

Strongly correlated classical plasmas under external forcing and dissipation - an example using Molecular Dynamics

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Abstract. Systems with excess of average potential energy per particle than its kinetic energy develop strong correlations. It is well known that such systems are not amenable to standard procedures of BBGKY hierarchy. This results in failure of both kinetic and fluid models. Phenomenology is the normal way out. If such a strongly correlated system is further subjected to strong drive and/or dissipation, “near first principles” computational methods such as Molecular Dynamics become necessary. Formation of Rayleigh-Bénard convection cells (RBCC), where a liquid is under the action of external gravity and external temperature gradient, is one such phenomena. We report here, the formation of RBCC in 2-dimensional strongly coupled Yukawa liquids, characterized by coupling strength Γ (ratio of average potential energy to kinetic energy per particle) and screening parameter κ (ratio of average inter particle distance to Debye length). We observe the existence of a critical external temperature difference, beyond which RBCC are seen to emerge. Beyond this critical external temperature difference, the strength of the maximum convective flow velocity is shown to exhibit a new, linear relationship with external temperature difference and with a slope independent of (Γ, κ) . The time taken for the transients to settle down (τ_s) is found to be 10,000 to 20,000 ω_{pd}^{-1} , where ω_{pd} is dust plasma frequency. At very high values of Γ and/or low values of κ , RBCC are seen to get suppressed.

1. Introduction

Strongly coupled plasmas (SCP) can be created in laboratories by immersing dust particles/grains of size of few micrometers and mass of the order of 10^{-13} kg in conventional glow discharge plasmas. Dust grains can acquire charge upto $Q \approx 10^4 e$, where e is the electronic charge, grain temperature $T \approx 0.01$ eV and grain plasma frequency $f_d \approx 1$ -50 Hz. SCPs can exhibit very high potential energy over kinetic energy per particle. SCP are found in variety of the systems in nature, for example, in dusty (complex) plasma [1], astrophysical plasmas [2], charged colloidal suspension and ultra-cold plasma [3] to mention a few. Due to the large mass and low temperature, grain medium exhibits a slow time response than the background plasma. An average inter-grain distance “ a ” can be of few millimeters [4, 5]. These stretched time and long length scales of strongly coupled plasmas make it possible to study the “kinetic level” dynamics [6] while at the same time address large scale hydrodynamic phenomena.

Depending on the value of the potential energy over kinetic energy per particle, dusty (complex) plasma can exist in variety of states, for example if the potential energy is very high then dusty (complex) plasma can form “crystalline phase” [4]. In the recent years



dusty plasmas have been a keen area of interest in experimental studies of the fundamental phenomena, for example, formation [4] and melting of Coulomb crystal [7], Mach cones excited by laser in Coulomb crystal [8], dynamics of 3-dimensional Yukawa balls [9], shear bending of the Yukawa liquids [10], head-on collision of the dust-acoustic solitons [11] to mention a few. There have been also very interesting simulation studies, for example, large scale Molecular Dynamics (MD) simulations of 2D strongly coupled Yukawa liquids have been performed to study “hydrodynamics” instability such as Kelvin-Helmholtz instability [12] and coherent dipole and tripole structures [13] as initial value problems.

Formation of the pattern such as Rayleigh-Bénard convection cells (RBCC) is one the fundamental non-equilibrium phenomena in a driven dissipative system. In the past simulations studies have been performed for the analysis of RBCC in the conventional fluids described by Lenard-Jones (LJ) potential, for example, formation of RBCC has been addressed by MD simulations [14, 15] and Direct Simulation Monte Carlo [16].

MD simulation of strongly coupled plasmas is a challenging problem with compounded difficulties in the presence of drive and dissipation. An MPI based molecular dynamics code in two and three dimensions has been developed to address the above said issues [12, 13, 17, 18]. The code is modular and is capable of handling a variety of model classical interaction potentials, external forcing, dissipation and a range of boundary conditions. Here we try to address the effect of strong coupling on the formation of the steady state RBCC, where dusty (complex) plasma is subjected to an external temperature gradient [19], in the presence of gravity [20] lead to steady state RBCC. A more detailed description of the work can be found in Ref. [21], where the effect of strong coupling, results for different values of aspect ratio, effect of dust-neutral drag, results for the smaller degrees of freedom etc. have also been addressed.

