Symmetrical Quasi-Classical Model for Classical Molecular Dynamics Simulations of Electronically Non-Adiabatic Processes

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Abstract

A recently described symmetrical windowing methodology [*J. Phys. Chem. A* **117**, 7190 (2013)] for quasi-classical trajectory simulations is applied here to the Meyer-Miller [*J. Chem. Phys.* **70**, 3214 (1979)] model for the electronic degrees of freedom in electronically non-adiabatic dynamics. Results generated using this classical approach are observed to be in very good agreement with accurate quantum mechanical results for a variety of test applications, including cases where coherence effects are significant and also the challenging asymmetric spin-boson system.