Chapter 7

Numerical Approach to Dynamical Structure Factor of Dusty Plasmas

Aamir Shahzad, Muhammad Asif Shakoori,
Mao-Gang HE and Yan Feng

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Abstract

The dynamical structure factor [$S(k,\omega)$] gives the information about static and dynamic properties of complex dusty plasma (CDPs). We have used the equilibrium molecular dynamic (EMD) simulations for the investigation of $S(k,\omega)$ of strongly coupled CDPs (SCCDPs). In this work, we have computed all possible values of dynamical density with increasing and decreasing sequences of plasma frequency (ω_p) and wave number (k) over a wide range of different combinations of the plasma parameters (κ, Γ). Our new simulation results show that the fluctuation of $S(k,\omega)$ increases with increasing Γ and it decreases with an increase of κ and N. Moreover, investigation shows that the amplitude of $S(k,\omega)$ increases by increasing screening (κ) and wave number (k), and it decreases with increasing Γ. Our EMD simulation shows that dynamical density of SCCDPs is slightly dependent on N; however, it is nearly independent of other parameters. The presented results obtained through EMD approach are in reasonable agreement with earlier known results based on different numerical methods and plasma states. It is demonstrated that the presented model is the best tool for estimating the density fluctuation in the SCCDPs over a suitable range of parameters.

Keywords: plasma parameter, current correlation function, dynamical structure factor, strongly coupled complex (dusty) plasmas, equilibrium molecular dynamics, complex dusty plasma

1. Introduction

Dynamical structure factor $S(k,\omega)$ is very actively investigated through theoretical, experimental and computer simulation for simple liquids as well as complex systems (dusty plasmas). The

$S(k,\omega)$ of the dusty plasmas is very significant to understand the dynamic behavior of dust particles in the complex plasmas. The subject of dusty plasma containing micron-size charged condensed particles has recently been actively investigated in the fields of science and technology. In addition, the investigation of dynamical behaviors is also studied in the areas of physics and chemistry of plasmas, ionized gases, and the space environment, environmental sciences, semiconductor plasma processing industries, nuclear energy generation and materials research. Dust in the atmosphere and in the entire universe exists in different shapes and sizes. Mostly dust particles are observed in solid form and sometimes also in liquid and gaseous forms. Current correlations and wave spectra's in the dusty plasma are generated due to dynamic motion of charged dust particles. The dust particles increase remarkable and unique fundamental physical property of ionized gases and dense plasma. Further dust particle increases future application of dusty plasma in industrial fields including nuclear fusion energy, material modification, and synthesis, environmental remediation, nano, aerospace and medical technologies.

1.1. History of dusty plasma

Current research on the dusty (complex) plasma becomes an interesting field in sciences and technologies. The term "plasma" was first used by the Langmuir in 1924. The most thrilling events in the field of dusty plasmas were occurred in 1980 for planet Saturn mission. Mendis in 1997 observed the bright comet in distant ancestor, which was the excellent cosmic laboratory for the investigation of dusty plasma and their dynamical and physical consequences. The other appearances of dusty plasmas were zodiacal light, the origin nebula, the noctilucent clouds, etc. At the laboratory level, dusty plasma is available in terrestrial laboratory at the remote past. Lyman Spitzer along with Hannes Alfven was recognized that dust in the universe was not merely a hindrance to a visual opinion but it was an essential component of the universe. A dust particle image taken a shape of spokes that rotating around Saturn ring and last surveys designated that these spokes were fine dust material. In 2005, Cassini spacecraft was made a new and improved observation of spokes with a feature that would provide an improved considerate of their source. In 1992, the European spacecraft Ulysses flew by the planet Jupiter and detected the dust particles and measured their masses and impact speed. Again in 1995, NASA spacecraft, Galileo perceived the origin of dust streams around Jupiter. The current enormous interest in complex plasmas started in the mid of 1980s, and started by laboratory investigation of dynamical structure factor of dusty plasmas. Current situation (2000–2017) of dusty plasma is stable in laboratory conditions and it is very significant in industries, science, and technology, medical science, and energy sectors, etc. Different characteristics of dust particles are investigating via theoretical, computer simulation and experimental techniques [1, 2].

