

Negative entropy-production rate in Rayleigh-Benard Convection in two-dimensional Yukawa liquids

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According to the second law of thermodynamics, the entropy-production rate is always positive. However, this is true only for an average behavior of a system. One can observe negative entropy-production rate in small systems observed for a finite time. Such rare events constitute the violations of the second law of thermodynamics. Evans, Morris and Cohen proposed a Fluctuation theorem (FT), known as ECM fluctuation theorem¹, which gives the relative probability of occurrence of these negative entropy production events for a non-equilibrium system in a steady-state. The validity of this FT has been verified in many near-equilibrium systems², however, no conclusive test was performed on far-from-equilibrium systems³.

In this work, we consider Rayleigh-Benard Convection in Yukawa liquids as an example of far-from-equilibrium system and test the validity of ECM fluctuation theorem using two-dimensional molecular dynamics simulations. When a thin layer of Yukawa liquid is placed under external gravity, g and external temperature difference, ΔT between the top and bottom plates, the system forms Rayleigh-Benard convection cells (RBCC) in its steady state beyond a critical value of ΔT ⁴. In this steady state, we calculate instantaneous microscopic vertical heat flux⁵ and the resulting instantaneous entropy production rate in a small subsystem chosen at the center of our system (Fig. 1). The instantaneous entropy production rate, $\sigma(t)$ so obtained shows both positive and negative fluctuations

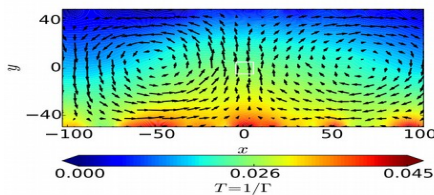


Fig.1 Fluid velocity (arrows) and kinetic temperature (colorbar) plot showing the RBCC formed in the system in its steady state and the subsystem chosen for calculating instantaneous entropy production is shown by white box at the center of our system.

about some positive mean value. The time-averaged entropy production rate, σ_τ (obtained by dividing the time-domain into segments, each of duration τ) is then used to find the probability of positive and negative entropy production rate events. We have found that the ratio of probability of these two entropy production rate events satisfies the ECM fluctuation theorem without requiring any additional fitting parameter (Fig. 2)⁶. The convergence time τ , for which FT is valid, is found to be either comparable to or greater than the time taken by particles to traverse the subsystem under consideration. We have also found that the probability of the negative entropy production rate events decreases with increase in subsystem size, the details of which will be presented.

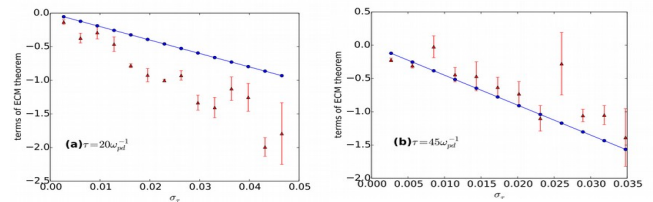


Fig. 2 LHS (red) and RHS (blue) of ECM fluctuation theorem as a function of σ_τ for two τ values (a) $\tau = 20\omega_{pd}^{-1}$ (b) $\tau = 45\omega_{pd}^{-1}$. LHS and RHS converges within error bars for longer τ value in accordance with ECM theorem.

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