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Monte Carlo simulation in a strongly coupled linear chain

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Abstract. Monte Carlo simulation is conducted for a strongly coupled one-dimensional confined-particles system. We deal with an infinite chain of positively charged dust particles. The particles interact through the Yukawa screened potential. It is found that a critical value exists for the number of closest neighbors that are involved in the interaction. The inter-particle distance at equilibrium is found. Using these results, we study the dust-acoustic as well as the dust-lattice modes for two situations. In the first we neglect the friction force while in the second situation the presence of an ambient gas in plasma is considered.

1. Introduction

Strongly coupled dusty plasma is a system in which the Coulomb interaction energy exceeds the kinetic energy. In such a situation the particles are able to organize themselves into an ordered structure, i.e. a Coulomb or plasma crystal [1]. From the first theoretical prediction of Wigner there has been increasing theoretical as well as experimental works on two- and three-dimensional plasma crystals [2, 3]. Using the usual plasma of ions and electrons it is difficult to observe such systems in the laboratory. More attention has been paid to the study of the strongly coupled system of dust grain particles. These particles, owing to their big charge, are often in a strongly coupled regime [4]. In this case it is possible to have the particles self-organized, yielding the formation of plasma crystals. The plasma crystals show a fascinating range of physical phenomena making them suitable model systems for fundamental physics research. The background configurations, phase transition or new mode excitation are examples of such phenomena [5]. In addition, dust crystals can be formed from man-made micro-sized dust grains and can be observed in real-time directly or by means of a charge coupled device (CCD) camera [6].

Recently it has been possible to make one-dimensional chains from condensed matter with low dimensionality [7, 8]. The chain is formed from massive highly charged dust particles which can be positively or negatively charged. Owing to different charging processes it is possible to have both charged dust particles in the same situation [9]. Thus, the one-dimensional crystals support different kinds of waves such as acoustic or lattice waves [10, 11]. The dust lattice waves result from the oscillation of regularly spaced particles in the horizontal direction. It has been shown that the grain oscillation in the vertical direction can lead to a low-frequency mode characterized by an inverse optic mode-like dispersion [12]. This

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suggests that the dust crystals can be used to study the properties of crystalline solids related to phase transition and wave propagation. Moreover, the presence of dust particles in plasma can alter the high-frequency modes by changing the ions or electrons drift velocities when charging processes occur on the dust surface. However, the low-frequency modes are governed by the dust dynamics. The dust-acoustic mode is one of the most widely investigated analytically or numerically in both weakly and strongly coupled plasmas [13]. In dust crystals, the dust-acoustic waves (DAWs) can be excited by low-voltage pulses and can be used to determine the dust characteristics. In the laboratory the direct measurement of DAWs in a strongly coupled regime has been performed for krypton plasma. Low-frequency compressional waves were also observed. The shielding length and dust plasma frequency have been measured directly [14].

For many dust-particle systems, Monte Carlo simulations have been used in different situations to find the background configuration or the melting process. Using a Monte Carlo method, it has been possible to study the background configuration of finite classical two-dimensional systems. In this case the particles which are electrons or ions are confined by hard-wall or parabolic potential. Such a system shows a shell structure which depends on the total number of particles [15]. Monte Carlo simulation has also been used in quasi-one-dimensional systems of charged particles interacting through the screened Yukawa potential. The Yukawa systems are of special interest, the interaction depends on the screening parameter which allows the behavior to vary between systems governed by short-range and long-range forces [16]. The dust characteristics can allow the force to change from attractive to repulsive. This situation leads to more difficulties in finding the distance between particles, in particular when the number of particles is large.

Monte Carlo simulation has also been used to investigate the ground-state configuration and structural transition in a quasi-one-dimensional multi-chain with an infinite number of classically charged particles. The particles crystallize in a certain number of chains [17]. The effect of friction on the normal mode of a quasi-one-dimensional system has been studied, and it was shown that the free oscillations of the system are exponentially damped in time [18]. In this paper we deal with a one-dimensional chain of an infinite number of positively charged dust particles. The particles interact through Yukawa potential. In Sec. 2 we derive the dispersion relation for dust-acoustic and dust-lattice modes. Section 3 is devoted to outlining the numerical simulation method and commenting on the results while in Sec. 4 we give a summary of the results.

