Special points in the two-dimensional Brillouin zone*

S. L. Cunningham†
Physics Department, University of California, Irvine, California 92664
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Using the method of Chadi and Cohen, we present, for each of the two-dimensional lattice types, the mean-value point, the set of generating wave vectors, and the sets of special points in the two-dimensional Brillouin zone which are the most efficient in finding accurate averages of a periodic function over the Brillouin zone.

I. INTRODUCTION

Many calculations involving crystal surfaces require averaging a periodic function of wave vector parallel to the surface over the two-dimensional Brillouin zone. Examples include calculations of the charge density, the self-consistent potential, the surface mean-square displacement, and the surface Debye-Waller factor. Usually, these averages are determined by sampling the function at a discrete set of points and summing with an appropriate weight for each point.

Recently, an important method has been introduced by Baldereschi[1] and developed by Chadi and Cohen[2,3] for determining special sets of wave-vector points in three-dimensional Brillouin zones which are the most efficient in finding these averages. By "efficient" we mean determining the average of a function to an arbitrary degree of accuracy with the least number of sampled wave-vector points. Attaining this efficiency is extremely important for two-dimensional Brillouin-zone calculations because evaluating the desired periodic function for a surface for a single wave-vector point can be several orders of magnitude more expensive than for the three-dimensional counterpart. In this note, we follow the discussion of Chadi and Cohen[3] and present the special point sets for the two-dimensional Brillouin zones associated with each of the five two-dimensional lattice types.

We briefly present the essential ingredients of the argument (modified for two dimensions) given by Chadi and Cohen.[3] A periodic function $f(\vec{k})$ can be expanded as

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

where

$$A_m(\vec{k})=\sum_{|\vec{R}|=c_m} e^{i\vec{k}\cdot\vec{R}}, \quad m=1,2,\ldots , \qquad (2)$$

and where $\vec{k}$ and $\vec{R}$ are the two-dimensional wave vector and lattice vector, respectively. The sum in Eq. (2) is over all lattice vectors of equal magnitude, i.e., those lattice vectors directed to lattice points on a ring about the origin. The terms $A_m(\vec{k})$ are ordered in m so that increasing m corresponds to increasing magnitude of $\vec{R}$. There is a slight difference between the sum in Eq. (2) and the sum over only equivalent lattice vectors which are related to each other by the set $\{T_j\}$ of two-dimensional point symmetry operations of the lattice. The distinction arises because it is possible for nonequivalent lattice points to be an equal distance from the origin. In practice, this distinction is unimportant since the only effect is to sometimes take a single function $A_m(\vec{k})$ from Eq. (2) and split it into two parts.

The *exact* average over the two-dimensional Brillouin zone of the function in Eq. (1) is equal to f_0 since the second term vanishes. The question we want to answer then is as follows: What is the best set of points $\{k_i\}$ and weighting factors $\{\alpha_i\}$ which can result in an accurate approximation to f_0?

To answer this question, we impose the following conditions on $\{k_i\}$ and $\{\alpha_i\}$:

$$\sum_i \alpha_i A_m(\vec{k}_i)=0, \quad m=1,2,\ldots,N , \qquad (3)$$

$$\sum_i \alpha_i=1 , \qquad (4)$$

where N is the number of functions $A_m(\vec{k})$ for which Eq. (3) is satisfied. By using Eq. (3) and (4) in Eq. (1), we find

$$f_0=\sum_i \alpha_i f(\vec{k}_i)-\sum_{m>N}^{\infty} f_m \sum_i \alpha_i A_m(\vec{k}_i) . \qquad (5)$$

If $f(\vec{k})$ is sufficiently smooth, then the coefficients f_m will decrease in magnitude as m increases. Consequently, the second term in Eq. (5), which only contributes for $m>N$, can be made small by choosing the sets $\{k_i\}$ and $\{\alpha_i\}$ for which N is large.

In addition to the above, Chadi and Cohen[3] have presented an important theorem. If $A_m(\vec{k}_1)=0$ for several values of m belonging to the set $\{N_1\}$, and if $A_m(\vec{k}_2)=0$ for values of m in set $\{N_2\}$, then Eq. (3) can be satisfied for m in both sets $\{N_1\}$ and

$\{N_2\}$ for the set of points

$$\vec{k}_i = \vec{k}_1 + T_i \vec{k}_2, \quad i = 1, 2, \ldots, n_T , \tag{6}$$

where i ranges over all the symmetry operations in the point group. The weighting factor α_i is $1/n_T$ where n_T is the number of elements in the point group. Repeating this procedure gives additional points. If $A_m(\vec{k}_3) = 0$ for m in the set $\{N_3\}$, then

$$\vec{k}_l = \vec{k}_i + T_j \vec{k}_3, \quad i, j = 1, 2, \ldots, n_T , \tag{7}$$

$$\alpha_l = (1/n_T)^2 . \tag{8}$$

In this manner, the set of special points can be obtained from knowledge of the "generating" wave vectors $\vec{k}_1, \vec{k}_2, \vec{k}_3, \ldots$.

