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Self-Diffusion of Dust Grains in Strongly Coupled Dusty Plasma Using Molecular Dynamics Simulation

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Abstract: *In this paper diffusion of dust particles in strongly coupled dusty plasma is investigated by using molecular dynamics simulations. Self-diffusion coefficients of complex plasmas are obtained for a wide range of plasma parameters using Green-Kubo expression which is based on integrated velocity autocorrelation function (VACF). It is assumed that dust particles interact with each other by Yukawa (i.e. screened Coulomb) potential. The study gives interesting results of dust particle diffusion in plasma.*
Keywords: *Dusty Plasma, Self-diffusion, Green-Kubo formula, Molecular dynamics simulation, Magnetic field*

I. Introduction

Dusty plasma represents [1-5] a mixture of ions, electrons, gas atoms and micron-sized charged grains. Dusty plasma is found in astrophysical environments like planetary rings, stars, nebulae, interstellar space, the solar system, cometary tails, molecular clouds etc. Terrestrial plasmas occur in lightning, a variety of laboratory experiments, and a growing array of industrial processes. Dust particles are produced as impurities in tokomak and their presence may lead to serious safety problem in tokomak operation. Moreover, such dust particles may affect the efficiency of tokomak. For future fusion devices including ITER, a proper understanding of dust transport in presence of magnetic field may be extremely important. Such study may help in removal of dust particles from fusion devices. Another very important area where transport of dust particles may key role is molecular cloud. Spectroscopic studies reveal that micron to nano-sized dust particles are present in molecular cloud and within these regions, star formation take place. Magnetic field present in molecular cloud may couple with the dust particles and this may play a very important role in formation and evolution of stars. The problem discussed in the present paper will give some idea about the transport properties of dust particles in such environments.

Self-diffusion of complex plasma refers to the motion of dust particles due to interaction with other dust particles. The micron-sized dust particles may be easily observed in laboratory and this gives an advantage to complex plasma for studying various phenomena like phase transition, structure formation and diffusion properties etc. The diffusion of dust particles is one of the most significant transport processes in complex plasma systems. It plays an important role in determining dynamical properties of many physical, chemical and biological systems. In the past decade, transport phenomena of Yukawa system have been studied both theoretically and experimentally. Molecular dynamics (MD) simulation is another very useful tool to study self-diffusion of a Yukawa system. The dynamical properties of the two-dimensional strongly coupled Yukawa systems were investigated by the molecular dynamics simulations [6-8]. Hamaguchi et al. [9] investigated the self-diffusion coefficient by the Green-Kubo formula over a wide domain of the Coulomb coupling (Γ) and screening (κ) parameters from MD simulations. Nuromura et al. [10] have performed a very interesting experiment in a capacitively coupled 13.56 MHz radio-frequency discharge to determine self-diffusion of liquid complex plasma. They found that self-diffusion co-efficient D increases linearly with time. In recent years, dusty plasma community has focused on the study of strongly coupled plasma in presence of magnetic field. [11,12,13,14,15,16]. The purpose of the present paper is to investigate the diffusion processes of strongly coupled 3D Yukawa system in a wide range of plasma parameters both in the presence and absence of external magnetic field. We have performed molecular dynamics (MD) simulations to determine the velocity autocorrelation function (VACF) and the self diffusion coefficient D by using the Green-Kubo expressions.

II. Theoretical Model

We consider a three dimensiona dusty plasma consisting of electrons, ions, gas atoms and micron-sized electrically charged dust particles. The interaction of dust particles is well described well by the Yukawa or Debye-Hückel potential [17-19]

$$\Phi(r_{ij}) = \frac{Q_d^{\,2}}{4\pi\varepsilon_0 r_{ij}} \exp(-\frac{r_{ij}}{\lambda_D}) \qquad (1)$$

where Q_d is the particle charge, λ_D is the screening length due to electrons and ions and r_{ij} is the distance between two particles. The dynamic properties of dusty plasma is characterized by two important parameters: Coulomb coupling parameter Γ and screening constant κ defined as

