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Anharmonic properties of solids within the stochastic self-consistent harmonic approximation

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Describing atomic vibrations from first-principles accurately is of paramount importance to understand the thermodynamic and transport properties of solids. Phonon dispersions are routinely calculated within the harmonic approximation, and transport properties can be studied by estimating the electron-phonon and phonon-phonon interactions within perturbation theory. Nevertheless, whenever the amplitude of the atomic displacements largely exceeds the range in which the harmonic potential is valid, the harmonic approximation completely fails without allowing a perturbative expansion.

The stochastic self-consistent harmonic approximation (SSCHA) that we have developed [1–4] offers an efficient method to calculate vibrational properties of solids even when the harmonic approximation completely collapses. The method is variational and takes into account quantum and thermal effects rigorously. With our recent developments on the SSCHA method [3], we show how phonon frequencies should be defined from the second derivative of the free energy, which allows calculating the transition temperature of structural second-order phase transitions. Moreover, the new developments [3] allow calculating third-order anharmonic force-constants, which determine thermal properties, beyond the perturbative limit. Also we are now capable of calculating the stress tensor including quantum/anharmonic effects and perform structural relaxations in this quantum/anharmonic energy landscape, in contrast to the classical calculations just focused on the classical Born-Oppenheimer energy surface.

In this lecture we will present the method and several applications of it in superconducting hydrides, charge-density-wave systems, and thermoelectric materials.

Refs

[1] I. Errea, M. Calandra and F. Mauri, Phys. Rev. Lett. {\bf 111}, 177002 (2013).
[2] I. Errea, M. Calandra and F. Mauri, Phys. Rev. B {\bf 89}, 064302 (2014).
[3] R. Bianco, I. Errea, L. Paulatto, M. Calandra and F. Mauri, Phys. Rev. B {\bf 96}, 014111 (2017).
[4] L. Monacelli, I. Errea, M. Calandra and F. Mauri, Phys. Rev. B {\bf 98}, 024106 (2018).

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