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2D Molecular Dynamics Simulation of Solitons Interaction in Dusty Plasma

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Abstract

Molecular Dynamics (MD) method is used to simulate a dusty plasma system as a one component plasma (OCP). The heavy dust particles are considered as discrete particles interacting with each other through the Yukawa potential. This assumption is justified by the screening effect due to the lighter plasma components (electrons and ions). Solitons excitation at different values of the Coulomb coupling parameter (Γ) is simulated. The formation of solitons in the system using electric field pulse in a narrow region is studied. Different scenarios of the interaction of solitons are studied for: A) Two solitons with the same amplitude and opposite directions. B) Two solitons with different amplitudes and opposite directions. C) Two solitons with different amplitudes and propagating in the same direction.

Keywords: Dusty plasma; Molecular Dynamics (MD); One Component Plasma (OCP); Yukawa Potential; Solitons.

1. Introduction

Solitons are type of nonlinear waves that have conserved shape, amplitude, and velocity, which is a result of the balancing between the nonlinearity of the wave and the dispersion of the medium that containing the soliton [1]. The soliton is the solution for some nonlinear differential equations such as nonlinear Schrödinger equation (NLSE) and Korteweg-de Vries equation (KdV). These equations are used to model nonlinear wave propagation [2, 3].

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Dusty plasma is one of the systems that encounter these nonlinear phenomena. Recently, dusty plasma and its nonlinear behavior get the attention of the scientific society because of its importance in the fields of space science and semi-conductor industry. Dust acoustic solitons were predicted by Rao and his colleagues [4] and observed experimentally by Samsonov and his colleagues [5]. The nonlinearity of the solitons is due to the inertia of dust heavy mass and is balanced by the dispersion of the system. Many experiments of dusty plasma observing dust acoustic solitons is theoretically described on the bases of the solution of the (KdV) which is as given:

$$\frac{\partial n_d}{\partial t} + C n_d \frac{\partial n_d}{\partial y} + D \frac{\partial^3 n_d}{\partial y^3} = 0 \qquad (1)$$

The second term represents the nonlinearity of the wave while the third term represent the dispersion of the medium, C and D depends on the density, temperature, and dust particle mass [6, 7]. It is difficult to simulate the dynamics of dust acoustic solitons by treating all the plasma components because of the large differences in there masses, so we will use the open source code of molecular dynamics ***LAMMPS*** which is the acronym of "***Large scale Atomic/Molecular Massively Parallel Simulator***" [8], and we will treat the dusty plasma as one component plasma (OCP) by considering the interaction among the dust particles as Yukawa potential form. What makes our consideration acceptable is that the lighter components (electrons and ions) work as screening medium between the dust particles [9]. The Yukawa potential has the following form:

$$U(r) = \frac{Q^2}{4\pi\epsilon_0 r} \exp\left(\frac{-r}{\lambda_D}\right) \qquad (2)$$

Where Q is the charge on the dust particle and equal to $-Z_d e$, where e is the electron charge, Z_d is the number of charges on the dust particle, r is the distance between two dust particles, λ_D is the dust Debye length. One component plasma is characterized by two parameters: Coulomb coupling parameter Γ , and screening parameter κ, and they have the following forms:

$$\Gamma = \frac{Q^2}{4\pi\epsilon_0 a_d k_B T_d} \qquad (3)$$

$$\kappa = \frac{a_d}{\lambda_D} \qquad (4)$$

where T_d is the dust temperature and a_d is the average distance between particles "Wigner-Seitz radius".

