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Correctly weighted tetrahedron method for *k*-space integration

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Abstract. The analytical integration of a linearly interpolated function commonly used in the tetrahedron integration (TI) method is not correct and the calculated quantities do not satisfy crystal symmetry. We propose an improved method wherein the integration is restricted to a minimal volume which covers the irreducible part of the Brillouin zone with microcubes in contrast to those by Kleinman and Hanke and co-workers. We also extend this to a hexagonal crystal. The *k*-points in the correctly weighted TI method are shown to have the characteristics of special points and give accurate values for an insulator. The efficiency of the present method is discussed in comparison with the conventional TI method.

1. Introduction

The tetrahedron integration (TI) method introduced by Lehmann and Taut [1] and Jepson and Anderson [2] has been used extensively for the $\boldsymbol{k}$-space integration of a function $f(\boldsymbol{k})$ in many theoretical studies of solid state physics. The integral over the irreducible part of the Brillouin zone (IBZ) is replaced by the sum of integrals over non-overlapping (micro)tetrahedra filling the IBZ [3] where the four vertices of a tetrahedron are on the mesh points setting appropriately in the BZ for which the values of $f(\boldsymbol{k})$ are given through some involved calculations, and inside the tetrahedron the integration is carried out analytically by using linear interpolation. Despite its efficiency, the TI method needs a relatively large number of $\boldsymbol{k}$-points to attain a desired accuracy. However, the number of $\boldsymbol{k}$-points is limited because the $\boldsymbol{k}$-space integration is a part of other large numerical calculations such as total energy or self-consistent bandstructure calculations. Recently, Kleinman [4] pointed out that the misweighting of the $\boldsymbol{k}$-points in the TI method produces an unexpectedly large error for the number of $\boldsymbol{k}$-points usually used in realistic calculations [5]. Furthermore, calculated quantities do not satisfy the crystal symmetry. To remedy this deficiency, Kleinman proposed that for cubic crystals the integration should be taken over the whole BZ of a cubic superlattice which contains one, two and four BZs of SC, FCC and BCC, respectively. This super BZ is divided into (micro)cubes by using a cubic mesh. Each of the cubes is further subdivided into six equal-volume tetrahedra to which the TI method is to be applied. However, since the volumes of integration are 48, 96 and 192 times larger than those of the TI method currently used [6–9] for SC, FCC and BCC, respectively, Kleinman's method is rather time consuming.

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For the FCC crystal, Hanke *et al* [10] give an improvement by using $\frac{1}{8}$ of the cubic super BZ where a cube is divided into non-equal-volume tetrahedra.

The misweighting problem results from the fact that the $\boldsymbol{k}$-points on or near the surfaces and corners of the IBZ are not treated correctly due to the use of linear interpolation. In this paper we will show that this problem can be avoided within the framework of linear interpolation by using the cubes which cover completely the IBZ and the superposition of twelve tetrahedra derived by two different schemes of division of a cube as will be shown in section 3: Kleinman substantially uses 48 tetrahedra for a cube derived by eight different schemes of division to attain the correct weighting for the $\boldsymbol{k}$-points in the SC IBZ. The present method also satisfies crystal symmetry. Numerical comparisons of the present method with the conventional TI method by Skriver [9] will be given in section 4. The application to non-cubic crystals will be discussed in the appendix.

2. Tetrahedron integration

We will now consider the calculation of the following integral over the BZ with the volume Ω by the TI method as

$$I = \frac{1}{\Omega}\int_{\mathrm{BZ}} f(\boldsymbol{k})\theta(\varepsilon_{\mathrm{F}} - \varepsilon(\boldsymbol{k}))\,\mathrm{d}\boldsymbol{k} \simeq \frac{1}{4\Omega}\sum_i w_i v_i \sum_{j=1}^{4} c_{ij}(\varepsilon_{\mathrm{F}}) f(\boldsymbol{k}_{ij}) \tag{2.1}$$

