NEW QUALITATIVE FEATURES IN INTRAMOLECULAR DYNAMICS: SIMPLE EXAMPLES

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Many simple quantum atomic or molecular systems possess several mutually commuting (exactly or approximately) observables (energy, angular momentum, ...). We will demonstrate that the patterns formed by joint spectra of mutually commuting operators show several specific qualitative features associated with bifurcations, monodromy, etc. Generic modifications of such patterns under the variation of one or several external parameters as well as their relation to the symmetry of the system will be discussed. As concrete systems, we will use the examples of hydrogen atom in the presence of small static electric and magnetic field[a], vibrational structure of triatomic linear molecules with Fermi resonance and small detuning[b] (CO_2, and CS_2 like molecules), rovibrational structure of tetrahedral molecules (such as methane or silane)[c]. Different patterns in the joint spectra of commuting operators (integrals of motion) are related to different dynamical regimes of the corresponding classical systems and to the presence of singularities of classical fibrations defined by the integrable approximations to these systems. In quantum analog systems, such singularities manifest themselves as *defects of regular lattices*. The difference between the standard defects used in solid state physics (dislocations, disclinations, vacancies) and defects which appear in the joint spectra due to the presence of monodromy will be explained.

[a] K. Efstathiou, D. Sadovskii, B. Zhilinskii. Proc. Roy. Soc. A, submitted.

[b] R. Cushman, H. R. Dullin, A. Giacobbe, D. D. Holm, M. Joyeux, P. Lynch, D.A. Sadovskii, B. Zhilinskii. Phys. Rev. Lett., **93** 024302-1-4 (2004)

[c] K. Efstathiou, D.A. Sadovskii and B.I. Zhilinskii. SIADS, **3**, 261-351 (2004).