

An ultrashort laser pulse photoionizing the molecule produces a superposition of a few cationic states. The coupling between the electrons and the nuclei has been predicted to cause fast decoherence. In this thesis, a two-dimensional model of coupled electron-nuclear dynamics in molecules is constructed. It is based on a harmonic potential in the nuclear degree of freedom and a double harmonic potential representing two centers that bind the electrons. The electronic potential's dependence on the nuclear configuration facilitates the coupling. Thanks to the simplicity of the model, it is numerically exactly solvable. We use the basis of its eigenstates to calculate the evolution of any initial state. Several quantities are used to measure decoherence and unravel the underlying mechanisms. Especially useful is the Wigner quasiprobability distribution. A few fundamental cases of the model are analyzed, and it is used to approximate the coherence dynamics in the normal modes of the H_2O^+ cation.