Finite-sum approximations to cubic Brillouin-zone integrals

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Techniques are given for representing a periodic function of cubic symmetry in terms of a sum over a finite set of orthogonal functions. General results for cubic lattices are tabulated in a form convenient for use in computation. The accuracy of an approximation may be improved systematically by augmenting an approximate set of points. The special points of Chadi and Cohen occur as a case in which the periodic function is evaluated at a sublattice of points. Other sublattices may also be used. Such sets of points are found to be in the spirit of the original Baldereschi special points because certain orthogonal functions in the expansion are identically zero for all sublattice points.

I. INTRODUCTION

Baldereschi proposed[1] that integrals of a periodic function over a Brillouin zone might be accurately approximated by evaluating the function at one point, the Baldereschi point (BP). Baldereschi and Tosatti[2] applied the technique with remarkable success to the calculation of the dielectric function for semiconductors and insulators and gave a comparison between calculations employing just the BP and more accurate approximations suggested by Chadi and Cohen[3] using finite sets of "special" points, which shall be referred to as CCP. As compared with the BP the CCP have the advantage of allowing arbitrary accuracy depending on the size of the set of CCP. Both the BP and CCP represent a tremendous savings in computation time and simplification of the calculation of Brillouin-zone integrals as compared to approaches involving interpolation between finite sets of points.[4] Since Brillouin-zone integrals occur in numerous contexts it is not surprising that the special-point techniques have been applied in many instances.[5]

Monkhorst and Pack[6] observed that the CCP are in fact finite sublattice sums, a point which was not self-evident from the original derivation.[3] It would then appear that the idea of a BP and CCP have nothing essential in common.

To be more explicit let $f(\vec{k})$ be a function which is invariant to translations $[f(\vec{k}+\vec{K})=f(\vec{k})]$ by reciprocal-lattice vectors $\vec{K}$ and to rotations by elements of point group G. Then, $f(\vec{k})$ may be expanded,

$$f(\vec{k})=\sum_m c_m A_m(\vec{k}), \tag{1}$$

in terms of the orthogonal set of symmetrized functions,

$$A_m(\vec{k})=\sum_{g\in G}\exp(i\vec{K}\cdot g\vec{R}_m)/G^0, \tag{2}$$

where the sum ranges over all elements of group G of order G^0. The vectors $\vec{R}_m$ are lattice vectors such that $\exp(i\vec{K}\cdot\vec{R}_m)=1$, and each vector $\vec{R}_m$ is a representative member of the set of ${}^0S_m$ distinct vectors $S_m=\{s\vec{R}_m\}$ generated from $\vec{R}_m$ with rotations of group G. An alternative to Eq. (2) is

$$A_m(\vec{k})=\sum_{s\in S_m}\exp(i\vec{k}\cdot s\vec{R}_m)/{}^0S_m, \tag{3}$$

in which all distinct vectors $(\vec{R}_m\neq s\vec{R}_m)$ are included once in the sum. It follows that

$$\int_{BZ} A_m(\vec{k})^* A_{m'}(\vec{k})d^3k=(A_m(\vec{k}),A_{m'}(\vec{k}))$$
$$=(\Omega/{}^0S_m)\delta_{m,m'}, \tag{4}$$

and that the coefficients in Eq. (1) are given by

$$c_m=(A_m(\vec{k}),f(\vec{k}))\,{}^0S_m/\Omega, \tag{5}$$

where Ω is the volume of the Brillouin zone (BZ) in $\vec{k}$ space. The integral in Eq. (4) is over the BZ. In the case $\vec{R}_0=\vec{O}$, $A_0(\vec{k})=1$, ${}^0S_m=1$, and

$$c_0=\int_{BZ} f(\vec{k})d^3k/\Omega \tag{6}$$

is the BZ average of function $f(\vec{k})$.

The BP is that point $\vec{k}_B$ for which as many $A_m(\vec{k}_B)\,m=1,2,\ldots,$ as possible are zero. Then, $c_0\cong f(\vec{k}_B)$, if the series converges with sufficient rapidity. The CCP are chosen to satisfy the conditions

$$\sum_i A_m(\vec{k}_i)\alpha_{i0}=0,\quad m=1,2,\ldots \tag{7}$$

and

$$\sum_i \alpha_{i0}=1. \tag{8}$$

A generalization of the Chadi-Cohen conditions is to choose the "weights" in the form of a matrix

$$\hat{\alpha}=\hat{A}^{-1}, \tag{9}$$

where matrix $\hat{A}$ has components

$$\hat{A}_{mi}=A_m(\vec{k}_i). \tag{10}$$

Then,

$$\sum f(\vec{k}_i)\alpha_{im}=c_m. \tag{11}$$

Obviously, this procedure is practicable only if the functions $A_m(\vec{k})$ in $\hat{A}$ are linearly independent with respect to the set of points $\{\vec{k}_i\}$, i.e., the inverse of matrix $\hat{A}$ must exist. The weights given by Eqs. (9) and (10) using the CCP and choosing the functions $A_m(\vec{k})$ to have the lowest possible magnitudes of $\vec{R}_m$ are exactly the weights described in Ref. 3: $\alpha_{i0}=\hat{\alpha}_{i0}$. The generalization allows all coefficients to be calculated and not just c_0. However, it is not an appealing scheme as a matrix inversion is needed.

