IMPERFECT QUANTUM BIFURCATIONS

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Rotational multiplets of isolated vibrational molecular states can manifest qualitative modifications of their structure under the variation of some parameters. For instance, the quantum bifurcations have been found in the spectra of the number of molecules when the rotational angular momentum increases[a]. There are only five different types of bifurcations depending on the symmetry of molecule when only one parameter is varied. The complete classification and the description of the universal behavior of a quantum systems near the bifurcation point has been given by Pavlichenkov and Zhilinskii[b].

In the present report, we study the evolution of bifurcations under the the symmetry breaking due to the slight isotopic substitutions. Lower molecular symmetry results in a reduced number of possible types of bifurcations. Thus some symmetrical bifurcations find their correspondence in the so-called imperfect bifurcations. The simplest four-atomic spherical top molecule A_4 is studied in details. This example enables us to make a correlation between the typical spherical top rotation level structure (T_d point symmetry) and the asymmetric top level structure (C_{2v} or C_s) and further with symmetric top level structure (C_{3v}). The basic bifurcations of the rotational energy surface of A_4, A_2A_2', $A_2A'A''$ and A_3A' molecules are considered and correlated with each other. The evolution of symmetrical bifurcations into less symmetrical or asymmetrical imperfect bifurcations is demonstrated.

[a] For recent review see B. Zhilinskii, Spectrochim. Acta, A, 52, 881 (1996)

[b] I. Pavlichenkov and B. Zhilinskii, Ann. Phys.(N.Y.) 184, 1 (1988).