2. Simulation setup

Our simulation has been carried out for a 2d system of point particles as the charged dust particles interacting through Yukawa form of potential energy. We created two setups one to simulate the formation and interaction of two opposite directions solitons. And the other is longer to simulate the interaction of the same direction solitons, both are 2d periodic boxes. The length of the first box $l_y = 500a_d$ and its width $l_x = 100a_d$. The length of the second box $l_y = 1200a_d$ and the width $l_x = 80a_d$. Parameters of the system is as the following: the mass of dust particle $m_d = 6.99 \times 10^{-13}$ Kg, charge on dust particle Q $= 11940$e , Wigner-Seitz radius $a_d = 4.18 \times 10^{-4}$ m Screening parameter $\kappa = 0.5$ which gives Debye length $\lambda_D = 8.36 \times 10^{-4}$ m. For these parameters, $E_0 = Q/4\pi\epsilon_0 a_d^2 = 98.39$ V/m and equilibrium density $(n_{d0})_{2d} = 1.821 \times 10^6\ m^{-2}$. The applied electric field for excitation will be expressed in terms of E_0, and will be less than 30 times E_0 because for electric fields greater than this limit the particles will escape the simulation box. The cutoff for particle interaction potential in the simulation here has been chosen to be at $20a_d$. Characteristic dust plasma frequency of the particles $\omega_{pd} = (Q^2/2\pi\epsilon_0 m a_d^3)^{1/2} \approx 35.84\ s^{-1}$, which corresponding to the dust plasma period to be 0.175 s. We have chosen simulation time step as $0.0072 \times 2\pi\omega_{pd}^{-1}$ s so that phenomena occurring at dust plasma frequency can be easily resolved. The distribution of particle positions and velocities created randomly. To avoid possible overlap between particles we ran microcanonical ensemble with limited traveling distance of particle, the ensemble named "NVE/limit". This procedure creates equilibrated system with maximum thermal velocity equal to (Xmax/time step). Now we need to set the temperature of the system to be T_d which correspond to the desired coupling parameter Γ. For that we used the canonical ensemble (NVT) Nose-Hoover thermostat [10, 11]. After reaching the temperature T_d we disconnected the canonical ensemble thermostat and ran the microcanonical ensemble (NVE) to check the stability of the equilibrium state at the temperature T_d. Now the system is ready to simulate the dynamics of the solitons. In this study we focused on the strongly coupled dusty plasma

which $\Gamma \gg 1$. For most of showed results we choose the value of $\Gamma = 60$. Also, we simulate the system with Γ slightly greater than crystallization coupling limit $\Gamma_C \approx 172$.

3. Results and discussions

3.1. Formation of single soliton

To produce a soliton in the system electric field E will be applied in a narrow rectangular region, that region oriented in the direction of x-axis as showed in figure (1), and the electric field was in negative y-direction inside that region. The applied electric field E exerts force $F_E = QE\vec{y}$ on the dust particles inside the region we referred before. The force acts in the positive y-direction as the dust particle has a negative charge $(-Q)$. that force excites a solitary wave propagates in the positive y-direction with amplitude proportional to the excitation field E.

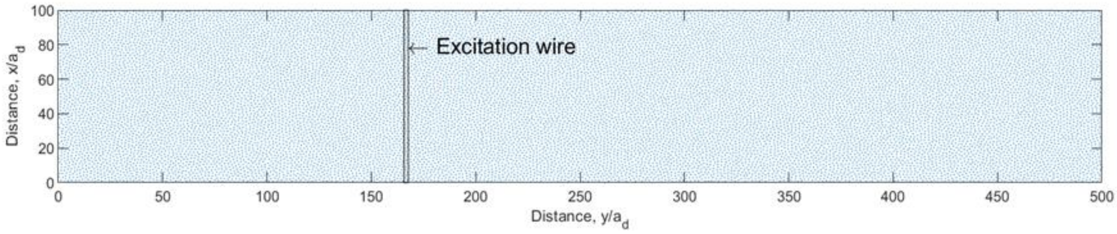


Figure 1: Illustration of the 2D simulation box with excitation wire of thickness $2a_d$ and the distribution of the dust particles.

The simulation box diagram is shown in the Figure (1), and the time evolution of density (n_d) is shown in Figure (2). The resultant soliton is consistent with the solution of the KdV equation. We observed formation of positive density soliton propagating in the positive y direction with constant velocity which its value depends on the amplitude of the excitation electric field as shown in figure (3).