One objective of this paper is to show that the coefficients α_{im} for the CCP can be evaluated in closed form. The CCP are found to be special in the spirit of the Baldereschi point. Certain symmetrized functions $A_m(\vec{k})$ which derive from points $\vec{R}_m$ on the surface of the zone in real space which delimits inequivalent vectors $\vec{R}_m$ are found to be identically zero for all CCP.

Do only CCP sublattice sums have special character? A second objective will be to answer this question. The derivation to be presented in Sec. III treats both lattice and sublattice sums in the same way. The results, Eqs. (19) and (20), are expressed as the finite sum analog to Eq. (4).

Since the development of Sec. III is quite compact, a one-dimension example is given in Sec. II. The purpose of Sec. II is to display the essential features of the derivation and notation in a context which is relatively free of complications. The main results for cubic systems presented in Sec. III are Eqs. (18)–(20), which contain parameters and are subject to conditions specified in Tables I–IV. It is intended that the results be in a form appropriate for immediate implementation on a computer and that the reader may work through the details of the derivation or not according to his desire. In Sec. IV some comments and conclusions are given.

II. FINITE SUMS IN ONE DIMENSION

With physically motivated artifacts removed the most complex mathematical structure involved is a finite geometric series

$$\sum_{m=0}^{N-1}\exp\left(\frac{im2\pi(n-n')}{N}\right)=NM(n,n';N), \tag{12a}$$

where m, n, n' are any integers and N is a positive

TABLE I. Notation for cubic lattice and sublattice points and zonal restrictions. Lattice (reciprocal-lattice) points are specified by upper- (lower-) case symbols. Zonal restrictions will be specified in terms of the $\frac{1}{48}$th zone wedge. Other points in the zone are generated by rotations of the cubic group. A zonal restriction on a set of points is indicated by the symbol for the points with the zonal restriction in parentheses. For example, $bu(f_N)$ designates those points of the reciprocal sublattice bu contained in the face-centered reciprocal-lattice zone f_N.

(A) Lattice and sublattice points.

$u=S=[(2,0,0),\ (0,2,0),\ (0,0,2)]$

$eu_1=ES_1=(1,0,0)+u,\quad eu_2=ES_2=(0,1,0)+u,$

$eu_3=ES_3=(0,0,1)+u,\quad eu=ES=eu_1+eu_2+eu_3$

$bu_1=FS_1=(0,1,1)+u,\quad bu_2=FS_2=(1,0,1)+u$

$bu_3=FS_3=(1,1,0)+u,\quad bu=FS=bu_1+bu_2+bu_3$

$fu=BS=(1,1,1)+u,\quad s=u+eu+bu+fu$

$b=u+bu,\quad B=S+BS$

$f=u+fu,\quad F=S+FS,\quad feu=fu+eu,\quad beu=bu+eu$

(B) Zonal restriction. A point (i,j,k) is contained in the $\frac{1}{48}$th zone wedge if integers $i\geq j\geq k\geq 0$ and

simple cubic zone: $s_N=S_N,\quad 2i\leq N$

body-centered zone: $b_N=F_N,\quad i+j\leq N$

face-centered zone: $f_N=B_N,\quad 2(i+j+k)\leq 3N$ and $i\leq N$

nonzero integer. The function $M(n,n';N)=1$ if $n=n'+jN$ for integer j, and $M(n,n';N)=0$ otherwise. In Sec. III the applications to lattices and sublattices of cubic systems involve triple products of linear combinations of such sums. A notation is needed which simply and clearly specifies such finite sums and the associated restrictions on the arguments n, n' of the summand. Further, it is desirable to be able to reorganize such sums easily. The immediate objective will be to reexpress sums in the form of Eq. (12a) in a compact notation.

The basic idea for the notation is to classify various infinite sets of points and then to select from these points a finite set by allowing only those points in the set which occur in a particular interval. The notation must distinguish between points which are summed and points which are the arguments of the sum.

For the one-dimensional example let $e=E=\{\ldots,-4,\ -2,\ 0,\ +2,\ +4,\ldots\}$ be the set of all even integers and $o=O=1+E$ be the set of all odd integers. Then the set of all integers is $s=S=E+O$. The convention is adopted that lower-case symbols $h=e$, o, or s refer to points which are to be summed and upper-case symbols $H=E$, O, or S refer to points associated with the arguments of a sum. The generalization of this idea for cubic systems is summarized in Table I(A).

Restrictions on sets of points will be imposed in a symmetric way, and the symmetry will be employed to abbreviate the notation. In the one-dimensional example, let $G=(E,I)$ be a two-element group having an identity operation E and an inversion operation I. In one dimension, inversion simply changes the sign of a number. Let $s_N=S_N$ represent an interval (or zone) of numbers m such that $0\leq m\leq N/2$, and where it is understood that this set of numbers is to be extended to include the numbers associated by symmetry operations of the group. Thus, the complete zone in this one-dimensional case is $-N/2\leq m\leq N/2$. Again, upper-case symbols are associated with arguments of the summand and lowercase symbols with the numbers to be summed. A restricted set of points will be represented by symbols of the form $h(s_N)$. For example, the symbol $o(s_5)$ represents the set of all odd points restricted to the zone s_5, $o(s_5)=(-1,1)$. The generalization of this concept for cubic systems is summarized in Table I(B). The zonal restrictions delimit basic 3-tuples of integers (i,j,k), which are then augmented by all transformations of the cubic group operating on the basic 3-tuples as Cartesian vectors. Thus, the cubic group operator c_x which involves a 180° rotation about the x axis adds $(i,-j,-k)$ to the basic set of 3-tuples.

