AN ALGEBRAIC METHOD FOR EXPLORING QUANTUM MONODROMY AND QUANTUM PHASE TRANSITIONS IN NON-RIGID MOLECULES

D. LARESE, *Department of Chemistry, Yale University, New Haven CT 06520-8107, USA*; F. IACHELLO, *Center for Theoretical Physics, Yale University, New Haven CT 06520-8120, USA*.

A simple algebraic Hamiltonian has been used to explore the vibrational and rotational spectra of the skeletal bending modes of HCNO, BrCNO, NCNCS, and other "floppy" (quasi-linear or quasi-bent) molecules. These molecules have large-amplitude, low-energy bending modes and champagne-bottle potential surfaces, making them good candidates for observing quantum phase transitions (QPT). We describe the geometric phase transitions from bent to linear in these and other non-rigid molecules, quantitatively analysing the spectroscopy signatures of ground state QPT, excited state QPT, and quantum monodromy.

The algebraic framework is ideal for this work because of its small calculational effort yet robust results. Although these methods have historically found success with tri- and four-atomic molecules, we now address five-atomic and simple branched molecules such as CH_3NCO and GeH_3NCO. Extraction of potential functions is completed for several molecules, resulting in predictions of barriers to linearity and equilibrium bond angles.