General formulae for the special points and their weighting factors in k-space integration

1992 J. Phys.: Condens. Matter 4 4583

(http://iopscience.iop.org/0953-8984/4/19/002)

J. Phys.: Condens. Matter 4 (1992) 4583–4594. Printed in the UK

General formulae for the special points and their weighting factors in k-space integration

Juichiro Hama† and Masaaki Watanabe‡

† Department of Materials Physics, Faculty of Engineering Science, Osaka University, Toyonaka, Osaka 560, Japan

‡ Faculty of Technology, Kinki University, Higashi-hiroshima, Hiroshima 729-17, Japan

Received 10 June 1991, in final form 2 January 1992

Abstract. General formulae are given for providing sets of the special points and their weighting factors for k-space integration without the use of a recurrence process for cubic, hexagonal and tetragonal lattices. The formulae are allowed to be used for intermediate numbers of k-points not considered in the method of Chadi and Cohen. It is shown that the special-point method is an open-type Lagrange quadrature of lowest order and that it gives accurate values for moderately varying functions but less accurate values for those with discontinuous derivatives at the Brillouin zone boundaries. In the present method it is possible to incorporate the second-order Lagrange quadrature and the Gaussian method. The efficiencies of these methods are discussed in comparison with the correctly weighted tetrahedron method.

1. Introduction

The special-point method proposed by Chadi and Cohen (CC) [1] has been used extensively in many theoretical studies of solid state physics for k-space integration of a periodic function $f(k)$ over the Brillouin zone (BZ). For a moderately varying function this method has made it possible to calculate the integral more accurately than the ordinary tetrahedron integration (TI) method for relatively small numbers of k-points selected appropriately in the irreducible BZ (IBZ), which is the smallest segment of the BZ reduced by the isogonal point-group symmetry of the lattice [2]. A set of the special points is derived from the recurrence process successively with the use of a seed point chosen deliberately in the IBZ for a next approximation, and their weighting factors are obtained by applying the symmetry operations to newly obtained k-points and counting the numbers of non-equivalent k-points.

Despite its efficiency the CC method has no general formulae for locating the special points in the IBZ and calculating their weighting factors, so that finding them becomes tedious for higher-order approximations. Owing to the non-uniqueness of the CC method, several different sets of the special points and their weighting factors are proposed [3, 4]. From an alternative approach, Monkhorst and Pack [5] have devised a method which generates the special points for the FCC and BCC lattices by using the super-cubic BZ of a simple-cubic lattice, although they did not give formulae for calculating the weighting factors. Recently Macot and Frank [6] have derived the general formulae which determine the special points and their weighting factors for the square and cubic lattices without use of the recurrence process. Their method,

0953-8984/92/194583+12$04.50

however, is confined to the CC scheme, so that possible numbers N_k of the special points are limited and N_k increases rapidly as the order of approximation becomes higher: $N_k = 1,2,10,60,408,\ldots$ and $1,2,8,40,240,\ldots$ for the FCC and BCC lattices, respectively. Thus general formulae for obtaining intermediate values of N_k may be useful because in many interesting cases of application the calculation of $f(\boldsymbol{k})$ is much more involved and time consuming than the numerical integration itself. In some applications of the special-point method the calculated values are very slowly convergent with respect to N_k, so that its improvement without loss of simplicity is also useful.

In this paper we shall present the general formulae for giving the special points in the IBZ and the corresponding weighting factors explicitly. In section 2 we describe the formalism and show that the special-point method is an open-type Lagrange quadrature of lowest order and propose a second-order improved scheme. In section 3 we apply the present method to the cubic lattices and show that it is possible to use the formulae for intermediate values of N_k. In section 4 and appendix 1 we show that the present method can be applied to the hexagonal and tetragonal lattices. In section 5 the efficiency of the special-point method is discussed in comparison with the correctly weighted TI method including quadratic interpolation scheme and the Gaussian method.

2. Formalism

We now express a wavevector $\boldsymbol{k}$ and a translation vector $\boldsymbol{R}$ in the direct lattice as

$$\boldsymbol{k} = \sum_\alpha q_\alpha \boldsymbol{b}_\alpha \qquad \boldsymbol{R} = \sum_\alpha l_\alpha \boldsymbol{t}_\alpha \tag{2.1}$$

where $\boldsymbol{b}_\alpha$ and $\boldsymbol{t}_\alpha$, respectively, denote the basis vectors of the reciprocal and direct lattices and l_α is an integer. A totally symmetric function $f(\boldsymbol{k})$ with the periodicity of the reciprocal lattice can be written as

$$f(\boldsymbol{k}) = \sum_{\boldsymbol{l}} F(\boldsymbol{l}) \frac{1}{N_S} \sum_S \exp(\mathrm{i}2\pi \boldsymbol{q}\cdot \boldsymbol{l}_S) \tag{2.2}$$

where S is an element of the symmetry group of the system with its order of N_S and $\boldsymbol{l}_S$ denotes a set of l_α for $S\boldsymbol{R}$. In the following, we suppress $N_S^{-1}\sum_S$ and express $\boldsymbol{l}_S$ as $\boldsymbol{l}$ for simplicity. From (2.2) the integral of $f(\boldsymbol{k})$ over the BZ with the volume Ω is written as

$$I = \frac{1}{\Omega}\int_\Omega f(\boldsymbol{k})\,\mathrm{d}\boldsymbol{k} = F(O). \tag{2.3}$$

Using N as the number of $\boldsymbol{k}$-points in the BZ, we express (2.3) as

$$I = \sum_{j=1}^{N} w(\boldsymbol{q}_j) f(\boldsymbol{q}_j) + R_N \tag{2.4}$$

where $w(q_j)$ is the weighting factor of a point q_j and is normalized to unity and the remainder R_N is given by

$$R_N = -\sum_{l}{}' F(l) \sum_{j=1}^{N} w(q_j) \exp(i2\pi q_j \cdot l) \tag{2.5}$$

where the prime means the exclusion of the $l = 0$ term. The central idea of the special-point method is to reduce R_N within a required accuracy by using the smallest set of q_j, because for many interesting cases of application the calculation of $f(k)$ is very time consuming.