Table 1: soliton parameters with $\Gamma = 100$ at time 45.24 $\omega_{pd}t$

E/E_0	M	$\delta n_d/n_{d0}$
20	1.147	0.269
25	1.203	0.323
30	1.234	0.341

In addition to the propagating soliton we observed a rarefactive density perturbations behind it which slowly damped. In Table (1) we present some calculated parameters of observed solitons where M is the Mach number which is the equal to v/C_s, where v is the soliton velocity and $C_s = 1.95 \times 10^{-2}\ m/s$ is the dust acoustic speed.

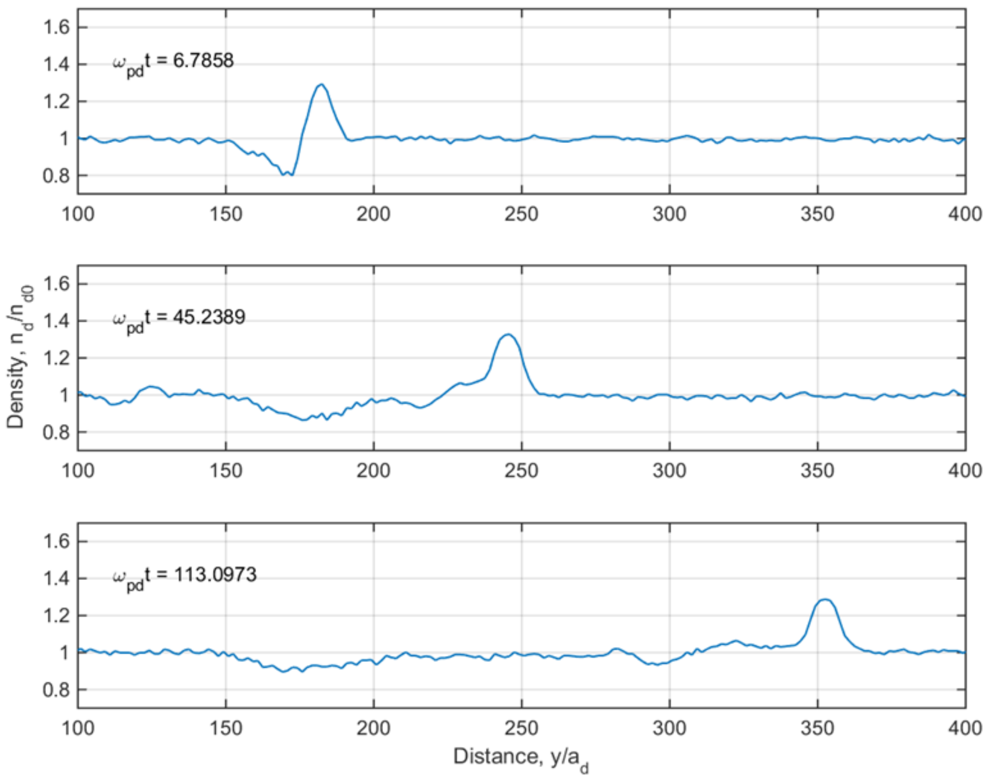
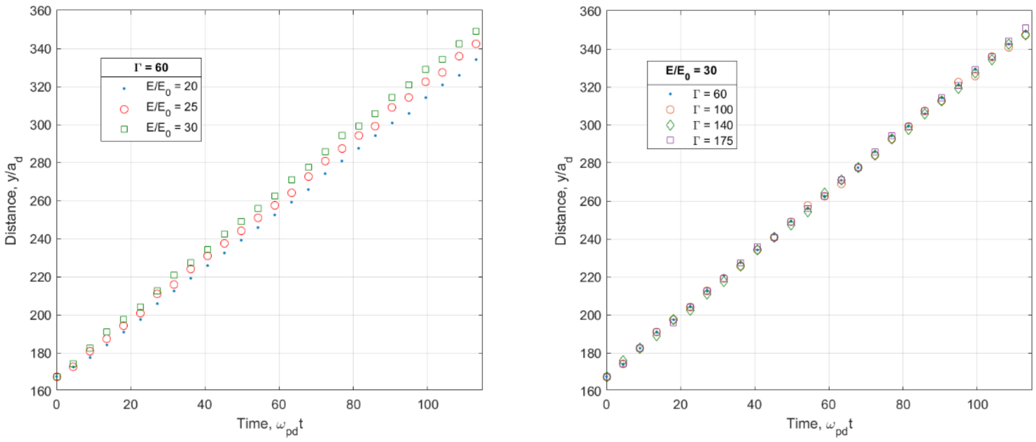


