

Ehrenfest dynamics is purity non-preserving: a necessary ingredient for decoherence

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We discuss the evolution of purity in mixed quantum/classical approaches to electronic nonadiabatic dynamics in the context of the Ehrenfest model. As it is impossible to exactly determine initial conditions for a realistic system, we choose to work in the statistical Ehrenfest formalism that we introduced in Ref. 1. From it, we develop a new framework to determine exactly the change in the purity of the quantum subsystem along the evolution of a statistical Ehrenfest system. In a simple case, we verify how and to which extent Ehrenfest statistical dynamics makes a system with more than one classical trajectory and an initial quantum pure state become a quantum mixed one. We prove this numerically showing how the evolution of purity depends on time, on the dimension of the quantum state space \mathcal{D} , and on the number of classical trajectories N of the initial distribution. The results in this work open new perspectives for studying decoherence with Ehrenfest dynamics.

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