1.2. Characteristics and types of dusty plasma

Dusty plasma is the plasma that contains an addition of dust charged particles along with electrons, ions, and neutral particles. The dynamical properties of plasma become more complex when we insert dust particle, so it is also known as complex plasma [3]. Dust particles are much larger in charge as compared to electrons, ions, and neutral particles and its size vary from hundreds of millimeter to 10 of nanometers and having a mass approximately 3×10^{-11} kg. The dynamic behaviors are easily observed experimentally by CCD camera. Dusty plasmas exist in space as well as in the laboratory and these dust particles are negatively charged but sometimes positive charge as well. It is charged through photoionization, electron bombardment, etc. the amount of charge on dust particles depends upon shape and size of dust particles. It has mostly spherical shape but sometimes also having rod type shape and irregular [4]. Dusty plasmas are classified on the basis of density, temperature, potential and thermal energies. The Coulomb coupling parameter describes the classification of complex dusty plasmas. The Coulomb coupling that is defined as "the ratio of average potential energy to the average thermal energy" and mathematically it can be expressed as: $\Gamma = \frac{P.E}{K.E} = \frac{Q^2}{4\pi\varepsilon_0} \frac{1}{k_B T}$ [5], where k_B is the Boltzmann constant, T is system temperature and ε_0 is permittivity of free space.

1.2.1. Weakly coupled dusty (complex) plasmas (WCCDPs)

When dust charged particles have average thermal energy due to neighboring particles much larger than the average potential energy, then that plasma is known as weakly coupled complex dusty plasma (WCDPs). The WCCDPs have a high temperature but low density and value of Coulomb coupling parameter less than 1 (mathematically $\Gamma < 1$). In case of WCCDPs, any structural form does not exist. The background of WCCDPs is considered as ionized gases.

1.2.2. Strongly coupled dusty (complex) plasma (SCCDPs)

The SCCDPs is speedily emerging filed from last three decades. It is very significant to astrophysical plasma and quickly progressing in laboratory experiments. In this type of dusty plasma average thermal energy of charged particles due to neighboring particles are much smaller than average potential energy and mathematically $\Gamma \geq 1$. In case of SCCDPs, it has high density and low temperature and can be specified in structural farm [6–8].

1.3. Dusty plasma in atmosphere and laboratory

There are many systems in the atmosphere where dust particles are established. Spaces between the stars are filled with a large amount of dust and gases. Dust particles in the interstellar region are metallic i.e. graphite, magnetite, and amorphous of carbon, dielectric material i.e. silicates and ices, etc. Comets, planetary space, planetary ring, and earth atmosphere are the region of our solar system. Gossamer ring, halo ring, and main rig are the three systems of Jupiter's ring. In the Saturn rings systems are mostly ices and its size vary from meter to micron. A Uranian rings system has major rings such as 6, 5, 4, 3, α, β, η, γ. In Neptune's ring systems appear in curios twisted materials and structure is dirty ice and composition such as iron, nickel, sulfur, earth atmosphere dusty ice, etc. [9]. A simple device for producing dusty plasmas is a dusty plasma device which is a single-ended *Q*-machine modified to allow the dispersal of dust grains. Dusty plasmas are produced by suspending micron-sized dust particles in a stratum of a dc neon glow discharge. Dusty plasma has been for the first time confined in cylindrical symmetric radio frequency plasma (RF) system also in the semiconductor industry.

1.4. Role of dust particles and applications

Dust particles have charge and chemically active species, it is formed and growth in dusty plasma devices. Sometimes in the form of a mixture of gases such as SiH_4, silane, oxygen, O_2, and Ar, etc.