Although we finally locate k-points in the IBZ, we adopt at present the parallelepiped zone whose three edges are given by b_1, b_2 and b_3. This is not usually the standard BZ but a primitive zone which has the same volume as the BZ. We define k-points in the zone by (2.1) with q_j-points given as

$$q_{j\alpha} = (1/n_\alpha)(j_\alpha - 1) + a_\alpha - \tfrac{1}{2} \qquad (j_\alpha = 1, 2, \ldots, n_\alpha) \tag{2.6}$$

where a_α takes an arbitrary value in the range $0 \leqslant a_\alpha \leqslant 1/n_\alpha$. The weighting factor of q_j is assumed to be $w(q_j) = 1/N$ with $N = n_1 n_2 n_3$. Using (2.6) we find

$$\sum_{j=1}^{N} w(q_j) \exp(i2\pi q_j \cdot l) = \frac{1}{N} \prod_{\alpha} (-)^{l_\alpha} \exp(i2\pi a_\alpha l_\alpha) \sum_{j_\alpha=1}^{n_\alpha} \exp\left(i \frac{2\pi}{n_\alpha} l_\alpha (j_\alpha - 1)\right). \tag{2.7}$$

Equation (2.7) shows that the second sum in the remainder R_N vanishes unless all l_α/n_α are equal to integers for $n_\alpha > 1$. Thus the set of k-points defined by (2.1) and (2.6) has the characteristics of the special points. The non-uniqueness of the special-point method results from the arbitrariness of the values of a_α. If we take $a_\alpha = 0$ or $1/n_\alpha$ with all even n_α-values and $a_\alpha = 1/2n_\alpha$, equation (2.6) corresponds to the scheme obtained by the correctly weighted TI method [8] and to that by Monkhorst and Pack, respectively. Owing to the lattice symmetry the several k-points given by (2.1) and (2.6) are equivalent if the values of a_α are chosen appropriately, so that we can restrict the non-equivalent k-points in the IBZ, although a slight modification in the treatment is necessary for non-primitive Bravais lattices. If the lattice has a second-order symmetry perpendicular to the axis b_α, the choice of $a_\alpha = 1/2n_\alpha$ is most preferable and that of $a_\alpha = 0$ or $1/n_\alpha$ is the next preferable choice in reducing the number of non-equivalent k-points in the IBZ.

From the derivation of the special points we found that the special-point method is simply an open-type Lagrange quadrature of lowest order and that the remainder is expressed in terms of partial derivatives of $f(q)$ as

$$R_N = \epsilon \sum_{\alpha} (D_\alpha)^p f(q)|_{q=\tilde{q}} \qquad D_\alpha = n_\alpha^{-1} \frac{\partial}{\partial q_\alpha} \tag{2.8}$$

where $p = 2$ and $\tilde{q}_\alpha$ takes a value in the range $-\frac{1}{2} < \tilde{q}_\alpha < \frac{1}{2}$ and $\epsilon = \frac{1}{24}$ and $-\frac{1}{12}$ for $a_\alpha = 1/2n_\alpha$ and $1/n_\alpha$, respectively. As is seen in (2.8), the convergence of the special-point method with respect to n_α is very slow. We can, however, show that, if

$f(q)$ is a well behaved function of class C_∞, it gives accurate values within a relatively small N_k by using the three-dimensional Euler–Maclaurin summation formula. Since the partial derivatives of any order are continuous and have the same values at the points separated by b_α-vectors, the magnitude of R_N is limited to

$$|R_N| \leqslant \int_\Omega \left| \prod_\alpha \frac{n_\alpha}{(2m_\alpha)!} B_{2m_\alpha} (D_\alpha)^{2m_\alpha} f(q) \right| \mathrm{d}q \tag{2.9}$$

where B_{2m} denotes the Bernoulli number with $B_0 = 1$ and $(D_\alpha)^0 = 1/n_\alpha$. In (2.9), m_α are the cut-off values in an asymptotic series chosen appropriately to reduce $|R_N|$ for a given set of n_α. This is a reason why the special-point method is effective because $|R_N|$ can be reduced to a very small value if $f(q)$ is a well behaved function. Equation (2.9) is also applicable to the correctly weighted TI method.

An improvement of the special-point method which takes quadratic interpolation into account is as follows. For simplicity we consider at present a one-dimensional integral

$$I = \int_{-1/2}^{1/2} f(q)\,\mathrm{d}q = \sum_{j=2}^{n-1} \int_{q_j-3h/2}^{q_j+3h/2} f(q)\,\mathrm{d}q \tag{2.10}$$

where $q_j = -\frac{1}{2} + jh$ with $h = 1/n$. We approximate $f(q)$ by using the three-point interpolation formula as

$$\begin{aligned} f(q) = f_j + (1/2h)\{f_{j+1} - f_{j-1} + \tfrac{1}{3}h[h^2 - (q-q_j)^2] f_j^{(3)}\}(q-q_j) + (1/2h^2)\{f_{j+1} \\ - 2f_j + f_{j-1} - \tfrac{1}{12}h^2[h^2 - (q-q_j)^2] f^{(4)}(\xi)\}(q-q_j)^2 \end{aligned} \tag{2.11}$$

with $q_j - 3h/2 < \xi < q_j + 3h/2$. Inserting (2.11) into (2.10), we have

$$\begin{aligned} I = (3/8n)[3(f_1 + f_4 + \ldots + f_{3n-2}) + 2(f_2 + f_5 + \ldots + f_{3n-1}) \\ + 3(f_3 + f_6 + \ldots + f_{3n})] + (21/640n^4) f^{(4)}(\xi). \end{aligned} \tag{2.12}$$

