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Energy, momentum, and angular-momentum transfer between electrons and nuclei

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Describing the coupled dynamics of electrons and nuclei beyond the adiabatic approximation is notoriously difficult. Starting from the full Hamiltonian of interacting electrons and nuclei, we first deduce an exact factorization [1] of the electron-nuclear wave function into a purely nuclear wave packet and a many-electron wave function which parametrically depends on the nuclear coordinates and which has the meaning of a conditional probability amplitude. The equation of motion for the nuclear factor is a standard Schrödinger equation featuring a vector potential and a scalar potential (both being N-body interactions). The time-evolution of the electronic conditional wave function is governed by a non-Hermitian "Hamiltonian"whose propagation nonetheless conserves the norm of the electronic wave function. This non-Hermiticity is essential for the correct description of decoherence [2,3]. For practical calculations, the equations of motion are "density-functionalized", leading to a coupled set of Kohn-Sham equation for the electrons and nuclei [4]. Furthermore, starting from the nuclear equation of motion of the exact factorization, we deduce subsystem Ehrenfest identities [5] characterizing the energy, momentum, and angular momentum transfer between electrons and nuclei. An electromagnetic-like force operator arising from the scalar and vector potentials in the nuclear equation of motion appears in all three Ehrenfest identities. The magnetic component leads to Lorentz-like forces which couple the motion of different nuclei to each other. Manifestations of these forces will be discussed.

[1] A. Abedi, N.T. Maitra, E.K.U. Gross, PRL 105, 123002 (2010).
[2] F. Agostini, S.K. Min, I. Tavernelli, E.K.U. Gross, J Phys Chem Lett 8, 3048 (2017).
[3] S.K. Min, F. Agostini, E.K.U. Gross, PRL 115, 073001 (2015).
[4] R. Requist, E.K.U. Gross, PRL 117, 193001 (2016).
[5] Chen Li, R. Requist, E.K.U. Gross, PRL 128, 113001 (2022).

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