

Note for the tetrahedron method in DFPT and electron-phonon calculations

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1 Definitions

- $\varepsilon_{kn\sigma}, \varepsilon_{k+qn'\sigma}, \dots$: Kohn-Sham eigenvalues
- ε_F : Fermi energy
- $\omega_{q\nu}$: Phonon frequency
- $g_{nkn'k+q}^{q\nu}$: electron-phonon vertex
- $N(\varepsilon_F)$: Density of states (for both spin) at the Fermi energy

2 Equations in DFPT and Electron-Phonon

We employ the tetrahedron method in the following equations in the DFPT with the ultrasoft pseudopotential [1]:

- $\delta(\varepsilon_F - \varepsilon_{i\sigma})$ in Eqn. (25). It is stored in a variable `dfpt_tetra_delta(1:nbnd,1:nks)` computed in subroutines `dfpt_tetra_main` and `dfpt_tetra_calc_delta`.
- $\theta(\varepsilon_F - \varepsilon_{kv\sigma})$ in Eqn. (B17). It is `wg(1:nbnd,ik)/wk(ik)`.
- Eqn. (B19),

$$w_{kv\sigma,k+qv'\sigma} = \theta(\varepsilon_F - \varepsilon_{kv\sigma})\theta(\varepsilon_{kv\sigma} - \varepsilon_{k+qv'\sigma}) + \theta(\varepsilon_F - \varepsilon_{k+qv'\sigma})\theta(\varepsilon_{k+qv'\sigma} - \varepsilon_{kv\sigma}). \quad (1)$$

It is stored in a variable `dfpt_tetra_ttheta(1:nbnd,1:nbnd,1:nks)` computed in subroutines `dfpt_tetra_main`, `dfpt_tetra_calc_beta1`, `dfpt_tetra_calc_beta2`, and `dfpt_tetra_average_beta`.

- Eqn. (B28),

$$\begin{aligned} \beta_{kv\sigma,k+qv'\sigma} = & \theta(\varepsilon_F - \varepsilon_{kv\sigma})\theta(\varepsilon_{kv\sigma} - \varepsilon_{k+qv'\sigma}) + \theta(\varepsilon_F - \varepsilon_{k+qv'\sigma})\theta(\varepsilon_{k+qv'\sigma} - \varepsilon_{kv\sigma}) \\ & + \alpha_{k+qv'\sigma} \frac{\theta(\varepsilon_F - \varepsilon_{kv\sigma}) - \theta(\varepsilon_F - \varepsilon_{k+qv'\sigma})}{\varepsilon_{kv\sigma} - \varepsilon_{k+qv'\sigma}} \theta(\varepsilon_{k+qv'\sigma} - \varepsilon_{kv\sigma}). \end{aligned} \quad (2)$$

It is stored in a variable `dfpt_tetra_beta(1:nbnd,1:nbnd,1:nks)` computed in subroutines `dfpt_tetra_main`, `dfpt_tetra_calc_beta1`, `dfpt_tetra_calc_beta2`, `dfpt_tetra_calc_beta3`, and `dfpt_tetra_average_beta`.

We also employ the tetrahedron method in calculations of the Flöhlich parameter

$$\lambda_{q\nu} = \frac{2}{N(\varepsilon_F)\omega_{q\nu}} \sum_{knn'} |g_{n'k+qnk}^\nu|^2 \delta(\varepsilon_{nk} - \varepsilon_F) \delta(\varepsilon_{n'k+q} - \varepsilon_F) \quad (3)$$

(when `electron_phonon="lambda_tetra"`), and

$$\lambda_{q\nu} = \frac{2}{N(\varepsilon_F)\omega_{q\nu}^2} \sum_{knn'} [\theta(\varepsilon_F - \varepsilon_{nk}) - \theta(\varepsilon_F - \varepsilon_{n'k+q})] \delta(\varepsilon_{n'k+q} - \varepsilon_{nk} - \omega_{q\nu}) |g_{nkn'k+q}^{q\nu}|^2 \quad (4)$$

(when `electron_phonon="gamma_tetra"`).