2. Strongly coupled (dusty/complex) plasma dynamics governed by Yukawa interaction

The inter-grain potential between two grains in a strongly coupled (dusty/complex) plasma is given by Yukawa potential $\phi(r) = [Q^2/(4\pi\epsilon_0 r)] \exp(-r/\lambda_D)$ where, Q is the charge on grain, “ r ” is inter-grain distance, ϵ_0 is the permittivity of vacuum, λ_D is the Debye length of the background plasma. Yukawa systems can be quantified [17] by two dimensionless parameters: (i) Coupling parameter $\Gamma = Q^2/(4\pi\epsilon_0 a k_B T)$ and (ii) Screening parameter $\kappa = a/\lambda_D$. Here “ a ” (Wigner-Seitz radius) $= 1/\sqrt{n\pi}$, T is dust grain temperature, “ m ” is mass of dust grain, k_B is Boltzmann constant and n is the 2-D aerial number density. The length, time and energy are normalized with a , ω_{pd}^{-1} and $Q^2/(4\pi\epsilon_0 a)$ respectively, where ω_{pd} is the dust-plasma frequency given by $[Q^2 n/(4\pi\epsilon_0 m a)]^{1/2}$. Other quantities in MD units are given in Table 1. For typical

Table 1. Reduced units used the current study

Reduced quantity	Reduced units
Distance (r)	$\frac{r}{a}$
Time (t)	$t\omega_{pd}$
Temperature (T)	$\frac{k_B T}{\left(\frac{Q^2}{4\pi\epsilon_0 a}\right)}$
Energy (E)	$\frac{E}{\left(\frac{Q^2}{4\pi\epsilon_0 a}\right)}$
Acceleration due to gravity (g)	$\frac{g}{(a\omega_{pd}^2)}$

laboratory dusty plasma parameters [22], earth’s gravity in our units is found to be $g_e \approx 0.063$.

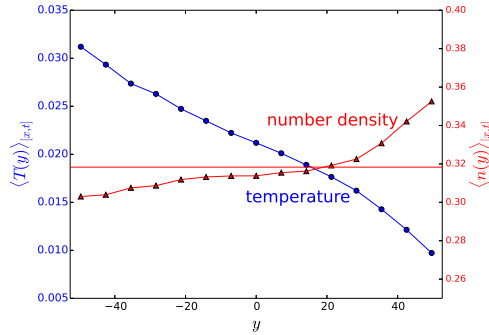


Figure 1. x -averaged density $\langle n(y) \rangle_{[x,t]}$ and temperature $\langle T(y) \rangle_{[x,t]}$ profile for $\Gamma = 50, \kappa = 4, g = 0.003g_e$ and $\frac{\Delta T}{T} = 1$.

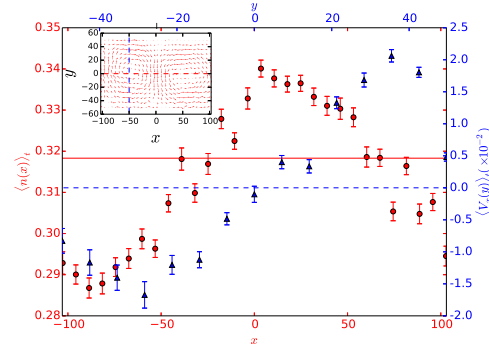


Figure 2. Averaged density $\langle n(x) \rangle_t$ variation with “ x ” at “ y ” ≈ 0 and horizontal component (“ x ”) of fluid velocity $\langle V_x(y) \rangle_t$ variation with “ y ” at “ x ” ≈ -50 . for $\Gamma = 50, \kappa = 4, g = 0.003g_e$ and $\frac{\Delta T}{T} = 1$.

In this work, we use $g \approx 0.0006 g_e$ to $0.03 g_e$ or “milli-gravity” values.

