactions, than MD methods. This is particularly true when the calculations are extended to multi-dimensions.

In an actual dusty plasma experiment, the strongly coupled crystalline state is fairly each to create, using rather large grains (5-10 µm radius). Smaller grains have less charge and hence Γ is reduced, but strong coupling ($\Gamma > 1$) can be realized in these systems as well. Dust acoustic waves provide a good diagnostic to measure properties of the dust, such as their charge and screening distance (7). This may be especially useful for smaller grains (< 1 µm), which are not readily detected by present laser scattering techniques.

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