Finally, the connection with conventional solid-state-physics notation is made. For cubic systems this will be done by assigning units to the quantities which appear in the sum Eq. (12a). The points that are summed will be associated with $\vec{k}$ vectors by assigning a unit $(2\pi/aN)$. Thus, for a set of points h ($h=e$, o, or s), $\{k\}=h(2\pi/aN)$ is the corresponding set of $\vec{k}$ vectors. Similarly, the arguments of the summand will be associated with lattice vectors by assigning unit a, the lattice constant. Thus, for a set of points H, $\{R\}=Ha$ is the corresponding set of lattice vectors. Since nothing essentially new has been done, the symbols representing restricted point sets will be used without decoration to represent restricted sets of $\vec{k}$ vectors and lattice vectors. Part of the point of this development is to emphasize that these assignments are quite arbitrary. One could have associated, equally well, the summed points with real space and the summand arguments with reciprocal space.

To reexpress Eq. (12a) in the restricted point set notation, the sum must be reorganized in a symmetric way and the function $M(n,n';N)$ must be reexpressed in the new language. The sum may be reorganized by replacing integers $N/2<m<N$ by $m'=m-N$. Then with the exception of the point $m=-N/2$ (which only occurs if N is even) the points in the sum are identical to the set $s(s_N)$. To make the sum symmetric it is convenient to introduce a weight function $w(k)$ which is defined relative to a zonal restriction as $w(k)=1$ when k is an interior point of the zone and $w(k)=\frac{1}{2}$ when k is a surface (or end) point of the zone. The generalization of function $M(n,n';N)$ is $\Delta(R,R';NS)=1$ if $R=R'+R_N$ for R_N contained in the lattice NS (NS indicates lattice S multiplied by N) and is zero otherwise. A new symbol has been used here because this function Δ is an extension of function M and is not identical to M. The reason is that whereas $\Delta(R,R';NS)$ is indeed just a scaled version of $M(n,n';N)$, the function Δ also carries meaning with arguments $\Delta(R,R';NO)$ while M does not. In this notation Eq. (12a) becomes

$$\sum_{s(s_N)} w(k)\exp[ik(R-R')]=N\Delta(R,R';NS). \quad (12b)$$

The notation has been devised to do more than just express a geometric sum in conventional solid-state notation. The notation also allows one to specify and evaluate sublattice sums. In the one-dimensional example only two sublattices e and o occur.

For even N the sum over even sublattice points is

$$\sum_{e(s_N)} w(k)\exp[ik(R-R')]=\frac{N}{2}\Delta\left(R,R';\ \frac{1}{2}NS\right). \quad (13)$$

Note that the restricted set of $\vec{k}$ vectors including the symmetry-related points involved is

$$e(s_N)=\{\ldots,2m,\ldots\}2\pi/(Na)$$
$$=\{\ldots,m,\ldots\}2\pi/(aN/2),\quad -N/2\leq 2m\leq N/2.$$

Thus, $e(s_N)=s(s_{N/2})$ and Eq. (12b) is identical to Eq. (13) if N in Eq. (12b) is replaced by $N/2$. In this sense we have shown that sums over $\vec{k}$ vectors in the sublattice e for N even does not lead to a new result. Conversely, the set of points $s(s_N)=e(s_{2N})$ serves as the basis for extending a lattice sum to larger N.

For even N the sum over odd sublattice points is

$$\sum_{o(s_N)} w(k)\exp[ik(R-R')]$$
$$=\frac{N}{2}\left[\Delta(R,R';NS)-\Delta(R,R';\tfrac{1}{2}NO)\right]. \quad (14a)$$

The direct evaluation of the sum in Eq. (14) gives

$$\exp[i(2\pi/Na)(R-R')]\Delta(R,R';\tfrac{1}{2}NS)$$
$$=\Delta(R,R';NS)-\Delta(R,R';\tfrac{1}{2}NO). \quad (14b)$$

The right member of Eq. (14b) explicitly reveals that the phase factor has the value -1 when $R-R'$ is in sublattice $\frac{1}{2}NO$ and has the value $+1$ for $R-R'$ in lattice NS.

Recall that the functions $\Delta(R,R';NS)$ have the value unity for lattice vectors which are equivalent with respect to the lattice NS (NS is lattice S scaled by N). Thus, the functions Δ imply a zonal restriction for inequivalent lattice vectors. For example, function $\Delta(R,R';\frac{1}{2}NS)$ implies that inequivalent lattice vectors are restricted to the zone $S_{N/2}$. The functions $\Delta(R,R';\frac{1}{2}NO)$ involving a sublattice $\frac{1}{2}NO$ always occur in the context of explicitly evaluating a sublattice sum as in Eqs. (13) and (14). Since

$$\Delta(R,R';\tfrac{1}{2}NS)=\Delta(R,R';NS)+\Delta(R,R';\tfrac{1}{2}NO)$$

the zonal restriction on lattice vectors associated with $\Delta(R,R';\frac{1}{2}NO)$ is also $S_{N/2}$. Also, note that combining additively Eqs. (13) and (14) reproduces Eq. (12b).