3. Simulation details

We use an upgraded version of two dimensional Multi Potential Molecular Dynamics (MPMD) [18, 20] code. We perform MD simulation of 7200 particles interacting through Yukawa potential. The \hat{x} boundaries are periodic and \hat{y} boundaries are specularly reflecting. The upper and lower \hat{y} boundaries are maintained at low and high temperature respectively. We choose a 2-dimensional vertical cross sectional area of a 3-dimensional system, with $L_x = 212a$ and $L_y = 106a$ which gives the aspect ratio $\beta = \frac{L_x}{L_y} = 2$, average number density $n = 7200/L_x L_y = 1/\pi$. As shown by Donkó et. al. [23], that for a given κ , viscosity of a strongly coupled Yukawa fluid is a convex function of Γ reaching a minimum for certain Γ . We choose a broad range of values of $\Gamma = 1, 25, 50, 100, 200, 500, 800, 1000$ and $\kappa = 0.5, 1, 2$ and 4 in the current study. These parameters are routinely attainable in laboratory conditions [4, 5]. We use Gaussian thermostat [24] in the presence of gravitational field to attain a desired bulk temperature T ($=1/\Gamma$) of the liquid. The time for thermalizing the system is $500 \omega_{pd}^{-1}$ and then we let the system to evolve micro-canonically for another $500 \omega_{pd}^{-1}$ at end of which it attains a thermal equilibrium corresponding to the desired Γ . A Leapfrog integrator with the time step size $\Delta t = 0.01$ is used such that the fluctuation in the total energy without the thermostat is $< 10^{-3}$ over an interval of $1000 \omega_{pd}^{-1}$. To generate a temperature gradient in the system we follow the method used by Vannitsem and Mareshchal [25]. In the present study we use relative temperature difference $\frac{\Delta T}{T}$ as a key parameter for deciding the onset of the convection cells, where \bar{T} is the average temperature.

4. Results

The system of particles is fluidized on to a 30×15 grid to analyze the “fluid” properties of the system. In FIG.-1 we plot “ x ”-averaged density and temperature profile for ($\Gamma = 50, \kappa = 4$), $g = 0.003g_e$ and $\frac{\Delta T}{T} = 1$. The density inversion due to the external temperature gradient is clearly seen in FIG.1, where density is seen to stay close to its mean value set at the start of the simulation. In FIG.-2 we plot the averaged horizontal “ x ”-fluid-velocity $\langle V_x(y) \rangle_t$ as a function of “ y ” at “ x ” ≈ -50 and density $\langle n(x) \rangle_t$ as a function of “ x ” at “ y ” ≈ 0 . In FIG.-3 we plot the “fluid” velocity field and local vorticity, constructed from the particle information. It is clearly

