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Nonadiabatic nuclear-electron dynamics: a quantum computing approach (15'+5')

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Abstract

The combined quantum electron-nuclear dynamics is often associated with the Born-Huang expansion of the molecular wave function and the appearance of nonadiabatic effects as a perturbation. On the other hand, native multicomponent representations of electrons and nuclei also exist, which do not rely on any a priori approximation. However, their implementation is hampered by prohibitive scaling costs and therefore quantum computers offer a unique opportunity for extending their use to larger systems. Here, we propose a quantum algorithm for the simulation of the time-evolution of molecular systems in the second quantization framework, which is applied to the simulation of the proton transfer dynamics in malonaldehyde. After partitioning the dynamics into slow and fast components, we show how the entanglement between the electronic and nuclear degrees of freedom can persist over long times if electrons are not adiabatically following the nuclear displacement.

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