Efficient thermostatting of semiclassical Hamiltonian lattice dynamics

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In this work, we propose mixed canonical-microcanonical equilibrium distribution and develop thermostat methods for semiclassical Hamiltonian lattice equations. In semiclassical Hamiltonian lattice models, the crystal lattice is described by classical Hamiltonian dynamics, whereas an extra charge (electron or hole) is modeled as a quantum particle within the tight-binding approximation. Such models are of significant scientific importance. A particular application is hyperconductivity, i.e., the experimental observation of charge transport without the presence of an external electric field when a silicate is bombarded with alpha particles. The charge is carried through the crystal by nonlinear lattice excitations. In the present work, the canonical equations for a semiclassical Hamiltonian describing the coupled lattice-charge dynamics are coupled to an efficient stochastic thermostat, which drives the system to the equilibrium distribution at a prescribed temperature with minimal perturbations to the Hamiltonian trajectories while at the same time ensuring the conservation of the charge probability. The properties of the proposed efficient thermostatting are explored and numerically demonstrated on a phenomenological semiclassical Hamiltonian lattice model.

References

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Acknowledgments

The authors acknowledge the following projects and grants:
Project from the Faculty of Physics, Mathematics and Optometry, University of Latvia (2024); MICINN PID2019-109175GB-C22, MICINN PID2022-138321NB-C22, and travel grants from VII PPITUS-2024 of the Universidad de Sevilla.