Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Exact factorization of the electron-nuclear wave function: General theory and applications FEDERICA AGOSTINI, ALI ABEDI, SEUNG KYU MIN, YASUMITSU SUZUKI, E.K.U. GROSS, Max Planck Institute of Microstructure Physics — The exact factorization of the molecular wave function [1, 2] to the product of an electronic factor, parametrically depending on nuclear positions, and a nuclear wave function is presented. This starting point is used to decomposed the time dependent Schrödinger equation into two equations, that generate the evolution of the electronic and nuclear components. In this formulation, time dependent scalar and vector potentials mediate the coupling between the two sets of degrees of freedom, in a formally exact way. They represent what is usually referred to as electronic "back-reaction" on the nuclei. In a model system for non-adiabatic electron transfer, we investigate the properties of the potentials [3] and we analyze the classical approximation [4] of nuclear dynamics, in comparison to exact dynamics. This last point will lead to the development of a practical scheme to deal with non-adiabatic dynamics in the mixed quantum-classical approximation.

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Date submitted: 15 Nov 2013 Electronic form version 1.4