Paul Bergold
(University of Surrey)

Thursday, February 1, 2024, 12:15

A New Computational Approach for Bridging the Quantum-Classical Divide in Molecular Dynamics

TUM Garching, room 02.08.011, Boltzmannstr. 3, 85748 Garching Forschungszentrum

Abstract: Although many-body quantum simulations have greatly benefited from high-performance computing facilities, large molecular systems continue to pose formidable challenges. Mixed quantum-classical models, such as Born-Oppenheimer molecular dynamics or Ehrenfest dynamics, have been proposed to overcome the computational costs of fully quantum approaches. However, current mixed quantum-classical models typically suffer from long-standing consistency issues. In this talk, we present a fully Hamiltonian theory of quantum-classical dynamics based on a geometric approach and Koopman wave functions. The resulting model appears to be the first to ensure a series of consistency properties, beyond the positivity of quantum and classical densities. We also exploit Lagrangian trajectories to formulate a finite-dimensional closure scheme for numerical implementations, the "Koopmon method". Numerical experiments demonstrate that the Koopmon method is able to capture effects beyond Ehrenfest dynamics in both the classical and the quantum sectors.