Special points for Brillouin-zone integrations*

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A method is given for generating sets of special points in the Brillouin zone which provides an efficient means of integrating periodic functions of the wave vector. The integration can be over the entire Brillouin zone or over specified portions thereof. This method also has applications in spectral and density-of-state calculations. The relationships to the Chadi-Cohen and Gilat-Raubenheimer methods are indicated.

I. INTRODUCTION

Many calculations in crystals involve integrating periodic functions of a Bloch wave vector over either the entire Brillouin zone (BZ) or over specified portions. The latter case arises, for example, in averages over states within the Fermi surface, and the calculation of the dielectric constant and generalized susceptibilities. To optimize the calculations it is helpful only to compute these functions at a carefully selected set of points in the BZ. This becomes more urgent in sophisticated calculations where the computational effort for each BZ point is substantial.

Methods for finding such sets of "special" points have been discussed by Chadi and Cohen[1] (hereafter referred to as CC). This paper presents an alternate approach which yields sets of points identical to those given by CC and additional sets with the same properties. It will be shown that the use of such points simply generates an expansion of the periodic function in reciprocal-space functions with the proper symmetries. This suggests an obvious, and rather accurate, interpolation of the function between the special points which is intrinsically more satisfactory than linear or quadratic methods. The relation to Gilat-Raubenheimer methods will be pointed out.

II. DERIVATION

In this section we will prove the existence of a set of periodic functions which are orthonormal on a uniformly spaced set of special points in the BZ.

Consider a lattice defined by the primitive translation vectors $\vec{t}_1, \vec{t}_2, \vec{t}_3$. A general lattice point is given by

$$\vec{R} = R_1\vec{t}_1 + R_2\vec{t}_2 + R_3\vec{t}_3 , \tag{1}$$

where R_1–R_3 are integers.

The associated primitive reciprocal-lattice vectors are given by

$$\vec{b}_1 = \frac{2\pi}{v}\,\vec{t}_2\times\vec{t}_3 , \quad \vec{b}_2 = \frac{2\pi}{v}\,\vec{t}_3\times\vec{t}_1 , \quad \vec{b}_3 = \frac{2\pi}{v}\,\vec{t}_1\times\vec{t}_2 . \tag{2}$$

v is the unit cell volume, and $\vec{b}_1$–$\vec{b}_3$ span the reciprocal lattice with BZ volume $8\pi^3/v$.

Let us define the sequence of numbers

$$u_r = (2r - q - 1)/2q \quad (r = 1, 2, 3, \ldots, q), \tag{3}$$

where q is an integer that determines the number of special points in the set. With the above u_r's we now define

$$\vec{k}_{prs} = u_p\vec{b}_1 + u_r\vec{b}_2 + u_s\vec{b}_3 . \tag{4}$$

This gives q^3 distinct points uniformly spaced in the BZ. Let $A_m(\vec{k})$ be given by

$$A_m(\vec{k}) = N_m^{-1/2} \sum_{|\vec{R}| = C_m} e^{i\vec{k}\cdot\vec{R}} , \tag{5}$$

where the sum is taken over all $\vec{R}$ vectors related by the operations of the lattice point group. This set of vectors is usually called a star. The C_m are in ascending order, starting with $C_1 = 0$. N_m is the number of members in the mth star of $\vec{R}$ [or the number of terms in the sum in Eq. (5)]. Note that $A_m(\vec{k})$ is totally symmetric under all point-group operations.

Let us now consider the quantity $S_{mn}(q)$ given by

$$S_{mn}(q) = \frac{1}{q^3} \sum_{p,r,s=1}^{q} A_m^*(\vec{k}_{prs}) A_n(\vec{k}_{prs}) . \tag{6}$$

Substituting Eq. (5) for A_m and A_n we can reduce $S_{mn}(q)$ to

$$S_{mn}(q) = (N_m N_n)^{-1/2} \sum_{a=1}^{N_m} \sum_{b=1}^{N_n} \prod_{j=1}^{3} W_j^{ab}(q) , \tag{7}$$

where

$$W_j^{ab}(q) = \frac{1}{q} \sum_{r=1}^{q} e^{(\pi i/q)(2r-q-1)(R_j^b - R_j^a)} . \tag{8}$$

