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Exact factorization of the full electron-nuclear wavefunction: A quantum-classical study FEDERICA AGOSTINI, ALI ABEDI, EBERHARD GROSS, Max-Planck-Institut für Mikrostrukturphysik — It was recently shown in [1] that the solution of the time-dependent Schrödinger equation for a molecular system can be exactly factorized to an electronic and a nuclear contribution. In [1], the authors derived exact equations of motion for the coupled evolution of the electronic and nuclear wavefunctions, which are a good starting point to develop approximations, systematically. Based on this exact decomposition of the electron and nuclear motion, we present a quantum-classical scheme for the coupled electron-nuclear dynamics. Nuclear degrees of freedom evolve along a classical trajectory, affecting electronic motion and inducing quantum transitions, which in turn alter nuclear dynamics. Applications of the proposed method to model systems will be presented.

[1] A. Abedi, N.T. Maitra and E.K.U. Gross, *Phys. Rev. Lett.* **105** 123002 (2010).

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