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Quantum Fidelity Susceptibility as a tool to characterize shape transitions in molecular bending spectra

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Molecular bending spectra can be broadly categorized into three physical cases, depending on the molecular equilibrium configuration: linear, bent, and nonrigid. We have studied the three cases in detail with an extended Hamiltonian (including up to four-body interactions) of the 2D limit of the Vibron Model (2DVM), and analyzed shape transitions such as bent to linear transition [1], and isomerization reaction between HCN and HNC isomers [2]. These Hamiltonians depend on different parameters according to the interactions taken into account to reproduce experimental data.

We purpose a method which allows to define a unique control parameter to drive the system from one dynamical symmetry to the other one [3]. This method has been proved to be useful in the study of precursors of excited states quantum phase transitions in the 2DVM [3,4] and in the Lipkin-Meshkov-Glick model [5].

Fixed the method, we need a physical quantity to study the dynamical structure of eigenstates. To solve this issue, authors have extended the usage of quantum fidelity susceptibility from the ground state to excited states domain. This quantity allows us not only to determine in an elegant and basis-independent way the linear or bent character of any excited state [3], but also to determine the transition state in isomerization reactions [4].

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