In Eq. (7) the a and b sums are over the members in the stars m and n, respectively. It can now easily be seen that the W_j^{ab} can assume the follow-

ing values:

$$W_j^{ab}(q)=\begin{cases}1 & \text{if } |R_j^b-R_j^a|=0,2q,4q,\ldots\\ (-1)^{q+1} & \text{if } |R_j^b-R_j^a|=q,3q,5q,\ldots\\ 0 & \text{otherwise.}\end{cases} \quad (9)$$

It should be remembered that q, R_j^b, and R_j^a are integers. If we now impose the restriction

$$|R_j^a|<q/2\,,\quad |R_j^b|<q/2\quad (j=1,2,3)\,, \quad (10)$$

then it follows that

$$W_j^{ab}(q)=\delta(R_j^a,R_j^b)\,. \quad (11)$$

From Eq. (7) it can now be seen that

$$S_{mn}(q)=\delta_{mn}\,. \quad (12)$$

In other words, all those functions $A_m(k)$ for which Eq. (10) is satisfied are orthonormal on the discrete set of BZ points $\vec{k}_{prs}$.

The lattice point-group symmetry can significantly reduce the number of distinct terms in the sums of Eq. (6). We can thus write

$$S_{mn}(q)=\frac{1}{q^3}\sum_{j=1}^{P(q)} w_j A_m(\vec{k}_j)A_n(\vec{k}_j)\,, \quad (13)$$

where $P(q)$ is the symmetry-dependent number of points $\vec{k}_j$ from the set of points $\{\vec{k}_{prs}\}$ in the irreducible wedge of the BZ. Equation (13) amounts to grouping together those terms in Eq. (6) that are identical because of point-group symmetry. Here w_j is the weight associated with $\vec{k}_j$ and is simply the ratio of the order of the entire point group to the order of the group of the wave vector at $\vec{k}_j$. For example, if $\vec{k}_j$ is a general point in the (1, 1, 1) direction of the simple-cubic lattice, then $w_j=\frac{48}{6}=8$. A description of the groups of $\vec{k}$ for various lattices is given by Koster.[2]

III. INTEGRATION, INTERPOLATIONS, AND ACCURACIES

Suppose we wish to integrate a function $f(\vec{k})$ that is totally symmetric and periodic in $\vec{k}$ space. $f(\vec{k})$ can be formally expanded in $A_m(\vec{k})$,

$$f(\vec{k})=\sum_{m=1}^{\infty} f_m A_m(\vec{k})\,, \quad (14)$$

where, because of the orthogonality of $A_m(\vec{k})$ on the BZ,

$$f_m=\frac{v}{8\pi^3}\int_{BZ} d\vec{k}\, A_m^*(\vec{k})f(\vec{k})\,. \quad (15)$$

Therefore the integral of $f(\vec{k})$ over the entire BZ leads to

$$\int_{BZ} d\vec{k}\, f(\vec{k})=\frac{8\pi^3}{v}f_1\,. \quad (16)$$

We could obtain approximations to f_m by the following sum over the set of $\vec{k}_j$ points:

$$\tilde{f}_m=\frac{1}{q^3}\sum_{j=1}^{P(q)} w_j f(\vec{k}_j)A_m(\vec{k}_j) \quad (17)$$

for all functions $A_m(\vec{k})$ corresponding to stars that satisfy Eq. (10). We thus obtain an approximate representation $\tilde{f}(\vec{k})$ for $f(\vec{k})$,

$$\tilde{f}(\vec{k})=\sum_m \tilde{f}_m A_m(\vec{k})\,, \quad (18)$$

where the sum is over functions that satisfy Eq. (10).

The BZ integrations like Eq. (16), using Eq. (17), will now be in error by the amount ϵ_{BZ} given by

$$\epsilon_{BZ}\equiv\int_{BZ} d\vec{k}\,[f(\vec{k})-\tilde{f}(\vec{k})]=\sum_{m>1} f_m N_m^{1/2} S_{m1}(q)\,, \quad (19)$$

where

$$S_{m1}(q)=\begin{cases}(-1)^{(q+1)(R_1+R_2+R_3)/q} & \text{if } R_1-R_3 \text{ are multiples of } q\\ 0 & \text{otherwise.}\end{cases} \quad (20)$$