It is important to note that the mean-value point (the best choice of a single wave-vector point) defined by Baldereschi[1] may or may not be one of the generating wave vectors. This is because the choice of generating wave vectors is dictated by finding the wave vectors for which the number of functions $A_m(\vec{k}) = 0$ is large. On the other hand, the mean-value point is determined by finding the single wave-vector point for which the first few functions $A_m(\vec{k}_0) = 0$, and the first nonzero function is minimized. This distinction is important for the cases of the oblique lattice and the hexagonal lattice as we shall see in the following results.

Therefore, in this paper we are distinguishing between three types of wave vector points. The first type is the mean value point $\vec{k}_0$. The second type is the set of generating vectors $\vec{k}_1, \vec{k}_2, \ldots$. The third type is the set of special points $\{k_i\}$ which are used in calculating the average over the Brillouin zone. The generating wave vectors, which are few in number, uniquely determine the special points, which may be rather large in number, by repeated use of Eq. (6).

II. RESULTS

In each of the following cases, the generating wave vectors are chosen in the following manner. First, we determine the wave vector that zeroes $A_1(\vec{k})$ (the first ring) and as many other functions $A_m(\vec{k})$ as possible. We label this wave vector $\vec{k}_1$. The idea is to choose $\vec{k}_1$ such that the set $\{N_1\}$ is as large as possible and includes the first ring. The second step is to determine the first function $A_m(\vec{k})$ which is not zeroed by $\vec{k}_1$. We then choose $\vec{k}_2$ to zero this function and as many others as possible. Third, we generate the set of points $\{\vec{k}_i\}$ by applying Eq. (6). Finally, we repeat the second and third step, each time finding the first nonzero function $A_m(\vec{k})$ and choosing the wave vector that makes it, and as many other functions as possible, zero. In this way, sets of special points of any size can be generated. How this works in practice will be shown below for each of the five two-dimensional lattice types.

A. Oblique lattice

A general oblique lattice can be defined by the primitive translation vectors

$$\vec{a}_1 = a(1, 0), \quad \vec{a}_2 = a(\delta, \beta) , \tag{9}$$

where $|\delta| \lesssim \frac{1}{2}$ and $\beta < 1$. Any arbitrary lattice point is given by

$$\vec{R} = l\vec{a}_1 + n\vec{a}_2 = a(l + n\delta, n\beta) , \tag{10}$$

where l and n are integers. The primitive reciprocal-lattice vectors are

$$\vec{b}_1 = (2\pi/a)(1, -\delta/\beta), \quad \vec{b}_2 = (2\pi/a)(0, 1/\beta) . \tag{11}$$

In Fig. 1(a) we show the Brillouin zone for the oblique lattice for the arbitrary choice of $\delta = 0.1$ and $\beta = 0.8$.

Every function $A_m(\vec{k})$ for the oblique lattice has the following form:

$$A_m(\vec{k}) = 2\cos[k_x(l + n\delta) + k_y n\beta]a . \tag{12}$$

For $\beta > \frac{1}{2}$, the functions $A_1(\vec{k})$ and $A_2(\vec{k})$, corresponding to (l, n) equal to (0, 1) and (1, 0), respectively, are zeroed by the unique value

