TOPOLOGICAL AND GROUP-THEORETICAL PREDICTIONS OF NOVEL ROVIBRATIONAL PATTERNS

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Description of generic qualitative features of the energy spectrum and of the internal dynamic of a quantum system is derived primarily from the global topological properties of the space of dynamical variables and their symmetry. In particular the classification of possible energy level patterns and of different ways of their modifications can be done without analyzing concrete molecular Hamiltonians. The scheme of such qualitative analysis developed and implemented recently for rotational, vibrational, rovibrational and electronic (Rydberg state) problems[a] includes the following steps:

- Construction of a classical limit for a model quantum Hamiltonian. Topological analysis of the corresponding phase space.
- Study of the symmetry group action on the phase space.
- Qualitative classification of the classical Hamilton functions. This step is based on Morse theory which gives the relation between topological properties of the phase space the system of stationary points and periodic orbits.
- Analysis of bifurcations and other possible qualitative modifications under the variation of control parameters, such as strict or approximate integrals of motion.
- Re-interpretation of the qualitative features of the classical dynamical system for the initial quantum operator.

The realization of the scheme on several simple examples related to the formation of unusual new patterns of rovibrational energy levels is given.

[a] For recent review see B. Zhilinskii, Spectrochim. Acta, A, 52, 881 (1996); D. Sadovskii and B. Zhilinskii, Phys. Rev. A, 47, 2653 (1993)