Anharmonic effects in superconductors, metallic hydrides, and layered materials from the stochastic self-consistent harmonic approximation

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Describing vibrations of atoms is of paramount importance in the physical properties of solids. Nowadays, phonon dispersions in the harmonic approximation are routinely calculated from first-principles. Nevertheless, whenever the displacements of the atoms largely exceed the range in which the harmonic potential is valid, the harmonic approximation completely fails.

Here we present a newly developed approach to treat strongly anharmonic systems named as the stochastic self-consistent harmonic approximation (SSCHA) [1,2]. The method is variational and takes into account quantum and thermal effects rigorously.

We demonstrate the validity of the SSCHA calculating the phonon spectra in agreement with experiments in palladium hydrides and demonstrating that their large isotope anomaly in the superconducting temperature is entirely due to the huge anharmonicity of hydrogen rattling modes. The method is suited as well to study the behavior of charge density waves (CDW) in layered metallic dichalcogenides like $NbSe_2$.

[1] Ion Errea, Matteo Calandra, and Francesco Mauri, PRL 111, 177002 (2013)
[2] Ion Errea, Matteo Calandra, and Francesco Mauri, PRB 89, 064302 (2014)