

Relaxation dynamics in isolated and open many-body quantum systems”

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We address the modeling of the ultrafast dynamics, after femtosecond laser pulse excitation, of both isolated and open many-body quantum systems by considering two test cases: the geometrical rearrangement of NO doped cryogenic Ne matrices upon photoexcitation of the impurity, and the vibrational relaxation of two CO molecules adsorbed on a copper substrate. The dynamical response of the Ne solid is investigated employing the multi-configurational time-dependent Hartree method. The approach is based on a multidimensional shell model, with the shell radii being the dynamical variables. It is shown that the inclusion of dynamical correlations modifies the high-dimensional wavefunction, however, mean values are well described within the mean-field ansatz. Pump-probe signals are calculated and found to be in good agreement with experimental results, allowing for a clear analysis of the ultrafast mechanism of the energy transfer into the solid. The simulation of the vibrational relaxation of two CO molecules approaching a Cu surface is performed within the reduced density matrix formalism in the Markovian regime, assuming a Lindblad form for the system-bath interaction. A factorizable ansatz is introduced for computing the relaxation rates and the associated operators, and benchmarked against the results obtained using the fully coupled spectral basis. The proposed procedure results in a much more advantageous scaling of the computational cost with respect to the increase of the dimensionality of the system. The factorizable method is found to provide an accurate description of the dissipative quantum dynamics of the model system on the whole range of intermolecular coupling strengths.