Figure 2: The propagation of soliton wave moving in the positive y-direction with excitation electric field (E/E_0 = 30) and ($\Gamma = 60$).



a) b)

Figure 3: The trajectory of the soliton with respect to the time, **a)** shows the increase of soliton velocity with the increase of the excitation electric field. **b)** shows that at different values of (Γ) but with the same excitation field the soliton velocity remains the same.

3.2. Interaction of two solitons

To simulate interaction between two solitons we added another excitation region but with opposite sign of excitation electric field to excite counter-propagating soliton as shown in figure (4).

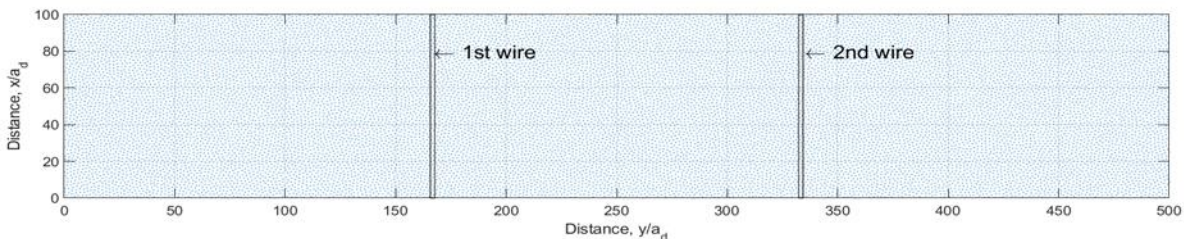


Figure 4: Illustration of the 2D simulation box with two excitation wires of thickness $2a_d$.

3.2.1 Collision of same amplitude solitons

When applying two opposite excitation electric fields one for each region, two counter-propagating solitons with the same amplitude appeared and collide with each other without change in amplitude or shape. The resultant amplitude while collision nearly equal to the sum of amplitudes of the two solitons as shown in figure (5), in contrast to earlier study carried by Sandeep and his colleagues [12] which found the resultant amplitude less than the sum. Each soliton experiences a phase shift δt inversely proportional to the solitons amplitude as shown in figure (6).

