Joint CQSE and CASTS Seminar

Weekly Seminar
Sep. 25, 2015 (Friday)

TIME Sep. 25, 2015, 14:30 ~ 15:30
TITLE Complex quantum Hamilton-Jacobi equation with Bohmian trajectories for wave packet dynamics
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Abstract

The CQHJE-BT method is introduced as a synthetic trajectory method for integrating the complex quantum Hamilton-Jacobi equation (CQHJE) for the complex action function by propagating an ensemble of real-valued correlated Bohmian trajectories (BT). Substituting the wave function expressed in exponential form in terms of the complex action into the time-dependent Schrodinger equation yields the CQHJE. We transform the CQHJE into the arbitrary Lagrangian-Eulerian (ALE) version with the grid velocity matching the flow velocity of the probability fluid. The ALE version describes the rate of change in the complex action transported along Bohmian trajectories. The ALE version of the CQHJE and the guidance equation for Bohmian trajectories are simultaneously integrated, and the time-dependent wave function is readily synthesized. The spatial derivatives of the complex action required for the integration scheme are obtained by solving one moving least squares matrix equation. In addition, the method is applied to a two-dimensional model chemical reaction and to the photodissociation dynamics of NOCl. Excellent computational results are obtained for the time-dependent reaction probabilities. The photodissociation dynamics of NOCl can be accurately described by propagating a small ensemble of trajectories. This study demonstrates that the CQHJE-BT method combines the considerable advantages of both the real and the complex quantum trajectory methods previously developed for wave packet dynamics.