Towards Modeling Coherent Control in Ab Initio Multiple Spawning Methods

TODD MARTINEZ, University of Illinois — Ab initio multiple spawning (AIMS) dynamics has been developed as a method to solve the nuclear and electronic Schrödinger equations simultaneously. In this talk, we present new extensions to the AIMS method which allow modeling light absorption with shaped laser pulses for the purposes of achieving coherent control. The new methods are tested on a variety of low-dimensional problems by comparison to numerically exact wavepacket dynamics.