Phonon, electron-phonon interaction and superconductivity from first-principles density functional theory

Gianni Profeta
Department of Physical and Chemical Sciences and CNR-SPIN
University of L'Aquila (ITALY)
gianni.profeta@aquila.infn.it

In this pedagogical lecture, we introduce a first-principles scheme to calculate adiabatic and nonadiabatic phonon frequencies in the full Brillouin zone by density functional methods.

First of all, we define the force constant functional and demonstrate the stationary properties of force-constant functional with respect to the first-order perturbation of the electronic charge density and on the localization of the deformation potential.

After the introduction of the Wannier function basis, the formalism will be re-written on this last basis. This allows for calculation of phonon-dispersion curves free from convergence issues related to Brillouin-zone sampling.
We present two examples of application of the method for the calculation of the phonon dispersion and electron-phonon coupling in two important superconducting materials MgB_2 and CaC_6. In both compounds we demonstrate the occurrence of several Kohn anomalies, absent in the previous state-of-the-art calculations, that are manifest only after careful electron- and phonon-momentum integration.

We present, then, the main line of the implementation of the above approach to calculate the superconducting critical temperature in BCS superconductors by the Eliashberg theory and the SuperConducting Density Functioanl Theory (SCDFT).