2. Model

The one-dimensional motion along the x-axis for a set of equally spaced identical particles is governed by the following equation of motion

$$\frac{d^2x_i}{dt^2} + \nu\frac{dx_i}{dt} = \frac{qE}{m}(x_i, t). \tag{1}$$

Each particle is a dust grain with positive charge $q = Ze$ and mass m. The second term on the left-hand side of (1) stands for the friction force acting on the particle. The coefficient ν is the friction frequency. The electric field $E(x_i, t)$ on each particle is the result of Coulomb interaction between the particle and the closest neighbors which are involved in the interaction. Let us consider only the closest N neighbor

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particles which have a significant contribution on the electric field. The dusty plasma is a sustained system, which needs the permanent presence of charged particles, i.e. electrons and ions. As a result the electric field is shielded beyond a distance greater than the Debye length λ_{D}. Hence, the expression of the electric field can be found from the Yukawa potential which stands for the screening effect:

$$V(r) = \frac{Ze}{4\pi\epsilon_0 r}\exp\left(-\frac{r}{\lambda_{\mathrm{D}}}\right), \tag{2}$$

where r is the distance between the particles with the rank in the chain i and l, $r = |x_i - x_l|$. The coordinates are measured from the center of the chain. In this work the screening parameters are given by

$$\frac{1}{\lambda_{\mathrm{D}}^2} = \frac{1}{\lambda_{\mathrm{De}}^2} + \frac{1}{\lambda_{\mathrm{Di}}^2}, \tag{3}$$

where $\lambda_{\mathrm{Di,e}} = (k_{\mathrm{B}}T_{\mathrm{i,e}}\epsilon_0/(n_{\mathrm{i,e}}e^2))^{1/2}$ correspond to the ion and the electron Debye length. In the case of quasi-neutrality and thermal equilibrium we have $\lambda_{\mathrm{D}} = 0.6$ mm, and the numerical values the densities $n_{\mathrm{i,e}}$ and temperatures $T_{\mathrm{i,e}}$ are those of [8].

First we neglect the friction force and put $\nu = 0$. The equation of motion is written as

$$\frac{d^2x_i}{dt^2} = \sum_{l\neq i}^{N}\frac{(Ze)^2}{4\pi\epsilon_0 m}\left(\frac{1}{|x_i - x_l|^2} + \frac{1}{|x_i - x_l|\lambda_{\mathrm{D}}}\right)\exp\left(-\frac{|x_i - x_l|}{\lambda_{\mathrm{D}}}\right). \tag{4}$$

The equation of motion (4) is re-written using the normalization $\widetilde{x} = x/x_0$ and $\widetilde{t} = \omega_0 t$, where

$$x_0 = \left(\frac{Z^2e^2}{\omega_0^2 m 4\pi\epsilon_0}\right)^{1/3} \quad \text{and} \quad \omega_0 = \left(\frac{nZ^2e^2}{\epsilon_0 m}\right)^{1/2}$$

is the *dust* plasma frequency, where n is the dust density. The equation of motion which is no longer depending on the specifics of the system is given by

$$\frac{d^2\widetilde{x}_i}{d\widetilde{t}^2} = \sum_{l\neq i}\left(\frac{1 + \mu|\widetilde{x}_i - \widetilde{x}_l|}{|\widetilde{x}_i - \widetilde{x}_l|^2}\right)\exp(-\mu|\widetilde{x}_i - \widetilde{x}_l|). \tag{5}$$

The parameter $\mu = \Delta/\lambda_{\mathrm{D}}$ depends on the inter-particle distance at equilibrium Δ, and we have assumed that all of the particles are regularly spaced.

The modes are generated by small perturbations of the electric field, and the particles in the chain are subject to small displacements $\widetilde{x}_i = i\Delta + \xi_i$ with $\xi_i \ll \Delta$.

To convert the equation of motion (5) into a wave equation we seek a solution of the form

$$\xi_i = \xi_0\exp[j(k\Delta - \omega t)], \tag{6}$$

where k and ω are the wave vector and frequency, respectively.

