First-Principle Perturbative Computation of Phonon Properties of Insulators in Finite Electric Fields

XINJIE WANG, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854-8019, USA — The methods of density-functional perturbation theory have been shown to provide a powerful tool for realistic calculations of lattice-vibrational, dielectric, elastic, and other response properties of crystals.\(^1\) Recently, a total-energy method for insulators in nonzero electric fields was proposed.\(^2\) However, the perturbative computation of phonon properties under a dc bias field has not previously been addressed. Here, we start from a variational total-energy functional with a field coupling term that represents the effect of the electric field on the crystal. The linear response of the field-polarized Bloch functions is obtained by minimizing the second-order derivative of the total-energy functional. Due to the presence of the electric field, the field-polarized Bloch functions at each k-point in the Brillouin zone are weakly coupled to those at the neighboring k-points. We implement the method in the ABINIT code and perform illustrative calculations of the phonon frequencies for III-V semiconductors.

1S. Baroni et al., Rev. Mod. Phys. 73, 515 (2001).
2I. Souza, J. Íniguez, and D. Vanderbilt, Phys. Rev. Lett. 89, 117602 (2002).