$$\vec{k}_0 = (\pi/a)(\tfrac{1}{2}, (1 - \delta)/2\beta) . \tag{13}$$

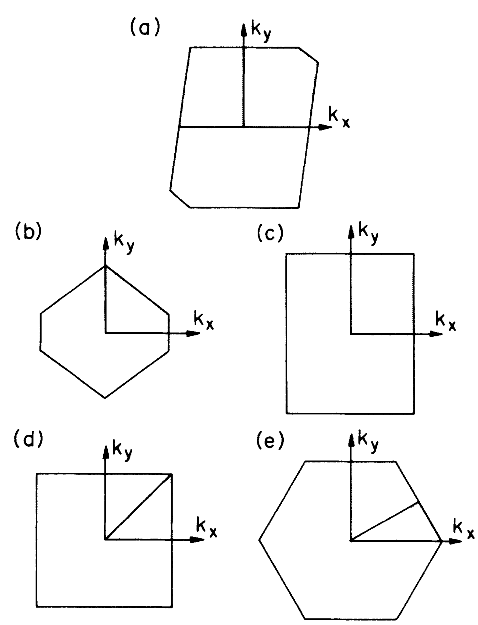

FIG. 1. Two-dimensional Brillouin zones and their irreducible segments (shaded) for the five two-dimensional lattice types. (a) Oblique ($\delta = 0.1$, $\beta = 0.8$), (b) centered-rectangular ($\beta = 0.75$), (c) primitive- rectangular ($\beta = 0.8$), (d) square, and (e) hexagonal.

This, then is the mean-value point.

The mean-value point $\vec{k}_0$ is not a good choice for the generating vector. This is because very few functions $A_m(\vec{k}_0)$ are zero. The best choice is

$$\vec{k}_1 = (\pi/a)(0, 1/2\beta) , \tag{14}$$

since this wave vector zeroes all functions given by Eq. (12) for which n is an odd integer.

The first nonzero function is $A_2(\vec{k})$ corresponding to the second ring which contains the lattice point $\vec{R} = a(1, 0)$. The second generating vector is

$$\vec{k}_2 = (\pi/a)(\tfrac{1}{2}, 0) , \tag{15}$$

which zeroes all functions for which l is odd and $n = 0$.

The point group for the oblique lattice contains only two operations—the identity operation and the π-rotation operation. Thus, application of Eq. (6) leads to two wave vector points which form the set of special points $\{\vec{k}_i\}$. They are

$$\vec{k} = (\pi/a)(\tfrac{1}{2}, 1/2\beta); \quad \vec{k} = (\pi/a)(-\tfrac{1}{2}, 1/2\beta) . \tag{16}$$

The two points are equally weighted with the value $\alpha = \frac{1}{2}$.

The position of the lattice point which is now in the ring of the first nonzero function $A_m(\vec{k})$ is $\vec{R} = a(2\delta, 2\beta)$. This corresponds roughly to a value $m = 5$ (the fifth ring). The designation of ring number is only approximate for the oblique lattice since the ordering depends on the sizes of the arbitrary length parameters δ and β. The best choice for the third generating wave vector is

$$\vec{k}_3 = (\pi/a)(0, 1/4\beta) . \tag{17}$$

Application of Eq. (7) [the iterated form of Eq. (6)] leads to four wave vectors in the special set. This is summarized in Tables I and II.

In Table I we present the first five generating wave vectors for the oblique lattice in column 2. In column 3 we give the number of points that will be in the special set of wave vectors after each generating wave vector is applied. Column 4 gives the position of the lattice point which is in the ring of the first nonzero function $A_m(\vec{k})$. The systematic behavior in each of these columns is apparent and the results for any number of points can be easily obtained. In column 4 we give an estimate of the number of the first nonzero ring. We see that with a set of 16 points in the special set, Eq. (3) is satisfied out to roughly the 30th neighbor.

In Table II we present the mean value point, the set of four special wave vectors, and the set of 16 special wave vectors with their respective weights for the oblique lattice.

In Fig. 2(a) we show the location of the 16 special wave-vector points in the irreducible segment of the Brillouin zone for the oblique lattice. It is possible that for some values of δ and β, the designated set may contain a point that falls outside the irreducible segment. If this occurs, it is always possible to translate the point by a reciprocal lattice vector or rotate by an operation in the point symmetry group to obtain the equivalent wave vector point within the irreducible segment.

TABLE I. First few generating wave vectors (column 2) for each of the five two-dimensional lattice types. In column 3 is the number of wave vectors that will appear in the set of special wave-vector points after the application of the generating wave vector. Column 4 gives the coordinates of the lattice point in the ring of the first nonzero function $A_m(k)$. Column 5 is the approximate value of m (ring number) for the coordinate in column 4.

