Seminar

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Institute for Plasma Research

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Title: Molecular Dynamics study of Convection Cells in 2D Yukawa liquids

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Date: 22nd December 2022 (Thursday)

Time: 11:00 AM

Venue: Seminar Hall, IPR

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Abstract

Equilibrium statistical mechanical systems, where many particles interact in the absence of external forces, are well understood. For example, a well-known governing principle is extremization of average entropy, which leads to an accurate prediction of various equilibrium phases. However, most of the systems around us are non-equilibrium, driven-dissipative in nature, such as living cells, coffee cups, tokamaks, oceans, planets, stars, galaxies etc, which are fundamentally different from the equilibrium systems in various aspects. For example, unlike equilibrium systems, there are no obvious governing principles to predict the dynamics of such driven-dissipative systems. Interestingly, these systems usually show the emergence of a diverse variety of fascinating macroscale structures or patterns under the effect of drive and dissipative forces. In view of their ubiquity, their fundamental and technological importance, it is imperative that one understands the dynamics of such far-from-equilibrium systems.

Using Yukawa liquids as a prototype, the present work is focused on understanding the dynamics of a minimal, non-equilibrium, driven-dissipative system, namely Rayleigh-Benard (RB) convection, where a fluid layer is subjected to an external temperature gradient in the presence of downward directed external gravity, which form patterns (macroscale structures or convection cells) beyond a critical value of the applied temperature gradient. Long length scales and slow times scales inherent to Yukawa liquids make them an excellent choice to study such fluid flow phenomena at the most fundamental kinetic level.

In this Thesis, by employing classical “first principles” 2D molecular dynamics simulations, the RB cells or patterns have been observed in Yukawa liquids, using just a few thousands of particles. In the quasi steady state of the RB system, where patterns form, a modern non-equilibrium entropic principle (also known as Fluctuation Theorem(s)) has been shown to operate, without assuming any fit parameters. Furthermore, the stability of convective patterns thus formed, is tested using particle-level perturbations and it has been found that the Rayleigh-Benard convection cells (or RBCCs) become unstable, giving way to a horizontal shear flow when subjected to certain particle-level velocity perturbations. The dynamics and stability of RB system have also been studied in the presence of particle-level charge-mass inhomogeneities and dust-neutral collisions. Cross-sectional aspect ratio is shown to play a crucial role in determining the stability of RBCCs. Using simple convection cells at various aspect ratios as initial conditions, important insights are obtained on understanding the stability of RBCCs. Several unresolved problems are identified, pointing towards plausible future work. Additionally, the possibility of realizing the present work in Complex plasma experiments will also be discussed.