First-principle phonon calculation

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February 10, 2023

1 The molecular dynamics approach

See [1]. The idea is rather simple: the phonon spectrum just illustrates the vibration modes of atoms, so if we just let atoms move (with an average kinetic energy that agrees with the temperature T in question), then the Fourier transform of the orbitals of the atoms gains high intensity on the dispersion relations. This seems to be the most *ab initio*method I've ever learned about.

A more efficient way is the so-called temperature-dependent effective potential, which is obtained by curve-fitting of the atomic force fields in MD.

References

[1] Xiaohan Zhang et al. "Finite-temperature phonon dispersion and vibrational dynamics of BaTiO 3 from first-principles molecular dynamics". In: *Physical Review B* 105.1 (2022), p. 014304.