Lattice:	Generating vector (units π/a)	Number of points	First non-zero R (units a)	Ring number m
Oblique	$\vec{k}_1 = (0, 1/2\beta)$	1	$(1, 0)$	2
	$\vec{k}_2 = (\frac{1}{2}, 0)$	2	$(2\delta, 2\beta)$	5
	$\vec{k}_3 = (0, 1/4\beta)$	4	$(2, 0)$	~7
	$\vec{k}_4 = (\frac{1}{4}, 0)$	8	$(4\delta, 4\beta)$	~23
	$\vec{k}_5 = (0, 1/8\beta)$	16	$(4, 0)$	~30
Centered-rectangular	$\vec{k}_1 = (1, 1/2\beta)$	1	$(1, 0)$	3
	$\vec{k}_2 = (\frac{1}{2}, 1/4\beta)$	4	$(2, 0)$	~11
	$\vec{k}_3 = (\frac{1}{4}, 1/8\beta)$	16	$(4, 0)$	~38
Primitive rectangular	$\vec{k}_1 = (\frac{1}{2}, 1/2\beta)$	1	$(0, 2\beta)$	4
	$\vec{k}_2 = (\frac{1}{4}, 1/4\beta)$	4	$(0, 4\beta)$	~11
	$\vec{k}_3 = (\frac{1}{8}, 1/8\beta)$	16	$(0, 8\beta)$	~45
Square	$\vec{k}_1 = (\frac{1}{2}, \frac{1}{2})$	1	$(2, 0)$	3
	$\vec{k}_2 = (\frac{1}{4}, \frac{1}{4})$	3	$(4, 0)$	9
	$\vec{k}_3 = (\frac{1}{8}, \frac{1}{8})$	10	$(8, 0)$	29
Hexagonal	$\vec{k}_1 = (\frac{2}{3}, 2/3t)$	1	$(0, t)$	2
	$\vec{k}_2 = (\frac{4}{9}, 0)$	3	$(3, 0)$	5
	$\vec{k}_3 = (\frac{2}{9}, 2/9t)$	6	$(0, 3t)$	12
	$\vec{k}_4 = (\frac{4}{27}, 0)$	18	$(9, 0)$	31

B. Centered-rectangular lattice

The centered-rectangular lattice is the special case of the oblique lattice where $\delta = \frac{1}{2}$. The primitive translation vectors are

$$\vec{a}_1 = a(1, 0), \quad \vec{a}_2 = a(\tfrac{1}{2}, \tfrac{1}{2}\beta) , \tag{18}$$

where we can always choose our axes such that $\beta < 1$. An arbitrary lattice point is given by

$$\vec{R} = l\vec{a}_1 + n\vec{a}_2 = a(l + \tfrac{1}{2}n, \tfrac{1}{2}n\beta) , \tag{19}$$

and the reciprocal-lattice vectors are

$$\vec{b}_1 = (2\pi/a)(1, -1/\beta), \quad \vec{b}_2 = (2\pi/a)(0, 2/\beta) . \tag{20}$$

For the choice of $\beta = \frac{3}{4}$, the Brillouin zone appears

TABLE II. Mean-value point and two of the first few sets of special wave-vector points for each of the five two-dimensional lattice types. Wave vectors are in units of π/a. The weighting factor α is also given.

