Nonadiabatic Dynamics in Open Quantum-Classical Systems: Forward-Backward Trajectory Solution

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A new approximate solution to the quantum-classical Liouville equation is derived starting from the formal solution of this equation in forward-backward form. The time evolution of a mixed quantum-classical system described by this equation is obtained in a coherent state basis using the mapping representation, which expresses N quantum degrees of freedom in a 2N-dimensional phase space. The solution yields a simple non-Hamiltonian dynamics in which a set of N coherent state coordinates evolve in forward and backward trajectories while the bath coordinates evolve under the influence of the mean potential that depends on these forward and backward trajectories. It is shown that the solution satisfies the differential form of the quantum-classical Liouville equation exactly. Relations to other mixed quantum-classical and semi-classical schemes are discussed.

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