The third-order derivative in (2.11) disappears in the course of integration. Incorporation of the quadratic interpolation to the special-point method can be done readily by multiplying $w(q_j)$ by the following factor:

$$(\tfrac{3}{16})^3 \prod_\alpha \{5 + (-)^{s_\alpha}\} \qquad s_\alpha = j_\alpha - 3\,[\tfrac{1}{3}(j_\alpha + 2)] + 2 \tag{2.13}$$

where $[x]$ denotes the Gauss symbol. For this case, R_N is also expressed by (2.8) with $p = 4$ and $\epsilon = \frac{7}{640}$. Note that $n_\alpha = 3m_\alpha$ with m_α as a positive integer. Thus the convergence is greatly improved if the magnitudes of partial derivatives higher than the fourth order decrease steadily. We have shown that the quadratic interpolation is incorporated easily into the present formalism, so that we shall consider only the linear cases in the next two sections.

3. Application to the cubic lattices

We shall apply the scheme presented in the previous section to the SC, FCC and BCC lattices. Although the treatments are essentially equivalent to those by Monkhorst and Pack except for giving general formulae of the weighting factors, we shall describe the method briefly because those for the FCC and BCC lattices are good references in treating the non-primitive tetragonal and orthorhombic lattices.

3.1. SC lattice

Owing to the O_h symmetry we can restrict j_α defined by (2.6) to the region $n \geqslant j_1 \geqslant j_2 \geqslant j_3 \geqslant \frac{1}{2}(n+1)$ where we take $n_\alpha = n$ and $a_\alpha = 1/2n$. With this choice we can confine the non-equivalent q_j to the IBZ. We find the weighting factor to be

$$w_{SC}(q_j) = \frac{1}{N}\{[3-\delta(j_1,j_2)][3-\delta(j_2,j_3)]-3\}\prod_\alpha [2-\delta(2j_\alpha, n+1)] \tag{3.1}$$

where $\delta(i,j)$ denotes the Kronecker delta and $N = n^3$.

In order to obtain simple schemes for finding general formulae for the special points and their weighting factors for non-primitive Bravais lattices, we take the BZ of the SC lattice having the lattice constant $a = \frac{1}{2}a_0$ with a_0 as the lattice constant of the respective non-primitive lattices. The BZ of the SC lattice is twice and four times those of the BZs of the FCC and BCC lattices, respectively. Note that a wavevector is expressed in units of $2\pi/a$. Since the scheme with an odd n cannot reduce the non-equivalent k-points in comparison with the SC case, we confine ourselves to the scheme with an even n in the following.

3.2. FCC lattice

We now consider a point q in the SC IBZ and introduce a point r_q defined by $(\frac{1}{2}-q_3, \frac{1}{2}-q_2, \frac{1}{2}-q_1)$. The point r_q is equivalent to the point q owing to the translational symmetry in the reciprocal lattice. If we take q in the FCC IBZ given by $n \geqslant j_1 \geqslant j_2 \geqslant j_3 \geqslant \frac{1}{2}(n+1)$ and $j_f \leqslant \frac{3}{4}(3n+2)$ with $j_f = j_1 + j_2 + j_3$, the r_q-points express all the points not included in the FCC IBZ but included in the SC IBZ. In order to exclude the equivalent points which appear on the surface of the FCC IBZ, we impose the further constraint that $j_2 \geqslant \frac{1}{4}(3n+2)$ for $j_f = \frac{3}{4}(3n+2)$. Thus we can confine the non-equivalent points to the FCC IBZ and write their weighting factors as

$$\begin{aligned} w_{FCC}(q_j) = {} & (8/N)\{6-3[\delta(j_1,j_2)+\delta(j_2,j_3)]+\delta(j_1,j_2)\delta(j_2,j_3)\} \\ & \times [2-\delta(4j_f, 9n+6)\delta(4j_2, 3n+2)]. \end{aligned} \tag{3.2}$$

3.3. BCC lattice

Similarly we can confine all the non-equivalent points to the IBZ of the BCC lattice defined by $n \geqslant j_1 \geqslant j_2 \geqslant j_3 \geqslant \frac{1}{2}(n+1)$ and $j_b \leqslant (\frac{3}{2})n+1$ with $j_b = j_1 + j_2$. A point q inside the BCC IBZ has at most three equivalent points not included in the BCC IBZ but included in the SC IBZ which are given by $x_q = \{\frac{1}{2}-q_2, \frac{1}{2}-q_1, q_3\}$, $y_q = \{\frac{1}{2}-q_3, \frac{1}{2}-q_1, q_2\}$ and $z_q = \{\frac{1}{2}-q_3, \frac{1}{2}-q_2, q_1\}$ where the braces denote that the components are arranged in descending order. Considering the cases when some of these points including the point q itself are mutually equal, we can express the weighting factor as

$$\begin{aligned} w_{BCC}(q_j) = {} & (8/N)\{24-12[\delta(j_1,j_2)+\delta(j_2,j_3)]+4\delta(j_1,j_2)\delta(j_2,j_3) \\ & -\delta(2j_b, 3n+2)[12-6\delta(j_1,j_2)-4\delta(j_2,j_3)+\delta(j_1,j_2)\delta(j_2,j_3)]\}. \end{aligned} \tag{3.3}$$

In table 1 we tabulate the numbers N_k of non-equivalent points for the special-point and TI methods. Although there are other possibilities for generating the special points and weighting factors, the present scheme with an even n gives the smallest number of points for the same order of approximation (2.5). The special points obtained by the CC method correspond to the present points with $n = 2^m, m = 1, 2, \ldots$.

