Exact quantum dynamics for electron-phonon coupled systems with multi-set matrix product states

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Electron-phonon coupling is at the heart of many important phenomena in physics and chemistry, but challenges the applicability of analytical and numerical methodologies. We present a numerically exact method allowing to describe electron-phonon coupled quantum systems in their single-electron sector with unprecedented efficiency [1,2]. The approach is based on a tensor network decomposition applied to vibrational wavefunctions in a multi-set ansatz where the wavefunctions is expanded as a sum over products of electronic states and their associated vibrational wavefunctions. We apply our method to explore electron dynamics in the Holstein model in one and two spatial dimensions. The dynamics of (vertical) Franck-Condon excitations in the regime where Holstein-coupled vibrational modes mix strongly with electronic degrees of freedom is shown to sharply contrast with the known self-localized behavior of vibrationally relaxed excitations. Instead, the strongly-coupled modes are found to periodically induce resonances between interacting electronic sites, during which effective excitation transfer occurs, allowing Franck-Condon excitations to attain substantial mean square displacements under conditions where relaxed excitations are essentially trapped to a single site.

References

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2. Y. Kurashige, *The Journal of Chemical Physics* 149, 194114 (2018).