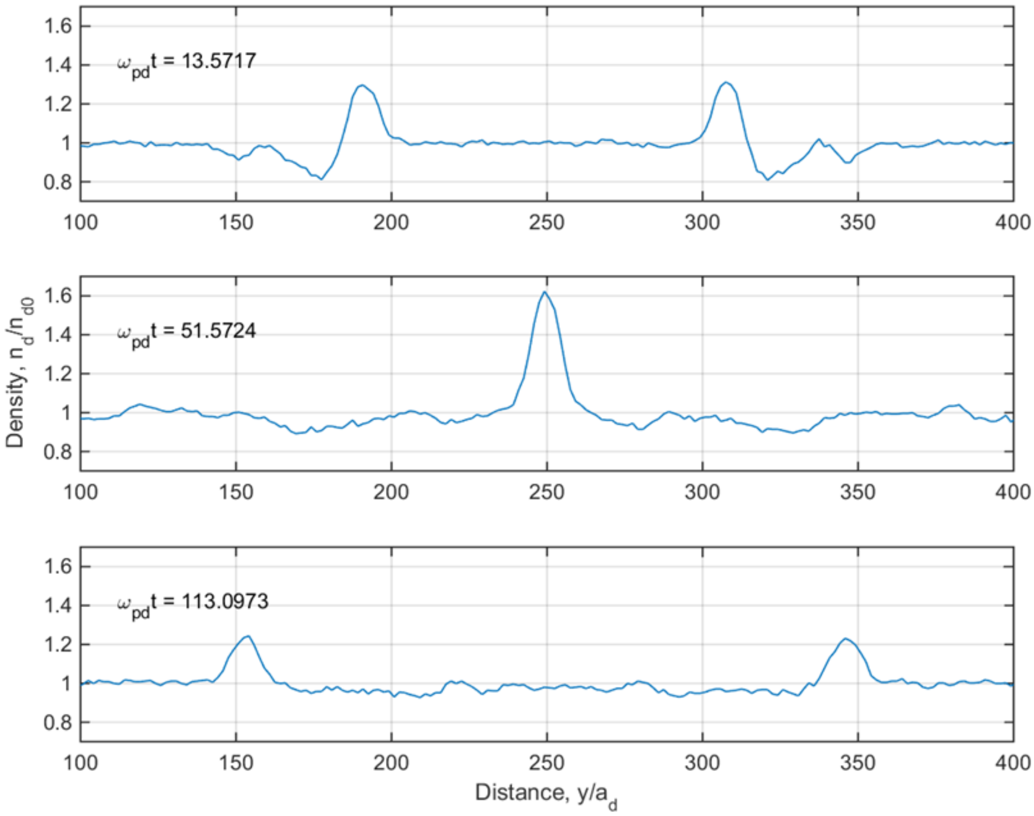
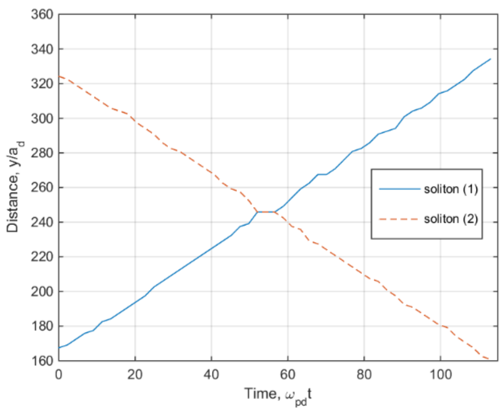
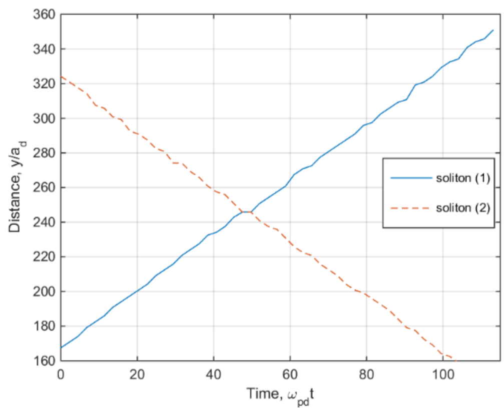


Figure 5: Collision of two counter-propagation solitons with the same amplitude with excitation electric field ($E/E_0 = 25$) and ($\Gamma = 60$).



a)



b)

Figure 6: The trajectory of two counter-propagating solitons with respect to the time, **a)** shows the phase shift ($\delta t = 4.53\ \omega_{pd}t$) at ($E/E_0 = 20$). **b)** shows the phase shift ($\delta t = 2.26\ \omega_{pd}t$) at ($E/E_0 = 30$).

3.2.2 Collision of different amplitudes solitons

When applying opposite excitation electric fields but with different amplitudes, two solitons with different amplitudes generated and collide with each other as shown in figure (7). The two solitons remain unchanged after collision but the soliton with smaller amplitude dragged back slightly in the direction of the larger soliton as shown in the figure (8), in agreement with the study of Surabhi and his colleagues [13]. Both solitons shifted in phase in agreement with Surabhi but in contrast with Sandeep and his colleagues [12] which the large soliton experience no phase shift.