Table 1. Numbers of the non-equivalent points N_k of the special-point and correctly weighted tetrahedron integration (TI) methods in the same order of approximations for the respective (cubic and hexagonal) lattices. Except for the SC case in the special-point method n is an even integer and for the hexagonal lattice, n_3 is an even integer, $m_1 = [\frac{1}{2}n_1]$ and $m_2 = [\frac{1}{3}n_1]$.

Special-point method
SC $\frac{1}{6}(n-[\frac{1}{2}n])(n-[\frac{1}{2}n]+1)(n-[\frac{1}{2}n]+2)$
FCC $\frac{1}{96}(n+2)(n^2+10n-24[\frac{1}{4}n])$
BCC $\frac{1}{192}(n+4)(n^2+14n-24[\frac{1}{4}n])$
Hexagonal $\{m_1(n_1-m_1)-\frac{1}{2}m_2(2n_1-3m_2-3)+1\}(\frac{1}{2}n_3)$
TI method
SC $\frac{1}{48}(n+2)(n+4)(n+6)$
FCC $\frac{1}{96}(n+4)(n^2+2n+24[\frac{1}{4}n]+24)$
BCC $\frac{1}{192}(n+6)(n^2+6n+24[\frac{1}{4}n]+32)$
Hexagonal $\{m_1(n_1-m_1)-\frac{1}{2}m_2(2n_1-3m_2-3)+1\}(\frac{1}{2}n_3+1)$

4. Application to non-cubic lattices

Owing to lower symmetries the application of the CC method to non-cubic lattices becomes more tedious than to the cubic lattices [1, 7]. We can, however, show that the general formulae for non-cubic lattices are derived easily by using the scheme presented in section 2.

For the hexagonal lattice we take the basis vectors of the reciprocal lattice as

$$b_1 = (2\pi/a)(1,-1/\sqrt{3},0) \qquad b_2 = (2\pi/a)(1,1/\sqrt{3},0)$$
$$b_3 = (2\pi/c)(0,0,1). \tag{4.1}$$

In the reciprocal space we introduce the primitive zone constructed by b_1, b_2 and b_3 which is 24 times larger than the IBZ of the hexagonal lattice. In this zone we define $N(=n_1^2n_3)$, the number of k-points, by (2.1) and (2.6) where $a_\alpha = \frac{1}{2}$ for $\alpha = 1, 2$ with $n_1 = n_2$ and $a_3 = 1/2n_3$. With this choice the remainder R_N vanishes except for the points $(\frac{1}{2}(m_1+m_2)n_1a, -\frac{1}{2}\sqrt{3}(m_1-m_2)n_1a, m_3n_3c)$ where m_1, m_2 and m_3 are arbitrary integers. Using the rotational and translational symmetries of the hexagonal lattice, we can show that the non-equivalent k-points are expressed by the points in the IBZ defined by

$$\tfrac{1}{2}n_1 + 1 \geqslant j_2 \geqslant j_1 \geqslant 1 \qquad j_1 + 2j_2 \leqslant n_1 + 3 \qquad n_3 \geqslant j_3 \geqslant \tfrac{1}{2}(n_3+1). \tag{4.2}$$

Here we take n_3 to be an even integer because for the same N_k the scheme with an even n_3 gives a higher-order approximation than that with an odd n_3. The weighting factor for a point q_j can be derived readily as

$$w_{\text{hex}}(q_j) = (2/N)\{[3\delta(j_1,1) + 2\delta(j_1,j_2) - 6]\delta(j_1 + 2j_2, n_1 + 3) - 6[\delta(j_1,1) + \delta(j_1,j_2)] + \delta(j_1,1)\delta(j_2,1) + 12\}. \tag{4.3}$$

The number of non-equivalent points is listed in table 1.

According to the present formalism the special points obtained by CC method can be derived very easily without the use of the tedious recurrence process. Let us consider the parallelepiped zone constructed by $b_1 + b_2$, b_2 and b_3 and define the k-points in the zone as $k = q_1(b_1 + b_2) + q_2 b_2 + q_3 b_3$. The CC method uses two sets of q_j:

$$\begin{aligned}
&(\text{A}): q_1 = (j_1 - 1)/3^{m_1} \qquad j_1 = 1,2,\ldots,3^{m_1} \\
&\qquad q_2 = (3j_2 - 2)/3^{m_1} \quad (3j_2 - 1)/3^{m_1} \qquad j_2 = 1,2,\ldots,3^{m_1-1} \\
&(\text{B}): q_1 = (3j_1 - 2)/3^{m_1} \quad (3j_1 - 1)/3^{m_1} \qquad j_1 = 1,2,\ldots,3^{m_1-1} \\
&\qquad q_2 = (j_2 - 1)/3^{m_1-1} \qquad j_2 = 1,2,\ldots,3^{m_1-1}
\end{aligned}$$

where, for both cases, q_3 is the same as (2.6) with $a_3 = 1/2n_3$ and $n_3 = 2^{m_3}$ and m_1 and m_3 are positive integers. The non-equivalent q are given by $3q_1 + 2q_2 \leqslant 1$ and $0 \leqslant q_3 \leqslant \frac{1}{2}$. The quantities N_k and R^2 with R as the shortest lattice vectors for the non-vanishing R_N are given as