Oblique	Centered-rectangular	Primitive rectangular	Square	Hexagonal
$[\frac{1}{2}, (1-\delta)/2\beta]$	$(1, 1/2\beta)$	$(\frac{1}{2}, 1/2\beta)$	$(\frac{1}{2}, \frac{1}{2})$	$(0.76, 0)$
$\alpha=1$	$\alpha=1$	$\alpha=1$	$\alpha=1$	$\alpha=1$
$(\frac{1}{2}, 1/4\beta)$	$(\frac{1}{2}, 1/4\beta)$	$(\frac{1}{4}, 1/4\beta)$	$(\frac{1}{4}, \frac{1}{4})$	$(\frac{10}{9}, 2/3t)$
$(\frac{1}{2}, 3/4\beta)$	$(\frac{3}{2}, 1/4\beta)$	$(\frac{1}{4}, 3/4\beta)$	$(\frac{3}{4}, \frac{3}{4})$	$(\frac{8}{9}, 0)$
$(-\frac{1}{2}, 1/4\beta)$	$(\frac{1}{2}, 3/4\beta)$	$(\frac{3}{4}, 1/4\beta)$	$(\frac{1}{4}, \frac{3}{4})$	$(\frac{4}{9}, 0)$
$(-\frac{1}{2}, 3/4\beta)$	$(\frac{1}{2}, 5/4\beta)$	$(\frac{3}{4}, 3/4\beta)$	$\alpha_{1,2}=\frac{1}{4}$	$\alpha=\frac{1}{3}$
$\alpha=\frac{1}{4}$	$\alpha=\frac{1}{4}$	$\alpha=\frac{1}{4}$	$\alpha_3=\frac{1}{2}$	
$(-\frac{3}{4}, 1/8\beta)$	$(\frac{1}{4}, 1/8\beta)$	$(\frac{1}{8}, 1/8\beta)$	$(\frac{1}{8}, \frac{1}{8})$	$(\frac{2}{9}, 2/9t)$
$(-\frac{1}{4}, 1/8\beta)$	$(\frac{3}{4}, 1/8\beta)$	$(\frac{3}{8}, 1/8\beta)$	$(\frac{3}{8}, \frac{3}{8})$	$(\frac{4}{9}, 4/9t)$
$(\frac{1}{4}, 1/8\beta)$	$(\frac{5}{4}, 1/8\beta)$	$(\frac{5}{8}, 1/8\beta)$	$(\frac{5}{8}, \frac{5}{8})$	$(\frac{8}{9}, 8/9t)$
$(\frac{3}{4}, 1/8\beta)$	$(\frac{7}{4}, 1/8\beta)$	$(\frac{7}{8}, 1/8\beta)$	$(\frac{7}{8}, \frac{7}{8})$	$(\frac{2}{3}, 2/9t)$
$(-\frac{3}{4}, 3/8\beta)$	$(\frac{1}{4}, 3/8\beta)$	$(\frac{1}{8}, 3/8\beta)$	$(\frac{3}{8}, \frac{1}{8})$	$(\frac{8}{9}, 4/9t)$
$(-\frac{1}{4}, 3/8\beta)$	$(\frac{3}{4}, 3/8\beta)$	$(\frac{3}{8}, 3/8\beta)$	$(\frac{5}{8}, \frac{1}{8})$	$(\frac{10}{9}, 2/9t)$
$(\frac{1}{4}, 3/8\beta)$	$(\frac{5}{4}, 3/8\beta)$	$(\frac{5}{8}, 3/8\beta)$	$(\frac{7}{8}, \frac{1}{8})$	$\alpha_{1-3}=\frac{1}{9}$
$(\frac{3}{4}, 3/8\beta)$	$(\frac{7}{4}, 3/8\beta)$	$(\frac{7}{8}, 3/8\beta)$	$(\frac{5}{8}, \frac{3}{8})$	$\alpha_{4-6}=\frac{2}{9}$
$(-\frac{3}{4}, 5/8\beta)$	$(\frac{1}{4}, 5/8\beta)$	$(\frac{1}{8}, 5/8\beta)$	$(\frac{7}{8}, \frac{3}{8})$	
$(-\frac{1}{4}, 5/8\beta)$	$(\frac{3}{4}, 5/8\beta)$	$(\frac{3}{8}, 5/8\beta)$	$(\frac{7}{8}, \frac{5}{8})$	
$(\frac{1}{4}, 5/8\beta)$	$(\frac{5}{4}, 5/8\beta)$	$(\frac{5}{8}, 5/8\beta)$	$\alpha_{1-4}=\frac{1}{16}$	
$(\frac{3}{4}, 5/8\beta)$	$(\frac{1}{4}, 7/8\beta)$	$(\frac{7}{8}, 5/8\beta)$	$\alpha_{5-10}=\frac{1}{8}$	
$(-\frac{3}{4}, 7/8\beta)$	$(\frac{3}{4}, 7/8\beta)$	$(\frac{1}{8}, 7/8\beta)$		
$(-\frac{1}{4}, 7/8\beta)$	$(\frac{1}{4}, 9/8\beta)$	$(\frac{3}{8}, 7/8\beta)$		
$(\frac{1}{4}, 7/8\beta)$	$(\frac{3}{4}, 9/8\beta)$	$(\frac{5}{8}, 7/8\beta)$		
$(\frac{3}{4}, 7/8\beta)$	$(\frac{1}{4}, 11/8\beta)$	$(\frac{7}{8}, 7/8\beta)$		
$\alpha=\frac{1}{16}$	$\alpha=\frac{1}{16}$	$\alpha=\frac{1}{16}$		

as in Fig. 1(b).

For this lattice, the mean value point and the first generating vector are the same. They are given by

$$\vec{k}_0=\vec{k}_1=(\pi/a)(1, 1/2\beta)\ . \tag{21}$$

This point zeroes the functions $A_m(\vec{k})$ for any ring containing a lattice point with n odd or $\frac{1}{2}n$ odd integer (all values of l). This includes the first two rings, but not the third with the lattice point $\vec{R}=a(1, 0)$. The second generating vector is

$$\vec{k}_2=(\pi/a)(\tfrac{1}{2}, 1/4\beta)\ . \tag{22}$$

The point group for the centered-rectangular lattice contains four operations. As a consequence, from Eq. (6) we find that the first two generating vectors result in a set of four special wave-vector points, each having a weight of $\alpha=\frac{1}{4}$.

