Special points for Brillouin-zone integrations

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The efficiency of two different methods for obtaining "special" points useful for Brillouin-zone integrations of periodic functions is compared. We find that for some Bravais lattices (such as body-centered cubic and hexagonal), the method suggested by Monkhorst and Pack leads to different and sometimes less efficient point sets than those previously obtained by Chadi and Cohen. For a two-dimensional oblique lattice, special points twice as efficient as those suggested by Cunningham are given.

Two different methods, one by Chadi and Cohen[1] (CC) and the other by Monkhorst and Pack[2] (MP), for generating "special" point sets for Brillouin-zone integration of periodic functions of wave vector have been suggested so far. In their paper MP state that their method gives sets of points identical to those of CC and additional intermediate sets. By applying their method to cubic Bravais lattices which they consider, we find this statement to be true for the simple cubic and face-centered-cubic lattices but not for the body-centered-cubic lattice or for other Bravais lattices such as a hexagonal lattice. For the latter we find the CC point sets to be more efficient than those obtained by applying the method of MP. In the following we briefly review the major features of each method and discuss the reasons for the difference in the point sets they generate. At the end of the paper we also give the special points for a two-dimensional oblique lattice. These points are twice as efficient as those given by Cunningham.[3]

The special points method is related to obtaining the average over the Brillouin zone of a periodic function

$$f(\vec{k}) = f_0 + \sum_{m=1}^{\infty} f_m A_m(\vec{k}) , \qquad (1)$$

where

$$A_m(\vec{k}) = \sum_{|\vec{R}| = c_m} e^{i\vec{k} \cdot \vec{R}} , \qquad (2)$$

with $0 < c_m \leq c_{m+1}$. By summing over the inequivalent members of the star of $\vec{k}$, a periodic function $f(\vec{k})$ can always be made to have the full symmetry of the Bravais lattice as in (1). The Brillouin-zone average of $f(\vec{k})$ is equal to f_0; we are, therefore, interested in the points k_i for which

$$f_0 \simeq \sum_{i=1}^{n} \alpha_i f(\vec{k}_i) \qquad (3)$$

is a good approximation, with α_i being the weighting factor of $\vec{k}_i$. To accomplish this we need

$$\sum_{i=1}^{n} \alpha_i = 1 \qquad (4)$$

and

$$\sum_{i=1}^{n} \alpha_i A_m(\vec{k}) = 0 , \quad m = 1, 2, \ldots, N \qquad (5)$$

for N as large as possible. The special points have been defined[1] to be those which result in the largest N for a given number of points.

The method of CC is based on the idea that if $A_m(\vec{k}_1)$ and $A_m(\vec{k}_2)$ are equal to zero for certain values of m denoted by $\{M_1\}$ and $\{M_2\}$, respectively, then a new set of points can be generated[1] from $\vec{k}_1$ and $\vec{k}_2$ such that (5) is satisfied for m in both $\{M_1\}$ and $\{M_2\}$. The new points are related to $\vec{k}_1$ and $\vec{k}_2$ by[4]

$$\vec{k}_i = \vec{k}_1 + T_i \vec{k}_2 , \qquad (6)$$

where T_i runs over the point-group operations of the Bravais lattice. Successive applications of (6) using the $\vec{k}_i$'s instead of $\vec{k}_1$ and a new point $\vec{k}_3$ (instead of $\vec{k}_2$), which sets $A_m(\vec{k}_3)$ equal to zero for values of m not covered by $\vec{k}_1$ and $\vec{k}_2$, lead to successively larger point sets. The weighting factor for each point is determined only by the symmetry of that point, as discussed in Ref. 1.

MP[2] have suggested another interesting method for generating special points. Their method reduces the three-dimensional problem to three one-dimensional problems. To show this we write

$$e^{i\vec{k} \cdot \vec{R}} = e^{i2\pi n_1 k_\alpha} e^{i2\pi n_2 k_\beta} e^{i2\pi n_3 k_\gamma} , \qquad (7)$$

where, if $\{\vec{t}_1, \vec{t}_2, \vec{t}_3\}$ and $\{\vec{G}_1, \vec{G}_2, \vec{G}_3\}$ are the primitive translation vectors in real and reciprocal space, we have

$$\vec{R} = n_1 \vec{t}_1 + n_2 \vec{t}_2 + n_3 \vec{t}_3 , \qquad (8)$$

$$\vec{k} = k_\alpha \vec{G}_1 + k_\beta \vec{G}_2 + k_\gamma \vec{G}_3 . \qquad (9)$$

To eliminate $\exp(i\vec{k} \cdot \vec{R})$ from the Fourier transform of $f(\vec{k})$ by using a sum over points $\vec{k}_i$, it is possible and sufficient to consider the three one-dim-

ensional problems associated with each exponential on the right-hand side of (7). If we take

$$k_\alpha = (2r - N_\alpha - 1)/2N_\alpha , \quad r = 1, 2, \ldots, N_\alpha , \quad (10)$$

and similarly for $k_\beta(s)$ and $k_\gamma(t)$, then the sum $\exp(i\vec{k} \cdot \vec{R})$ over the points

$$\vec{k}_{rst} = k_\alpha^{(r)} \vec{G}_1 + k_\beta(s) \vec{G}_2 + k_\gamma(t) \vec{G}_3 ; \quad r = 1, \ldots, N_\alpha$$

$$s = 1, \ldots, N_\beta ; \quad t = 1, \ldots, N_\gamma , \quad (11)$$

is zero for all $\vec{R}$ for which at least one of the following conditions is satisfied: $0 < |n_1| < N_\alpha$, or $0 < |n_2| < N_{\beta_1}$ or $0 < |n_3| < N_\gamma$; [the relation between the n's and $\vec{R}$ being given by (8)]. The size of the resulting point set is determined by the numbers N_α, N_β, and N_γ.

