DYNAMICS OF LOCALIZED ANGULAR MOMENTUM AND MULTI-SURFACE ROTATIONAL ENERGY ANISOTROPY FOR INTERNAL-ROTOR MOLECULES AND POSSIBLE SYMMETRY CONVERSION EFFECTS

JUSTIN C. MITCHELL, WILLIAM G. HARTER, *Department of Physics, University of Arkansas, Fayetteville, AR 72701*.

Rigid or semi-rigid rotors with attached gyroscopes approximately model dynamics and spectra of molecules with internal rotation [a] or rovibrational coupling [b]. Classical dynamics of axially constrained rotors are approximated by intersecting rotational-energy-surfaces (RES) that have (J-S).B.(J-S) forms in the limit of constraints that do no work. Improved semi-classical eigen-RES have avoided crossings that make concentric nested surfaces whose anisotropy determines approximate levels, symmetries and dynamics [c]. Semi-classical eigensolutions are compared to those found by direct diagonalization. Possible application to spectra of methyl-rotor molecules are discussed.

[a] J. Ortigoso, I. Kleiner, and J. Hougen, J. Chem. Phys. 110, 11688 (1999).
[b] H. S. Yoo, M. J. DeWitt, and B. H. Pate, J. Chem. Phys, 108, 1348 (2004).
[c] W. G. Harter, Comp. Phys. Reports 8, 320-393(1988) Sections 6.2-3.