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Simulation Coherent Quantum Processes in Many-Body Systems Using Classical Trajectories CRAIG MARTENS, University of California, Irvine — We describe a method for the simulation of coherent quantum dynamics in many-body systems. The approach is based on the semiclassical limit of the multistate quantum Liouville equation and solution using classical trajectory ensembles. The method is applied to modeling nonadiabatic quantum dynamics and the creation, evolution, and decay of quantum coherence in condensed phase systems. The role of environmental interactions in inducing—or delaying—ultrafast electronic decoherence of molecules in condensed phases is investigated. In addition, simulations of vibrational dephasing of an I_2 diatomic molecule in cryogenic rare gas matrices are described. For I_2 in Kr, excellent agreement with recent experimental results is obtained.

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