$$\begin{aligned}
&(\text{A}): N_k = 3^{m_1-1}(3^{m_1-1} + 1)2^{m_3-2} \qquad R^2 = \min(3^{2m_1-1}a^2, 2^{2m_3}c^2) \\
&(\text{B}): N_k = 3^{m_1-1}(3^{m_1-2} + 1)2^{m_3-2} \qquad R^2 = \min(3^{2m_1-2}a^2, 2^{2m_3}c^2)
\end{aligned}$$

respectively, where min means that the smaller value in the arguments is taken. Since the CC method uses (A) and (B) one after the other, the derivations of the special points becomes more complicated and N_k increases rapidly as the order of approximation becomes higher in comparison with the present method. Scheme (A) is essentially equivalent to the present method with $n_1 = 3^{m_1}$ and $n_3 = 2^{m_3}$, but scheme (B) is less accurate than the present method for the same N_k. The general formulae for the primitive tetragonal (PT) and body-centred tetragonal (BCT) lattices can be derived more easily in the present method than in the method of Lin-Chung, which will be discussed in appendix 1.

In our previous paper [8] we have presented the general formulae for locating the k-points in the IBZ and their weighting factors of the correctly weighted TI method. For the hexagonal lattice, however, they do not have the characteristics of the special points, although they are correct in view of the correctly weighted TI method. In appendix 2 we shall give an improved scheme which has the characteristics of the special points using the method presented in this section.

5. Numerical comparison and discussion

On application of the special-point method it is expected implicitly that the magnitudes of the Fourier coefficients $F(l)$ decrease more rapidly as R becomes large.

However, as shown in section 2 for a moderately varying function of C_∞ class the special-point method is much more accurate than expected. In table 2 we show the relative errors of the integrated values over the SC BZ versus N_k for the function with a sharp peak at $q = 0$ given by (figure 1)

$$f_1(q) = \ln\left(1 - \tfrac{2}{3}g\sum_\alpha \cos(2\pi q_\alpha) + g^2\right). \tag{5.1}$$

The results show that, as the peak becomes weak, the special-point method becomes accurate. For the same N_k the special-point method is much more effective than the TI method owing to the use of an open-type integration formula.

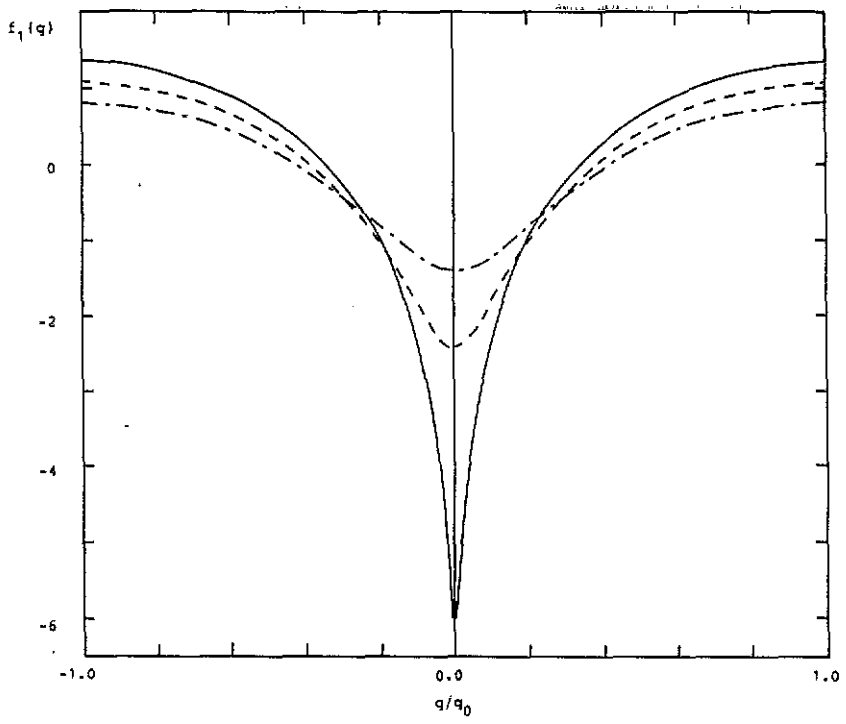

Figure 1. Variation in $f_1(q)$ along the [111] direction with $g = 0.95$ (——), 0.70 (– – –) and 0.50 (– · –) and $q_0 = \frac{1}{2}\sqrt{3}$.

If the function, however, has discontinuous derivatives at the BZ boundaries, the accuracy reduces to that obtained by a lowest-order Lagrange quadrature of open type, which is essentially equivalent to the correctly weighted TI method although the N_k used is larger than the special-point method. The TI method is a closed-type Lagrange quadrature with linear interpolation and its extension to quadratic interpolation is possible to incorporate by multiplying $w(q_j)$ by a factor $\prod_\alpha[1 + \frac{1}{3}(-)^{j_\alpha}]$. The error for the TI method with quadratic interpolation is expressed in the form (2.8) with $p = 4$ and $\epsilon = \frac{1}{180}$. To compare the accuracy of the special-point method with that of other methods, we calculated the integrals over the SC BZ of the following two types of function: one has a sharp peak at the centre of the BZ and the other rapidly

Table 2. Relative errors (absolute values) of the integrated values over the SC BZ of $f_1(q)$ with $g = 0.95$, 0.70 and 0.50 versus the number N_k of non-equivalent points: S, special-point method; T, tetrahedron method; G, Gaussian method.