In Table I we present the three generating wave vectors needed to obtain the sixteen-point set of special wave vectors. These points satisfy Eq. (3) out to roughly the 38th neighbor. The generalization to larger numbers of generating vectors is obvious from the table.

In Table II we present the mean-value point, the four-point and sixteen-point sets of special wave vectors, along with the corresponding weights. The sixteen-point set is shown in Fig. 2(b). Again, points that may fall outside the irreducible segment of the Brillouin zone can always be moved to fall within it.

C. Primitive rectangular lattice

The primitive translation vectors, lattice vector, and reciprocal lattice vectors for the primitive

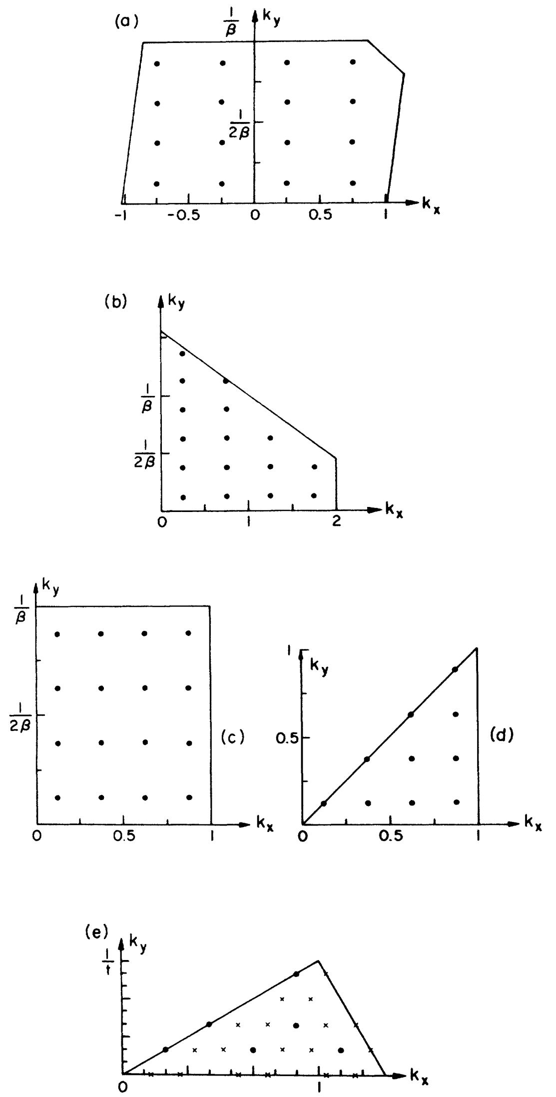

FIG. 2. Irreducible segments of the five two-dimensional Brillouin zones showing one of the sets of special wave vector points. (a) Sixteen-point set for the oblique lattice, (b) sixteen-point set for the centered-rectangular lattice, (c) sixteen-point set for the primitive-rectangular lattice, (d) ten-point set for the square lattice, (e) six-point set (dots) and eighteen point set (crosses) for the hexagonal lattice.

rectangular lattice are given, respectively, by

$$\vec{a}_1 = a(1, 0), \quad \vec{a}_2 = a(0, \beta), \quad \vec{R} = a(l, n\beta) ,$$
$$\vec{b}_1 = (2\pi/a)(1, 0), \quad \vec{b}_2 = (2\pi/a)(0, 1/\beta) . \tag{23}$$

As in the case of the centered-rectangular lattice, the mean-value point and the first generating wave vector are the same. They are given by

$$\vec{k}_0 = \vec{k}_1 = (\pi/a)(\tfrac{1}{2}, 1/2\beta) . \tag{24}$$

This point zeroes all functions $A_m(\vec{k})$ for any ring containing a lattice point with either l or n odd. This includes the first three rings but not the fourth which passes through the position vector $\vec{R} = a(0, 2\beta)$. The second generating vector is

$$\vec{k}_2 = (\pi/a)(\tfrac{1}{4}, 1/4\beta) , \tag{25}$$

which zeroes all functions $A_m(\vec{k})$ related to a lattice point where either $\frac{1}{2}l$ or $\frac{1}{2}n$ is an odd integer. These vectors, along with the third generating vector, are given in Table I. As in the previous case, three generating vectors result in a set of 16 wave vectors in the special set. Again, because β is arbitrary ($\beta < 1$), the value of m designating the ring number of the first nonzero function $A_m(\vec{k})$ is only approximate. The values in Table I are for a value of $\beta \sim 0.75$.