Consider now the case where we integrate over a portion of the BZ, such as the volume enclosed by the Fermi surface (FS). Then the integral can be represented by

$$\int_{<FS} d\vec{k}\, f(\vec{k})\approx\sum_m \tilde{f}_m I_m\,, \quad (21)$$

where the summation is over functions corresponding to stars which satisfy Eq. (10) and

$$I_m=\int_{<FS} d\vec{k}\, A_m(\vec{k})\,. \quad (22)$$

Here the error is given by

$$\epsilon_{FS}\equiv\int_{<FS} d\vec{k}\,[f(\vec{k})-\tilde{f}(\vec{k})]$$

$$=\sum_m (f_m-\tilde{f}_m)I_m+\sum_{m'} f_{m'}I_{m'}\,, \quad (23)$$

where the prime indicates stars which do *not* satisfy Eq. (10). The quantities I_m are typically of the order 1 and vary in sign. We found this way of integrating over the volume within the FS very efficient and accurate once the $f(\vec{k})$ was computed over the $\vec{k}_j$ throughout the irreducible wedge of the BZ.[3]

A satisfactory analysis of the errors incurred in the above two cases is hard to give. This obviously depends critically on the function $f(\vec{k})$. In CC it is argued that ϵ_{BZ} decreases proportional to C_m^{-3}. This is based on the observation that for a smoothly varying $f(\vec{k})$ a Taylor expansion

around $\vec{k}=0$ converges well. However, in actual calculations on some simple crystals the convergence for both ϵ_{BZ} and ϵ_{FS} is much more favorable.[3] This is most likely due to the periodic behavior of $f(\vec{k})$, which causes the Taylor expansion to be slowly convergent for $\vec{k}$ close to the BZ boundaries. Although $f(\vec{k})$ will be largely parabolic near $\vec{k}=0$, $f(\vec{k})$ must level off towards the BZ boundaries. Most of the contribution to the BZ integral comes near the BZ boundary. Hence CC's analysis becomes rather irrelevant for realistic $f(\vec{k})$ functions. In fact, it might be more appropriate to point to the relationship between the f_m values and the tight-binding interpretation of the Fourier expansion of Eq. (14). It is then clear that f_m should converge more like overlap and/or energy integrals over atomic-orbital basis functions. Typically one would expect then to find

$$f_m \propto C_m^P e^{-\alpha C_m}, \quad C_m \to \infty \tag{24}$$

the power P and exponent α being dependent on $f(\vec{k})$. It is clear that the behavior can lead to a decrease in ϵ faster than C_m^{-3}. In practice one simply monitors the convergence of both the actual value of f_m as q increases, and the rapidity with which their magnitudes fall off for increasing m values.

In some lattices it is preferable to restrict q to even integers. This is especially true in the case of the cubic lattices. Take, for example, the simple-cubic lattice. The smallest star for which $S_{mn}(q)\neq\delta_{mn}$ is the one corresponding to $\vec{R}=(q,0,0)$. Now $\tilde{f}(\vec{k})$ is an approximation to $f(\vec{k})$ consisting of a linear combination of orthogonal functions. If $q=2$, $\tilde{f}(\vec{k})$ is a linear combination of four orthogonal functions, whereas if $q=1$, $\tilde{f}(\vec{k})$ consists of a single term. Since the fit using four functions is presumably better than a fit to a single term, and in both cases only one k point is used, $q=2$ is preferable to $q=1$. Similarly, for cubic lattices, $q=2l$ is preferable to $q=2l-1$ since

$$P(2l-1)=P(2l)=l(l+1)(l+2)/6\,. \tag{25}$$

Incidently, the point given by $q=2$ is the mean-value point described by Baldereschi.[4]

In the general derivation the same value of q was used in all three dimensions; however, for less-symmetric Bravais lattices this is not necessary. In fact it might be advantageous to change q in one direction to reduce the number of $\vec{k}$ points without loss of overall accuracy.

The nonprimitive fcc and bcc lattices are discussed in the Appendix. In particular, it is pointed out how the "special points" of CC form a subset of those obtained by us. Also the equivalence of our points and those used in the Gilat-Raubenheimer scheme is discussed.