N_k	4	10	20	35	56
0.95 S	1.9×10^{-2}	4.7×10^{-3}	1.8×10^{-3}	8.7×10^{-4}	4.7×10^{-4}
T	1.3	1.1×10^{-1}	2.5×10^{-2}	8.4×10^{-3}	3.5×10^{-3}
G	5.0×10^{-3}	6.6×10^{-4}	1.2×10^{-4}	2.2×10^{-5}	2.2×10^{-6}
0.70 S	1.6×10^{-2}	1.8×10^{-3}	2.8×10^{-4}	5.2×10^{-5}	1.1×10^{-5}
T	7.0×10^{-1}	2.6×10^{-2}	2.5×10^{-3}	3.5×10^{-4}	5.9×10^{-5}
G	2.4×10^{-4}	4.1×10^{-4}	5.6×10^{-6}	4.0×10^{-6}	1.0×10^{-8}
0.50 S	8.3×10^{-3}	3.1×10^{-4}	1.6×10^{-5}	9.5×10^{-7}	6.3×10^{-8}
T	5.8×10^{-1}	9.5×10^{-3}	3.3×10^{-4}	1.6×10^{-5}	9.5×10^{-7}
G	1.3×10^{-2}	8.7×10^{-5}	1.1×10^{-5}	7.7×10^{-7}	2.4×10^{-8}

decreases near the BZ boundaries; both of these have discontinuous derivatives at the BZ boundaries given by (figure 2)

$$f_2(q) = \tan^{-1}\left(\frac{2g}{3(1-g^2)}\sum_\alpha \cos(\pi q_\alpha)\right) \tag{5.2}$$

$$f_3(q) = \left(1 + \tfrac{2}{3}g\sum_\alpha \cos(\pi q_\alpha) + g^2\right) \Big/ \left(1 - \tfrac{2}{3}g\sum_\alpha \cos(\pi q_\alpha) + g^2\right) \tag{5.3}$$

where $\cos(\pi q_\alpha)$ is interpreted as $\frac{1}{2}[1 + \cos(2\pi q_\alpha)]^{1/2}$ in order for $f(q)$ to be a periodic function. Table 3 shows the relative errors of the integrated values over the SC BZ. The results show that the convergence of the special-point method with respect to N_k is much slower than the improved schemes. Although the TI method is also used frequently for k-space integration, its accuracy is not good for a small number N_k. Note that the ordinal TI method is less accurate than the correctly weighted TI method [8].

For k-space integration, almost all the theories adopt equally spaced abscissae. There is, however, no positive reason that we must use them except for simplicity, so that it is interesting to apply the Gaussian integration method with non-equally spaced abscissae, which uses an interpolation scheme based on orthogonal polynomials, to the present problem. Its incorporation into the present formalism can be done readily by multiplying the weighting factors resulting from orthogonal polynomials [9]. Using the Legendre polynomials, we have calculated the integrals for f_1, f_2 and f_3. The results given in tables 2 and 3 show that the Gaussian method is excellent. It also gives much better values than the special-point method does for such a function with a divergent point in the BZ as $f_4 = [1 - \frac{1}{3}\sum_\alpha \cos(2\pi q_\alpha)]^{-1}$ which was treated by Macot and Frank. The relative errors for the Gaussian (special-point) method are $1.24\times10^{-2}, 2.56\times10^{-3}, 5.63\times10^{-4}, 1.37\times10^{-4}$ and 3.43×10^{-5} ($1.47\times10^{-1}, 6.97\times10^{-2}, 3.45\times10^{-2}, 1.72\times10^{-2}$ and 8.60×10^{-3}) for $N_k = 4$, 20, 120, 816 and 5984, respectively. However, the Gaussian method with the Chebyshev polynomials of first kind is less effective than the special-point method.

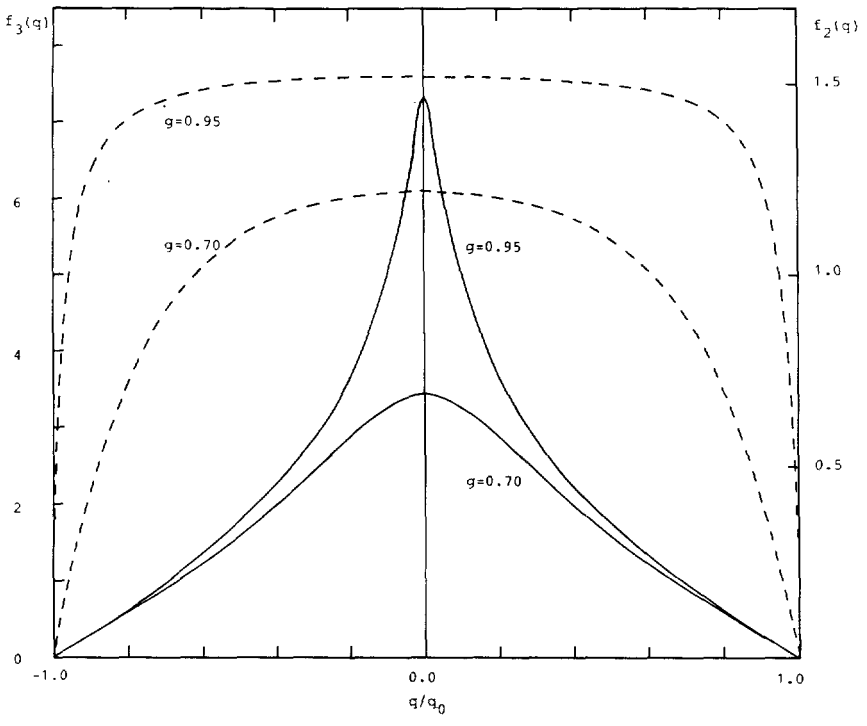

Figure 2. Variation in $f_2(q)$ (– – –) and $f_3(q)$ (——) along the [111] direction with $q_0 = \frac{1}{2}\sqrt{3}$.