$$\Gamma = \frac{Z^2 e^2}{4\pi\varepsilon_0 a K_B T_d} \tag{2}$$

$$\kappa = \frac{a}{\lambda_D} \tag{3}$$

where $a = \left(\frac{3}{4\pi n_d}\right)^{1/3}$ is the mean inter-particle distance, T_d is the temperature of the dust grains, n_d is the dust number density. The system is called "strongly coupled" if the coulomb coupling parameter i.e., the ratio of the average inter particle potential energy to the average kinetic energy, is comparable with or greater than unity. An external magnetic field B is applied along z-direction. The dynamics of the plasma particles is affected by the magnetic field and as a result the interaction potential among dust particles becomes anisotropic in presence of the field. In the xy-plane, perpendicular to the magnetic field, the interaction potential around a test dust particle with a charge Q_d in presence of external magnetic field is [20,21] taken as

$$\Phi(r) = \frac{Q_d^{\ 2}}{4\pi\varepsilon_0 r_{ij} f_1} \exp\left(-r_{ij}/\rho_s\right) \tag{4}$$

where $f_1 = 1 + f$ and $f = \left(\omega_{pi}^2/\omega_{ci}^2\right)$, ω_{pi} and ω_{ci} beings the ion plasma and ion gyro-frequencies respectively, $\rho_s = \sqrt{f_1}\lambda_{De} \equiv \left(C_S/\omega_{ci}\right)$ is the ion-acoustic gyro-radius, λ_{De} is the electron Debye radius, and $C_S = \lambda_{De}\omega_{pi}$ is the ion-acoustic speed. The interaction potential has been taken as normal Debye-Hückel along z-direction. The presence of magnetic field affects the shielding of dust particles and this indirectly leads to modification of the two controlling parameters Γ and κ to Γ_m and κ_m respectively, where

$$\Gamma_m = (\Gamma / f_1) = \frac{Q_d^{\ 2}}{4\pi\varepsilon_0 a f_1} \frac{1}{K_B T_d} \tag{5}$$

$$k_m = \left(a/\rho_s\right) = \left(\frac{a}{\sqrt{f_1}\lambda_{De}}\right) \tag{6}$$

Self-diffusion of dust particles can be studied with the help of MD simulation using either Einstein's formula or Green-Kubo integral method. In the Einstein plot method, they are evaluated from the slope of the mean-squared displacement in the long-time limit. In the Green-Kubo integral method, transport coefficient may be obtained as integral under the time correlation functions and the relevant thermodynamic fluxes. The self-diffusion co-efficient D of a system of particles in three dimensional cases can be calculated using velocity autocorrelation function (VACF) through the Green-Kubo integral formula [22]

$$D = \frac{1}{3}\int_0^{\alpha} Z(t)dt \tag{7}$$

where VACF= $Z(t) = \left\langle v_j(t) \cdot v_j(0) \right\rangle$ (8)

The brackets <…....> in Eq. (8) represent the canonical ensemble average over all particles. The integrand Z(t) is the velocity autocorrelation function, which measures the temporal development of particles that are tracked individually, as they collide with others and it is the fluctuating velocity. The VACF is calculated over all segments of the ensemble average of the velocity products at time t and an initial time t_0.

III. Simulation Technique

The Molecular dynamics (MD) simulation code [20] is developed using a 3D cubic simulation box of side L and periodic boundary conditions. The normalized size of simulation box is taken to be equal to 9.792616. The velocity autocorrelation function (VACF) and Green-Kubo formula have been incorporated to estimate the diffusion coefficient of dust particles. The simulation is performed with 500 particles for FCC crystal structure. Each grain is assigned an initial random velocity such that the average kinetic energy corresponds to the chosen temperature T_d. The Newton equation of motion and the Velocity- verlet algorithm used to calculate the new position and velocities from the computed forces. The conservation of energy and momentum is verified to check whether the simulation is self consistent, and can be used for new interaction models. The space, mass, time, velocity, energy and external magnetic field are normalized by λ_D, m_d, $1/\omega_{pi}$, $\sqrt{m_d\lambda_D^2/K_BT_d}$, K_BT_d and $\sqrt{m_d/4\pi\varepsilon_0 a^3}$

