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Exact Factorization of the Electron-Nuclear Wavefunction: Exact Electronic Potentials in Coupled Electron-Ion Dynamics YASUMITSU SUZUKI, ALI ABEDI, Max Planck Institute of Microstructure Physics, NEEPA T. MAITRA, Hunter College and the City University of New York, KOICHI YAMASHITA, The University of Tokyo, E.K.U. GROSS, Max Planck Institute of Microstructure Physics — We develop a novel approach to the coupled motion of electrons and ions that focuses on the dynamics of the electronic subsystem. Usually the description of electron dynamics involves an electronic Schrödinger equation where the nuclear degrees of freedom appear as parameters or as classical trajectories. Here we derive the exact Schrödinger equation for the subsystem of electrons, staying within a full quantum treatment of the nuclei. This exact Schrödinger equation features a time-dependent potential energy surface for electrons (e-TDPES). We demonstrate that this exact e-TDPES differs significantly from the electrostatic potential produced by classical or quantum nuclei.

[1] Y. Suzuki, A. Abedi, N. T. Maitra, K. Yamashita and E. K. U. Gross, e-print arXiv:1311.3218v1

Yasumitsu Suzuki
Max Planck Institute of Microstructure Physics

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