Secondly dust particles are formed in devices when atoms and molecules are spurted from walls and electrodes into the plasma by electron and ion bombardment. Moreover, the growth of dust particles in the plasma is coagulation, nucleation and surface growth. Thermal fluctuations and Coulomb interaction play the significant role for determination structure of SCCDPs. When the values of Γ (>1) increase then system organized from nonideal gases phase to ordered condensed phase. Dust particles are suspended in the gaseous plasma phase with few electrons temperature and charge up to 10^4 ordered. Interestingly, the dust clouds in a dusty plasma formed into the structural form even at room temperature. Dust particle has large mass as compared to ion and an electron which gives the results slowly downtime scale and it can easily observed the macroscopic structure and its dynamical behavior directly study in space and real time [10]. Dusty plasma used for nanocrystalline silicon particles grow in the silane plasmas used to increase efficiency and lifetime of the silicon solar cells. It is used for thin film coating applied in plasma-enhanced chemical vapor deposition (PECVD) for the improvement of material surface properties. Carbon-based nanostructure growth in the hydrocarbon plasmas or fluorocarbons used to produce thin carbon films. It is used to improve material properties such as chemical inertness, high hardness and wear resistance. Self-lubrication coating and wear resistance using different compound as a dust particle (MoS_2). Ar/CH_4 plasma used for making the nanocrystalline diamond films fabricated which as exceptional properties such as chemical inertness, high hardness, and extreme smoothness which used to improve the performance of cutting tools. Diamond whiskers fabricated by the etching in RF plasmas for the enhancement of electron field emission. The reactive ion etching (RIE) process are used to a precise efficiently sharpen micro-tips of diamond [11]. Complex (dusty) plasmas (CDPs) have various advantages in a different industries, technologies, and energy sector due to the existence of dust particles. CDPs are stable under the laboratory condition. The CDPs can also be used for the diagnostic purpose because dust particles are trapped at the room temperature and keep their desire dynamical state for hours. Dusty plasma frequency in the range several hertz and easily observed through CCD cameras. It is produced in the gas discharge tube with natural gas pressure range that varies from 1 to 100 pa, which is subject to moderate damping [8]. Moreover, magnetized dustyplasma device used to produce a number of the verity of magnetic fields configuration with the help of four independent superconducting coils [12]. Magnetized glow discharge dusty plasma device, RF plasma device, ISS experiment and DC glow discharge devices used for different applications in industries and diagnostic purpose of dusty plasma. Dust particles are found in a tokamak (fusion plasma) and dusty plasmas depositions techniques devices [11, 13].

1.5. Dynamical structure factor

The dynamical structure factor $S(k,\omega)$] gives the information about static and dynamic properties of the fluid in simple and complex systems. In hydrodynamic condition, the $S(k,\omega)$ provides experimental calculable quantities such as the thermal diffusivity, adiabatic sound velocity and the ratio of specific heats [8]. These properties of the fluids are measured through light scattering, x-ray and inelastic neutron experiments on a substance such as dense plasmas, liquids, and glasses. Sound waves are generated through $S(k,\omega)$ in strongly coupled CDPs (SCCDPs) and density is more strongly damped at liquid phase [14, 15]. The SCCDP is many body dynamical systems that show different collective excitations and their properties investigated through numerical simulation and theoretical approaches [16]. In condensed matter physics, the pair correlation function usually cannot be determined directly. Rather, the structure factor is determined by scattering of x-rays or neutrons. In dusty plasmas, we are able to measure the pair correlation function directly and to calculate the structure factor in order to compare with condensed matter experiments. The $S(k,\omega)$ is just the Fourier transform of the pair correlation function. Fluctuation of the dynamical density of dusty plasma generates current correlation spectra such as longitudinal and transverse currents [17]. Dynamic ion structure factor of warm dense matter and dense plasma consist of the complete information of ions in strongly interacting systems and also influenced by the electrons property. It is closely associated with density fluctuation, thus determines transport properties and many relaxations such as electrons ion temperature equilibrium and stopping power and also the equation of state. It is also used for diagnostics of the extreme states of matter like a warm dense matter of x-ray Thomson scattering [18]. Dynamical scattering function is given through times correlation function, fluctuated density of liquid argon and light scattering function [19].

2. Numerical model and simulation techniques

In this section, we have implemented molecular dynamic (MD) simulation code with Ewald summation for forces and energies which makes it possible to account the long-range Coulomb interparticle interactions. We trace the motion of single charge species and integrated through leapfrog method and assume that the presence of neutralizing homogenous background. In this plasma environment, random fluctuating forces and friction forces are acting on a charged particle in addition to which forces initiating from the interaction of charged particle. Length of simulation cubic box is defined as $\left(\frac{4\pi N}{3}\right)^{1/3}$ and particles have a random spatial configuration for the beginning of simulation [15, 20]. Fluctuation of microscopic density is observed for different plasma parameters approaching near the equilibrium state [21]. The presented study includes the solution of the equation of motion of a system and particle interacts with each other through Yukawa potential. Provided that an accurate potential can be established for the system of attention under study and equilibrium MD (EMD) can be used irrespective of the phase condition and thermodynamic of the system involved. Yukawa potential is most commonly used potential (screened Coulomb) for SCCDPs including many physical systems such as physics of chemical and polymer, medicine and biology systems, astrophysics, environmental, etc. Major advantage for using this potential is that it reduces the calculation time compared other potentials [22]. The interaction potential energy of a charged particle in Yukawa liquid is given

$$\phi(\mathbf{r}) = \frac{Q^2}{4\pi\varepsilon_o}\frac{e^{\frac{-r}{\lambda_D}}}{|\mathbf{r}|} \tag{1}$$

