Forward-Backward Semiclassical Dynamics

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Forward-backward semiclassical dynamics (FBSD) provides a practical methodology for including quantum mechanical effects in classical trajectory simulations of polyatomic systems. FBSD expressions for time-dependent expectation values or correlation functions take the form of phase space integrals with respect to trajectory initial conditions, weighted by the coherent state transform of a corrected density operator. It is shown that the initial density in finite temperature expressions can be fully quantized by employing the discretized path integral representation of statistical mechanics, thus ensuring a proper treatment of zero point effects and capturing important imaginary components that are absent from purely classical trajectory methods. Optimal sampling is achieved through Monte Carlo or molecular dynamics techniques. Applications to polyatomic clusters and condensed phase processes are presented.