2.1 Tetrahedron method for DFPT

First, we cut out one or three tetrahedra where $\theta(\varepsilon_F - \varepsilon_{nk}) = 1$ from tetrahedron T and evaluate $\varepsilon_{nk}, \varepsilon_{n'k+q}$ at the corners of T'' (See Appendix A and B of the previous study[2]). Second, we perform the following integration in each tetrahedra [Eqn. (C3) in that paper] :

$$\begin{aligned} W_i &= 6V'' \int_0^1 dx_1 \int_0^1 dx_2 \int_0^1 dx_3 \int_0^1 dx_4 \frac{x_i \delta(x_1 + x_2 + x_3 + x_4 - 1)}{d_1 x_1 + d_2 x_2 + d_3 x_3 + d_4 x_4} \\ &= -V'' \sum_{j=1, j \neq i}^4 \frac{d_j^2 \left(\frac{\ln d_j - \ln d_i}{d_j - d_i} d_j - 1 \right)}{\prod_{k=1, k \neq j}^4 (d_j - d_k)}, \end{aligned} \quad (5)$$

where d_i is $\varepsilon_{n'k+q} - \varepsilon_{nk}$ at the corner of the trimmed tetrahedron.

For avoiding a numerical error, we should not use the above formula as is. Practically, we use the following formulae according to the degeneracy of d_1, \dots, d_4 .

- When d_1, \dots, d_4 are different each other,

$$\begin{aligned} A_2 &= \left(\frac{\ln(d_2) - \ln(d_1)}{d_2 - d_1} d_2 - 1 \right) \frac{d_2}{d_2 - d_1}, & A_3 &= \left(\frac{\ln(d_3) - \ln(d_1)}{d_3 - d_1} d_3 - 1 \right) \frac{d_3}{d_3 - d_1}, \\ A_4 &= \left(\frac{\ln(d_4) - \ln(d_1)}{d_4 - d_1} d_4 - 1 \right) \frac{d_4}{d_4 - d_1}, & B_2 &= \frac{A_2 - A_3}{d_2 - d_3} d_2, & B_4 &= \frac{A_4 - A_3}{d_4 - d_3} d_4, \\ W_1 &= \frac{B_4 - B_2}{d_4 - d_2}. \end{aligned} \quad (6)$$

- When $d_1 = d_4$,

$$\begin{aligned} A_2 &= \left(\frac{\ln(d_2) - \ln(d_1)}{d_2 - d_1} d_2 - 1 \right) \frac{d_2^2}{d_2 - d_1} - \frac{d_1}{2}, & B_2 &= \frac{A_2}{d_2 - d_1}, \\ A_3 &= \left(\frac{\ln(d_3) - \ln(d_1)}{d_3 - d_1} d_3 - 1 \right) \frac{d_3^2}{d_3 - d_1} - \frac{d_1}{2}, & B_3 &= \frac{A_3}{d_3 - d_1}, \\ W_1 &= \frac{B_3 - B_2}{d_3 - d_2}. \end{aligned} \quad (7)$$

- When $d_3 = d_4$,

$$\begin{aligned} A_2 &= \frac{\ln(d_2) - \ln(d_1)}{d_2 - d_1} d_2 - 1, & B_2 &= \frac{d_2 A_2}{d_2 - d_1}, & A_3 &= \frac{\ln(d_3) - \ln(d_1)}{d_3 - d_1} d_3 - 1, & B_3 &= \frac{d_3 A_3}{d_3 - d_1}, \\ C_2 &= \frac{B_3 - B_2}{d_3 - d_2}, & C_3 &= \frac{\ln(d_3) - \ln(d_1)}{d_3 - d_1} d_3 - 1, & D_3 &= 1 - \frac{2C_3 d_1}{d_3 - d_1}, & E_3 &= \frac{D_3}{d_3 - d_1}, \\ W_1 &= \frac{d_3 E_3 - d_2 C_2}{d_3 - d_2}. \end{aligned} \quad (8)$$

