PARTICIPATION RATIO AND QUANTUM FIDELITY SUSCEPTIBILITY AS TOOLS TO CHARACTERIZE BENT-TO-LINEAR SHAPE TRANSITIONS

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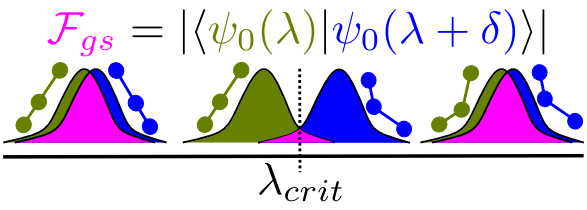
Molecular bending spectra can be broadly categorized into three physical cases, depending on the molecular equilibrium configuration: linear, bent, and nonrigid. We have studied the three cases in detail with an extended Hamiltonian (including up to four-body interactions) of the 2D limit of the Vibron Model (2DVM). We have obtained bending band origin predictions within experimental accuracy as well as the corresponding eigenstates for several molecules [a].



The particular spectroscopic signatures characterizing states that straddle the barrier to linearity in nonrigid molecules have been pinpointed with the quantum monodromy and the Birge-Sponer plots. In addition, we propose a characterization of the obtained bending eigenstates making use of the Participation Ratio and the Quantum Fidelity Susceptibility [b]. The first quantity has already proved useful in determining linearity barriers in molecular bent-to-linear transitions, as well as characterizing transition states in isomerization reactions, e.g., HCN-HNC bond-breaking system [c]. Besides, the second quantity allows us to determine in an elegant and basis-independent way the linear or bent character of any excited state.

As an application, we have studied, using the above mentioned quantities, the bending spectra of several molecules of interest in different fields: HNC, OCCCO, CH_3NCO, ClCNO, NCNCS, and Si_2C.

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[a] J. Khalouf-Rivera, F. Pérez-Bernal, M. Carvajal, *J. Quant. Spectrosc. Radiat. Transfer* (2021) 261, 107436.

[b] J. Khalouf-Rivera, M. Carvajal, F. Pérez-Bernal, SciPost Physics (2021) submitted (arXiv:2102.12335).

[c] J. Khalouf-Rivera, M. Carvajal, L. F. Santos, F. Pérez-Bernal, J. Phys. Chem. A (2019) 123, 44, 9544-9551.