where ε_{F} and $\varepsilon(\boldsymbol{k})$ denote, respectively, the Fermi energy and the band energy of a wave vector $\boldsymbol{k}$, θ denotes the unit step function and the suffix i runs over non-equivalent tetrahedra in the BZ. In (2.1) v_i and w_i are the volume and multiplicity of the ith tetrahedron with the wave vectors at its vertices given by $(\boldsymbol{k}_{i1}, \boldsymbol{k}_{i2}, \boldsymbol{k}_{i3}, \boldsymbol{k}_{i4})$. Hereafter we assume that all tetrahedra have the same volume v_{t} and that the vertices are rearranged in the order of $\varepsilon_1 \leqslant \varepsilon_2 \leqslant \varepsilon_3 \leqslant \varepsilon_4$ with $\varepsilon_j = \varepsilon(\boldsymbol{k}_{ij})$ and the coefficients $c_{ij}(\varepsilon_{\mathrm{F}})$ become 0 for $\varepsilon_{\mathrm{F}} < \varepsilon_1$ and 1 for $\varepsilon_{\mathrm{F}} \geqslant \varepsilon_4$, respectively. When the Fermi surface is present inside the ith tetrahedron, c_{ij} can be calculated by using the linear interpolations $\varepsilon(\boldsymbol{k}) = \varepsilon_j + \boldsymbol{a}\cdot(\boldsymbol{k} - \boldsymbol{k}_j)$ and $f(\boldsymbol{k}) = f_j + \boldsymbol{b}\cdot(\boldsymbol{k} - \boldsymbol{k}_j)$ where $\boldsymbol{a}$ and $\boldsymbol{b}$ are determined by the values ε_j and f_j at the four vertices of the tetrahedron. Here we suppressed the suffix i for simplicity. The results are given as follows

(i) for $\varepsilon_1 \leqslant \varepsilon_{\mathrm{F}} < \varepsilon_2$:

$$c_j = \left[4\delta_{j1} + \sum_{m=1}^{4}(\delta_{mj} - \delta_{j1})\Delta_{m1}\right]\Delta_{21}\Delta_{31}\Delta_{41} \tag{2.2}$$

(ii) for $\varepsilon_2 \leqslant \varepsilon_{\mathrm{F}} < \varepsilon_3$:

$$\begin{aligned} c_j = {} & [1 + (\delta_{j1} - \delta_{j4})\Delta_{14}]\Delta_{41} - [\delta_{j3} + \Delta_{j,5-j} + (\delta_{j1} + \delta_{j3})\Delta_{j,4-j}]\Delta_{13}\Delta_{23}\Delta_{41} \\ & + [\delta_{j2} + \Delta_{j,5-j} + (\delta_{j2} + \delta_{j4})\Delta_{j,6-j}]\Delta_{14}\Delta_{32}\Delta_{42} \end{aligned} \tag{2.3}$$

(iii) for $\varepsilon_3 \leqslant \varepsilon_{\mathrm{F}} < \varepsilon_4$:

$$c_j = 1 - \left[4\delta_{j4} + \sum_{m=1}^{4}(\delta_{mj} - \delta_{j4})\Delta_{m4}\right]\Delta_{14}\Delta_{24}\Delta_{34} \tag{2.4}$$

where $\Delta_{jj'} = (\varepsilon_{\mathrm{F}} - \varepsilon_{j'})/(\varepsilon_j - \varepsilon_{j'})$ and δ_{ij} denotes the Chronecker delta. Equations (2.2)–

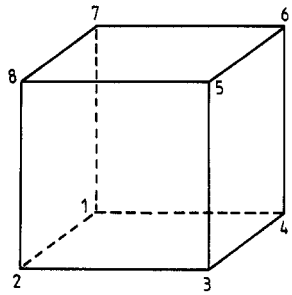

Figure 1. Numbering scheme for the eight vertices of a cube and a prism.

Table 1. Schemes of division of a cube and a prism into six equal-volume tetrahedra. A set of four integers represents a tetrahedron in the cube or the prism whose vertices are numbered according to figure 1.

