Rovibrational modes and classification of triply excited states of atoms

C. D. Lin

J. R. Macdonald Laboratory, Department of Physics,
Kansas State University, Manhattan, KS 66506

It is well understood that electron correlation plays a major role in determining the properties of multiply excited states of atoms. The shell model does not describe these states and alternative quantum numbers are needed to classify them. For doubly excited states, classification of these states in terms of new quantum numbers, $(K, T)^A$, have been available since the 1980's. The K, T and A are used to describe the collective bending and stretching motion of the two excited electrons, in analogy to the bending and breathing motion of a linear triatomic molecule. New spectral regularity emerges and propensity rules in processes involving doubly excited states have been found when they are ordered according to the new quantum numbers.

In the past few years we have been investigating the classification of triply excited states of atoms. We have developed a computational package for treating three-electron atoms in hyperspherical coordinates, but the emphasis in recent years has been on the classifications. *We have succeeded in classifying the intrashell triply excited states*. For example, there are eight intrashell triply excited states when all the three electrons are in the n=2 manifold, the so-called 2l2l'2l" triply excited states. The eight states have been separated into three groups. Within each group the three electrons perform motion akin to the vibrational motion of an XY_3 molecule with X being the nucleus and Y the electron, and the states within the group are identified as the rotational excited states of a symmetric top. The identification of the internal vibrational normal mode is supported by displaying the joint electronic density plots in appropriate coordinates and by analyzing the internal nodal surfaces of the wave functions as imposed by the quantum symmetries. Density plots for the three groups of the 2l2l'2l" triply excited states are shown as A, B and C in the plots here. As will be explained in the talk, in A the three electrons form a coplanar equilateral triangle with the nucleus at the center, in B the three electrons perform motion like that of an ammonia molecule and in C the three electrons can form an isosceles triangle while the equilateral triangle geometry is forbidden. Most recently we have extended the classification to the **sixty-four** 3l3l'3l" triply excited states. For this purpose we study the classification of a model atom with three electrons on the surface of a sphere. We have succeeded in classifying all these 64 states. Besides the fundamental A, B and C normal modes, excited vibrational modes such as Ab, Ac, Bb, etc., have been identified, see figure. We will show that the triply excited states of N^{2+} and N^{4+} can indeed be classified using the present scheme. Extension of the classification to intershell triply excited states is underway.