Equation (14) is a new result which leads to the one-dimensional analog of CCP. The "special" nature of CCP only manifests itself in the context of sums over symmetrized functions. In one dimension the relevant symmetrized functions are $\cos(kR)$ and $\sin(kR)$. For cosine functions, Eq. (14) is applied to evaluate the cosine sum

$$\sum_{o(s_N)} w(k)\cos(kR)\cos(kR')$$
$$=(N/4)[\Delta(R,-R';NS)-\Delta(R,-R';\tfrac{1}{2}NO)$$
$$+\Delta(R,R';NS)-\Delta(R,R',\tfrac{1}{2}NO]. \quad (15)$$

The right member of Eq. (15) may be evaluated explicitly when R and R' are restricted to lattice vectors R,R' in $S(S_{N/2})=\{o\leq m\leq N/4\}a$. Note that symmetry-related (negative) points do not produce independent symmetrized functions. The key observation here is that should the point $R=R_M=(N/4)a$ exist (N must be divisible by 4), the right-hand member of Eq. (15) is identically zero. The only way that this can happen is if $\cos(kR_M)=0$ for each k in the sum. Exactly, the same situation occurs in three dimensions, and this is what is "special" about CCP.

All one-dimensional sums may be expressed in the form of finite-sum analogs to Eq. (4),

$$\sum_{h(s_N)} w(k)\cos(kR_m)\cos(kR'_m)=N_0(h(s_N))\,\frac{M(h,m)\delta_{m,m'}}{{}^0S_m}, \quad (16a)$$

where ${}^0S_m$ [see Eq. (3)] is ${}^0S_m=2$ for $R_m>0$ and ${}^0S_0=1$ for $R_0=0$. The quantity $N_0(h(s_N))$ is the number of inequivalent points in the sum

$$\sum_{h(s_N)} w(k)=N_0(h(s_N)). \quad (16b)$$

$N_0(s(s_N))=N$ and $N_0(o(s_N))=N/2$. The normalization factor $M(h,m)$ is always unity for R_m interior to the zone of inequivalent lattice vectors. $M(s,m)=2$ if a R_m is a zone-surface point $R_m=(N/2)a$. Such a surface point exists only if N is even. $M(o,m)=0$ if R_m is a zone-surface point $R_m=(N/4)a$. The odd sum has meaning only for even N, and a zone-surface point $R_m=(N/4)a$ occurs only if N is divisible by 4.

There are more parallels that may be drawn between the one-dimensional case and the cubic systems. The main complications in proceeding to cubic systems are the difficulty in visualizing the three-dimensional geometry and the increased number of possible restricted point sets.

III. FINITE CUBIC LATTICE SUMS

The objective of this section will be to outline an explicit derivation of lattice and sublattice sums over a Brillouin zone in which for each set of points in the $\vec{k}$-space sum there will correspond a specific set of lattice vectors $\{\vec{R}_m\}$. The results summarized in Tables I–IV apply to Eqs. (18)–(20) of the text.

Notation for specifying (sub)lattices of points is given in Table I(A). As in one dimension, upper-case symbols are associated with space (sub)lattices and lower-case symbols with reciprocal (sub)lattices. It may be helpful to note the mnemonics used in naming the sublattices. Of course, s, b, and f refer to simple, body centered, and face centered. The conventional usage is followed

where the lattice reciprocal to a given space lattice is given the same name as the space lattice. For example, f is a body-centered-cubic lattice of points, but it occurs as a lattice reciprocal to a face-centered space lattice. The prefix e in eu is a reminder that these are edge points. The reciprocal lattice u is a universal lattice in that it is a sublattice of all three cubic reciprocal lattices.

A finite set of (sub)lattice points is specified by allowing only those points which lie within or on the surface of a "zone." Such zonal restrictions are specified in Table I(B). Thus, $g(h_N)$ symbolizes $\vec{k}$ vectors in the form $\vec{k}=(k_1, k_2, k_3)$, where 3-tuples of integers $\vec{k}$ are points in (sub)lattice g and they are restricted to a zone h_N. Units for $\vec{k}$ vectors are $2\pi/Na$, where a is the lattice constant for the conventional cube. The $\vec{k}$-vector restrictions are just BZ restrictions. Similarly, $H(L_N)$ represents the set of lattice vectors $\vec{R}_m=(m_1, m_2, m_3)$ with 3-tuples of integers m_j in (sub)lattice H which are restricted to the zone L_N. Units for lattice vectors are $a/2$.