- When $d_4 = d_1$ and $d_3 = d_2$,

$$\begin{aligned} A_1 &= 1 - \frac{\ln(d_2) - \ln(d_1)}{d_2 - d_1} d_1, & B_1 &= -1 + \frac{2d_2 A_1}{d_2 - d_1}, & C_1 &= -1 + \frac{3d_2 B_1}{d_2 - d_1}, \\ W_1 &= \frac{C_1}{2(d_2 - d_1)}. \end{aligned} \quad (9)$$

- When $d_4 = d_3 = d_2$,

$$\begin{aligned} A_1 &= 1 - \frac{\ln(d_2) - \ln(d_1)}{d_2 - d_1} d_1, & B_1 &= -1 + \frac{2d_2 A_1}{d_2 - d_1}, & C_1 &= -1 + \frac{3d_2 B_1}{d_2 - d_1}, \\ W_1 &= \frac{C_1}{2(d_2 - d_1)}. \end{aligned} \quad (10)$$

- When $d_4 = d_3 = d_1$,

$$\begin{aligned} A_1 &= -1 + \frac{\ln(d_2) - \ln(d_1)}{d_2 - d_1} d_2, & B_1 &= -1 + \frac{2d_2 A_1}{d_2 - d_1}, & C_1 &= -1 + \frac{3d_2 B_1}{2(d_2 - d_1)}, \\ W_1 &= \frac{C_1}{3(d_2 - d_1)}. \end{aligned} \quad (11)$$

- When $d_4 = d_3 = d_2 = d_1$,

$$W_1 = \frac{1}{4d_1}. \quad (12)$$

- Other weights are calculated by using the permutation.

3 Tetrahedron method for electron-phonon

3.1 Eqn. (3)

First, we cut out one or two triangles where $\varepsilon_{nk} = \varepsilon_F$ from a tetrahedron and evaluate $\varepsilon_{n'k+q}$ at the corners of each triangles as

$$\varepsilon_i'^{k+q} = \sum_{j=1}^4 F_{ij}(\varepsilon_1^k, \dots, \varepsilon_4^k, \varepsilon_F) \varepsilon_j^{k+q}. \quad (13)$$

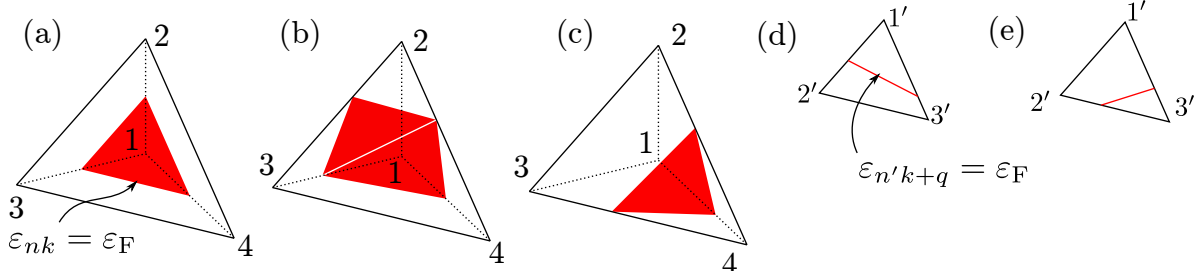


Figure 1: How to divide a tetrahedron in the case of $\epsilon_1 \leq \epsilon_F \leq \epsilon_2$ (a), $\epsilon_2 \leq \epsilon_F \leq \epsilon_3$ (b), and $\epsilon_3 \leq \epsilon_F \leq \epsilon_4$ (c).