S_1	1247	2346	2368	2467	2678	3568
S_2	1238	1345	1358	1457	1578	4567
S_3	1237	1345	1456	1567	2378	3578
S_4	1246	1267	2348	2678	3458	4568
S_5	1246	1267	2346	2356	2568	2678
S_6	1248	1478	2348	3458	4568	4678

(2.4) create no calculational problem even if some of the values of ε_j have the same values in the respective cases. For the integration on the Fermi surface the coefficients of $f(\boldsymbol{k}_{ij})$ are given by $\partial c_{ij}/\partial \varepsilon_F$.

3. Application to cubic crystals

For an insulator, $f(\boldsymbol{k}_{ij})$ at the four vertices of a tetrahedron have the same weights (volume elements reduced by Ω) due to the use of the linear interpolation. Thus the results obtained depend upon the way in which the IBZ is divided into tetrahedra, since every vertex of a cube does not have the same weight when equation (2.1) is applied to six equal-volume tetrahedra in a cube in contrast to the three-dimensional trapezoidal rule which is a correct linear approximation: in the conventional TI [9] and Kleinman's methods the weights associated with $f(\boldsymbol{k}_{ij})$ for the eight vertices of a cube become 6, 2, 2, 2, 6, 2, 2, 2 and 1, 5, 3, 3, 1, 5, 3, 3, respectively, all in units of $v_t/4\Omega$ (see figure 1). Therefore, we must pay particular attention to the $\boldsymbol{k}$-points on or near the surfaces of the IBZ when we apply (2.1) to the integration over the IBZ. The situation is unchanged when the Fermi surface is present.

Following Kleinman, we take a cubic super BZ with the edge length of $4\pi/\lambda a$ where λ is taken to be equal to 2 for SC and 1 for FCC and BCC, respectively, and a is the lattice constant of the respective crystals. We divide it into $(2N)^3$ cubes with edge length of $2\pi/\lambda Na$ and number the vertices of each cube as shown in figure 1. If we subdivide each cube with the volume $v_c = \Omega/(2N)^3$ into six equal-volume tetrahedra according to the two schemes S_1 and S_2 shown in table 1 and superpose these with a weighting factor $\frac{1}{2}$,

then we have the same weights $p_{ij} = v_c/8\Omega$ for each vertex of the ith cube in accordance with the three-dimensional trapezoidal rule. This allows us to reduce the domain of the integration to $\frac{1}{8}$ of the cubic super BZ. The wavevector of the vertex 1 of the ith cube is written in the Cartesian coordinates as

$$\boldsymbol{k}_{i1} = (2\pi/\lambda Na)(n_{i1}, n_{i2}, n_{i3}) \tag{3.1}$$

with $0 \leqslant n_{ij} < N$. We represent the ith cube by the triplet (n_1, n_2, n_3) where the suffix i is suppressed. Since the cubes having the triplets obtained by permutations of (n_1, n_2, n_3) give the equivalent contributions to the integral, we can restrict the integer n_j further to $N > n_1 \geqslant n_2 \geqslant n_3 \geqslant 0$. The multiplicity $w_s(n_1, n_2, n_3)$ of a non-equivalent cube becomes 8, 24, 24 and 48, respectively, for $n_1 = n_2 = n_3$, $n_1 = n_2 \neq n_3$, $n_1 \neq n_2 = n_3$ and otherwise. The number of non-equivalent $\boldsymbol{k}$-points, N_k, is given by $(N+1)(N+2)(N+3)/6$. For a cube for which more than two of the n_j are equal, some vertices are outside the IBZ. In this case we rearrange (n_1, n_2, n_3) of these vertices to (n_1', n_2', n_3') with $n_1' \geqslant n_2' \geqslant n_3'$ by a permutation using the cubic symmetry.

