Higher Order Propagators for Path-integral Monte Carlo Study: Application to Quantum Quadrupolar Rotors

S. Park and Y. Kwon

Division of Quantum Phases and Devices, School of Physics, Konkuk University, Seoul, Korea

For quantum Monte Carlo simulations the primitive propagator whose time step error is proportional to τ^3, has been widely employed. A fourth-order propagator Chin proposed some years ago could produce more accurate results with small enough time step since it involves a time step error proportional to τ^5. Its application, however, requires a great deal of computer time increase, limiting its efficiency. Zillich et al.[1] recently developed extrapolated higher-order propagators which could allow more efficient calculations to be carried out. In their scheme any even-order propagator can be generated through the multi-product (MP) expansion of the primitive propagator, whose accuracy and efficiency were systematically tested for liquid ^{4}He. We here apply the MP higher-order propagators to path-integral Monte Carlo (PIMC) simulations on asymmetric quadrupolar rotors, which is a model system to study orientational ordering in a molecular solid of hydrogen deuteride at low temperatures under high pressures. Through comparison of the accuracy of these new calculations with the ones of using the old propagators, we investigate availability of MP propagators to a quantum-many system with rotational degrees of freedom. Finally we present PIMC phase diagrams of quantum quadrupolar rotors fixed at the face-centered cubic lattice sites and compare them with the one determined experimentally for solid hydrogen deuteride.

[1]R. E. Zillich, J. M. Mayrhofer, and S. A. Chin, J. Chem. Phys. **132**, 044103 (2010).