Here Q is the charge on dust particle, r is the distance between interacting particles, λ_D is Debye screening length that accounts for the screening of interaction of other plasma species and ε_o is permittivity of free space. The scaling (dimensionless) parameters, which fully characterized the system, one is known as Coulomb coupling parameter [23],

$$\Gamma = \frac{Q^2}{4\pi\epsilon_o}\frac{1}{a_{ws}k_B T} \quad (2)$$

where, a_{ws} is the “Wigner-Seitz” radius and it is defined as $\pi n^{\frac{-1}{2}}$ with n is the equilibrium dust number density, k_B is the Boltzmann constant and T is absolute system temperature. It is noted that the Γ is measured as the ratio of average potential energy to average kinetic energy per particle. Second scaling parameter is Debye screening parameter and it is given as $\kappa = a_{ws}/\lambda_D$.

The EMD simulations are performed for a particle number that is chosen between 500 and 1000 particles in a microcanonical ensemble using periodic boundary conditions and minimum image convention of the dust particles. It is to be mentioned that the number density (n) is defined as $n = N/V$, here N is the number of particles and V is the volume of simulation box and it is calculated as $V = 4\pi N/3$. On our case, most of simulations are performed for $N = 500$ and it is observed that the mentioned number of particles is suitable for EMD computations with statistical uncertainty limits. In presented case, the simulation time step is dt = 0.0001 and total simulation time limit was 425,000 step units. The EMD simulations are run between 4.25 10^6 ($1/\omega_p$) to 3.25 10^6 ($1/\omega_p$) time units for each combination of (Γ, κ) in the series of recording dynamical structure factor (DSF), $S(k,\omega)$, of SCCDPs. It can be seen that the first patch of $S(k,\omega)$ results is obtained after the time limit of (38000) step unit. For our case, 13 patches of $S(k,\omega)$ results are obtained and results show that each patch has nearly behavior of $S(k,\omega)$ showing the accuracy of numerical algorithm. In this work, the dynamical structure factor computations of SCCDPs are reported for a wide range of Coulomb coupling parameters Γ ≡ (1, 200) and the Debye screening strength κ ≡ (1.4, 4).

2.1. Model of DSF [$S(k,\omega)$]

The number density of single species also known as mass density and dimensionless quantity in molecular dynamic units can be written as

$$\rho(r, t) = \sum_j \delta(r - r_j(t)) \quad (3)$$

here r is the point at time t. from the practical point of view, it is known as local density. The average occupancy in the small volume of r space and it calculates over the short interval of time. The definition of density is satisfied matter conserved requirement.

$$f\rho(r, t)dr = N_m \quad (4)$$

The space and time-dependent density correlation are explain from the van Hove correlation function which is define as $G(r, t) = G_s(r, t) + G_s(r, t)$ and further detail is given in Ref. [23]. Fourier transform of density fluctuation and new expression is given as

$$\rho(k, t) = f\rho(r, t)\, e^{-ik.r}\, dr = \sum_j e^{-ik.r(t)} \quad (5)$$

where k is the wave number and becomes equal to $k = 2\pi/L$ and L is the length of simulation box. The intermediate function can be defined as

$$F(k, t) = \langle \rho(k, t)\rho(\text{-}k, t) \rangle \quad (6)$$

The relation between static structure factors with the dynamic structure factor is

$$S(k,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(k,t)\, e^{i\omega t}\, dt \tag{7}$$

This satisfies the sum rule as

$$\int_{-\infty}^{\infty} S(k,\omega) d\omega = S(k) \tag{8}$$

The dynamical structure function is related to longitudinal current correlation function, which is expressed as [22].

$$S(k,\omega) = \frac{1}{\omega^2} C_L(k,\omega) \tag{9}$$

3. Results and discussion

The EMD simulation has been used for the calculation of $S(k,\omega)$ to understand the dynamic phenomenon of particles for 3D SCCDPs. We have analyzed our simulation results of $S(k,\omega)$ in term of frequency, amplitude and fluctuation rate with respect to these parameters (κ, Γ, and k).