The equation of motion for the i[th] dust particles may be written as

$$m_d \frac{d^2\vec{r}_i}{dt^2} = \vec{F}_i(t) \tag{9}$$

where $\vec{F}_i(t) = -Q_d \sum \nabla_i \Phi(r_{ij}) + Q_d \vec{v}_i(t)\times\vec{B}$ for i= 1, 2, 3,..., N and $j \neq i$. Here, m_d is mass of the dust grain, r_i is the position of the grain i, F_i is the force acting on the i_{th} particle and $\phi(r_{ij})$ represents Debye-Hückel type of interaction potential. For our MD simulation we have taken dust grain mass $m_d = 4.0\times10^{-15}$ Kg, ion mass $m_i=1.6726\times10^{-27}$Kg, dust density $n_d = 3.74\times10^{10}\text{m}^{-3}$, ion density $n_i = 1.0\times10^{14}\text{m}^{-3}$, electron and ion charge $q_e= q_i = 1.602200\times10^{-19}$C, electron temperature T_e=2320K, dust charge $Q_d=1.77952\times10^{-16}$C and dust grain radius $r_d = 2.0\times10^{-6}$m. The simulation is performed with 500 particles for FCC crystal structure. Periodic boundary condition is applied

IV. Results and Discussion

Based on the expressions as described in section II and using MD simulation, values of self-diffusion coefficient are obtained for different dust grain radius r_d and the results are plotted in Fig.1 with Coulomb coupling parameter Γ = 200, 370, 500 and 800. The screening parameter is kept constant at κ =1.27. It is seen from the graph that self-diffusion coefficient D decrease with the increase in dust size. Higher values of self-diffusion coefficient for lower values of Γ indicating that self-diffusion decreases as the system goes to the strongly coupled regime.

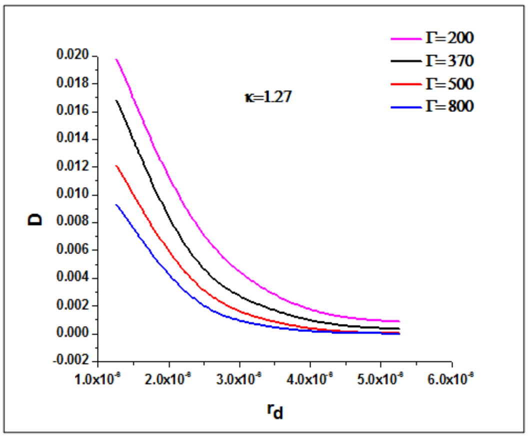

Figure 1: Plot of self-diffusion coefficient D vs. dust radius r_d for different Coulomb coupling parameter Γ at constant screening parameter κ = 1.27.

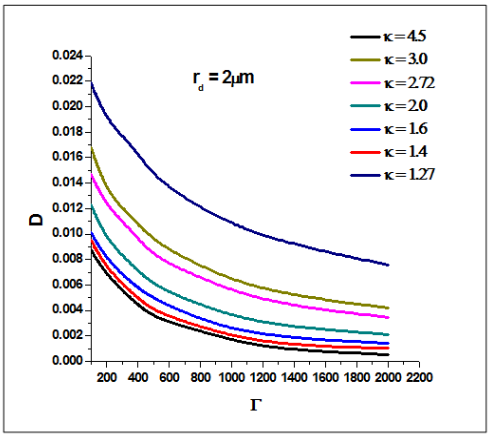

Figure 2: Self-diffusion coefficient D as a function of Coulomb coupling parameter Γ plot for screening parameter =1.27, 1.4, 1.6, 2.0, 2.72, 3.0 and 4.5 respectively.