In Table II we present the coordinates of the mean-value point, the four- and sixteen-point special wave-vector sets and their respective weights, for the primitive rectangular lattice. The sixteen-point set is shown in Fig. 2(c). The generalization to larger numbers of points is straightforward.

D. Square lattice

The square-lattice results can be obtained directly from the primitive rectangular-lattice results by setting the parameter $\beta = 1$. There is one difference, however. The irreducible segment of the square lattice is smaller than what one would obtain merely by setting $\beta = 1$ for the rectangular lattice. Consequently, many of the points in the primitive rectangular set for $\beta = 1$ are equivalent to each other through operations of the square-lattice point group. This results in a reduced number of wave vectors in the special sets and a distinction, heretofore not needed, in the weights of each point. In Table II these reduced sets are presented along with the various weights for each point. We see that the wave vector points that fall on the diagonal of the square Brillouin zone have half of the weight of the other points. The ten-point set is shown in Fig. 2(d). Another distinction, since the square lattice is unique, is that the values of m in Table I are no longer approximate.

E. Hexagonal lattice

The primitive translation vectors for the hexagonal lattice are

$$\vec{a}_1 = a(1, 0), \quad \vec{a}_2 = a(\tfrac{1}{2}, \tfrac{1}{2}t) , \tag{26}$$

where $t = \sqrt{3}$ is introduced for notational convenience. The reciprocal-lattice vectors are

$$\vec{b}_1 = (2\pi/a)(1, -\tfrac{1}{3}t), \quad \vec{b}_2 = (2\pi/a)(0, \tfrac{2}{3}t) . \tag{27}$$

The Brillouin zone and the irreducible segment are shown in Fig. 1(e).

The hexagonal lattice is unique among the five two-dimensional lattices because it is not possible to find a single wave-vector point which zeroes the function $A_m(\vec{k})$ for the first two rings. These two functions are

$$\begin{aligned} A_1(\vec{k}) &= 2\cos k_x a + 4\cos\tfrac{1}{2}k_x a \cos\tfrac{1}{2}tk_y a \\ A_2(\vec{k}) &= 2\cos tk_y a + 4\cos\tfrac{3}{2}k_x a\cos\tfrac{1}{2}tk_y a . \end{aligned} \tag{28}$$

To obtain the mean value point, we want to find the wave vector $\vec{k}_0$ for which $A_1(\vec{k}_0) = 0$ and for which $|A_2(\vec{k}_0)|$ is minimum. The result is

$$\vec{k}_0 = (\pi/a)(0.7614, 0) , \tag{29}$$

where the numerical factor is obtained from the solution of the equation

$$\cos k_x a = 1 - t . \tag{30}$$

The mean value point $\vec{k}_0$ is not a good choice for the first generating vector since only a few functions $A_m(\vec{k})$ are zeroed.

The first four generating wave vectors are shown in Table I. Generalization to more is obvious. We see that the set of 18 wave vectors, which results from applying the four generating vectors, satisfies Eq. (3) out to the 31st neighbor. The coordinates of the mean value point and the three- and six-point sets of special wave vectors are given in Table II. As in the case of the square lattice, the weights of each point are not the same; those points on the boundary of the irreducible segment are weighted exactly half as much as the points within the irreducible segment.

In Fig. 2(e) we show the positions of the wave vectors in the six-point set (dots) along with the positions of the wave vectors in the eighteen-point set (crosses).

Recently, Appelbaum and Hamann[4] performed a calculation of the surface of silicon which requires a sum over the hexagonal two-dimensional Brillouin zone. They performed the sum by choosing two wave vector points, the Γ point at the zone center $[\vec{k}_1 = (0, 0)]$ and the J point at the center of the zone edge $[\vec{k}_2 = (1, 1/t)\pi/a]$ (also called the M point). With this choice, Eq. (3) can be satisfied for the first two rings ($m = 1, 2$) by setting $\alpha_1 = \frac{1}{4}$ and $\alpha_2 = \frac{3}{4}$ [see Eqs. (28)]. Equation (3) is not satisfied for $m = 3$.

