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Semiclassical description of non-adiabatic dynamics - Part II

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Dept. of Chemistry, U. C. Berkeley — Semiclassical IVR is a classical trajectory based method that is used to incorporate quantum effects into classical MD simulations. This, in combination with the classical electron analog model of Meyer and Miller allows us to describe the dynamics on coupled electronic states. The classical electron analog model treats the relevant electronic and nuclear degrees of freedom of a system on the same footing. This achieves dynamical consistency which mixed quantum-classical approaches tend to lack. In joint work with Ananth and Miller, we are studying different IVR approaches to describe non-adiabatic dynamics. One such formulation is “The Exact Forward-Backward IVR”; this has no other approximation other than the semiclassical description of quantum dynamics. Applications of this approach to various model problems will be presented.

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