Formulas for the Chadi-Cohen process

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For the square and cubic lattices, formulas are designed which yield, for **k**-space summations over the Brillouin zone, the special points in the irreducible Brillouin zone and the corresponding weighting factors prescribed by the Chadi-Cohen method. For the simple-cubic and fcc lattices these formulas at stage ν correspond to those of Monkhorst and Pack at stage 2^{ν}. These formulas allow one to compute the summations to any order of approximation, not necessarily successively. It is demonstrated how extrapolation in the inverse of the number of special points may be used to speed up the calculations. Furthermore, the formulas are shown to be useful for numerically evaluating the integrals of singular functions in two dimensions.

I. INTRODUCTION

Chadi and Cohen[1] (to be referred to as CC) proposed both a method and a process for evaluating **k**-space integrals numerically. The main idea of the *method*, basically a Gaussian numerical integration method, is to relate the integral sought to a combination of appropriately weighted values of the integrand at some "special" points in the irreducible Brillouin zone (IBZ: the smallest segment of the first Brillouin zone that would cover the whole Brillouin zone when properly rotated about the origin). The *process* required to implement the CC method (i.e., to find a set of special points and their weighting factors) is not unique; alternate processes are possible based on different choices from among the zeros of the symmetrized plane waves which enter the theory. The specific recursion process proposed by Chadi and Cohen allows one to obtain the required points together with their weighting factors, successively and up to any order of approximation, in a very simple and direct fashion. The main drawback of this process has been that no general formulas exist for locating the special points in k space, so that calculations soon become tedious; calculations are rarely carried through beyond the fourth or even the third order.

In the absence of formulas, other authors[2,3] (reviewed by Evarestov and Smirnov[3]) have taken advantage of the nonuniqueness of the CC process to design other processes within the CC method. Some of these authors do find formulas which generate (alternate) special points and their weighting factors. Monkhorst and Pack[3] have devised formulas which generate special points with weighting factors equal to unity, which for the simple-cubic (sc) and fcc cases give at stage 2^{ν} essentially the CC νth-stage points. These points have not been reduced to the IBZ, or even to the first Brillouin zone, making the computations unnecessarily lengthy. The CC process thus remains by far the one used most frequently in the literature. For this reason it is of interest and importance to develop formulas for the CC process for the bcc and SQ (square) lattices as well.

We have found that, for the three cubic lattices and the square lattice, formulas can be designed whereby the special points and their corresponding weighting factors are obtained. These formulas can be easily implemented in a computation program; successive orders of approximation (not necessarily starting at the first order) can be obtained. Moreover, having all points in the IBZ reduces the computation time considerably below that required when, as in Monkhorst and Pack's formula, the points vary over the entire Brillouin zone and even beyond. It is shown that, if need be, the points may be extrapolated to provide a substantial gain of precision while reducing computer time. In addition the method, with appropriate modifications, has been found useful in evaluating the integrals of singular functions in two dimensions.

In Sec. II we briefly review the basic theory, following CC. Section III describes the recursive process of CC. In Sec. IV we present our formulas for the square lattice and the three cubic lattices. In Sec. V we present the extrapolation procedure and, as an example, the evaluation of the Watson sum[4] in the simple-cubic lattice for which the exact result is known. Section VI presents a treatment of integrable diverging functions in two dimensions. Section VII contains some concluding remarks.

II. REVIEW OF CHADI-COHEN THEORY

It is desired to calculate

$$F=(1/N)\sum_{\mathrm{BZ}} f(\mathbf{k}) ,$$

where $f(\mathbf{k})$ is a periodic function of the wave vector $\mathbf{k}$ with the periodicity of the reciprocal lattice. $f(\mathbf{k})$ can be written as a symmetrized-plane-wave (SPW) expansion:

$$f(\mathbf{k})=f_0+\sum_{m=1}^{\infty} f_m A_m(\mathbf{k}) , \tag{2.1}$$

where the

$$A_m(\mathbf{k})=\sum_{\mathbf{R}\in\{T\mathbf{R}_m\}} \exp(i\mathbf{k}\cdot\mathbf{R}) \tag{2.2}$$