For the FCC and BCC crystals we can reduce the number of non-equivalent cubes further than in the SC crystal. In the case of FCC cubes (n_1, n_2, n_3) and $(N - n_3 - 1, N - n_2 - 1, N - n_1 - 1)$ give equivalent contributions to the integral, so we can restrict n_j further to $n_1 + n_2 + n_3 < \frac{3}{2}N$. Since the cubes with $n_1 + n_2 + n_3 \leqslant \frac{3}{2}N - 3$ and those with $\frac{3}{2}N - 3 < n_1 + n_2 + n_3 < \frac{3}{2}N$ have one and no equivalent cube, the multiplicities $w(n_1, n_2, n_3)$ of these cubes are given by $2w_s$ and w_s with w_s as the quantity defined in the SC case. N_k is given by $(N+2)(N^2 + N + 6[N/2] + 6)/12$ with [x] as the Gauss symbol. For BCC, a cube (n_1, n_2, n_3) has three equivalent cubes given by $\{n_1, N - n_2 - 1, N - n_3 - 1\}$, $\{N - n_1 - 1, n_2, N - n_3 - 1\}$ and $\{N - n_1 - 1, N - n_2 - 1, n_3\}$ where $\{n_1, n_2, n_3\}$ means that the components are taken to be in descending order. Thus we can restrict n_j further to $n_1 + n_2 < N$ and $w(n_1, n_2, n_3) = 4w_s$ for $n_1 + n_2 \leqslant N - 2$. For a cube (n_1, n_2, n_3) with $n_1 + n_2 = N - 1$, w is given by w_s, $\frac{4}{3}w_s$ and $2w_s$ for $n_1 = n_2 = n_3$, $n_1 \neq n_2 = n_3$ and otherwise, respectively, and $N_k = (N+3)(N^2 + 3N + 6[N/2] + 8)/24$. Though for both cases there appear to be instances where some vertices of a cube are outside the IBZ, the values of ε_j and f_j for these vertices can be expressed by those inside the IBZ by using the cubic symmetry.

As can be seen from the above discussions, for FCC and BCC the $\boldsymbol{k}$-points are not necessarily on the surfaces or corners of the respective IBZ, i.e. we can choose N to be an arbitrary integer in contrast to the TI method currently used [6–9]. Though there are, of course, other possibilities to attain the correct weighting by using, for example, the two schemes S_3 and S_4 shown in table 1, these give substantially the same results: there are small differences in determination of the Fermi surface inside each cube.

4. Discussion

For interesting cases in the application of $\boldsymbol{k}$-space integration, $f(\boldsymbol{k})$ is a totally symmetric function of the system considered and has the translational symmetry in the reciprocal lattice. In this case $f(\boldsymbol{k})$ can be written in terms of the Fourier series of the direct lattice as

$$f(\boldsymbol{k}) = \sum_l F(\boldsymbol{R}_l) g_l(\boldsymbol{k}) \tag{4.1}$$

$$g_l(\boldsymbol{k}) = \sum_S{}' \exp(\mathrm{i}\boldsymbol{k} \cdot S\boldsymbol{R}_l) \tag{4.2}$$

Table 2. Comparison of $\langle g_l(\boldsymbol{k})\rangle_\varepsilon$ calculated by the present method with those of Skriver's by the single tight-band models with $\varepsilon = \varepsilon_b + 0.7W$. The symbol S denotes the values by Skriver's method and the correct values are calculated by using more than 10^4 points in the respective crystals. The averaged absolute errors (in units of 10^{-2}) of the density of state $\langle|\Delta D(\varepsilon)|\rangle$ are obtained from 200 energy points.

N_k	$R_l[l_1, l_2, l_3]$					$\langle\|\Delta D(\varepsilon)\|\rangle$
FCC	000	110	200	211	220	
44	0.62	2.55	0.08	−0.72	−0.41	1.5
85	0.62	2.62	0.07	−0.77	−0.43	1.0
85 S	0.61	2.53	−0.02	−0.58	−0.20	1.2
Correct	0.62	2.67	0.08	−0.85	−0.48	
BCC	000	111	200	220	311	
55	1.76	1.15	−0.71	−0.60	0.40	0.6
55 S	1.77	1.16	−1.04	0.14	0.71	1.1
Correct	1.75	1.24	−0.76	−0.64	0.39	
HCP	000	100	001	210	101	
64	0.41	5.18	−0.02	−0.75	−4.39	1.6
64 S	0.42	5.16	−0.07	−0.40	−0.36	1.9
Correct	0.41	5.34	−0.02	−0.89	−4.99	
DIA	000	110	200	211	220	
44	2.87	−2.31	0.86	1.30	−0.06	2.5
85	2.86	−2.40	0.92	1.47	−0.11	1.6
85 S	2.87	−1.70	0.86	2.65	0.83	2.0
Correct	2.86	−2.45	0.97	1.60	−0.12	