Then we calculate $\delta(\epsilon_{n'k+q} - \epsilon_F)$ in each triangles and obtain weights of corners. This weights of corners are mapped into those of corners of the original tetrahedron as

$$W_i = \sum_{j=1}^3 \frac{S}{\nabla_k \epsilon_k} F_{ji}(\epsilon_1^k, \dots, \epsilon_4^k, \epsilon_F) W'_j. \quad (14)$$

F_{ij} and $\frac{S}{\nabla_k \epsilon_k}$ are calculated as follows ($a_{ij} \equiv (\epsilon_i - \epsilon_j)/(\epsilon_F - \epsilon_j)$):

- When $\epsilon_1 \leq \epsilon_F \leq \epsilon_2 \leq \epsilon_3 \leq \epsilon_4$ [Fig. 1(a)],

$$F = \begin{pmatrix} a_{12} & a_{21} & 0 & 0 \\ a_{13} & 0 & a_{31} & 0 \\ a_{14} & 0 & 0 & a_{41} \end{pmatrix}, \quad \frac{S}{\nabla_k \epsilon_k} = \frac{3a_{21}a_{31}a_{41}}{\epsilon_F - \epsilon_1} \quad (15)$$

- When $\epsilon_1 \leq \epsilon_2 \leq \epsilon_F \leq \epsilon_3 \leq \epsilon_4$ [Fig. 1(b)],

$$F = \begin{pmatrix} a_{13} & 0 & a_{31} & 0 \\ a_{14} & 0 & 0 & a_{41} \\ 0 & a_{24} & 0 & a_{42} \end{pmatrix}, \quad \frac{S}{\nabla_k \epsilon_k} = \frac{3a_{31}a_{41}a_{24}}{\epsilon_F - \epsilon_1} \quad (16)$$

$$F = \begin{pmatrix} a_{13} & 0 & a_{31} & 0 \\ 0 & a_{23} & a_{32} & 0 \\ 0 & a_{24} & 0 & a_{42} \end{pmatrix}, \quad \frac{S}{\nabla_k \epsilon_k} = \frac{3a_{23}a_{31}a_{42}}{\epsilon_F - \epsilon_1} \quad (17)$$

- When $\epsilon_1 \leq \epsilon_2 \leq \epsilon_3 \leq \epsilon_F \leq \epsilon_4$ [Fig. 1(c)],

$$F = \begin{pmatrix} a_{14} & 0 & 0 & a_{41} \\ a_{13} & a_{24} & 0 & a_{42} \\ a_{12} & 0 & a_{34} & a_{43} \end{pmatrix}, \quad \frac{S}{\nabla_k \epsilon_k} = \frac{3a_{14}a_{24}a_{34}}{\epsilon_1 - \epsilon_F} \quad (18)$$

Weights on each corners of the triangle are computed as follows [$(a'_{ij} \equiv (\epsilon'_i - \epsilon'_j)/(\epsilon_F - \epsilon'_j))$]:

- When $\epsilon'_1 \leq \epsilon_F \leq \epsilon'_2 \leq \epsilon'_3$ [Fig. 1(d)],

$$W'_1 = L(a'_{12} + a'_{13}), \quad W'_2 = La'_{21}, \quad W'_3 = La'_{31}, \quad L \equiv \frac{a'_{21}a'_{31}}{\epsilon_F - \epsilon'_1} \quad (19)$$

- When $\varepsilon'_1 \leq \varepsilon'_2 \leq \varepsilon_F \leq \varepsilon'_3$ [Fig. 1(e)],

$$W'_1 = La'_{13}, \quad W'_2 = La'_{23}, \quad W'_3 = L(a'_{31} + a'_{32}), \quad L \equiv \frac{a'_{13}a'_{23}}{\varepsilon'_3 - \varepsilon_F} \quad (20)$$

3.2 Eqn. (4)

In this case, we cut tetrahedra in the same manner to the case of

$$\frac{\theta(\varepsilon_F - \varepsilon_{kv\sigma}) - \theta(\varepsilon_F - \varepsilon_{k+qv'\sigma})}{\varepsilon_{kv\sigma} - \varepsilon_{k+qv'\sigma}} \theta(\varepsilon_{k+qv'\sigma} - \varepsilon_{kv\sigma}) \quad (21)$$

in the DFPT calculation. Then we evaluate $\delta(\varepsilon_{n'k+q} - \varepsilon_{nk} - \omega_{q\nu})$ in the trimmed tetrahedra.

References

- [1] A. Dal Corso, Phys. Rev. B **64**, 235118 (2001).
- [2] M. Kawamura, Phys. Rev. B **89**, 094515 (2014).