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Semiclassical Description of Non-Adiabatic Dynamics - Part I

NANDINI ANANTH, CHARULATHA VENKATARAMAN, WILLIAM MILLER, University of California Berkeley — Molecular dynamics simulations of systems that involve non-adiabatic transitions has always been challenging as this involves following the coupling between quantum states of the system. The behavior of such systems can best be modeled by making sure that the method used can not only provide a way to incorporate quantum effects, but can also ensures the equivalent treatment of the electronic and nuclear degrees of freedom. We use the classical electron model (Meyer-Miller) to do the latter ; while time evolution using the semiclassical initial value representation (SC-IVR) ensures the inclusion of quantum effects. We are currently studying the viability of this approach with a few test systems. In order to further study the effectiveness of this approach, we are working on several variations of the SC-IVR. For instance, the Forward Backward IVR (FB-IVR) is a variation of the SC-IVR that presents a simplified formulation for correlation functions with a double propagator. The Linearized IVR (LSC-IVR) is yet another variation which results in a more 'classical' formulation of the problem. Our observation and results obtained will be presented.

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