Electron-Nuclear Correlation via the Exact Factorization Approach

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The exact factorization approach enables the definition of exact potentials driving the dynamics of a quantum subsystem coupled to other quantum subsystems. These potentials yield insight into correlations and provide a useful starting point for new approximate methods e.g. for electronic structure embedding for strong correlation, for mixed quantum-classical dynamics of electrons and ions, and for photon-matter coupling. We briefly review recent progress in these areas, and highlight some success in predictions of exact-factorization-based methods compared with traditional methods, as well as some on-going improvements to the methods. Some of our recent work has focussed on electronic coherences, which are key to understanding and controlling photo-induced molecular transformations. While the evolution of electronic coherences is known to depend on nuclear motion, the exact nature of this electron-nuclear correlation has not yet been well-understood: are inherently quantum aspects of nuclear motion significant, or does an essentially classical picture capture the physics? We discuss the importance of the projected nuclear quantum momenta, and how spatial-resolution influences predictions of experiments even when they measure only spatially-integrated coherences. While traditional trajectory-basedsimulation schemes are blind to the quantum momenta, exact-factorization-based methods approximate these correlation terms, and correctly capture electronic coherences in a range of situations.