The dispersion equation is obtained using a recursive relation. We take the first nearest neighbors and derive the dispersion relation than include the second closest neighbors and so on. For a set of N nearest neighbors, the dispersion relation can be written as follows:

$$\omega^2 = 2(1 + \mu)\sum_{i=1}^{N}\exp(-i\mu)4\sin^2\left(\frac{ik\Delta}{2}\right), \tag{7}$$

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which can be written as

$$\omega^2 = 2(1+\mu)\sum_{i=1}^{N}\exp(-i\mu)[2-\exp(jik\Delta)-\exp(-jik\Delta)]. \tag{8}$$

We use the identity $\sum_{i=0} S^i = 1/|1-S|$ when $|S| < 1$ and $N \to \infty$ in (8) and normalize k by $\Delta^- < 1$ to obtain

$$\omega^2 = 2(1+\mu)\left[\frac{1}{1-e^{-\mu}} - \frac{1}{1-\exp(-\mu+jk)} - \frac{1}{1-\exp(-\mu-jk)}\right]. \tag{9}$$

From (9) and taking into consideration the situation when $\mu \ll 1$ and $k \ll 1$ one obtains the dispersion relation for the DAWs

$$\omega^2 = 4(1+\mu)\left[\frac{k^2}{\mu(\mu^2+k^2)}\right]. \tag{10}$$

On the other hand when $\mu > 1$ we have $(e^{-\mu})^i \to 0$ as $i \to \infty$, we can limit the summation in (7) to a finite number. For example, if we take only the first term we have

$$\omega^2 = 2(1+\mu)\exp(-i\mu)4\sin^2\left(\frac{k}{2}\right), \tag{11}$$

which is the dust-lattice wave (DLW) dispersion relation. However, in our case we consider the DLW dispersion relation from a summation over a fixed number as is explained in the next section.

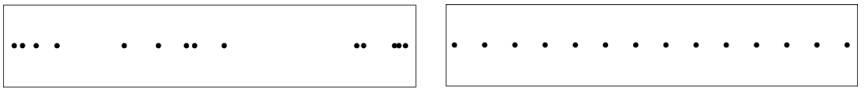
3. Numerical results

The numerical simulation is conducted for an infinite number of particles in the chain. Infinite and finite systems are very different, so it is worth knowing how large the system must be to yield the behavior of an infinite system. In our case we consider a small number of particles in a simulation cell called a box. The box is of finite length L and is repeated periodically along the chain. This length is given by $L = N\Delta$, and Δ has to be calculated using Monte Carlo simulation. At the starting point we give a random position for each particle as shown by Fig. 1(a) for the half space $x > 0$. Then a random displacement is generated. To keep the number of particles in the box constant and equal to N at all times we make the following transformations:

$$x \to \begin{cases} x - L/2 & \text{if } x > L/2, \\ x + L/2 & \text{if } x < -L/2. \end{cases}$$

The effect of periodicity on the interaction is considered through the calculation of the distance between particles. By means of a Monte Carlo method with the standard metropolis algorithm, the total energy is calculated for the configuration obtained after performing random displacements. The new configuration is accepted if the total energy is less than the previous old configuration. In the other case the new configuration is accepted if $\exp(-|E_{\text{new}} - E_{\text{old}}|T)$ is less than a given uniformly distributed number. We have found the configuration at very low temperatures. To avoid metastable configurations, the given temperature is reached using the technique of simulated annealing. The system is heated up and cooled down [13]. The corresponding equilibrium configuration is shown in Fig. 1(b).

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(a) (b)

Figure 1. Half space $x > 0$ particle configurations in a box of length L: (a) random configuration and (b) at equilibrium.

