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Anharmonic phonons and second-order phase-transitions by the stochastic self-consistent harmonic approximation

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Abstract

The harmonic approximation provides the basic approach to study structural and dynamical properties of systems. Nevertheless, anharmonic effects are crucial in order to take into account several physical phenomena, such as finite values of thermal conductivity and thermal expansion in solids. Anharmonicity can generally be treated within perturbation theory on top of the harmonic results. However, such an approach is inappropriate when the harmonic solution is dynamically unstable or when the anharmonic corrections of the phonon energies are larger than the harmonic frequencies themselves. Notably, this situation occurs near lattice-related second-order phase-transitions such as charge-density-wave (CDW) or ferroelectric instabilities or in H-containing materials, where the large zero-point motion of the protons results in a violation of the harmonic approximation. Interestingly, even in these cases, phonons can be observed, measured, and used to model transport properties. In order to treat such cases, we developed a stochastic implementation of the self-consistent harmonic approximation valid to treat anharmonicity in the nonperturbative regime [1]. The method allows to obtain, from first-principles, the structural, thermodynamic and vibrational properties of strongly anharmonic systems and, in particular, study the properties of structural second-order phase-transitions.

In this talk I will describe the method developed. I will also show some applications to the hydrogen-bond symmetrization transition in the superconducting hydrogen sulfide system, the system exhibiting the highest T_c reported for any superconductor so far [2]. With this method we are able to predict the transition pressure and the evolution of phonons with pressure.

References

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[2] I. Errea, M. Calandra, C. J. Pickard, J. R. Nelson, R. J. Needs, Y. Li, H. Liu, Y. Zhang, Y. Ma, F. Mauri, Nature 532, 81 (2016)