are the symmetrized plane waves. The summation in

(2.2) is to be carried out over all points $\mathbf{R}$ related to some particular typical lattice point $\mathbf{R}_m$ by an element of the point-group operation T. Since the integral over the Brillouin zone (BZ) of each $A_m(\mathbf{k})$ vanishes, the calculation of F amounts to the evaluation of f_0. This is emphasized by writing (2.1) in the form, for a particular $\mathbf{k}_i$:

$$f_0 = f(\mathbf{k}_i) - \sum_{m=1}^{\infty} f_m A_m(\mathbf{k}_i) . \tag{2.3}$$

The original idea[5] was to choose a single point $\mathbf{k}_1$ such that the largest number of terms in the summation in (2.3) vanishes; hoping that the nonvanishing terms of (2.3) would contribute negligibly to f_0, in CC (Ref. 1) it is shown that results can be improved if one takes more than one point, namely, the n' values of $\mathbf{k}_i^{(\nu)}$ (at order of approximation ν), distributed over the BZ, such that

$$\sum_{i=1}^{n'} A_m(\mathbf{k}_i^{(\nu)}) = 0, \quad m = 1,2,\ldots,M . \tag{2.4a}$$

$M+1$ is the lowest value of m for which (2.4a) is not satisfied. Since the SPW's are invariant under the operations which transport a given point from the BZ into the IBZ, the summation in (2.4a) may be restricted to $\mathbf{k}_l^{(\nu)}$ in the IBZ; since, however, more than one point in the BZ might well map onto each $\mathbf{k}_l^{(\nu)}$ in the IBZ, one must then introduce weighting factors $\alpha_l^{(\nu)}$ (which may be taken to sum to unity):

$$\sum_{l=1}^{n} \alpha_l^{(\nu)} A_m(\mathbf{k}_l^{(\nu)}) = 0, \quad m = 1,2,\ldots,M , \tag{2.4b}$$

where n is the number of special points in the IBZ. Equation (2.3) then generalizes at order ν to

$$f_0^{(\nu)} = \sum_{l=1}^{n} \alpha_l^{(\nu)} f(\mathbf{k}_l^{(\nu)}) - \sum_{l=1}^{n} \alpha_l^{(\nu)} \sum_{m>M}^{\infty} f_m A_m(\mathbf{k}_l^{(\nu)}) . \tag{2.5}$$

Assuming that the terms for $m > M$ can be neglected, one has

$$f_0^{(\nu)} \cong \sum_{l=1}^{n} \alpha_l^{(\nu)} f(\mathbf{k}_l^{(\nu)}) . \tag{2.6}$$

Equation (2.6) is the central equation of the method.

The problem is now to obtain the special points $\mathbf{k}_l^{(\nu)}$ and their weighting factors $\alpha_l^{(\nu)}$. For that purpose Chadi and Cohen proposed and proved the theorem (returning to the full BZ): If $A_m(\mathbf{k}) = 0$ is satisfied by $\mathbf{k} = \mathbf{k}_1$ for $m = m_1$ and by $\mathbf{k} = \mathbf{k}_{\text{seed}}$ for $m = m_2 > m_1$, then the set of points

$$\mathbf{k}_i = \mathbf{k}_1 + T_i \mathbf{k}_{\text{seed}}, \quad i = 1,2,\ldots,n_T \tag{2.7}$$

(where $\{T\}$ is the symmetry operation group of the lattice and n_T is the number of elements in that group) satisfies

$$\sum_{i=1}^{n_T} A_m(\mathbf{k}_i) = 0 \quad (m = m_1, m_2) . \tag{2.8}$$

The CC theorem has here been restated in an equivalent but convenient form. For general order ν, (2.7) is replaced by

$$\mathbf{k}_{(j)l}^{(\nu)} = \mathbf{k}_l^{(\nu-1)} + T_j \mathbf{k}_{\text{seed}}^{(\nu)} . \tag{2.9}$$

Though $\mathbf{k}_{\text{seed}}^{(\nu)}$ and $\mathbf{k}_l^{(\nu-1)}$ are chosen to lie in the IBZ, the $\mathbf{k}_{(j)l}^{(\nu)}$ are generally not in the IBZ. The latter are next brought by translation and group rotation (if necessary) into the IBZ. We let $\mathbf{k}_l^{(\nu)}$ be the set of distinct values of the latter points. They are the points to be used for order ν. The weighting factors $\alpha_l^{(\nu)}$ are then

$$\alpha_l^{(\nu)} = n_l \Big/ \sum_l n_l , \tag{2.10}$$

where n_l is the number of points in the BZ that map onto the point $\mathbf{k}_l^{(\nu)}$ by the point-group operations.

