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Quantum anharmonicity in solids: from high Tc superconductivity to muon spectroscopy.

Atoms in a crystal are quantum particles that oscillate even at zero temperature.

The quantum behavior of the atoms makes them very different from classical particles as they are not point charges and they do not necessarily sit at the minimum of the static energy potential. In other words, the vibrational energy associated to the quantum oscillations can strongly modify the static energy landscape, even changing the ground state derived from the Born-Oppenheimer energy surface minimum.

The description of the quantum nature of the atoms is usually carried out by using quantum Monte Carlo simulations or path integral molecular dynamics.

These techniques are, however, very expensive and limited to a small number of particles.

In this talk I will present the Stochastic Self-Consistent Harmonic Approximation[1,2,3,4] developed by our team. This technique allows for a precise treatment of quantum and anharmonic effects beyond the perturbative limit in a very efficient way even for periodic systems having some hundreds of atoms and with ab initio accuracy. I will show with several examples that correctly acounting for quantum effects and non-perturbative anharmonicity is crucial in many different fields ranging from Hight Tc superconductivity [5,6] to charge density waves [7], from thermal transport [8] to muon spectroscopy [9].

References:

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