Fig.2 shows self-diffusion coefficient D as a function of Coulomb coupling parameter Γ plot for screening parameter κ =1.27, 1.4, 1.6, 2.0, 2.72, 3.0 and 4.5 respectively at constant dust radius r_d = 2μm. Self-diffusion coefficient D as a function of screening parameter κ for Coulomb coupling parameter Γ = 200, 370, 500, 800 and 1200 respectively at constant dust radius r_d = 2μm has been plotted in Fig.3. As the value of κ increases thermal motion of dust grains increases and self-diffusion coefficient increases. On the other hand with the increase in the value of Γ the system moves from disordered state to ordered state and as a result self-diffusion coefficient decreases.

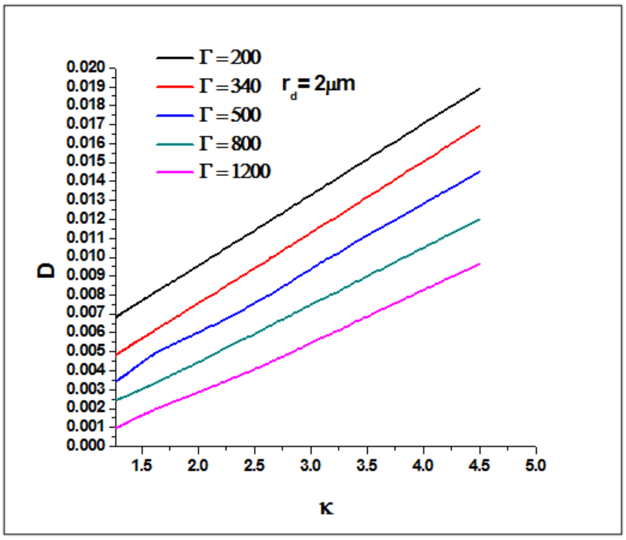

Figure 3: Self-diffusion coefficient D as a function of screening parameter κ plot for Coulomb coupling parameter Γ = 200, 370, 500, 800 and 1200 respectively at constant dust radius r_d = 2μm.

Fig.4 shows a comparison between variation of self-diffusion coefficient D in presence of magnetic field and in its absence. These curves show that diffusion of dust particles across the magnetic field slows down in presence of magnetic field.

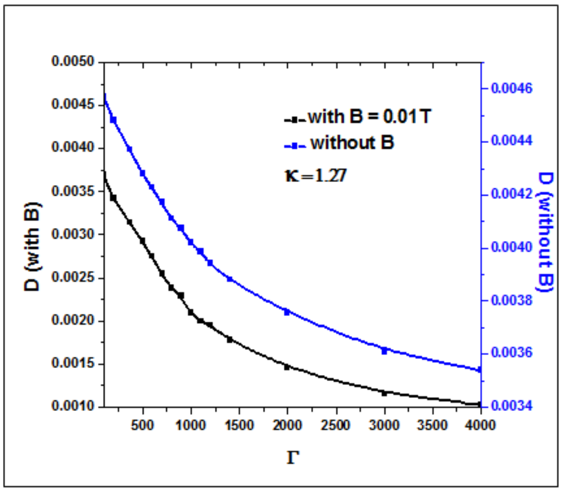

Figure 4: Plot shows a comparison of self-diffusion coefficient D as a function of Coulomb coupling parameter Γ without magnetic field (blue color) and with magnetic field B = 0.01T (black color) at constant screening parameter κ = 1.27.

The presence of magnetic field along z-direction, introduces anisotropy to the system. Self-diffusion coefficient (SDC) D has been splitted into two terms, SDC(⊥) defined as D⊥ and SDC(‖) defined as $D_{\parallel}$, perpendicular and parallel to the magnetic field respectively. D⊥ has been evaluated on the basis of xy-co-ordinates of the dust grains whereas $D_{\parallel}$ has been evaluated from z-co-ordinates of the particles. In Fig.5, D⊥ and $D_{\parallel}$ have been plotted against Coulomb coupling parameter Γ for constant value of magnetic field B = 0.005T. From the graph it has been observed [16] that perpendicular component of self-diffusion coefficient of dust grains D⊥ is greater than parallel component $D_{\parallel}$.

