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

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1 Definitions

- $\varepsilon_{kn\sigma}, \varepsilon_{k+qn'\sigma}, \cdots$: Kohn-Sham eigenvalues
- ε_{F} : Fermi energy
- $\omega_{q\nu}$: Phonon frequency
- $g^{q\nu}_{nkn'k+q}$: electron-phonon vertex
- $N(\varepsilon_{\mathrm{F}})$: 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]:

- $\delta(\varepsilon_{\mathrm{F}} - \varepsilon_{i\sigma})$ 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`.
- $\theta(\varepsilon_{\mathrm{F}} - \varepsilon_{kv\sigma})$ in Eqn. (B17). It is `wg(1:nbnd,ik)/wk(ik)`.
- Eqn. (B19),

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

  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),

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

  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

$$\lambda_{q\nu} = \frac{2}{N(\varepsilon_{\rm F})\omega_{q\nu}} \sum_{knn'} |g^{\nu}_{n'k+qnk}|^2 \delta(\varepsilon_{nk} - \varepsilon_{\rm F})\delta(\varepsilon_{n'k+q} - \varepsilon_{\rm F}) \tag{3}$$

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

$$\lambda_{q\nu} = \frac{2}{N(\varepsilon_{\rm F})\omega_{q\nu}^2} \sum_{knn'} [\theta(\varepsilon_{\rm F} - \varepsilon_{nk}) - \theta(\varepsilon_{\rm F} - \varepsilon_{n'k+q})]\delta(\varepsilon_{n'k+q} - \varepsilon_{nk} - \omega_{q\nu})|g^{q\nu}_{nkn'k+q}|^2 \tag{4}$$

(when `electron_phonon="gamma_tetra"`).

2.1 Tetrahedron method for DFPT

First, we cut out one or three tetrahedra where $\theta(\varepsilon_{\rm F} - \varepsilon_{nk}) = 1$ 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] :

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

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 $d_1, \cdots d_4$.

- When $d_1, \cdots d_4$ are different each other,

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

- When $d_1 = d_4$,

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

- When $d_3 = d_4$,

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

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

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

- When $d_4 = d_3 = d_2$,

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

- When $d_4 = d_3 = d_1$,

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

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

$$
W_1 = \frac{1}{4 d_1}. \tag{12}
$$

- 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 $\varepsilon_{nk} = \varepsilon_{\mathrm{F}}$ from a tetrahedron and evaluate $\varepsilon_{n'k+q}$ at the corners of each triangles as

$$
\varepsilon_i'^{k+q} = \sum_{j=1}^{4} F_{ij}(\varepsilon_1^k, \cdots, \varepsilon_4^k, \varepsilon_{\mathrm{F}}) \epsilon_j^{k+q}. \tag{13}
$$

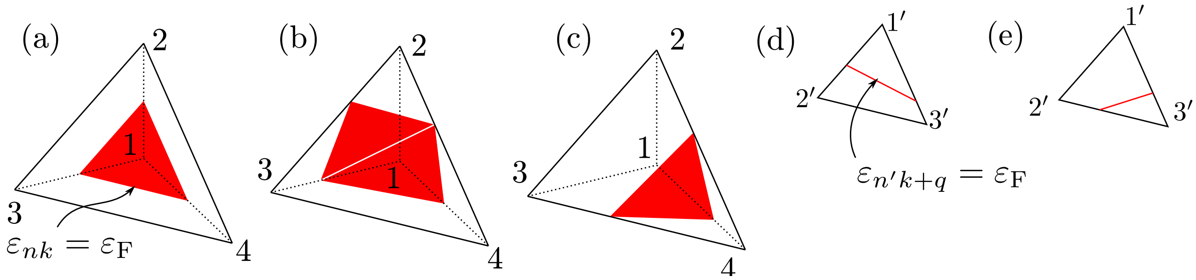

Figure 1: How to divide a tetrahedron in the case of $\epsilon_1 \leq \varepsilon_{\rm F} \leq \varepsilon_2$ (a), $\varepsilon_2 \leq \varepsilon_{\rm F} \leq \varepsilon_3$ (b), and $\varepsilon_3 \leq \varepsilon_{\rm F} \leq \varepsilon_4$ (c).