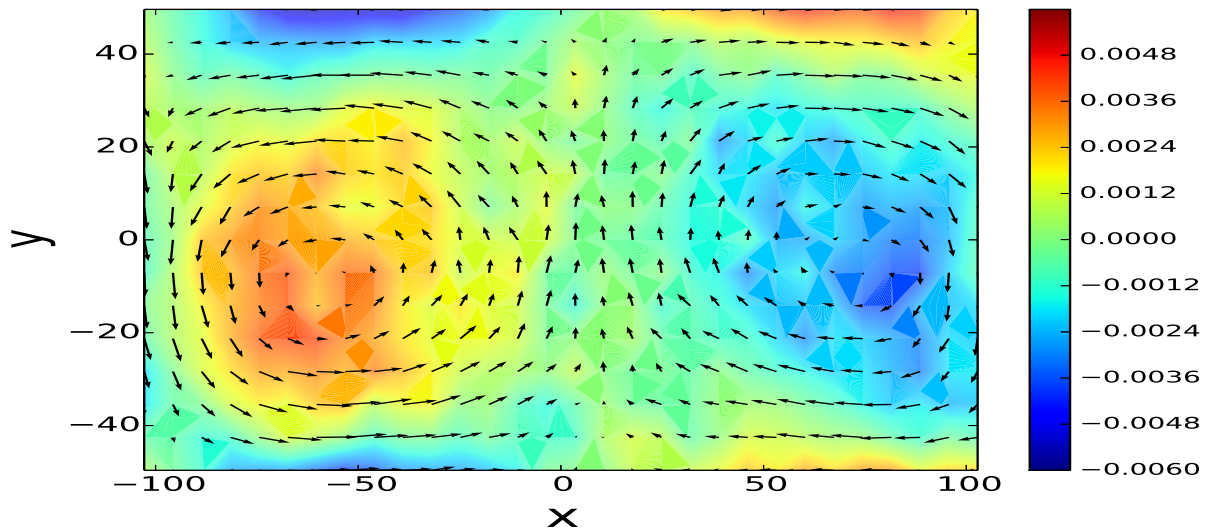


Figure 3. The snapshots show vorticity ($\vec{\omega} = \vec{\nabla} \times \vec{v}$) plot of the system. Blue and red regions correspond to negative and positive vorticity, respectively, and the color-map label shows the magnitude of local vorticity. Arrows indicate direction of the local “fluid” velocity for $\Gamma = 50, \kappa = 4, g = 0.005g_e$ and $\frac{\Delta T}{T} = 1.7$. The quantities are obtained by taking the successive time averages, for the period of $20,000 \omega_{pd}^{-1}$. Grain velocities in the region are fluidized through a 30×15 grid with 16 particles per cell, to construct local vorticity and velocities.

seen that after the system has reached steady state, the system exhibits a two roll structure for $\beta = 2$. The convection cells do not emerge quickly but go through different transient stages and eventually attain a steady state of one or two rolls of convection cells depending on the value of β ($= \frac{L_x}{L_y}$). For the range of (Γ, κ) and $\frac{\Delta T}{T}$ values considered here, typical time for the transients to settle down (τ_s) to a steady state RBCC is found to be about $10,000$ - $20,000 \omega_{pd}^{-1}$ or 1-2 million time steps. As shown in FIG.4, relative temperature difference ($\frac{\Delta T}{T}$) is seen to scale with maximum horizontal flow velocity ($\langle V_x \rangle_t^{max}$). It is evident from FIG.-5 that RBCC are seen to emerge after the system has reached its steady state, where the total energy is not changing too much around its equilibrium values. It is observed that for a given (Γ, κ) , there exists a critical value of relative temperature difference ($\frac{\Delta T}{T}$)_c beyond this value RBCC are seen to emerge and the horizontal convective flow velocity ($\langle V_x \rangle_t^{max}$) increases linearly with $\frac{\Delta T}{T}$. It is interesting to note that the slopes are independent of (Γ, κ) and appear to be “universal” for the Yukawa liquids. This novel linear dependency is demonstrated perhaps for the first time for the strongly coupled systems. The quantities in FIG.1 and 2 are obtained by taking the time average for the period of $20,000 \omega_{pd}^{-1}$ and are obtained for $\Gamma = 50, \kappa = 4$ and $\frac{\Delta T}{T} = 1$. However for very strongly coupled systems, meaning for high Γ (and/or low κ) values the system does not form the steady state RBCC. For example at high Γ (say ≥ 500) we find that the transient phase prolongs up to $\tau_s \approx 100,000 \omega_{pd}^{-1}$ and the formation of steady state RBCC is rendered difficult even at very high values of $\frac{\Delta T}{T}$ [see FIG.-6]. In FIG.-6 we plot the velocity field plot for $\Gamma = 1000$ and $\kappa = 4$, as we can see the strong coupling effect is seen to suppress the formation of steady state RBCC. We believe this could be due to a complex dependence of the non-equilibrium transport coefficients at high Γ . We also observe formation of steady state RBCC for a range of β values for Yukawa fluid [not shown here, for details see Figure 12 and

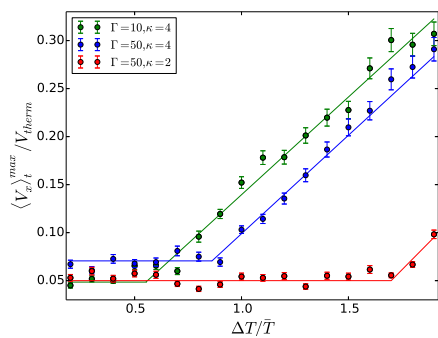


Figure 4. The averaged maximum horizontal convective flow velocity $\langle V_x \rangle_t^{max} / V_{therm}$ as a function of relative temperature difference ($\Delta T / \bar{T}$) for different values of (Γ, κ) .