Appendix 1

Special points and their weighting factors for the tetragonal lattices are considered in this appendix.

A1.1. Primitive tetragonal lattice

Let us introduce $N(= n_1^2 n_3)$ number of k-points given by (2.1) and (2.6) in the BZ where $a_\alpha = 1/2n_\alpha$, $n_1 = n_2$ and the basis vectors are defined by $b_1 = 2\pi(1/a, 0, 0)$, $b_2 = 2\pi(0, 1/a, 0)$ and $b_3 = 2\pi(0, 0, 1/c)$ with a and c as the lattice constants. From symmetry considerations we can show that all the non-equivalent points are expressed by the points in the IBZ defined by $\frac{1}{2} \geqslant q_1 \geqslant q_2 \geqslant 0$ and $\frac{1}{2} \geqslant q_3 \geqslant 0$. The weighting factor for a point q is written as

$$w_{\mathrm{PT}}(q_j) = (1/N)[2 - \delta(q_1 - q_2)] \prod_{\alpha} [2 - \delta(q_\alpha)] \tag{A1.1}$$

where $\delta(q) = 1$ and 0 for $q = 0$ and otherwise, respectively.

A1.2. Body-centred tetragonal lattice

We consider the PT BZ whose lattice constants given by $a = \frac{1}{2}a_0$ and $c = \frac{1}{2}c_0$ with a_0 and c_0 as those of the BCT lattice. In the PT BZ we introduce N, the number of k-points, similarly to the method in section A1.1 where we assume that n_1 and n_3 are even integers. The non-equivalent k are expressed in the BCT IBZ by

$$\tfrac{1}{2} \geqslant q_1 \geqslant q_2 \geqslant 0 \qquad \tfrac{1}{2} \geqslant q_1 + q_2 \qquad \tfrac{1}{2} \geqslant q_3 \geqslant 0 \qquad \tfrac{1}{4}(c^2 + a^2) \geqslant c^2 q_1 + a^2 q_3. \tag{A1.2}$$

Table 3. Relative errors (absolute values) of the integrated values over the SC BZ for $f_2(q)$ and $f_3(q)$ with $g = 0.95$ and 0.70. The notation is the same as in table 2 and the subscripts 1 and 2 attached to the S and T mean the linear and quadratic interpolation schemes, respectively.

N_k	4	10	20	35	56
			$f_2(q)$		
0.95 S_1	4.3×10^{-3}	2.2×10^{-3}	1.3×10^{-3}	9.0×10^{-4}	6.5×10^{-4}
S_2	3.3×10^{-3}	7.1×10^{-4}		2.6×10^{-4}	1.2×10^{-4}
T_2	3.5×10^{-2}	3.8×10^{-3}	9.7×10^{-4}	3.6×10^{-4}	1.6×10^{-4}
G	2.8×10^{-4}	1.5×10^{-5}	1.1×10^{-7}	2.7×10^{-7}	2.6×10^{-8}
0.70 S_1	2.0×10^{-2}	8.9×10^{-3}	5.0×10^{-3}	3.2×10^{-3}	2.2×10^{-3}
S_2	8.2×10^{-3}	2.4×10^{-4}		1.1×10^{-5}	1.2×10^{-5}
T_2	2.0×10^{-2}	5.2×10^{-4}	2.5×10^{-5}	2.7×10^{-5}	1.5×10^{-5}
G	1.5×10^{-4}	1.2×10^{-8}	$<1.0 \times 10^{-9}$	$<1.0 \times 10^{-9}$	$<1.0 \times 10^{-9}$
			$f_3(q)$		
0.95 S_1	2.1×10^{-2}	1.0×10^{-2}	5.9×10^{-3}	3.9×10^{-3}	2.7×10^{-3}
S_2	4.3×10^{-2}	7.2×10^{-3}		2.2×10^{-3}	8.2×10^{-4}
T_2	8.3×10^{-1}	1.3×10^{-2}	1.7×10^{-2}	1.6×10^{-3}	2.4×10^{-3}
G	1.7×10^{-2}	4.6×10^{-3}	1.8×10^{-3}	8.5×10^{-4}	4.5×10^{-4}
0.70 S_1	2.6×10^{-2}	1.2×10^{-2}	6.4×10^{-3}	4.1×10^{-3}	2.1×10^{-3}
S_2	5.2×10^{-2}	3.3×10^{-3}		4.8×10^{-4}	4.1×10^{-5}
T_2	2.4×10^{-1}	7.6×10^{-3}	1.4×10^{-3}	1.1×10^{-4}	5.5×10^{-5}
G	5.9×10^{-3}	5.5×10^{-4}	6.9×10^{-5}	1.2×10^{-5}	3.9×10^{-6}

In order to exclude several equivalent points appearing on the surface of the BCT BZ, we impose a further constraint on (A1.2) given by

$$\tfrac{1}{4} \geqslant q_3 \text{ for } c^2 q_1 + a^2 q_3 = \tfrac{1}{4}(a^2 + c^2) \qquad \tfrac{1}{4} \geqslant q_3 \text{ for } q_1 = q_2 = \tfrac{1}{4} \tag{A1.3}$$