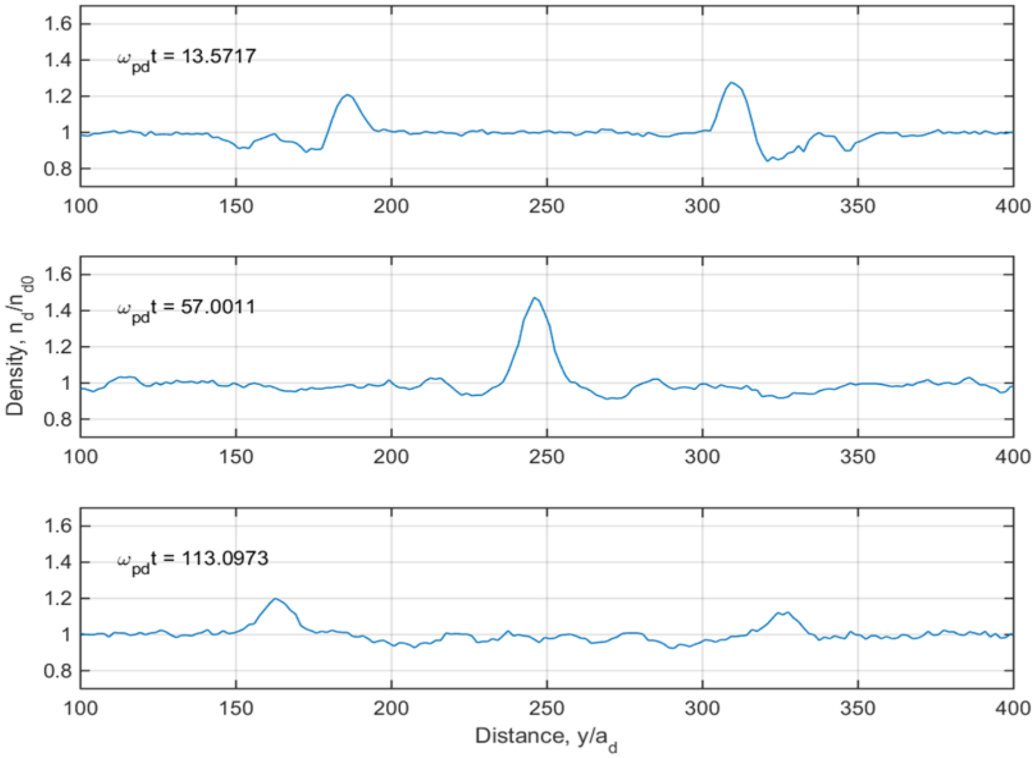


Figure 7: Collision of two counter-propagation solitons with different amplitudes with excitation electric fields ($E_L/E_0 = 15$) for the left soliton, ($E_R/E_0 = -20$) for the right one and ($\Gamma = 60$).

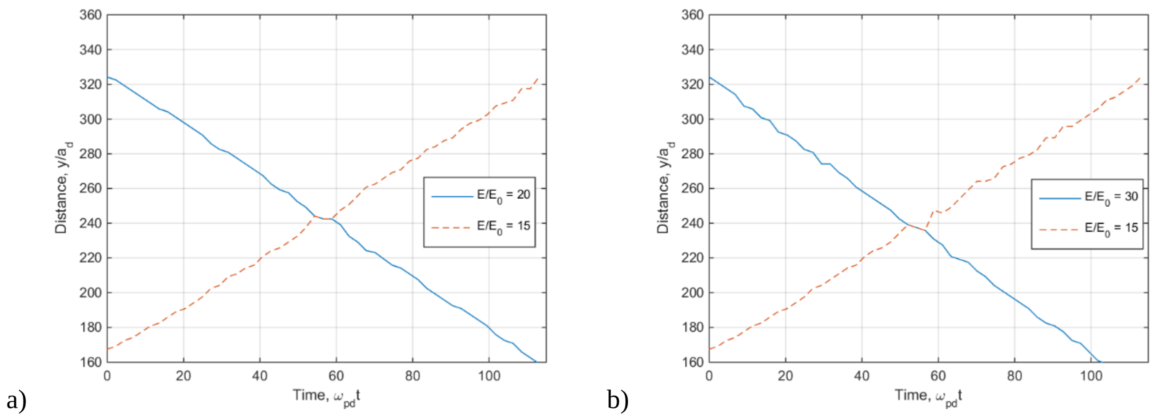


Figure 8: The trajectory of two counter-propagating solitons with different amplitudes with respect to the time at ($\Gamma = 60$), **a)** shows the backward drag distance of the smaller soliton ($\delta y = 1.7\ a_d$). **b)** shows the backward

drag distance of the smaller soliton ($\delta y = 3.4\ a_d$). Both with phase shift ($\delta t = 4.52\ \omega_{pd} t$).