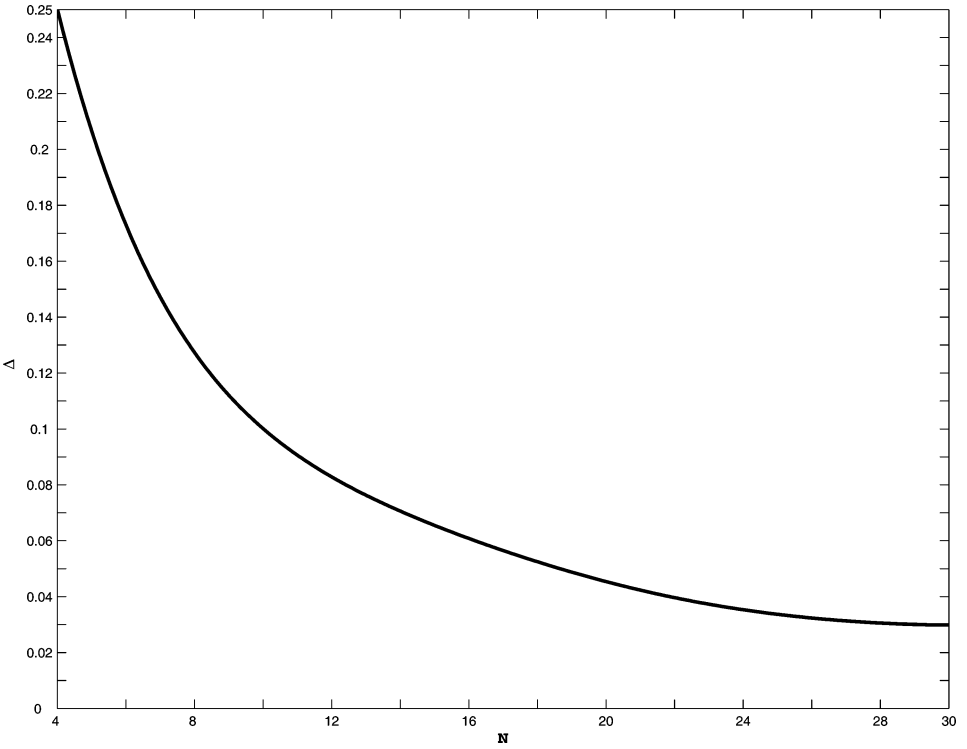


Figure 2. The inter-particle distance Δ versus the number of particles in the box N.

From the numerical investigation, using our Monte Carlo code we have performed the simulation for different numbers of particles in the simulated box. When we change the number of particles, i.e. change the nearest neighbors involved in the interaction, we obtain the inter-particle distance Δ at equilibrium. The variation of Δ versus N is represented in Fig. 2. This figure reproduces the well-known result for a strictly one-dimensional chain, the dependence of Δ is $1/N$. However, the problem is regarding the number of particles which should be considered in the box. For a low value of N the inter-particle distance decreases very quickly, we have to consider more nearest neighbors which make a significant contribution to the total electric field acting on the test particle. As N approaches a critical value, we have found an asymptotic limit for Δ. The corresponding value is $N_c = 28$ beyond which there is almost no change in Δ. The number of particles included in the interaction can be roughly limited to N_c. The latter result is a consequence of the short-range interaction: each grain interacts at a distance shorter than the Debye length. The characteristic shielding distance depends only on the background plasma. Liu

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et al. [7] have studied the phonon in a one-dimensional chain experiment. The experimental investigation was conducted for negatively charged dust particles. The maximum number of particles in the chains was $N = 28$. Numerical simulation shows that the interaction has no effect if a larger number of particles is considered. It can be a general result: there is no scaling parameter such as mass or charge values, so it depends only on the nature of the interaction between particles and the plasma components.

Finding the inter-particle distance and the length of the box at equilibrium we have calculated the parameter $\mu = \Delta/\lambda_{\mathrm{D}}$ then plotted the dispersion relation $\omega = f(k)$ for the DAW given by (10) and for the DLW from (7). In the latter case we limit the summation to N. To investigate the effect of the number of particles in the box two cases have been considered: $N = 14$ and $N = 28$ (Fig. 3(a) and (b)). We note that the dust lattice mode is subject to the most important change, in particular when we compare our results with those of Otani et al. [11] where the limit $N \to \infty$ was considered. In their investigation, the analytical model was based on a long-range interaction. We have shown that we can limit the interaction to N_{c} neighbors. This result can be used for both finite and infinite one-dimensional chains where the interaction is of Yukawa type. For the infinite case we have to use the periodical boundary condition. Thus, limiting the number of particles in the box yields a change in the DLW characteristics. This wave is a result of the collective effect of the shielded Coulomb interaction between particles. When the interaction reaches its cut-off range the contribution of all other particles beyond this cut-off is not important, the amplitude of ω does not change when N increases. The profile of the DAW which is created by the pressure gradient of the ambient plasma was not affected by the number of particles considered in the box.