A point (q_1, q_2, q_3) defined by (A1.2) and (A1.3) have at most three equivalent points in the PT IBZ given by $(\frac{1}{2} - q_2, \frac{1}{2} - q_1, q_3)$, $(\frac{1}{2} - q_1, q_2, \frac{1}{2} - q_3)$ and $(\frac{1}{2} - q_2, q_1, \frac{1}{2} - q_3)$. Note that the reciprocal-lattice vectors are expressed in terms of the basis vectors of the PT lattice. Considering cases in which some of these including the point q are identical, we get the weighting factor as

$$w_{\mathrm{BCT}}(q) = (8/N)[2 - \delta(q_1 - q_2)][2 - \delta(q_1 + q_2 - \tfrac{1}{2})]\{1 + [1 - \delta(q_1 - \tfrac{1}{4})\delta(q_3 - \tfrac{1}{4})] \times [1 - \delta(q_1 - q_2)\delta(q_1 + q_2 - \tfrac{1}{2})\delta(q_3 - \tfrac{1}{4})]\}. \tag{A1.4}$$

The non-vanishing points for R_N are given by $\boldsymbol{R} = (m_1 n_1 a, m_2 n_1 a, m_3 n_3 c)$ with m_1, m_2 and m_3 as integers. The application of the present method becomes simpler if we set $a = c$ in (A1.2) and (A1.3) although some of the special points are outside the BCT IBZ. The present method is more general and easier for obtaining the special points and their weighting factors than Lin-Chung's method which corresponds to the present method with $n_1 = n_3 = 2^m, m = 1, 2, \ldots$.

Appendix 2

In reciprocal space we take the parallelepiped zone whose three edges are given by b_1, b_2 and $\frac{1}{2}b_3$ and locate k-points defined by (2.1) in this zone where $q_\alpha = j_\alpha / n_\alpha$

with $n_1 = n_2$ and $j_\alpha = 0, 1, \ldots, n_\alpha$. If we take n_3 to be one half of n_3 given in section 4, we have the same order of the approximation as the special-point method. In the following we express k_j as (j_1, j_2, j_3). From symmetry we can show that the following points are equivalent: (j_1, j_2, j_3), $(n_1 - j_1,\ n_1 - j_2,\ j_3)$, $(n_1 - j_1 - j_2,\ j_2,\ j_3)$, $(j_1, n_1 - j_1 - j_2, j_3)$ and those with interchange of j_1 with j_2. For a point (j_1, j_2, j_3) we introduce two types of regular triangular prism whose six vertices are on the mesh points given by

$$\begin{aligned}&\text{(a)}: (j_1, j_2, j_3 + p), (j_1 + 1, j_2, j_3 + p), (j_1, j_2 + 1, j_3 + p)\\ &\text{(b)}: (j_1 + 1, j_2, j_3 + p), (j_1, j_2 + 1, j_3 + p), (j_1 + 1, j_2 + 1, j_3 + p)\end{aligned} \tag{A2.1}$$

with $p = 0, 1$. From symmetry considerations we can show that all the non-equivalent prisms of (a) and (b) are expressed by the points in the IBZ of the hexagonal lattice defined by $n_1 > j_1 + 2j_2$, $\frac{1}{2}n_1 > j_2 \geqslant j_1 \geqslant 0$ and $n_3 > j_3 \geqslant 0$. The weighting factors of the prisms (a) and (b) for a point (j_1, j_2, j_3) are given by

$$\begin{aligned}w_a(k_j) = 2[6 &- 3\delta(j_1, j_2) - 3\delta(j_1 + 2j_2, n_1 - 1) - \delta(2j_1 + j_2, n_1 - 1)\\ &+ 2\delta(j_1, j_2)\delta(3j_1, n_1 - 1)]\end{aligned} \tag{A2.2}$$

$$\begin{aligned}w_b(k_j) = 2[6 &- 3\delta(j_1, j_2) - 3\delta(j_1 + j_2, n_1 - 2) - \delta(2j_1 + j_2, n_1 - 2)\\ &+ 2\delta(j_1, j_2)\delta(3j_1, n_1 - 2)][1 - \delta(j_1 + j_2, n_1 - 1)]\end{aligned} \tag{A2.3}$$

respectively. We now number the vertices of the prisms (a) and (b) as 1, 2, 3 for $p = 0$ and 4, 5, 6 for the corresponding vertices of $p = 1$ in the order written in (A2.1) and divide these prisms into three tetrahedra with equal volume $v_t = (\sqrt{3}/18n_1^2 n_3)[(2\pi)^3/a^2 c]$ following two schemes:

(A) 1235, 1345, 3456
(B) 1236, 1246, 2456.

Superposing (A) and (B) with equal weights of $\frac{1}{8}$, we can express the integral (2.3) as

$$I = \frac{v_t}{4\Omega} \sum_j \sum_{p=a,b} w_p(k_j) \sum_{l=1}^{3} \sum_{m=1}^{4} f(k_{jplm}) \tag{A2.4}$$

where k_{jplm} denotes the wavevector of the mth vertex of the lth tetrahedron of the pth type of prism which belongs to a point k_j. Equation (A2.4) has the characteristics of the special points. Application of (A2.4) to the calculation for $f(k)$ inside the Fermi surface or on the constant-energy surface can be done readily [8].

References

[1] Chadi D J and Cohen M L 1973 *Phys. Rev.* B **8** 5747
[2] Bradley C J and Cracknell A P 1972 *The Mathematical Theory of Symmetry in Solids* (Oxford: Clarendon)
[3] Mignen J 1976 *J. Physique* **37** 925
[4] Evarestov R A and Smirnov V P 1980 *Phys. Status Solidi* b **99** 463
[5] Monkhorst H J and Pack J D 1976 *Phys. Rev.* B **13** 5188
[6] Macot L and Frank B 1990 *Phys. Rev.* B **41** 4469
[7] Lin-Chung P J 1978 *Phys. Status Solidi* b **85** 743
[8] Hama J, Watanabe M and Kato R 1990 *J. Phys.: Condens. Matter* **2** 7445
[9] Abramowitz M and Stegun I A (ed) 1968 *Handbook of Mathematical Functions* (New York: Dover)