TOR VERGATA
UNIVERSITÀ DEGLI STUDI DI ROMA

Dipartimento di Fisica

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Seminar

Wednesday, 12 June 2024 - h. 14:30

Fisica della Materia room (Department of Physics)

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The Chinese University of Hong Kong - Southern University of Science and Technology

"From molecular dynamics to the hydrodynamic limit using the Distinguishable Kinetic Ising Model"

Abstract

The lattice Boltzmann method (LBM) is based on the discretization of the Boltzmann transport equation in time, space and momentum. Assuming a convergence to a local Maxwell-Boltzmann distribution, the momentum-space discretization is obtained by means of Gauss-Hermite quadratures which are supposed to capture the equilibrium diffusive/ballistic dynamics of a homogeneous system at thermal equilibrium. However, when trying to derive such discretization from molecular dynamics (MD), i.e. by means of the molecular-dynamics-lattice-gas (MDLG) mapping [1], one can only approximately recover the standard LBM stencils, for certain values of the coarse-graining parameters. Furthermore, while LBM is concerned with the expectation value of the discrete distribution (populations), by means of MDLG one can study their fluctuations displaying non-trivial scaling features [2].

I will introduce a kinetic Ising model with distinguishable particles which offers a possible alternative to the need of extensive and computationally demanding MD simulations required to investigate the different regimes of the MDLG mapping: one can leverage the equivalence between the Ising model and the lattice gas to define a discrete version of MD allowing for phase-separation (still in the correct universality class) and consistent thermodynamic fluctuations.

Distinguishability is necessary to reconstruct the coarse-grained discrete probability distribution (populations) while allowing for local momentum conservation. The model is compliant with the results obtained in [1] and [2] while extending the analysis to different scaling regimes. I will also show that the MDLG populations can capture both a Gaussian and a non-Gaussian statistics according to the value of the coarse-graining parameters, demonstrating non-trivial scale transformation properties that are related to the framework of the Renormalization Group.

[1] : Parsa, M. R. and Wagner, A. J., PRE, 96, 013314 (2017).
[2] : Parsa, M. R. and Wagner, A. J., PRL, 124, 234501 (2020).

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