3.1. Effect of friction

The injection of a neutral beam to sustain the dusty plasma provides an additional force in the equation of motion (1). In the presence of noble gases (argon or neon) the friction frequency is given by [19]

$$\nu_{\mathrm{fr}} = \frac{C_v P}{a \cdot \rho} \tag{12}$$

where C_v is the specific heat, a is the dust radius, P is the pressure of the gas and ρ is the dust mass density of the grains. At ambient temperature we have $\nu = 1.17 \times 10^4\ \mathrm{s}^{-1}$.

The dispersion relations for the situation when the friction is not neglected $\nu \neq 0$ is obtained using the same calculation as in Sec. 2, one finds

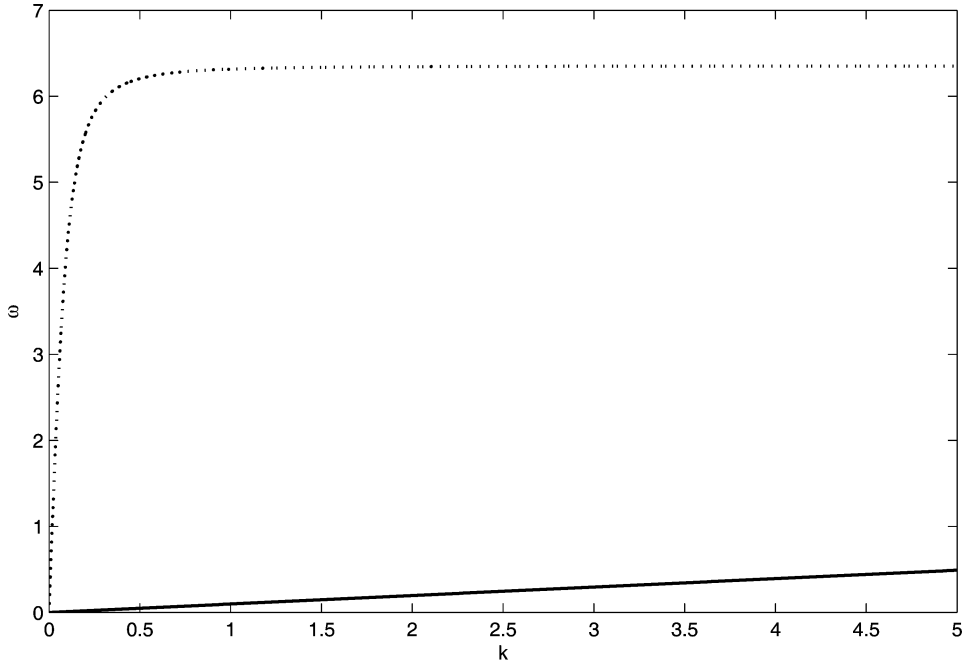
$$\omega(\omega + j\nu) = 4(1+\mu)\left[\frac{k^2}{\mu(\mu^2 + k^2)}\right] \tag{13}$$