This section shows an overview of our results obtained through EMD simulations for dynamical structure factor $S(k,\omega)$ function of SCCDPs at $\kappa = 1, 2, 3$ and 5 with $N = 500$. **Figures 1–4** shown our results for $S(k,\omega)$ over a wide suitable range of plasma states (Γ, κ) at four values of wave vectors $\boldsymbol{k}$ = (0, 1, 2 and 3). A sequence of dynamical structure factor in increasing of wave vector ($\boldsymbol{k}$) is computed to determine the suitable equilibrium values of $S(k,\omega)$. We have performed 16 EMD simulation with $N = 500$ for each screening parameters at different four values of $\boldsymbol{k}$. There are 64 simulations are carried out for different combination of plasma parameters in order to observe complete behaviors of DSF $S(k,\omega)$ at higher varying frequency (ω_p) as compared to earlier simulation results [16]. It is observed that the presented results obtained through EMD simulations for varying parameters have suitable signal-to-noise ratio of the DSF. Our results are satisfactory good agreement with earlier EMD estimations and show that the presented EMD results at higher ω_p and earlier EMD simulations have comparable performance with small system size, both yielding the close values of the DSF $S(k,\omega)$. Moreover, the system temperature ($1/\Gamma$), strength of Debye screening (κ), system run time (total time), system size (N), and wave vector ($\boldsymbol{k}$) are changed to observe how efficiently the presented EMD method computes the DSF $S(k,\omega)$ of SCCDPs.

In addition, in each panels of **Figures 1–4**, we have shown the behaviors of $S(k, \omega)$ at four values of $\boldsymbol{k}$. All these data are excellent due to the good statistics and allow the analysis of the structure–function within a broad dynamical range. It is examined that the peaks of $S(k,\omega)$ are decay at lower Γ values for different four values of κ and $\boldsymbol{k}$. It can be noted that the peaks survive up to higher k values at intermediate to higher Γ values and shift toward the higher frequency (ω_p). It is further observed that the wave spectra of $S(k,\omega)$ shifts toward sinusoidal waves form, at the intermediate values of $\Gamma = 50$ and wave spectra shifts toward square type waves forms at higher values of ($\Gamma = 100,200$). Moreover, the panels (a) to (d) of each figures represent the results of $S(k,\omega)$ in nonideal gases state to liquid and crystalline order state

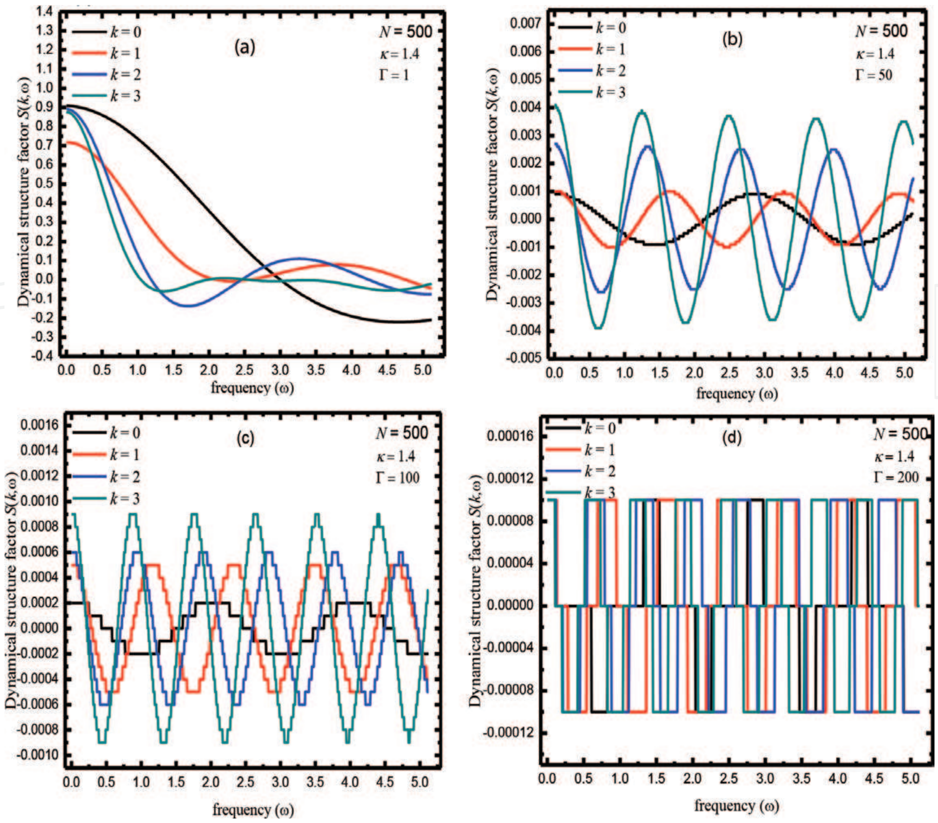

Figure 1. Variation of dynamical structure factor $S(k,\omega)$ as a function of plasma frequency (ω) of strongly coupled complex plasma at $\kappa = 1.4$, $N = 500$ and waves number $k = 0$, 1, 2, and 3 for (a) $\Gamma = 1$, (b) $\Gamma = 50$, (c) $\Gamma = 100$, (d) $\Gamma = 200$.

