Numerical integration of thermostated semiclassical Hamiltonian lattice equations

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Abstract: In this work, we develop computationally efficient splitting methods for semiclassical Hamiltonian lattice equations, where crystal lattice models are 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 by nonlinear lattice excitations. In the present work, the canonical equations for a semiclassical Hamiltonian describing the coupled lattice-charge dynamics are coupled to a gentle stochastic thermostat, which drives the system to the canonical 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 splitting methods are explored and numerically demonstrated on a phenomenological semiclassical Hamiltonian lattice model.

Keywords: semiclassical Hamiltonian dynamics; splitting methods; lattice models; stochastic thermostats; charge transfer; nonlinear localized excitations.

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Acknowledgments: The authors acknowledge the following projects and grants: J. Bajārs: project from the Faculty of Physics, Mathematics and Optometry, University of Latvia (2024); J.F.R. Archilla: MICINN PID2022-138321NB-C22, and travel grants from VII PPITUS-2024 of the Universidad de Sevilla.