A better choice for the two-wave-vector point sample and weights would be

$$\begin{aligned} \vec{k}_1 &= (\pi/a)(\tfrac{1}{2}, 1/2t), \quad \alpha_1 = \tfrac{1}{2} \\ \vec{k}_2 &= (\pi/a)(1, 0), \quad \alpha_2 = \tfrac{1}{2} . \end{aligned} \tag{31}$$

This sample satisfies Eq. (3) for both the first and second ring. The reason this sample is better than that used by Applebaum and Hamann (all other considerations being equal[5]) is that the size of the first nonzero term ($m = 3$) is smaller. For this term, the sum in Eq. (3) is equal to 6 for the sample points used by Appelbaum and Hamann, whereas the sum is equal to -2 for the sample points in Eqs. (31). This is also true for the sixth ring ($m = 6$) which is the second nonzero term in the set. Thus, the error in the average due to choosing the two wave-vector points in Eqs. (31) is approximately one-third the error due to choosing Applebaum and Hamann's sample. Incidentally, neither of these sets will be determined by the systematic method presented in this paper.

III. DISCUSSION

We have applied the method of Chadi and Cohen[3] to the determination of sets of special wave vectors (the points which are the most efficient in averaging a periodic function over the Brillouin zone) for each of the five two-dimensional lattice types. For each lattice we have found the mean-value point, as defined by Baldereschi,[1] and a few of the smallest sets of special wave-vector points. The generalization to larger sets is a trivial extension of the results presented here. These sets of special wave-vector points are very important in calculations concerning surface properties where, for some cases, considerations of numerical efficiency are the determining factors in performing the calculation.

The accuracy with which any set of points gives the average of a periodic function is determined by the "smoothness" of the function in reciprocal space. A discussion of accuracy is given by Chadi and Cohen.[3] Basically, the smoother the periodic function, the faster is the decay in magnitude of the expansion coefficients f_m. In favorable cases, the use of the mean-value point alone can give accurate results for the averages over the Brillouin zone.

If the analytic dependence on wave vector $\vec{k}$ of the periodic function $f(\vec{k})$ is not known (as is usually the case), then the accuracy of the averaging process can only be determined by successive calculations using two different wave vector samples. If this test of the accuracy is not performed, then the results of the calculation will always be open to criticism. For example, Applebaum and Hamann[4] have argued that the two-wave-vector point sample for their silicon calculation[4] is adequate due to the tight-binding nature of silicon and to the fact that the charge distribution is localized. However, they also claim that the surface state band is only partially filled. If this is true then the periodic function $f(\vec{k})$ cannot be smooth but must have a discontinuity at the wave-vector point where the surface-state band crosses the Fermi energy. This implies that the two-point sample may be too small to give accurate results. The only way to resolve this question of accuracy is to repeat the calculation with a different sample of wave-vector points, and examine the differences in the results.

For the primitive rectangular lattice and the square lattice, the sets of wave-vector points and weights are the same as those one obtains from a "displaced" mesh. By this we mean the following: Starting from the origin, generate the mesh of points in the Brillouin zone where each point is separated by $1/M$ (M is an integer) of the distance to the zone boundary. Then displace each point in the mesh in the direction of the zone diagonal by half the distance to the next point. The points in Figs. 2(c) and 2(d) are displaced meshes for the value $M=4$. The set of points in Figs. 2(a) and 2(b) are similar (but not equivalent) to a displaced mesh. The set of points for the hexagonal lattice [Fig. 2(e)], is totally unrelated to a displaced mesh.

Finally, whereas there are many sets of points of various sizes generated by the scheme presented in this paper, there are other possible sets which will not be found. For example, a displaced mesh with the value $M=3$ and appropriate weights can satisfy Eqs. (3) and (4) for both the square and rectangular lattice. It is possible to obtain this set from generating vectors, but the generating vectors would not be found by the systematic scheme presented in this paper. The important advantage of the method in this paper is that once a set of points of a certain size is obtained, we know that it is the optimum set of that size for efficiently finding the average over the Brillouin zone.

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†Present address: Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, Calif. 91125.

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[5] Another consideration which may influence the choice of sample is the difficulty in calculating the function $f(\vec{k})$ for various wave-vector points. For high-symmetry points, $f(\vec{k})$ may be easier to calculate, and this fact may dictate which sample is used. A third possible choice of two wave-vectors which is also better than the choice of Appelbaum and Hamann is $\vec{k}_1=(\pi/a)(\frac{2}{3},0)$ and $\vec{k}_2=(\pi/a)(\frac{4}{3},0)$ with $\alpha_1=\frac{3}{4}$ and $\alpha_2=\frac{1}{4}$. This choice is not as good as Eqs. (31).