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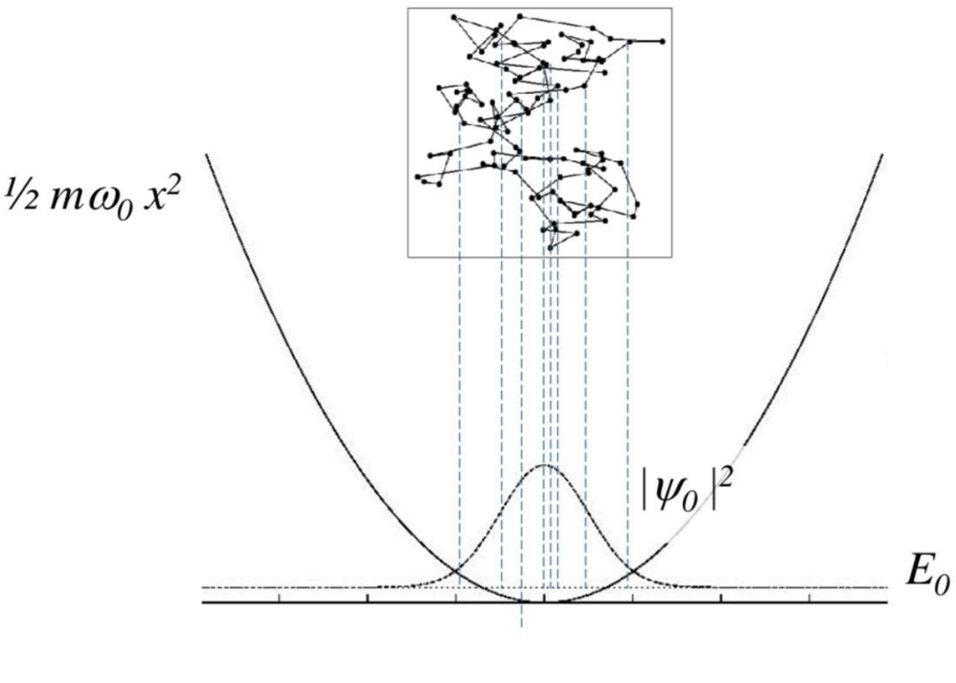
Nuclear quantum effects in condensed matter

It becomes nowadays possible to conceive and design materials with specific properties, almost from scratch. Matter consists of an assembly of electrons and nuclei. Although much heavier than electrons, light nuclei, mainly hydrogen, exhibit quantization of the vibrational levels, zero-point energy and tunnelling. These so-called Nuclear Quantum Effects (NQE) can have a large impact on the structure and the dynamics of materials. NQE are also crucial for describing heavier nuclei at low temperatures and other phenomena, such as isotope effects, that escape a purely classical frame.

The behaviour of systems that are at the borderline between the classical and quantum worlds is in general complex. The genuine quantum characteristics might be spoiled by electric fields, high disorder, etc. I will illustrate through selected examples some paradoxical effects that can be encountered in condensed matter : ice and exotic phases of methane hydrates at extreme pressures, typical of those inside giant icy planets of the solar system. I will also show the spectacular isotope effects in the phase transition of Sodium Hydroxide, which has hindered its explanation for about 40 years. I will conclude by discussing the importance of simulation methods that are able to account for the quantum dynamics of nuclei. In the last decade, in our group we have developed numerical models and theories that account for nuclear quantum effects, at various approximation levels. for instance in the semi-classical regime, in the framework of the generalized Langevin equation.



The advent of machine-learning based techniques has opened the way to refine models for describing the inter-atomic forces, and the nuclear quantum effects, even if modest, might change the statistical properties appreciably.
Their explicit inclusion in simulations is an emerging field of research, with impact on many fields, spanning materials science, geophysics, physical chemistry and biochemistry.