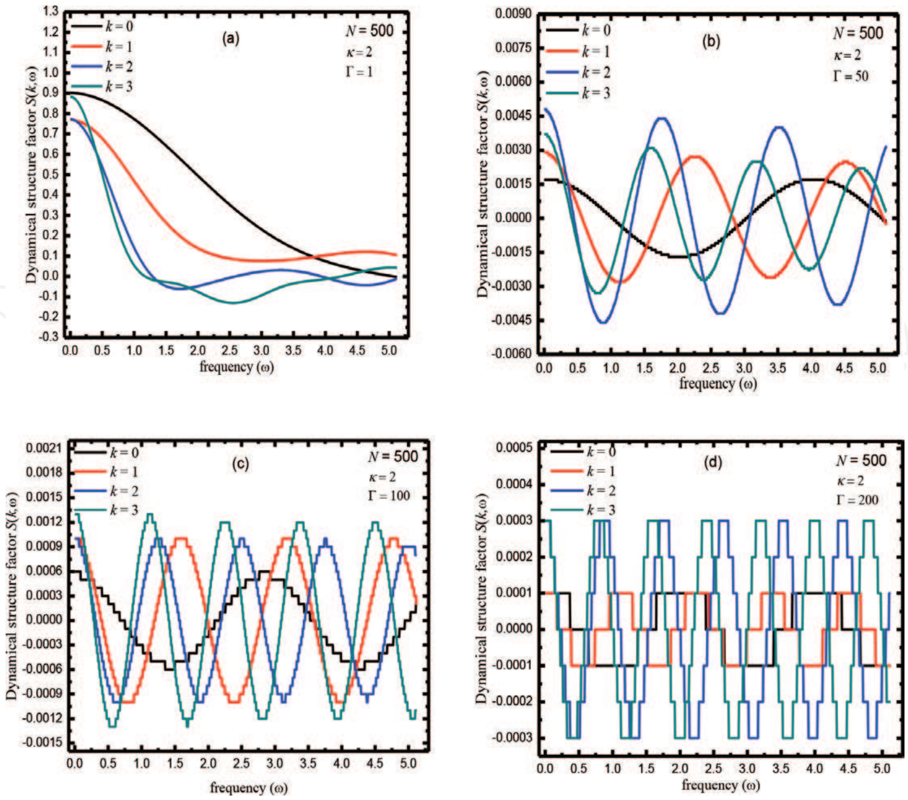

Figure 2. Variation of dynamical structure factor $S(k,\omega)$ as a function of plasma frequency (ω) of strongly coupled complex plasma at $\kappa = 2$, $N = 500$ and waves number $k = 0$, 1, 2, and 3 for (a) $\Gamma = 1$, (b) $\Gamma = 50$, (c) $\Gamma = 100$, (d) $\Gamma = 200$.