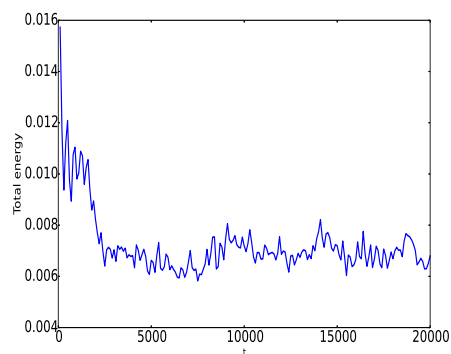


Figure 5. Long time evolution of total energy for $\Gamma = 50, \kappa = 4$ (transient phase) and $\frac{\Delta T}{T} = 1.7$.

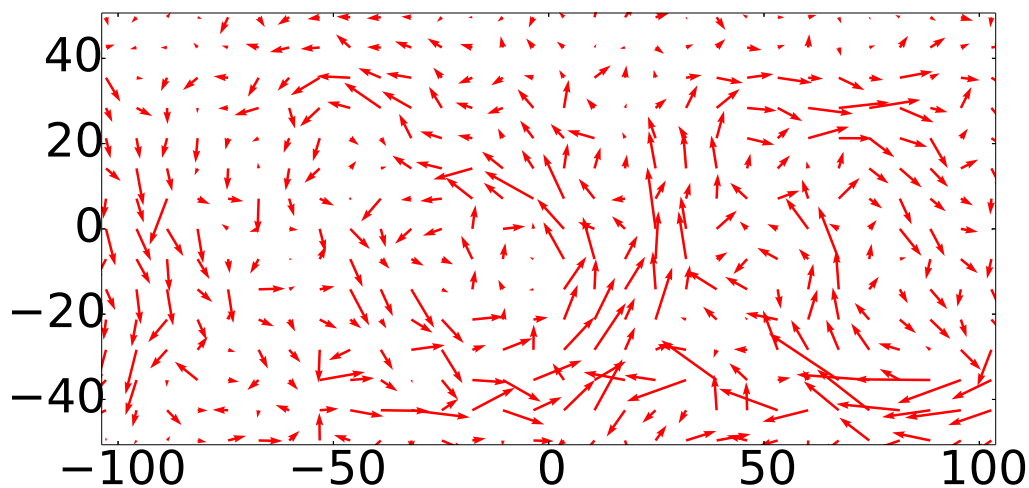


Figure 6. Fluid velocity field for $\Gamma = 1000, \kappa = 4, g = 0.00025g_e$ (transient phase) and $\frac{\Delta T}{T} = 1.8$. The velocities shown here are averaged over the period $(100,000 \omega_{pd}^{-1})$.

13 of [21]].

5. Summary

The phenomena of Rayleigh-Bénard instability in strongly coupled Yukawa liquids using molecular dynamics simulations has been addressed. The convection cells take a time period called, transient period τ_s , for the full development. The time taken for the steady state to form is found to be $\tau_s \approx 10,000 - 20,000 \omega_{pd}^{-1}$. A linear relationship between average maximum convective horizontal velocity and relative temperature is found for strongly coupled Yukawa liquids and slopes are found to be independent of (Γ, κ) values. The strong coupling effects are seen to suppress the formation of steady state convective cells and the transient phases are seen to prolong for up to $100,000 \omega_{pd}^{-1}$ or more. Steady state RBCC is also seen for a range of values of aspect ratio β .

In future many unanswered observations will be addressed, for example, physical reason behind origin of linear relationship between average maximum convective horizontal velocity and relative temperature difference and universality of slope etc.

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