Statistical mechanics far from equilibrium: prediction and test for a sheared system

A. BAULE, R. M. L. EVANS, R. A. SIMHA, P. D. OLMSTED, University of Leeds — Beginning from a description of the forces of interaction between microscopic particles in motion, equilibrium statistical mechanics can predict both the statistical properties of their resulting configurations and the properties of the fluid (or other material) that they constitute. Despite the existence of statistical steady states of complex fluids under continuous shear flow, with intriguing similarities to equilibrium phase behaviour, a similarly complete statistical solution has hitherto been unobtainable away from thermodynamic equilibrium. Instead, theorists have had to resort to artificial models with simple dynamics (e.g. some invented set of microscopic transition rates) or, alternatively, to use near-equilibrium approximations. We report the first complete statistical treatment of a collection of particles interacting via Newtonian forces in the presence of continuous boundary-driven flow, arbitrarily far from equilibrium [1]. Our investigation is based on a non-equilibrium counterpart to detailed balance [2] which leads to a set of simple constraints for the driven transition rates in our model system. We have tested the predictions in simulations, by numerically solving and time-stepping the force-balance equations. [1] R. M. L. Evans, R. A. Simha, A. Baule and P. D. Olmsted, to be submitted. [2] R. M.L. Evans, Phys. Rev. Lett. 92, 150601 (2004).

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