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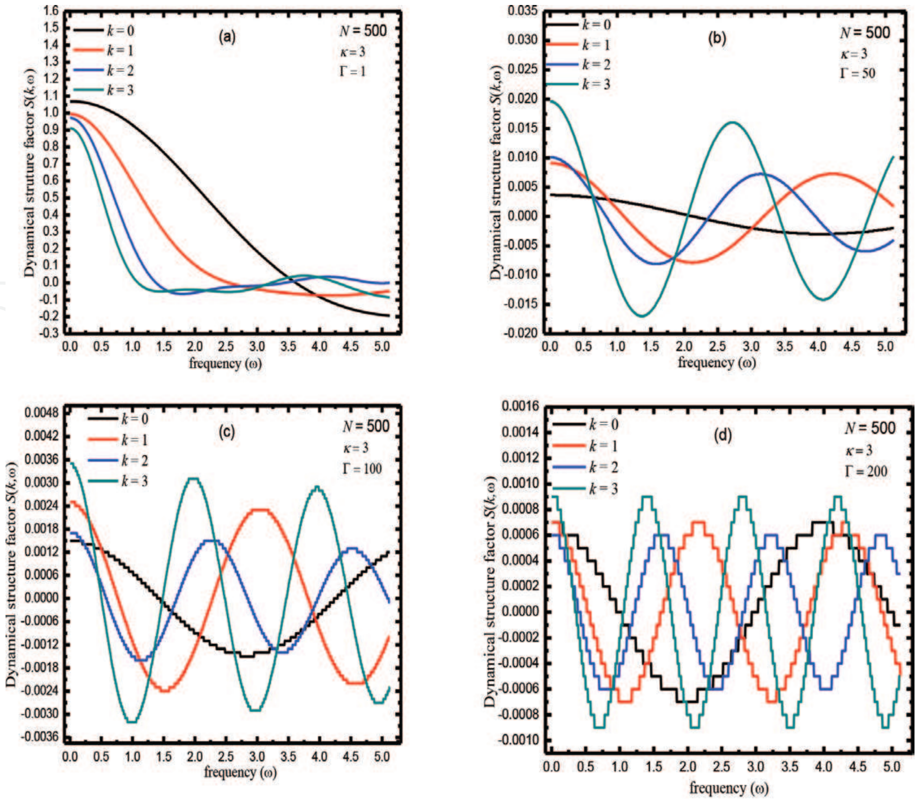

Figure 3. Variation of dynamical structure factor $S(k,\omega)$ as a function of plasma frequency (ω) of strongly coupled complex plasma at $\kappa = 3$, $N = 500$ and waves number $k = 0, 1, 2,$ and 3 for (a) $\Gamma = 1$, (b) $\Gamma = 50$, (c) $\Gamma = 100$, (d) $\Gamma = 200$.

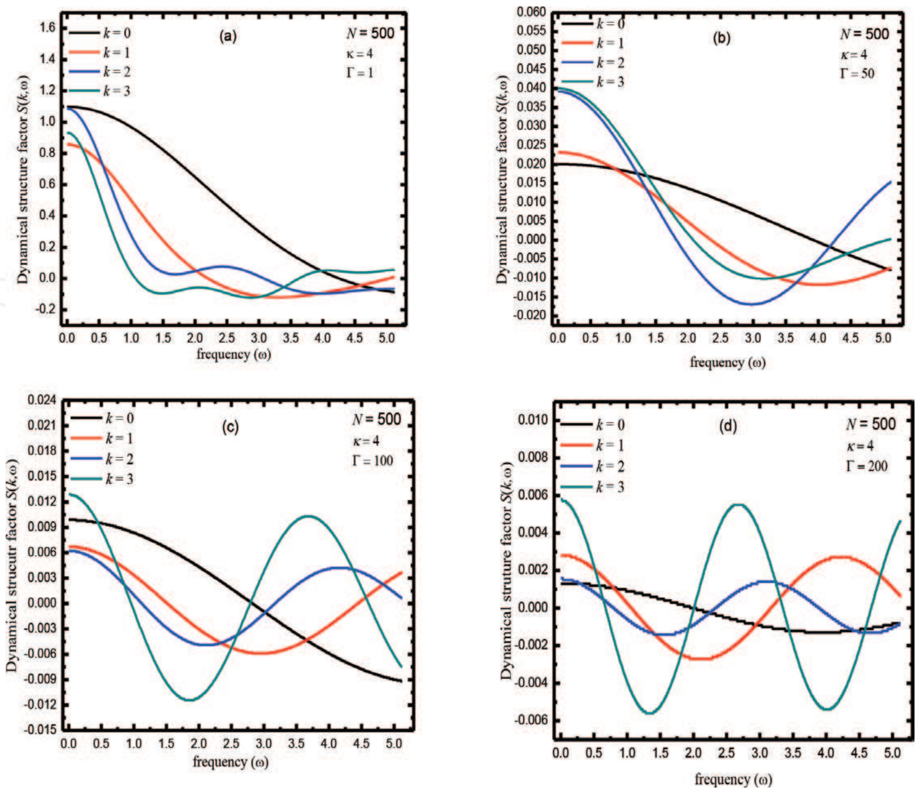

Figure 4. Variation of dynamical structure factor $S(k,\omega)$ as a function of plasma frequency (ω) of strongly coupled complex plasma at $\kappa = 4$, $N = 500$ and waves number $k = 0, 1, 2,$ and 3 for (a) $\Gamma = 1$, (b) $\Gamma = 50$, (c) $\Gamma = 100$, (d) $\Gamma = 200$.