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

$$W_i = \sum_{j=1}^{3} \frac{S}{\nabla_k \varepsilon_k} F_{ji}(\varepsilon_1^k, \cdots, \varepsilon_4^k, \varepsilon_{\rm F}) W'_j. \tag{14}$$

F_{ij} and $\frac{S}{\nabla_k \varepsilon_k}$ are calculated as follows ($a_{ij} \equiv (\varepsilon_i - \varepsilon_j)/(\varepsilon_{\rm F} - \varepsilon_j)$):

- When $\varepsilon_1 \leq \varepsilon_{\rm F} \leq \varepsilon_2 \leq \varepsilon_3 \leq \varepsilon_4$ [Fig. 1(a)],

$$F = \begin{pmatrix} a_{12} & a_{21} & 0 & 0 \\ a_{13} & 0 & a_{31} & 0 \\ a_{14} & 0 & 0 & a_{41} \end{pmatrix}, \qquad \frac{S}{\nabla_k \varepsilon_k} = \frac{3 a_{21} a_{31} a_{41}}{\varepsilon_{\rm F} - \varepsilon_1} \tag{15}$$

- When $\varepsilon_1 \leq \varepsilon_2 \leq \varepsilon_{\rm F} \leq \varepsilon_3 \leq \varepsilon_4$ [Fig. 1(b)],

$$F = \begin{pmatrix} a_{13} & 0 & a_{31} & 0 \\ a_{14} & 0 & 0 & a_{41} \\ 0 & a_{24} & 0 & a_{42} \end{pmatrix}, \qquad \frac{S}{\nabla_k \varepsilon_k} = \frac{3 a_{31} a_{41} a_{24}}{\varepsilon_{\rm F} - \varepsilon_1} \tag{16}$$

$$F = \begin{pmatrix} a_{13} & 0 & a_{31} & 0 \\ 0 & a_{23} & a_{32} & 0 \\ 0 & a_{24} & 0 & a_{42} \end{pmatrix}, \qquad \frac{S}{\nabla_k \varepsilon_k} = \frac{3 a_{23} a_{31} a_{42}}{\varepsilon_{\rm F} - \varepsilon_1} \tag{17}$$

- When $\varepsilon_1 \leq \varepsilon_2 \leq \varepsilon_3 \leq \varepsilon_{\rm F} \leq \varepsilon_4$ [Fig. 1(c)],

$$F = \begin{pmatrix} a_{14} & 0 & 0 & a_{41} \\ a_{13} & a_{24} & 0 & a_{42} \\ a_{12} & 0 & a_{34} & a_{43} \end{pmatrix}, \qquad \frac{S}{\nabla_k \varepsilon_k} = \frac{3 a_{14} a_{24} a_{34}}{\varepsilon_1 - \varepsilon_{\rm F}} \tag{18}$$

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

- When $\varepsilon'_1 \leq \varepsilon_{\rm F} \leq \varepsilon'_2 \leq \varepsilon'_3$ [Fig. 1(d)],

$$W'_1 = L(a'_{12} + a'_{13}), \qquad W'_2 = L a'_{21}, \qquad W'_3 = L a'_{31}, \qquad L \equiv \frac{a'_{21} a'_{31}}{\varepsilon_{\rm F} - \varepsilon'_1} \tag{19}$$

- When $\varepsilon'_1 \leq \varepsilon'_2 \leq \varepsilon_{\mathrm{F}} \leq \varepsilon'_3$ [Fig. 1(e)],

$$W'_1 = La'_{13}, \qquad W'_2 = La'_{23}, \qquad W'_3 = L(a'_{31} + a'_{32}), \qquad L \equiv \frac{a'_{13}a'_{23}}{\varepsilon'_3 - \varepsilon_{\mathrm{F}}} \tag{20}$$

3.2 Eqn. (4)

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

$$\frac{\theta(\varepsilon_{\mathrm{F}} - \varepsilon_{kv\sigma}) - \theta(\varepsilon_{\mathrm{F}} - \varepsilon_{k+qv'\sigma})}{\varepsilon_{kv\sigma} - \varepsilon_{k+qv'\sigma}}\theta(\varepsilon_{k+qv'\sigma} - \varepsilon_{kv\sigma}) \tag{21}$$

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).