3.2.3 Overtaking of two solitons

In this case we perform the simulation in different setup because its need to longer simulation box to show the overtaking of the two solitons. The new setup is illustrated in figure (9). We observed that the smaller soliton did not merge in the bigger soliton, but they look like as if they exchange their positions as shown in figure (10). The trajectory of the two solitons shows the exchange action as in figure (11).

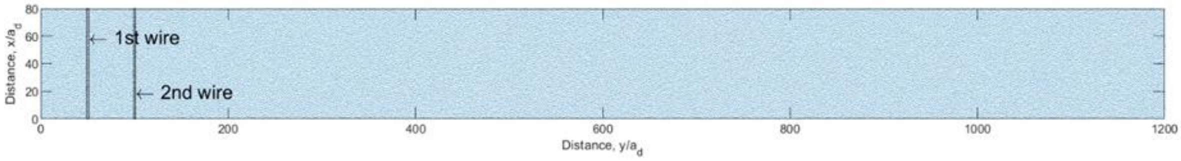


Figure 9: Illustration of the 2D simulation box with two excitation wire of thickness $2a_d$ to excite two co-propagating solitons.

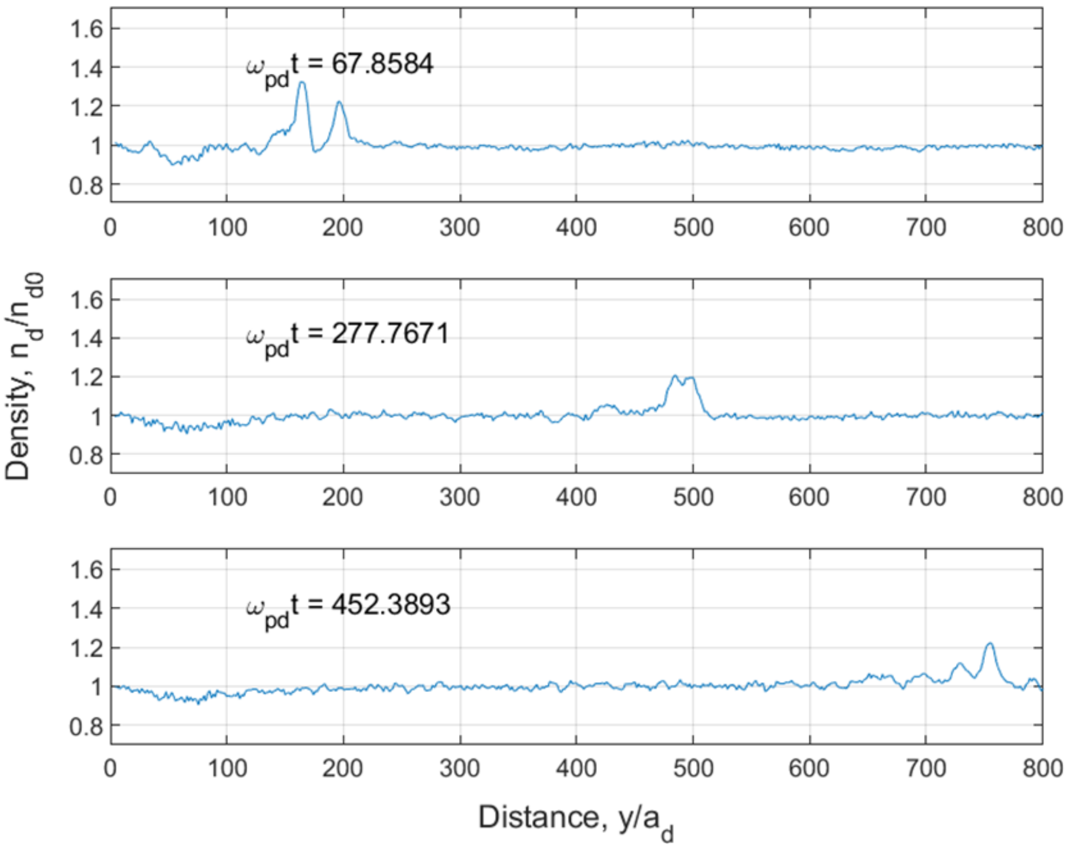


Figure 10: Collision of two co-propagation solitons with different amplitudes with excitation electric field $(E/E_0\ = 30)$, $(E/E_0\ = 15)$ and $(\Gamma = 175)$.