For the simple cubic and face-centered-cubic Bravais lattices, the method of MP outlined above gives special point sets identical to those obtained by CC and also additional intermediate sets. For the body-centered-cubic (bcc) structure, however, the point sets resulting from the two methods are different. For example, CC find the two points (units of $2\pi/a$, where a is the lattice constant)

$$\vec{k}_1 = (\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}) , \quad \vec{k}_2 = (\tfrac{3}{4}, \tfrac{1}{4}, \tfrac{1}{4}) , \quad (12)$$

with weighting factors α of $\tfrac{1}{2}$ for each point, whereas the method of MP gives

$$\vec{k}_1 = (\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}) , \quad \vec{k}_2 = (\tfrac{1}{2}, 0, 0) ,$$
$$\alpha_1 = \tfrac{1}{4} , \quad \alpha_2 = \tfrac{3}{4} . \quad (13)$$

The first set of points is slightly more efficient for Brillouin-zone integrations than the second set; they eliminate the first five nearest-neighbor shells from the Fourier transform of $f(\vec{k})$ as compared to the first four shells for the second set of points. The larger point sets obtained from either method, although always different, appear to be roughly equivalent[5] in their efficiency: The eight-point set of CC fails for $\vec{R} = (4, 0, 0)a$; the six-point set[6] obtained by applying MP's method fails for $\vec{R} = (2, 2, 2)a$. The difference in the special point sets obtained by CC and MP results from the

fact that in picking a "generating wave vector" CC choose points that set the *sum* of $\exp(i\vec{k} \cdot \vec{R})$ over related lattice vectors equal to zero, whereas by construction MP set each exponential term individually equal to zero. The latter procedure may not always lead to the best possible point sets. For example, for the same accuracy a straight-forward application of MP's method for a hexagonal lattice leads to larger point sets than those of CC, although it may be possible to modify MP's method to obtain the same results.

We now discuss special points for two-dimensional Brillouin-zone integrations. Cunningham[3] has obtained the special point sets for two-dimensional zones. However, the point sets he gives for the oblique lattice are not the optimal ones. Defining a general oblique lattice by the primitive translation vectors

$$\vec{t}_1 = a(1, 0) , \quad \vec{t}_2 = a(\delta, \beta) ,$$

the special points in ascending order of accuracy are for set 1

$$\vec{k} = (1, (1 - \delta)/\beta) \quad \text{(units of } \pi/2a) , \quad \alpha = 1 ;$$

for set 2 in units of $\pi/2a$

$$\vec{k}_1 = (1, (1 - \delta)/\beta) , \quad \vec{k}_2 = (1, (1 + \delta)/\beta) ,$$

$$\alpha_1 = \alpha_2 = \tfrac{1}{2} ;$$

for set 3 in units of $\pi/4a$

$$\vec{k}_1 = (1, (1 - \delta)/\beta) , \quad \vec{k}_2 = (1, -(1 + \delta)/\beta) ,$$

$$\vec{k}_3 = (1, (3 - \delta)/\beta) , \quad \vec{k}_4 = (1, -(3 + \delta)/\beta) ,$$

$$\vec{k}_5 = (3, 3(1 - \delta)/\beta) , \quad \vec{k}_6 = (3, -3(1 + \delta)/\beta) ,$$

$$\vec{k}_7 = (3, (1 - 3\delta)/\beta) , \quad \vec{k}_8 = (3, -(1 + 3\delta)/\beta) ,$$

$$\alpha_1 = \cdots = \alpha_\gamma = \tfrac{1}{8} .$$

The last two sets given above have the same accuracy as those given by Cunningham[3] but are a factor of 2 more efficient. The method of MP can also be used to determine intermediate point sets for the two-dimensional case.

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

[2]H. J. Monkhorst and J. D. Pack, Phys. Rev. B **13**, 5188 (1976).

[3]S. L. Cunningham, Phys. Rev. B **10**, 4988 (1974).

[4]The same set of points results if $\vec{k}_2 + T_i \vec{k}_1$ is taken instead of (6).

[5]For the bcc Bravais lattice the star of $\vec{k}$ points obtained by applying the method of MP (Ref. 2) contains fewer points than those of CC (Ref. 1). For functions $f(\vec{k})$ which do not have the full symmetry of the lattice, it may, therefore, be preferable to use the MP point sets. Since in an extended-zone scheme the special point sets for all cubic lattices [whether simple cubic or face-centered-cubic (fcc) or body-centered cubic]

are identical, the bcc points of MP can also be used for other cubic lattices. For example, for the fcc lattice the points equivalent to those given in Eq. (13) would be $\vec{k}_1 = (\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2})$, $\vec{k}_2 = (\tfrac{1}{2}, 0, 0)$, $\vec{k}_3 = (1, \tfrac{1}{2}, 0)$, with $\alpha_1 = \tfrac{1}{4}$, $\alpha_2 = \alpha_3 = \tfrac{3}{8}$. For the bcc lattice $\vec{k}_3$ and $\vec{k}_2$ are equivalent points. For a function having the full symmetry of the Bravais lattice, the two-point scheme of CC gives more accurate results than the three points given above.

[6]For the bcc lattice the expression given by MP (Ref. 2) for the number of special points in a given set does not actually apply to the sets derived by applying their method. It applies correctly, however, to the special point sets that can be obtained by transforming the simple cubic special points into the bcc Brillouin zone.