Quantum dynamics of confined molecules

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We will provide an account of the available methodologies designed to simulate the quantum dynamics of confined molecules. We are interested in providing an interpretation of spectroscopic experiments that probe to rotational, vibrational, and translational motions of molecules trapped in quantum fluids and nano-cavities. Of particular interest is the behaviour of molecular rotors as probes of superfluidity in helium and hydrogen clusters and droplets [1,2,3]. The quantum nature of hydrogen molecules trapped in clathrate hydrates and the dynamics of water molecules trapped in matrices such as C60 cages will also be considered. For the latter case, issues such as nuclear spin conversion will be addressed. The formal and computational tools that enable these investigations range from exact basis set methods for few degrees of freedom systems, to path integral based techniques for larger system sizes. Both finite temperature and ground state path integral methods will be described. Observables such as effective rotational constants, vibrational shifts, the superfluid fraction, and quantum entanglement entropies can be obtained from such techniques and will help shed light on the nature of confined quantum systems.

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