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Anharmonic effects from the self-consistent harmonic approximation: the example of simple cubic calcium

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Abstract: Although the harmonic approximation is in many cases enough to accurately describe vibrational properties of solids, it sometimes breaks down. Whenever the dynamical behavior of the solid is not determined by the second derivatives of the potential at equilibrium but by higher order terms, the harmonic approximation may lead not only to wrong numerical values for the phonon frequencies and the free energy, but to a misleading interpretation of the stability of the system. For instance, a structure might show imaginary phonons in the harmonic approximation but might be perfectly stable due to anharmonic stabilization. In these last cases anharmonicity needs to be taken into account in the dynamical description of the solid beyond perturbation theory. We propose that the self-consistent harmonic approximation (SCHA) is the appropriate framework to tackle these problems as it seeks the physically well-defined Gibbs-Bogoliubov inequality and allows us to define the anharmonic problem through a variational procedure. We apply the SCHA to the high-pressure simple cubic phase of calcium that is unstable in the harmonic approximation but is found experimentally. The SCHA has been applied fully ab initio including all coefficients in the dynamical potential up to fourth order. According to our results [1], the anharmonic phonon spectrum is stable and, therefore, we can state that anharmonicity stabilizes this phase. Moreover, our phonon spectrum allow us to estimate the superconducting transition temperature in this system and we found a good agreement with experimental results.
[1] Ion Errea, Bruno Rousseau, and Aitor Bergara, Physical Review Letters 106, 165501 (2011).