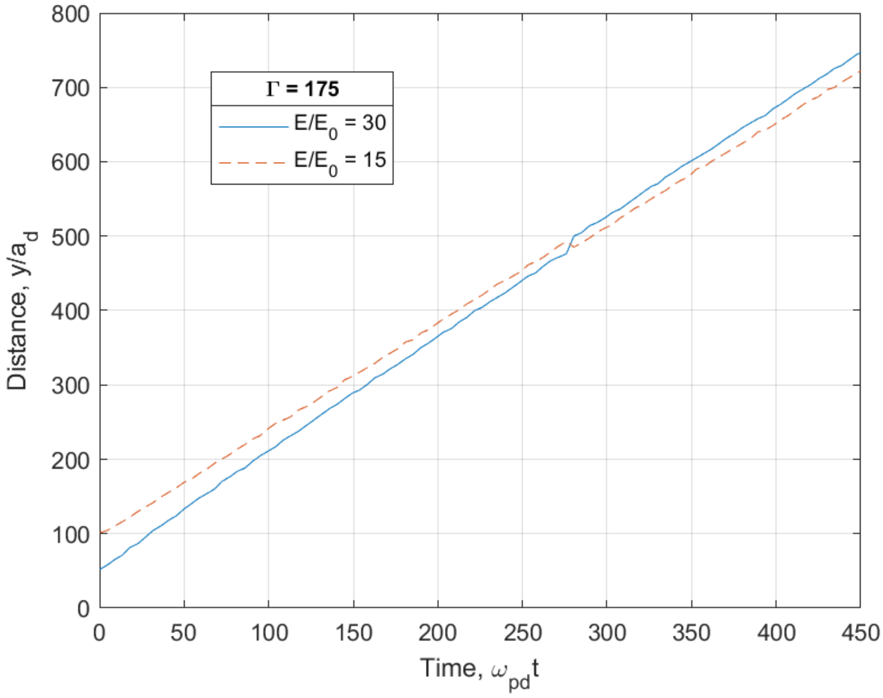


Figure 11: The trajectory of the two co-propagating solitons with different amplitudes with respect to the time at ($\Gamma = 175$), the two solitons exchange their path with phase shift ($\delta t = 4.5\ \omega_{pd} t$).

4. Conclusion

In this study, we performed a simulation of a system of dusty plasma using molecular dynamics and considered the system to be a one component plasma and the potential energy between particles in the form of Yukawa potential. We used a sharp pulse of electric field to excite the solitons. These solitons were observed moving at velocities that depend on their amplitude, but these velocities do not depend on the value of the coupling parameter. In the case of collision of two solitons with the same amplitude and moving to each other, we noticed that their shapes and speed did not change after the collision, but during the collision a phase shift occurred. This phase shift is inversely proportional to the amplitude value of solitons, and this is consistent with previous simulations of Sandeep and his colleagues [12], but it differs with the practical observations of Sharma and his colleagues [7], and the theoretical study of Surabhi and his colleagues [13]. In the case of two solitons, the soliton with a lower amplitude suffers a backward drag in the direction of the larger soliton and both suffer from a phase shift, in agreement with the study of Surabhi and his colleagues [13]. In the case of two solitons moving in the same direction, the larger soliton overtakes the smaller soliton without showing an emerging between them, but they appear as if they are exchanging path, and the largest amplitude during overtaking is less than the larger soliton amplitude, in agreement with the study of Jerry and his colleagues [14].

5. Recommendations

We recommend more experimental and theoretical studies of the interactions of solitons in dusty plasma systems, also simulations that consider the effects of ions and neutrals on the motion of the dust particles. The effect of coupling parameter Γ on soliton velocity need more studies especially considering values greater than the crystallization limit Γ_C.

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