Shape-phase transitions in quantum many-body systems

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A quantum statistical analysis of the regular and chaotic dynamics of medium-mass even-even nuclei within the framework of the interacting boson model-2 (IBM-2) has been carried out. In the SU(3) to U(5) shape-phase transition from deformed to vibrational spherical isotopes a broad nearly regular region has been observed, while the SU(3)* - corresponding to triaxial shape – to U(5) one shows a unexpected completely regular behavior. These results confirm and extend the observations previously made by other authors in the frame of IBM-1, strengthening the hypothesis of the basic role played by the partial dynamical symmetries as well as recently introduced symmetries at the critical point in the shape transitions in preserving regular motion patterns even far from the usual dynamical limits of IBM-2. A new important feature of the SU(3)* limit has also been found, confirming the importance of this symmetry of IBM in studying nuclear structure properties, mainly of isotopes far from the stability valley.

Furthermore, I present main results of molecular dynamics simulations carried out to investigate structural and thermodynamics properties of polyamidoamine (PAMAM) dendrimers. In last ten years, many progresses have been made in the analysis of structural properties of a special class of branched polymers, named dendrimers. Owing to their extremely particular structure and physical behaviour, these macromolecules have important applications in many fields such as material science, pharmacology, medicine (for istance, improvement of cancer therapy), nanochemistry, viscosity modification and biochemistry (for example, micelle, liposome and biomolecule mimics).

The internal structure of dendrimers has been thus investigated from both a theoretical and experimental point of view. In this work the study of structural (radius of gyration, structure function, and so on) and thermodynamics (for instance, energies and temperature) properties of these non-ionic dendrimers is presented and critically discussed with reference to available experimental data. By comparing the data obtained from our MD simulations with the literature ones, a structural transition is found from an internal self-similar structure to a spherical one. These results confirm the PAMAM dendrimer structure proposed by experiments performed by means of SAXS and quasi elastic light scattering (QELS) techniques.