for the DAW and

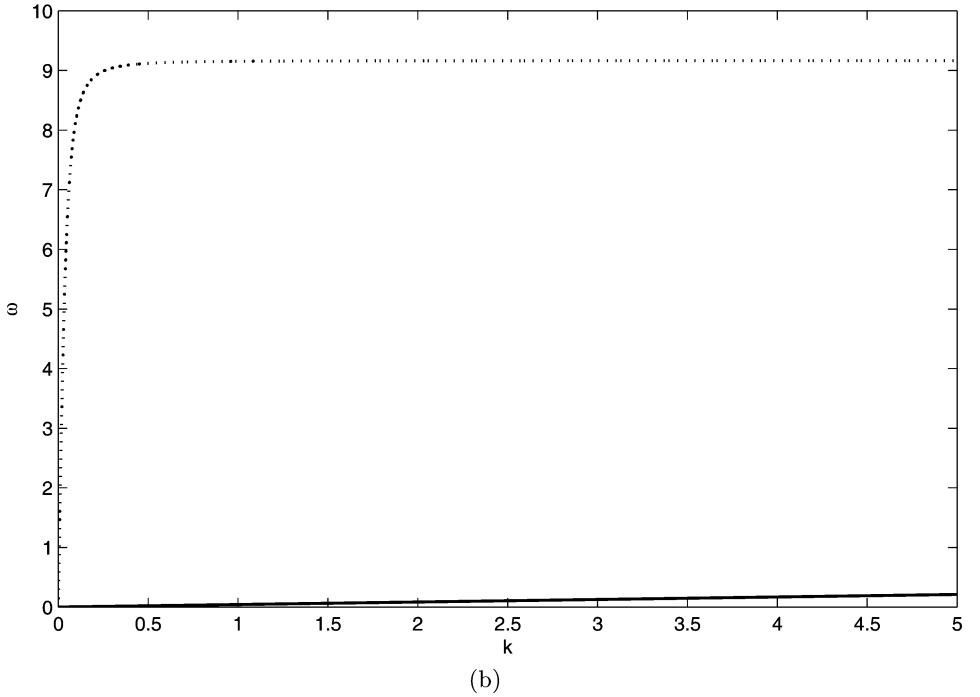
$$\omega(\omega + j\nu) = 2(1+\mu)\sum_{i=1}^{N} \exp(-i\mu) 4 \sin^2\left(\frac{ik\Delta}{2}\right) \tag{14}$$

for the DLW. Owing to the external excitation of the wave, the frequency ω is purely real, thus the wave number has two parts $k = k_{\mathrm{r}} + jk_{\mathrm{i}}$. The imaginary part k_{i} is associated with the wave spatially damping when it propagates as is observed in the experiments [7]. From dispersion relations (13) and (14) and using the inverse function calculation, we plot the real k_{r} and the imaginary k_{i} parts versus ω. Figures 4(a)

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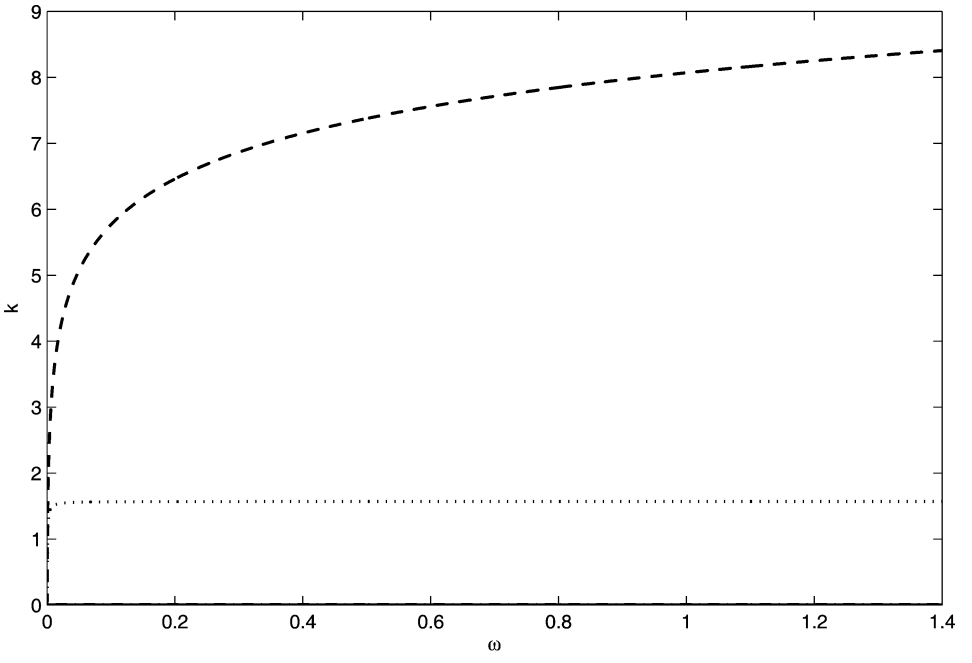
(a)