where $F(\boldsymbol{R}_l)$ is the Fourier coefficient and $\boldsymbol{R}_l$ denotes the representative or star of the translation vectors connected mutually through $\boldsymbol{R}_{l'} = S\boldsymbol{R}_l$ where S acts as the point group parts of the symmetry operations and the prime on the summation means that the operations $\boldsymbol{R}_l = S\boldsymbol{R}_l$ are excluded except for the identity. The $\boldsymbol{k}$-space integration of (4.1) is written as

$$\langle f(\boldsymbol{k})\rangle_{\varepsilon_F} = F(\boldsymbol{0}) + \sum_{l=1}^{\infty} F(\boldsymbol{R}_l)\langle g_l(\boldsymbol{k})\rangle_{\varepsilon_F} \tag{4.3}$$

where we take l as $0 < |\boldsymbol{R}_1| \leq |\boldsymbol{R}_2| \leq \ldots$ and $g_0(\boldsymbol{k}) = 1$. In cubic crystals we write $\boldsymbol{R}_l$ in the Cartesian coordinates as $(\lambda/2)(l_1, l_2, l_3)a$ with λ defined in section 3 and in a hexagonal crystal we write it as $l_1\boldsymbol{t}_1 + l_2\boldsymbol{t}_2 + l_3\boldsymbol{t}_3$ with $\boldsymbol{t}_1$, $\boldsymbol{t}_2$ and $\boldsymbol{t}_3$ as the basis vectors of the direct lattice defined, respectively, by $(\sqrt{3}/2, -1/2, 0)a$, $(0, 1, 0)a$ and $(0, 0, 1)c$ with a and c as the lattice constants where l_j is an integer for all cases. Hereafter we express $\boldsymbol{R}_l$ by $[l_1, l_2, l_3]$. From equations (3.1), (4.2) and (A.1) we can see that for an insulator $\langle g_l(\boldsymbol{k})\rangle_{\varepsilon_F}$ vanishes except for $[2Nl_1, 2Nl_2, 2Nl_3]$ and $[N_1(l_1 + l_2), N_1(2l_1 - l_2), 2N_3l_3]$ in cubic and hexagonal crystals, respectively. Therefore the integral (4.3) is represented accurately by $F(\boldsymbol{0})$ when N_k becomes large: the $\boldsymbol{k}$-points in the present method have the characteristics of the special points [11, 12]. In Skriver's method [9] the non-vanishing terms in the summation of (4.3) start from [1, 1, 0], [1, 1, 0], [1, 1, 1] and [1, 0, 0] for SC,

Table 3. Some of the interpolated values $\varepsilon'(\boldsymbol{k})$ (in Ryd) of 55 $\boldsymbol{k}$-points for the first conduction band of BCC iron and of 85 $\boldsymbol{k}$-points for the second one of FCC copper obtained by using the values of 14 and 19 $\boldsymbol{k}$-points as the input data for the respective crystals. The original data $\varepsilon(\boldsymbol{k})$ are taken from [13] and [14], respectively and $\boldsymbol{k} = (k_x, k_y, k_z)$ is given in units of $\pi/4a$.

BCC iron			FCC copper		
$\boldsymbol{k}$	$\varepsilon'(\boldsymbol{k})$	$\varepsilon(\boldsymbol{k})$	$\boldsymbol{k}$	$\varepsilon'(\boldsymbol{k})$	$\varepsilon(\boldsymbol{k})$
110	0.155	0.154	110	0.292	0.291
221	0.297	0.286	300	0.263	0.265
300	0.300	0.297	432	0.284	0.291
421	0.430	0.426	520	0.235	0.236
441	0.418	0.418	543	0.284	0.284
521	0.479	0.467	632	0.252	0.253
610	0.459	0.455	730	0.245	0.237
700	0.425	0.424	821	0.220	0.218

FCC, BCC and hexagonal crystals, respectively. Thus the quantities calculated by the conventional TI method do not satisfy crystal symmetry.