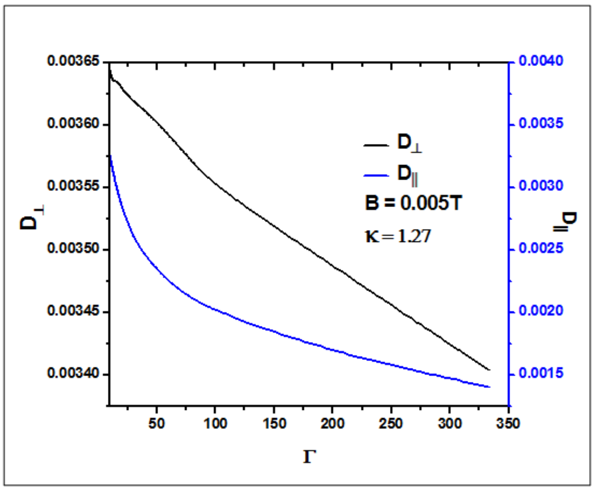

Figure 5: Plot shows a comparison of components of self-diffusion coefficient , D⊥ (blue color) and $D_{\|}$ (black color) as a function of Coulomb coupling parameter Γ at constant screening parameter κ = 1.27.

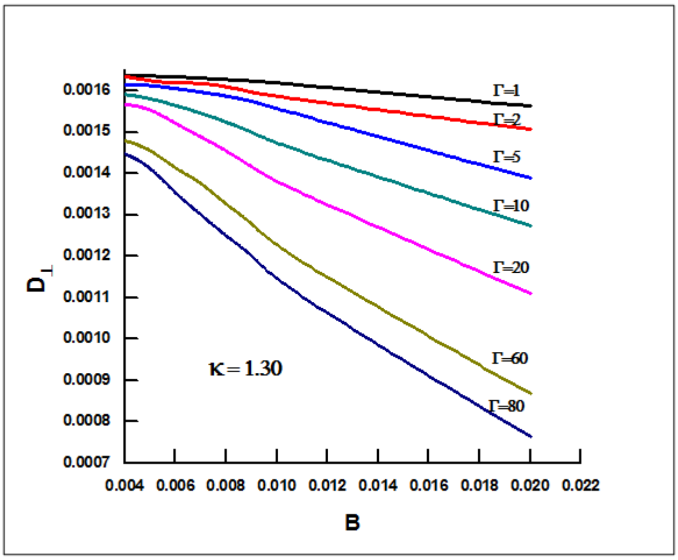

Figure 6: Self-diffusion coefficient D⊥ as a function of magnetic field strength B plot for lower values of Coulomb coupling parameter Γ at constant screening parameter κ = 1.30.

To see the dependence of self-diffusion coefficient on magnetic field, we have plotted D⊥ across magnetic field B in Fig.6 for lower values of Coulomb coupling parameter Γ. As the magnetic field is increased, self-diffusion coefficient D⊥ gradually decreases [16]. The particles are confined due to the magnetic field and this result in the reduction in diffusion.

V. Conclusions

We have performed extensive molecular dynamics (MD) simulation of a three dimensional dusty plasma both in the presence and absence of external magnetic field. The diffusion coefficients have been computed for a number of values of the plasma parameter and the magnetic field strength. Our study gives an idea about the dependence of self diffusion of dust particles on various parameters including magnetic field. The main results found in this study can be summarized as follows:

1. Diffusion increases for higher values of κ or lower values of Γ indicating that diffusion decreases as the system goes to the strongly coupled regime.
2. As the magnetic field B is increased from 0.001T to 0.02T, diffusion gradually decreases. The particles are confined due to the magnetic field and this result in the reduction in diffusion.
3. Parallel component of self-diffusion coefficient $D_{\|}$ is smaller than the perpendicular component D⊥.

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