

First-principle phonon calculation

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1 Feynman diagrams for phonons

1.1 Single-phonon Green function

The general definition of the Green function for a real bosonic field is

$$D(\mathbf{q}, t - t') = -i \langle \mathcal{T} A_{\mathbf{q}}(t) A_{\mathbf{q}}(t') \rangle, \quad (1)$$

where

$$A_{\mathbf{q}} = a_{\mathbf{q}} + a_{-\mathbf{q}}^{\dagger}. \quad (2)$$

In the non-interactive case, we have

$$\begin{aligned} D^{(0)}(\mathbf{q}, t - t') &= -i \langle \mathcal{T} (a_{\mathbf{q}} e^{-i\omega_{\mathbf{q}} t} + \text{h.c.}) (a_{\mathbf{q}} e^{-i\omega_{\mathbf{q}} t'} + \text{h.c.}) \rangle \\ &= -i(\theta(t - t') e^{-i\omega_{\mathbf{q}}(t - t')} + \theta(t' - t) e^{i\omega_{\mathbf{q}}(t - t')}). \end{aligned} \quad (3)$$

Then we can evaluate the Fourier transform of it and get

$$D^{(0)}(\mathbf{q}, \omega) = \int_{-\infty}^{\infty} e^{i\omega(t - t')} D^{(0)}(\mathbf{q}, t - t') = \frac{1}{\omega - \omega_{\mathbf{q}} + i0^+} - \frac{1}{\omega - \omega_{\mathbf{q}} - i0^+} = \frac{2\omega_{\mathbf{q}}}{\omega^2 - \omega_{\mathbf{q}}^2 + i0^+}. \quad (4)$$

This also works for phonons. Note the fact that even when we have zero phonon in the ground state, we still have two terms in the propagator: it comes from the fact that $A_{\mathbf{q}}$ always contains both annihilation and creation operators and thus $D^{(0)}$ is always non-zero regardless of the sign of $t - t'$. Also note the minus sign between $1/(\omega \pm \omega_{\mathbf{q}})$: it comes from the fact that we are dealing with bosons and not fermions. For phonons, $A_{\mathbf{q}}$ is proportional to $X_{\mathbf{q}}$; this enables us to link phonon Green function with displacement correlation function.

Just like the case for electrons, we can do self-energy correction to the phonon propagator. Suppose we have already done a Dyson resummation and find

$$D^{-1}(\mathbf{q}, \omega) = (D^{(0)}(\mathbf{q}, \omega))^{-1} - \Pi(\mathbf{q}, \omega). \quad (5)$$

We have

$$D(\mathbf{q}, \omega) = \left(\frac{\omega^2 - \omega_{\mathbf{q}}^2 - 2\omega_{\mathbf{q}}\Pi + i0^+}{2\omega_{\mathbf{q}}} \right)^{-1} = \quad (6)$$

2 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 BaTiO₃ from first-principles molecular dynamics". In: *Physical Review B* 105.1 (2022), p. 014304.