IV. APPLICATION TO SPECTRAL CALCULATIONS

Many solid-state calculations involve computing certain spectral properties of solids. This usually involves the evaluation of integrals similar to

$$I(\omega)=\int_{BZ} d\vec{k}\, F(\vec{k})\delta(\omega-\omega(\vec{k}))\,. \tag{26}$$

Also of interest is the special case when $F(\vec{k})=1$, where $I(\omega)$ becomes a density-of-states calculation.

Several methods have been devised to perform such integrations.[5] In cases where the calculation of $F(\vec{k})$ and $\omega(\vec{k})$ is very expensive it is advantageous to calculate $F(\vec{k})$ and $\omega(\vec{k})$ on a fine mesh of points, denoted by $\{\vec{k}_i\}$, based on their values on a coarse grid, denoted by $\{\vec{k}_j\}$. The "linear analytic" method of Gilat and Raubenheimer[5] is then applied to each minicell about each of the fine-mesh points. If these functions are reasonably smooth then it seems quite natural to generate their values on the fine mesh by the method described in this paper.

$$F(\vec{k}_i)=\sum_m F_m A_m(\vec{k}_i)\,, \tag{27}$$

$$\omega(\vec{k}_i)=\sum_m \omega_m A_m(\vec{k}_i)\,, \tag{28}$$

where F_m and ω_m are calculated from the coarse grid:

$$F_m=\frac{1}{q^3}\sum_{j=1}^{P(q)} w_j F(\vec{k}_j)A_m(\vec{k}_j)\,, \tag{29}$$

$$\omega_m=\frac{1}{q^3}\sum_{j=1}^{P(q)} w_j \omega(\vec{k}_j)A_m(\vec{k}_j)\,. \tag{30}$$

Unlike the local interpolation and integration methods reviewed by Gilat,[5] the above procedure is based on a global BZ fit, but nevertheless it belongs to the class of "hybrid methods" which Gilat shows to be highly successful.

APPENDIX: SPECIAL CONSIDERATION FOR CUBIC LATTICES

A. Face-centered cubic (fcc)

Consider two cubic lattices: first, a simple-cubic lattice with spacing parameter $a=a_0$, and second, an fcc lattice with $a=2a_0$. For a given q, which will be even for reasons discussed previously, there are q^3 uniformly spaced points $\{\vec{k}_i\}$ in the sc BZ, placed on a cubic grid. The BZ for the fcc lattice has just half the volume of the sc BZ and careful counting reveals there are exactly half as many points associated with the fcc BZ. In fact, for each fcc $\vec{k}$ point there is another outside the fcc BZ (but within the sc BZ) related by an

fcc reciprocal-lattice vector. For the sc lattice

$$\frac{1}{q^3}\sum_{i=1}^{q^3} A_m^*(\vec{k}_i)A_n(\vec{k}_i)=\delta_{mn}\,, \tag{A1}$$

where both m and n correspond to stars of $\vec{R}$ which satisfy Eq. (10). Now let us further restrict m and n to correspond to stars the sum of whose components is even (i.e., 000, 110, 200, 211, 220, 310, 222, ...), which are the stars of fcc lattice vectors.

Regrouping Eq. (A1) we find

$$\frac{1}{q^3}\sum_{j=1}^{q^3/2}[A_m^*(\vec{k}_j)A_n(\vec{k}_j)+A_m^*(\vec{k}_j+\vec{G}_j)A_n(\vec{k}_j+\vec{G}_j)]=\delta_{mn}\,, \tag{A2}$$

where the j sum is over points associated with the fcc BZ, and $(\vec{k}_j+\vec{G}_j)$ are the corresponding points related by the fcc reciprocal-lattice vector $\vec{G}_j$. Since $A_m(\vec{k}_j+\vec{G}_j)=A_m(\vec{k}_j)$, we find

$$\frac{2}{q^3}\sum_{j=1}^{q^3/2} A_m^*(\vec{k}_j)A_n(\vec{k}_j)=\delta_{mn}\,. \tag{A3}$$

The 48-fold symmetry of the O_h point group allows us to consider only points in the irreducible wedge given by

$$0\le k_z\le k_y\le k_x\le 2\pi/a\,, \tag{A4}$$

$$k_x+k_y+k_z\le 3\pi/a\,. \tag{A5}$$

Equation (A3) reduces to

$$\frac{2}{q^3}\sum_{j=1}^{P(q)} w_j A_m^*(\vec{k}_j)A_n(\vec{k}_j)=\delta_{mn}\,, \tag{A6}$$

where

$$P(q)=\begin{cases}(q/96)(q+2)(q+4) & \text{if } q/2 \text{ is even} \quad (A7)\\ \frac{1}{96}(q+2)(q^2+4q+12) & \text{if } q/2 \text{ is odd.} \quad (A8)\end{cases}$$