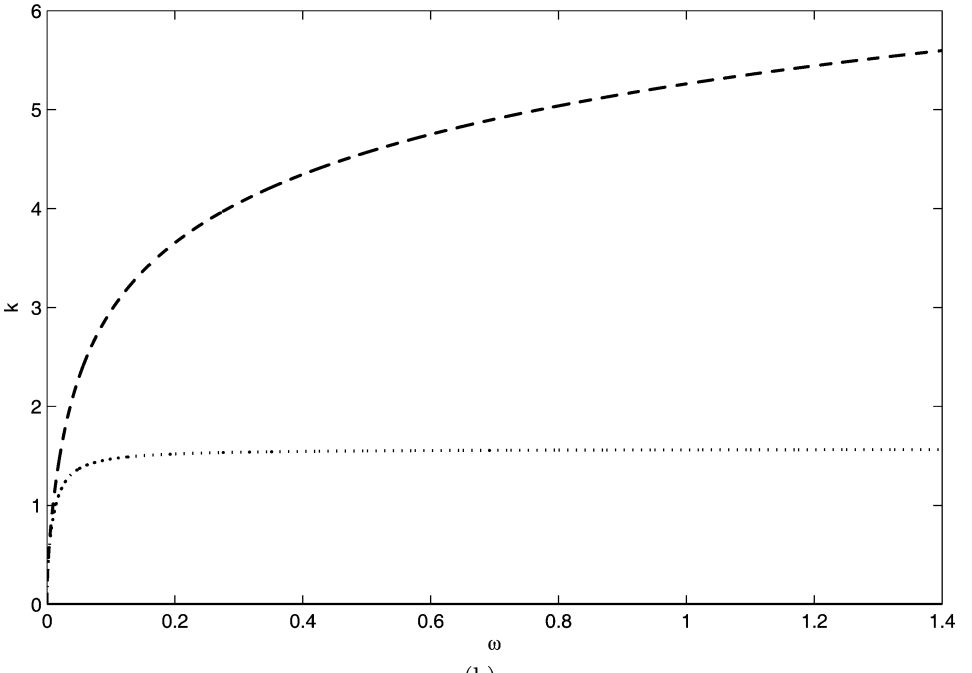
(b)

Figure 3. Dispersion relation for DAW (—) and DLW ($\cdots$) for (a) $N = 14$ and (b) $N = 28$.

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(a)



(b)

Figure 4. The imaginary $k_{\mathrm{i}}(---)$ and real $k_{\mathrm{r}}(\cdots)$ parts of the wave number for the DLW corresponding to (a) $N = 14$ and (b) $N = 28$.

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and (b), which correspond respectively to $N = 14$ and $N = 28$, show that there is no excitations small values of the wave number ($\omega \sim 0$), which means an overdamping until $k_\mathrm{i} > k^*$. The number of particles in the box, in particular for the low-frequency mode, plays an important role in this case: we have $k^*(N = 14)/k^*(N = 28) = 3$. As the frequency increases the amplitude of the k_i dependence on N is weaker. For $\omega = 0.2$ we have $k_\mathrm{i}(N = 28)/k_\mathrm{i}(N = 14) = 0.58$ while for $\omega = 1.4$ we have $k_\mathrm{i}(N = 28)/k_\mathrm{i}(N = 14) = 0.66$. Comparing the profile of k_r from Figs. 4(a) and (b), we found that it is not affected by the number of particles in the box. It is possible to say that for higher frequencies we will find the same behavior for k_i as N changes. We can conclude that an infinite chain behaves like a finite chain with the same spacing between particles. However, this is not true for low frequencies. The DAW is not seen in Figs. 4(a) and (b): it is totally damped in our case.

4. Conclusion

Monte Carlo simulation has been used to find the ground-state configuration of an infinite linear chain at low temperature. The chain is formed from positively charged dust grains. Using a variable length box, it was found that the inter-particle distance between interacting particles through the Yukawa screened potential depends on the number of particles in the box. Beyond a critical value of the number of particles N_c all other particles has no significant contribution on the total electric field on each particle. The inter-particle distance as well as the length of the box have been found. Using this result the effect of the number of particles in the simulated box has been investigated to study the DAW and DLW. The presence of a friction force was also considered.

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