In order to look into the effect of the Fermi or constant-energy surface on the TI, we have calculated $\langle g_l(\boldsymbol{k})\rangle_\varepsilon$ on the single tight-band models. The band energies of a wavevector $\boldsymbol{k} = (k_x, k_y, k_z)$ for FCC, BCC, HCP and diamond crystals are written, respectively, as

$$\varepsilon_{\mathrm{FCC}}(\boldsymbol{k}) = -4(\cos(\tfrac{1}{2}k_x a)\cos(\tfrac{1}{2}k_y a) + \cos(\tfrac{1}{2}k_y a)\cos(\tfrac{1}{2}k_z a) + \cos(\tfrac{1}{2}k_z a)\cos(\tfrac{1}{2}k_x a)) \tag{4.4}$$

$$\varepsilon_{\mathrm{BCC}}(\boldsymbol{k}) = -8\cos(\tfrac{1}{2}k_x a)\cos(\tfrac{1}{2}k_y a)\cos(\tfrac{1}{2}k_z a) \tag{4.5}$$

$$\varepsilon_{\mathrm{HCP}}(\boldsymbol{k}) = 2[\varepsilon_0(\boldsymbol{k}) \pm (\tfrac{3}{2} + \varepsilon_0(\boldsymbol{k}))^{1/2}]\cos(\tfrac{1}{2}k_z c) \times \varepsilon_0(\boldsymbol{k}) = 2\cos[(\sqrt{3}/2)\,k_x a]\cos(\tfrac{1}{2}k_y a) + \cos(\tfrac{1}{2}k_y a) \tag{4.6}$$

$$\varepsilon_{\mathrm{DIA}}(\boldsymbol{k}) = \pm 2(1 - \tfrac{1}{4}\varepsilon_{\mathrm{FCC}}(\boldsymbol{k}))^{1/2}. \tag{4.7}$$

In calculating $\langle g_l(\boldsymbol{k})\rangle_\varepsilon$ we take the energy as $\varepsilon = \varepsilon_b + 0.7W$ with ε_b and W as the bottom energies and widths of the respective bands and we include a spin factor of 2. In table 2 we compare the values calculated by the present method with those by Skriver's where the correct values are obtained by using more than 10^4 points for the respective crystals and for HCP we take N_3 in (A.1) to be $N_1/2$. The density of state $D(\varepsilon)$ can be obtained by (2.1) by replacing $c_{ij}(\varepsilon_F)$ and f_{ij} by $\partial c_{ij}(\varepsilon)/\partial\varepsilon$ and 1, respectively. In table 2 we also show the averaged absolute errors of $D(\varepsilon)$ estimated from 200 energy points. The results show that the present method gives more satisfactory values than Skriver's for all crystals considered.

For the integration of $f(\boldsymbol{k})$ over the BZ the present method gives accurate values even if N_k is small. However, when the Fermi surface is present we need a relatively large N_k so as to obtain correct values. For a case where only small numbers of calculated $\varepsilon(\boldsymbol{k})$ and $f(\boldsymbol{k})$ are available due to the involved calculations needed, (4.1) gives a simple and accurate interpolation formula which satisfies crystal symmetry: the Fourier series are

truncated in finite terms so as to determine $F(\boldsymbol{R}_l)$ from the available data by using a least-squares fitting method. Table 3 shows the interpolated values of $\varepsilon(\boldsymbol{k})$ for the first conduction band of BCC iron [13] with $N_k = 55$ and the second one of FCC copper [14] with $N_k = 85$ calculated by the augmented-plane-wave method. For the input data we use the values of 14 and 19 $\boldsymbol{k}$-points for BCC iron and FCC copper, respectively. The interpolation is satisfactory for both cases. Since for a small value of N_k the errors in the $\boldsymbol{k}$-space integration result from poor estimations of the constant-energy or Fermi surface, we can obtain more correct values if we calculate the integration for a larger N_k by using the interpolated values of $\varepsilon(\boldsymbol{k})$ and $f(\boldsymbol{k})$.