B. Body-centered cubic (bcc)

Let us again compare with an sc structure. Consider the sc lattice with $a=a_0$ and a bcc lattice with $a=2a_0$. The BZ for the bcc lattice has $\frac{1}{4}$ the volume of the sc BZ and by carefully counting we find $\frac{1}{4}$ as many points associated with the bcc BZ as with the sc BZ. For each bcc $\vec{k}$ point there are three others outside the bcc BZ (but within the sc BZ) related by a bcc reciprocal-lattice vector. Again for the sc lattice Eq. (A1) holds when both m and n correspond to stars of $\vec{R}$ which satisfy Eq. (10). Now we further restrict the components of the m and n stars to be either all even or all odd (000, 111, 200, 220, 311, ...), i.e., the stars of bcc lattice vectors.

Regrouping the terms of Eq. (A1) we see that

$$\frac{1}{q^3}\sum_{j=1}^{q^3/4}\left(A_m^*(\vec{k}_j)A_n(\vec{k}_j)+\sum_{l=1}^{3}A_m^*(\vec{k}_j+\vec{G}_j^l)A_n(\vec{k}_j+\vec{G}_j^l)\right)=\delta_{mn}\,, \tag{A9}$$

where $\vec{k}_j$ are grid points associated with the bcc BZ and $(\vec{k}_j+\vec{G}_j^l)$ are the three points related to $\vec{k}_j$ by bcc reciprocal-lattice vectors. Analogous to Eq. (A3) we find

$$\frac{4}{q^3}\sum_{j=1}^{q^3/4} A_m^*(\vec{k}_j)A_n(\vec{k}_j)=\delta_{mn}\,. \tag{A10}$$

Owing to O_h symmetry we need consider only those points associated with the irreducible wedge:

$$0\le k_z\le k_y\le k_x\le 2\pi/a\,, \tag{A11}$$

$$k_x+k_y\le 2\pi/a\,. \tag{A12}$$

Equation (A9) reduces to

$$\frac{4}{q^3}\sum_{j=1}^{P(q)} w_j A_m^*(\vec{k}_j)A_n(\vec{k}_j)=\delta_{mn}\,, \tag{A13}$$

where

$$P(q)=\begin{cases}(q/192)(q+4)(q+8) & \text{if } q/2 \text{ is even} \quad (A14)\\ \frac{1}{192}(q+2)(q+4)(q+6) & \text{if } q/2 \text{ is odd.} \quad (A15)\end{cases}$$

As mentioned earlier the $\vec{k}_j$ points generated here and those given by CC are identical except that for cubic structures the latter yields only those sets of points corresponding to $q=2^n$ ($n=1,2,3,4,\ldots$).

It is obvious from Eqs. (25), (A7), (A8), (A14), and (A15) that $P(q)$ increases rapidly as q increases. Of course the accuracy increases with q, but for some applications the computation of a function at many points may be very costly. If the convergence is not quite adequate for $q=2^n$ and the computation for $q=2^{n+1}$ is prohibitive, hopefully the intermediate values of q may be useful.

For cubic lattices the reader will note the equivalence of the sets of cubic grid points given here and those given by Janak for constructing the offset Gilat-Raubenheimer mesh.[6]

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[1]D. J. Chadi and M. L. Cohen, Phys. Rev. B 8, 5747 (1973).

[2]G. F. Koster, in *Solid State Physics*, edited by F. Seitz

and D. Turnbull (Academic, New York, 1957), Vol. 5, pp. 173–256.
[3]J. D. Pack, D. L. Freeman, and H. J. Monkhorst (unpublished).
[4]A. Baldereschi, Phys. Rev. B 7, 5212 (1973).
[5]G. Gilat, J. Comput. Phys. 10, 432 (1972).
[6]J. F. Janak, in *Computational Methods in Band Theory*, edited by P. M. Marcus, J. F. Janak, and A. R. Williams (Plenum, New York, 1971), pp. 323–339.