corresponding to Γ (1, 200). In case of crystalline order state, the amplitude of vibrating particle decreases significantly and it converts completely in square waveform. It is interesting to note that the fundamental behavior of dust particles is different and it shows decaying trends in nonideal gases state, sinusoidal form in liquid state and square wave form in crystalline state at fixed screening value. Figures show that the results of $S(k,\omega)$ depend on the plasma parameters (κ, Γ), as expected. Furthermore, it is investigated that in the ideal form of dusty plasma with high temperatures (low coupling values) the dust particles are exponentially decaying from high to low amplitude. One of justification is the dust particles transferred their energy to the surrounding particles that at high plasma temperature values. Furthermore, in panels (b) represent the EMD results of $S(k,\omega)$ in the liquefied state of dusty plasma. In this regime, dust particles comparatively less transfer their energy to the system. At this regime amplitude is maximum for simulation box size (L = max) and frequency of oscillating of dust particles is low and in the sinusoidal waveform. The frequency and amplitude of oscillating dust particles increase with increasing wave numbers k = 2, 3 and exhibit in the periodic wave form. Panels (c) show the results of $S(k,\omega)$ of dusty plasma in the nearly crystalline states. We have analyzed that in this regime the particles are tightly bound. In this case, the dust particles have small amplitude as compared to the gaseous and liquefy forms of dusty plasma.

It is observed from each panel of **Figures 1–4**, the dynamic of dust particles increases with increasing wave number. It is to be noted that the values of amplitude of the $S(k,\omega)$ are 3 = 0.7406, 0.6662, 0.8004 and 0.7902 respectively, for four wave numbers (k = 0, 1, 2, and 3) at the same values of κ, Γ and N. It is observed that the dynamical structure factor of SCCDPs depends on plasma parameters (κ, Γ). The frequency mode of $S(k,\omega)$ is high at low κ for SCCDPs. It is observed that κ is equally affecting on the dynamic of dust particles either the dusty plasma in any phase (gaseous, liquid and crystalline).

4. Summary

We have employed EMD simulations for the investigations of $S(k,\omega)$ over a wide range of Coulomb and Debye screening parameters (κ, Γ). It has been shown that the presented EMD technique and previous numerical methods have equivalent performance for the wide range of plasma state points, both yielding satisfactory data for plasma $S(k,\omega)$. New simulations provide more consistent and inclusive results for the plasma $S(k,\omega)$ over a complete range of Γ (1, 200) and κ (1.4, 4) than the previously known numerical results. Our investigations show that the dynamic of dust particles are exponentially decayed, sinusoidal form and crystalline form, respectively, in the gaseous, liquefy regime and crystalline states of SCCDPs. Moreover, the dynamical spectra of dusty plasma do not observe at very high values of Γ and low values of κ. Moreover, our results indicate that the dynamical structure factor in SCCDPs depends on κ, Γ and k. It has been shown that the presented simulation has comparable performance with the earlier simulation of $S(k,\omega)$ over the wide domain of plasma states. For future work, it is suggested that presented EMD technique based Ewald summation can be used to investigate and explore dynamical structure factor behaviors in other simple liquid, dipolar and ionic materials.

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Abbreviation and symbols

EMD	equilibrium molecular dynamics
MD	molecular dynamics
SCCDPs	strongly coupled complex dusty plasmas
WCCDPs	weakly coupled complex dusty plasmas
CDPs	complex (dusty) plasma
DSF	dynamical structure factor
PECVD	plasma-enhanced chemical vapor deposition
$S(k,\omega)$	dynamical structure factor
k	wave number
N	number of particles
ω_p	plasma frequency
κ	Debye screening strength
Γ	Coulomb coupling

Author details

Aamir Shahzad[1,2]*, Muhammad Asif Shakoori[1], Mao-Gang HE[2] and Yan Feng[3]

*Address all correspondence to: aamirshahzad_8@hotmail.com

1 Molecular Modeling and Simulation Laboratory, Department of Physics, Government College University Faisalabad (GCUF), Faisalabad, Pakistan

2 Key Laboratory of Thermo-Fluid Science and Engineering, Ministry of Education (MOE), Xi'an Jiaotong University, P. R. China

3 Center for Soft Condensed Matter Physics and Interdisciplinary Research, College of Physics, Optoelectronics and Energy, Soochow University, Suzhou, China

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