Note that for integer N, zone s_{2N} contains all $\vec{k}$ vectors in zones s_N, b_N, and f_N. The approach will be to perform the (sub)lattice sum $g(s_{2N})$ of $\exp(i\vec{k}\cdot\vec{R}_m)$ directly and then to reduce it to the appropriate BZ. Since it is conceptually simplest to consider all points within a particular zone of $\vec{k}$ space, a weighting scheme is devised whereby points on the surface are assigned a weight according to the fraction of the point (regarded as a finite sphere) which is contained in the volume. For the simple cubic zone an interior point $\vec{k}$ has weight $w(\vec{k})=1$; for face points $w(\vec{k})=\frac{1}{2}$; for edge points $w(\vec{k})=\frac{1}{4}$; and for vertex points $w(\vec{k})=\frac{1}{8}$. This weighting assures that equivalent surface points will be counted once only. The result is

$$\sum_{g(s_{2N})} w(\vec{k})\exp[i\vec{k}\cdot(\vec{R}-\vec{R}')] = N^3[n_0\Delta(\vec{R},\vec{R};NS)+n_1\Delta(\vec{R},\vec{R}';NES) + n_2\Delta(\vec{R},\vec{R}';NES)+n_3\Delta(\vec{R},\vec{R}';NBS)], \tag{17a}$$

where $\Delta(\vec{R},\vec{R}';NH)=1$ if $\vec{R}-\vec{R}'=N\vec{R}(H)$, where $\vec{R}(H)$ is any vector of (sub)lattice H and $\Delta(\vec{R},\vec{R}',NH)=0$ otherwise. The parameters n_j $(j=0, 1, 2, 3)$ depend on the (sub)lattice sum which has been performed and are specified in Table II.

It may be helpful for the reader to note that in Table II only the first four entries are fundamental. All remaining entries correspond to combinations of these sublattice sums. For example, to obtain the lattice sum b, one may simply combine sublattice sums u and bu. The coefficients n_j add columnwise.

TABLE II. Brillouin-zone sum parameters for Eqs. (18). The first three columns labeled $P(L)$ indicate restrictions on N for each of the space lattices. A (sub)lattice sum g which occurs nontrivially only for even N is indicated with an e, and a sum g which occurs nontrivially for both even and odd N is indicated with an o. The last column Z_N specifies zonal restrictions on lattice vectors.

$P(S)$	$P(B)$	$P(F)$	g	n_0	n_1	n_2	n_3	Z_N
e	e	e	u	1	1	1	1	S_N
e	e	e	eu	3	1	−1	−3	S_N
e	e	e	bu	3	−1	−1	3	S_N
e	e	e	fu	1	−1	1	−1	S_N
o	o	o	s	8	0	0	0	S_{2N}
e	o	e	b	4	0	0	4	B_N
e	o	e	feu	4	0	0	−4	B_N
e	e	o	f	2	0	2	0	F_N
e	e	o	beu	6	0	−2	0	F_N

From Table II and Eq. (17a) it is seen that the lattice sums simplify to

$$\sum_{h(s_{2N})} w(\vec{k})\exp[i\vec{k}\cdot(\vec{R}-\vec{R}')]=N^3n_0\Delta(\vec{R},\vec{R}';NL), \tag{17b}$$

where h $(h=u,\ s,\ b,\ f)$ is any reciprocal-lattice sum and L $(L=\frac{1}{2}S,\ S,\ B,\ F)$ is any space lattice. No such simplification is possible for sublattice sums. In the case of sublattice sums the first nonzero coefficient n_j $(j=1, 2, 3)$ implies the smallest zone Z_N in which inequivalent vectors $\vec{R}_m$ may be found. For $n_1\neq 0$, $Z_N=S_N$; for $n_2\neq 0$, $Z_n=F_N$; and for $n_3\neq 0$, $Z_N=B_N$. If $n_1=n_2=n_3=0$, then $Z_N=S_{2N}$.

All that remains in the sketch of the proof is to reduce the sums over points in s_{2N} to points within the appropriate BZ. The following observation makes this process straightforward. Conventional BZ's are formed subject to the requirement that all nonequivalent points be as close to the origin as possible.[7] Alternative restrictions on nonequivalent points are simpler to conceptualize in the cases of lattices reciprocal to the bcc and fcc space lattices. Let a "simple cube" have sides of unit length (reciprocal-lattice units are $2\pi/a$) which are parallel to the cubic axes: the [100], [010], and [001] directions. Of course, a simple cube centered about the origin is identical to the simple cubic BZ. It is easy to show directly that the BZ for the lattice reciprocal to the bcc space lattice is equivalent to two simple cubes, one centered at the origin and one centered at the point (1, 0, 0). Also, the BZ for the lattice recipro-

cal to the fcc space lattice is equivalent to four simple cubes, one centered at the origin and three centered about points (1, 0, 0), (0, 1, 0,), and (0, 0, 1).

