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Finite-Temperature Dynamical Properties of the Holstein Model: Hierarchical Equations of Motion Approach

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While ground-state properties of the Holstein model are well understood by now, the evaluation of its finite-temperature spectral properties has received more attention only recently [1, 2]. Here, we develop a hierarchical equations of motion (HEOM) approach to compute real-time single-particle correlation functions and thermodynamic quantities of the Holstein model at finite temperature [3]. We exploit the conservation of the total momentum of the system to formulate the momentum-space HEOM whose dynamical variables explicitly keep track of momentum and energy exchanges between the electron and phonons. Our symmetry-adapted HEOM enable us to overcome the numerical instabilities inherent to the commonly used real-space HEOM. The HEOM results for the electronic spectral function, obtained on chains containing up to ten sites, compare favorably to existing literature. To provide an independent assessment of the HEOM approach and to gain insight into the importance of finite-size effects, we devise a quantum Monte Carlo (QMC) procedure to evaluate finite-temperature single-particle correlation functions in imaginary time and apply it to chains containing up to twenty sites. QMC results reveal that finite-size effects are quite weak, so that the results on 5 to 10 site chains, depending on the parameter regime, are representative of larger systems.

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