REMARKS ON THE PHASE CHANGE OF THE ELECTRONIC WAVE FUNCTION UPON GOING ONCE AROUND A JAHN-TELLER CONICAL INTERSECTION IN VIBRATIONAL COORDINATE SPACE

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In this talk we revisit, with pedagogical emphasis for high-resolution spectroscopists, some presently existing discussions of phase factors for fixed-nuclei electronic wavefunctions in the Jahn-Teller problem. We give explicit examples, for a symmetric pyramidal NH_3-like molecular shape, of perfectly reasonable variants of such electronic wavefunctions that do not transform into their negatives upon going once around the conical intersection (i.e., that do not exhibit a Berry phase change of -1), as well as an example calculation for the pseudo-rotational energy levels and wavefunctions near the bottom of a deep Jahn-Teller moat that does not make use of half-integral quantum numbers and that does not require abandoning ordinary C_{3v} point group theory. Some cautionary remarks on drawing inappropriate conclusions from overly hasty Berry phase arguments will also be presented.