The reduction must be done separately for each space lattice. It is done by translating simple cubes and half cubes into the appropriate BZ simple cubes. Two types of translations occur: (1) Translations by $\vec{k}$ vectors in the universal lattice u, e.g., $\vec{k}-(2,0,0)=(-2N+k_1,k_2,k_3)/N$. Such translations do not affect the sublattice. (2) Translations by a primitive lattice vector. e.g., $\vec{k}-(1,1,0)=(-N+k_1,-N+k_2,k_3)/N$. If N is odd, the sublattice may be changed. The weighting scheme assures that the interior points have weight $w(\vec{k})=1$ and that surface points are apportioned according to the fraction of the point contained inside the BZ. All that must be done is to account for each translation. The BZ in the form of simple cubes is then rearranged into the symmetric BZ. In the case where N is odd each translation may introduce a new sublattice of points. Such cases are excluded as trivial. In nontrivial cases, the reduction simply introduces a space-lattice-dependent repetition factor M_L: $M_S=8$, $M_F=2$, and $M_B=4$. Equations (12) become

$$M_L\sum_{g(h_N)} w(\vec{k})\exp[i\vec{k}\cdot(\vec{R}-\vec{R}')] = N^3[n_0\Delta(\vec{R},\vec{R}';NS)+n_1\Delta(\vec{R},\vec{R}';NES) + n_2\Delta(\vec{R},\vec{R}';NFS)+n_3\Delta(\vec{R},\vec{R}';NBS)], \tag{18a}$$

and

$$M_L\sum_{g(h_N)} w(\vec{k})\exp[i\vec{k}\cdot(\vec{R}-\vec{R}')]=N^3 n_0\Delta(\vec{R},\vec{R}';NL). \tag{18b}$$

The relevant parameters are given in Table II. All sub(lattices) considered are invariant to cubic rotations.

The preceding discussion applies to cubic (sub)-lattice sums in general. Now, the scope is limited to applications for expansions of functions $f(\vec{k})$ which are invariant to cubic group rotations and to translations by reciprocal-lattice vectors as in Eq. (1). The result has the form

$$\sum_{g(h_N)} w(\vec{k})A_m(\vec{k})A_{m'}(\vec{k})=N_0(g(h_N))\frac{M(g,m)\delta_{m,m'}}{{}^0S_m} \tag{19a}$$

for all (sub) lattice sums g characterized in Table II, where the symmetrized functions defined by Eqs. (2) and (3) are constructed from translationally and rotationally inequivalent vectors $\vec{R}_m$ contained in zonal section Z_N. The quantity $N_0(g(h_N))$ is the number of inequivalent points in the (sub)lattice sum

$$\sum_{g(h_N)} w(\vec{k})=N_0(g(h_N))=\frac{n_0N^3}{M_L}. \tag{19b}$$

Before proceeding to discuss the normalization factor $M(g,m)$ and the use of symmetry in the sums, it is well to be sure that the meaning of Eq. (19a) is clear. Assume that N is given. The reciprocal lattice $h=\{\vec{k}\}$ is implied by the translational invariance of $f(\vec{k})$. In turn this implies that the relevant lattice vectors are $H=\{\vec{R}_m\}$ and the appropriate reduction factor is $M_L=M_H$. The sum over points $\vec{k}$ of (sub)lattice g [Table I(A)] is restricted to zonal section h_N [Table I(B)], but is otherwise independent of h. Any (sub)lattice sum may be used, provided N is even or it is nontrivial in the case of odd N. The inequivalent vectors of H are determined by the sum (Table II). The normalization factor $M(g,m)$ (Tables II–IV) for vector $\vec{R}_m$ depends on $\vec{R}_m$ and the sum.

The use of symmetry to reduce the sum and the evaluation of normalization factors involves similar considerations. Since the functions $A_m(\vec{k})$ are invariant to cubic group rotations all $\vec{k}$ vectors which are related by rotations may be combined into one term,

$$\sum_{g(rh_N)}{}' {}^0s(\vec{k})A_m(\vec{k})A_m(\vec{k})=N_0(g(h_N))\frac{M(g,m)\delta_{m,m'}}{{}^0S_m}, \tag{19c}$$

where rh_N is the symmetry-reduced zonal section or irreducible wedge (RBZ). If ${}^0d(\vec{k})$ is the number of $\vec{k}$ vectors in the set $d(\vec{k})$ of distinct vectors generated by cubic group rotations, then

$${}^0s(\vec{k})=w(\vec{k})\,{}^0d(\vec{k}). \tag{20}$$

The set of vectors $d(\vec{k})$ may include vectors $\vec{k}'=\vec{k}+\vec{K}$ which, therefore, are translationally equivalent to $\vec{k}$. Let $s(\vec{k})$ denote the set of vectors which are rotationally distinct from $\vec{k}$ and translationally inequivalent. For most $\vec{k}$ vectors in cubic systems the number of members of $s(\vec{k})$ is ${}^0s(k)$, as given by Eq. (20). For interior points $w(\vec{k})=1$ and ${}^0s(\vec{k})=d(\vec{k})$. For most face points the effect of points in $d(\vec{k})$ which are equivalent to $\vec{k}$ is to reunite the face points into whole points. The proof is by inspection. In cubic systems the only points in the RBZ for which Eq. (20) fails occur in the case of the symmetric RBZ for the lattice reciprocal to the fcc space lattice and which fall on the hexagonal face $2\vec{k}\cdot(1,1,1)=3$. For these points translation of a $\vec{k}$ vector rotated by a dihedral operation produces a relation between face points, and not an equivalence. These symmetry-related points lie on either side of the line between

TABLE III. Weights and normalization factors for (sub)lattice sums over the Brillouin zone in Eqs. (19). Eight different types of points are distinguished by cubic rotational symmetry. They are listed with their multiplicities ${}^0d(k)$ shown in parentheses: $(0,0,0),(1)$; $(x,0,0),(6)$; $(x,x,x),(8)$; $(x,x,0),(12)$; $(x,y,y),(x,x,z),(x,y,0),(24)$; $(x,y,z),(48)$, where $x>y>z>0$. Weights $w(\vec{k})$ and normalization factors $M(g,m)$ are given for each of the cubic zones defined in Table I. Points are specified by 3-tuples (i,j,k) where $i\geq j\geq k\geq 0$. A restriction to the hexagonal face $2(i+j+k)=3N$ is denoted HF. Any further restrictions are given explicitly. (Sub)lattic-dependent parameters of the normalization factor $M(g,m)$ are defined in Table II.