Appendix

An extension of the present method to tetragonal and orthorhombic crystals can be accomplished by replacing the cube by a rectangular prism. Some modifications, however, are necessary for a hexagonal crystal. We consider the TI over the parallelepiped constructed by the three vectors $\boldsymbol{u}_1 = (\boldsymbol{b}_1 + \boldsymbol{b}_2)/3$, $\boldsymbol{u}_2 = (2\boldsymbol{b}_1 - \boldsymbol{b}_2)/3$ and $\boldsymbol{u}_3 = \frac{1}{2}\boldsymbol{b}_3$ with $\boldsymbol{b}_i$ as the basis vectors of the reciprocal lattice orthogonal to $\boldsymbol{t}_i$ as defined in section 4. This domain is four-times larger than the IBZ. We divide it into $N_1^2 N_3$ (micro)prisms using the mesh given by

$$\boldsymbol{k} = (n_1/N_1)\boldsymbol{u}_1 + (n_2/N_1)\boldsymbol{u}_2 + (n_3/N_3)\boldsymbol{u}_3 \tag{A.1}$$

with the integers taken to be $0 \leqslant n_1, n_2 < N_1$ and $0 \leqslant n_3 < N_3$. The volume of a prism is given by $v_p = \Omega/(6N_1^2 N_3)$ with $\Omega = 16\pi^3/(\sqrt{3}\,a^2 c)$. For non-cubic crystals we define p_{ij} to be $(v_p/4\Omega)E(\hat{\boldsymbol{q}}_1, \hat{\boldsymbol{q}}_2, \hat{\boldsymbol{q}}_3)$ where E denotes the spherical excess in spherical trigonometry with $\hat{\boldsymbol{q}}_j$ as the unit vectors along the three edges associated to a vertex. The definition is in accordance with the weights given by the three-dimensional trapezoidal rule in the oblique coordinates. For the hexagonal crystal p_{ij} becomes $\frac{1}{12}$ and $\frac{1}{6}$ in units of v_p/Ω, respectively, for $j = 1, 3, 5, 7$ and $2, 4, 6, 8$ (see figure 1). If we subdivide each prism into six equal-volume tetrahedra according to the two schemes S_5 and S_6 given in table 1 and superpose these with the weighting factor $\frac{1}{2}$, then we have the correct weighting when we apply the TI to these tetrahedra. Considering that prisms (n_1, n_2, n_3) (n_2, n_1, n_3), $(N_1 - n_1 - 1,\ N_1 - n_2 - 1,\ n_3)$ and $(N_1 - n_2 - 1,\ N_1 - n_1 - 1, n_3)$ are equivalent, we can restrict n_j to the IBZ defined by $0 \leqslant n_2 \leqslant n_1 < N_1$, $n_1 + n_2 < N_1$ and $0 \leqslant n_3 < N_3$. For this case we have $w(n_1, n_2, n_3)$ given by 6 for $n_1 = n_2$ and $2n_1 + 1 = N_1$, 12 for $n_1 = n_2$ and $2n_1 + 1 \neq N_1$, 12 for $n_1 + n_2 = N_1 - 1$ and $2n_1 + 1 \neq N_1$, and 24 for otherwise, respectively, and $N_k = ([N_1/2] + 1)([N_1/2] - 1)(N_3 + 1)$. Since some vertices of the prisms with $n_1 = n_2$ and/or $n_1 + n_2 = N_1 - 1$ are outside the IBZ, we rearrange (n_1, n_2, n_3) of these vertices to (n_1', n_2', n_3') for $n_1 + n_2 < N_1$ and $(N_1 - n_2', N_1 - n_1', n_3)$ for $n_1 + n_2 \geqslant N_1$ where n_1' and n_2' denote, respectively, the larger and smaller ones of n_1 and n_2 in order to express $\varepsilon(\boldsymbol{k}_j)$ and $f(\boldsymbol{k}_j)$ by those of the $\boldsymbol{k}$-points inside the IBZ.

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