		$w(k)$	$M(g,m)$
(A)	*SC* Zone, S_N.		
(4)	$(N,N,N)/2$	$\frac{1}{8}$	$(n_0+3n_1+3n_2+n_3)/n_0$
(3)	$(N,N,2k)/2$, $N>2k\geq 0$	$\frac{1}{4}$	$(n_0+2n_1+n_2)/n_0$
(2)	$(N,2j,2k)/2$, $N>2j\geq 2k>0$	$\frac{1}{2}$	$(n_0+n_1)/n_0$
(1)	interior point	1	1
(B)	bcc zone, $b_N=F_N$.		
(5)	$(N,0,0)$	$\frac{1}{6}$	$(2n_0+4n_2)/n_0$
(4)	$(N,N,N)/2$	$\frac{1}{4}$	$(n_0+3n_2)/n_0$
(3)	$(i,N-i,N-i)$, $N>i>N/2$	$\frac{1}{3}$	$(n_0+2n_2)/n_0$
(2)	$(i,N-i,k)/2$, $N>i>N/2$; $N-i>k$	$\frac{1}{2}$	$(n_0+n_2)/n_0$
(1)	interior point	1	1
(C)	fcc zone, $f_N=B_N$.		
(5)	$(N,N/2,0)$	$\frac{1}{4}$	$(2n_0+2n_3)/n_0$
(4)	(N,j,k), $N/2>j\geq k\geq 0$	$\frac{1}{2}$	2
(3)	$(i,N/2,N-i)$, $N>i\geq N/2$	$\frac{1}{2}$	$(n_0+n_3)/n_0$
(2a)	(i,j,k), $N>i>N/2>j>N/4$; HF	1	1
(2b)	(i,j,k), $N>i>N/2;3N/4>j>N/2$; HF	0	0
(1)	interior point	1	1

points $W\,[\vec{k}=(1,\frac{1}{2},0)]$ and $L\,[\vec{k}=(\frac{1}{2},\frac{1}{2},\frac{1}{2})]$. Since such points are face points with $w(\vec{k})=\frac{1}{2}$, a way to handle the situation is to exclude one set of these points; (for example, those with $k_y>\frac{1}{2}$). Then, Eq. (19c) applies equally to all cubic systems, with the prime on the sum serving as a reminder to exclude the hexagonal face points described above in the case of the fcc space lattice. In practice it is simplest to determine ${}^0d(k)$ and then to use Eq. (20) to compute ${}^0s(\vec{k})$. The weights for face points in cubic systems are given in Table III.

To complete the discussion of Eq. (19) the normalization factor $M(g,m)$ remains to be derived. First, symmetry is used in Eq. (19a) to replace $A_m(\vec{k})$ by one plane wave,

$$\sum_{g(h_N)} w(\vec{k})A_m(\vec{k})A_{m'}(\vec{k}) = \sum_{g(h_N)} w(\vec{k})\exp(i\vec{k}\cdot\vec{R}_m)A_{m'}(\vec{k}) \qquad (21)$$
$$= \sum_s \sum_{g(h_N)} \frac{w(\vec{k})\exp[i\vec{k}\cdot(s\vec{R}_{m'}-\vec{R}_m)]}{{}^0S_m},$$

and the second equation follows using the definition of $A_{m'}$ in the form of Eq. (3). Then, Eqs. (18) are used to evaluate the sum. The face points on the zonal section must be treated separately. The results expressed as normalization factors are given for general (sub)lattice sums in Table III and are evaluated for the sums considered here in Table IV. The parameters have been checked by verifying Eq. (19c) by direct calculation on a computer.

IV. DISCUSSION

Several points merit further comment. In the case of the sublattice sum fu all $A_m(\vec{k})=0$ which are constructed with respect to surface points $\vec{R}_m$. These are Chadi-Cohen points and this is why they are special. Of the possible choices of sublattice sums, they are to be preferred because calculations using other symmetric sublattice points often involve more points in the sublattice sum than the number of independent coefficients c_m of Eq. (1) that they can approximate.

TABLE IV. Evaluation of normalization factors $M(g)$ for surface points. The various types of surface points are in listed Table III. Only the index will be given here.

(A) sc zone, $S_N(S_{2N})$.	$M(u)$	$M(eu)$	$M(bu)$	$M(fu)$	$[M(s)]$
(4)	8	0	0	0	8
(3)	4	$\frac{4}{3}$	0	0	4
(2)	2	$\frac{4}{3}$	$\frac{2}{3}$	0	2
(1)	1	1	1	1	1
(B) bcc zone, $b_N = F_N$.	$M(f)$	$M(beu)$			
(5)	6	$\frac{2}{3}$			
(4)	4	0			
(3)	3	$\frac{1}{3}$			
(2)	2	$\frac{2}{3}$			
(1)	1	1			
(C) fcc zone, $f_N = B_N$.	$M(b)$	$M(feu)$			
(5)	4	0			
(4)	2	2			
(3)	2	0			
(2a)	1	1			
(1)	1	1			

Any of the (sub)lattice sums above may be used to approximate specific Brillouin-zone integrals such as Eqs. (5) and (6). In general the number of independent coefficients c_m obtained is equal to or less than the number of rotationally and translationally inequivalent points used in approximating the coefficient. The finite-sum analog to Eq. (5),

$$M(g,m)c_m = {}^0S_m \sum_{g(rh_N)} \frac{{}^0s(\vec{k})A_m(\vec{k})f(\vec{k})}{N_0(g(h_N))} , \qquad (22)$$

is obtained using Eq. (19c) and Eq. (1). As an example of the use of the tables, consider the case where $f(\vec{k})$ is invariant to lattice vectors reciprocal to the fcc space lattice. Let $g = fu$, the CCP. Hence, from Table I(A), the $\vec{k}$ vectors will be of the form $\vec{k} = (1,1,1) + (2m, 2n, 2p)$ in units of $2\pi/(Na)$, where m, n, p are integers. Further, in Table I(B) they must be in the face-centered reduced zone f_N conditioned by

$$2m + 1 \geq 2n + 1 \geq 2p + 1 > 0 ,$$

$$2m + 1 \leq N, \quad 2(3 + 2m + 2n + 2p) \leq 3N .$$

The space-lattice repetition factor is $M_F = 2$.

From Table II, line 4, it is seen that N must be even and that the inequivalent lattice vectors are face-centered lattice vectors, restricted to a reduced zone S_N. The total number of points, Eq. (19b), is $N_0(fu(f_N)) = N^3/2$.

The weight factors ${}^0s(\vec{k})$ are determined from Eq. (20) and Table III(C). ${}^0S_m$ is the number of distinct lattice vectors generated by cubic rotations. The normalization factors $M(fu, m)$ are

TABLE V. Comparison of the number of points for simple cubic lattice sums $N(s(rf_N))$ to Chadi-Cohen sublattice sums $N(fu(rf_{2N}))$ of the same accuracy in estimating BZ integrals. The example refers to an fcc space lattice. N restricts the zonal section. N_0 is the total number of points in the Brillouin zone.

N	N_0	$N(s(rf_N))$	$N(fu(rf_{2N}))$
3	108	10	6
4	256	19	10
5	500	28	19
6	864	44	28
7	1372	60	44
8	2048	85	60
12	6912	231	182
16	16384	489	408

listed in Table IV(A), column 4. The fact that $M(fu, m)=0$ for lattice vectors $\vec{R}_M$ on the surface of zone S_N simply means that these coefficients c_m are not determined, since $A_m(\vec{k})=0$ for all points $\vec{k}$ of the type fu. The ratios $\alpha_{i0}={}^0s(\vec{k}_i)/N_0(fu(f_N))$ are exactly the weights described by Chadi and Cohen, Eqs. (7) and (8).

The sum with $g=s$ and with N replaced by $N/2$ would evaluate these same "internal" coefficients and the coefficients corresponding to the surface lattice vectors at the same level of accuracy. The application of CCP to the interpolation of functions throughout the Brillouin zone has attractive possibilities.

It is not difficult to derive formulas which "count" the number of inequivalent points in a $\frac{1}{48}$ zonal section. To illustrate the "surface" effect in CCP, a comparison is made in Table V between the number of CCP and the number of simple cubic lattice points which may be used to evaluate BZ integrals to the same accuracy. The comparison is made for the fcc space lattice.

However, it would be premature to conclude categorically that the CCP are the only sublattice sums that merit consideration. Other sublattices may prove valuable in expansions or in the evaluation of specific integrals involving symmetries other than the identity representation. Equations (18) provide the basis for an investigation of such expansions.

The derivation given here is specific to the cubic systems. In this respect it lacks the elegance of an approach which treats any space lattice on equal footing. A more general approach would have been to form $\vec{k}$-vector (sub)lattices with respect to the primitive $\vec{k}$ vectors, $\vec{b}_1, \vec{b}_2, \vec{b}_3$. For example, an odd set of $\vec{k}$ vectors would be $o_i=\{\ldots, -3, -1, 1, 3, \ldots\}\vec{b}_i/N$. The corresponding treatment for lattice vectors relates lattices and sublattices to the primitive lattice vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$ ($\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$). For cubic systems one obtains the same results as described above, but at the cost of considerable complication.

It would be of interest to see the effect of using CCP in applications to interpolation such as have been reported recently by Boyer.[8] Boyer's approach to evaluating an approximation is a very good one and can be used any time that Fourier-series techniques are applicable. It is to be preferred to the time-honored practice of pronouncing an approximation to a particular Fourier coefficient adequate if it appears to stabilize as the level of a approximation is increased.

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