III. CONSTRUCTION SCHEME

To obtain the special points $\mathbf{k}_l^{(\nu)}$ in the spirit of (2.9) one may proceed as follows:[1,2,6,7] Consider the first symmetrized plane wave function $A_1(\mathbf{k})$; choose a point $\mathbf{k}_{\text{seed}}^{(1)}$ with its three coordinates equal and which lies inside the IBZ, such that $A_1(\mathbf{k}_{\text{seed}}^{(1)}) = 0$. $\mathbf{k}_{\text{seed}}^{(1)}$ is the (only) special point in order 1.

The general process for going from order $\nu-1$ to order ν is as follows: Find the first SPW $A_{m_\nu}(\mathbf{k})$ that is nonvanishing at all of the points $\mathbf{k}_{\text{seed}}^{(1)}, \mathbf{k}_{\text{seed}}^{(2)}, \ldots, \mathbf{k}_{\text{seed}}^{(\nu-1)}$ (the CC theorem ensures that if an $A_m(\mathbf{k})$ vanishes at all the seeds up to a given order, its contribution to f_0 *automatically* vanishes at all higher orders in the present scheme); find a zero, $\mathbf{k}_{\text{seed}}^{(\nu)}$, in the IBZ and having all its coordinates equal, of that SPW; combine $\mathbf{k}_{\text{seed}}^{(\nu)}$ [using (2.9)] with all the points $\mathbf{k}_l^{(\nu-1)}$ generated at order $\nu-1$; bring the resulting points when necessary into the IBZ (they are now the $\mathbf{k}_l^{(\nu)}$) and obtain their weighting factors from (2.10). In the Appendix we give details of this construction for the bcc lattice up to order $\nu = 3$.

IV. FORMULAS

The construction scheme described in Sec. III, applied to the cubic lattices and to the square lattice, produces, at some approximation order ν, the following typical situation (a is the lattice constant):

$$\mathbf{k}_l^{(\nu)} = (b,c,d)(2\pi/a) \in \text{IBZ} ,$$

where $b \geq c \geq d \geq 0$ (Ref. 8) are rational numbers of the form $p/2^q$, p is an odd integer smaller than 2^q, and $q \geq 1$ is an integer. To go to the next order one needs, for example, $\mathbf{k}_1^{(\nu+1)} = (g,g,g)(2\pi/a)$ [following CC (Ref. 1), one always chooses a point having all its coordinates equal] where g is a rational number of the form $1/2^{q+1}$. The

TABLE I. First-order points.

Lattice	$\mathbf{k}_1^{(1)}$ (units of $2\pi/a$)	$\alpha_1^{(1)}$
SQ	$\frac{1}{4},\frac{1}{4}$	1
sc	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	1
fcc	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	1
bcc	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	1

TABLE II. Parameters and exponents to be used in formulas (4.2), (4.3), and (4.4) for CC order $\nu > 1$. Coordinates are in units of $2\pi/a$ in the sc and SQ lattices, and π/a in the bcc and fcc lattices.

Lattice	λ	β	γ	μ Exactly three coord. equal	μ Exactly two coord. equal	μ No two coord. equal
SQ	ν	$\nu+1$	$2\nu-2$		1	2
sc	ν	$\nu+1$	$3\nu-3$	1	3	6
fcc	ν	ν	$3\nu-4$	1	3	6
bcc	ν	ν	$3\nu-5$	1	If sum of any two coord. $=1$, $\mu=1$; otherwise $\mu=3$	If sum of any two coord. $=1$, $\mu=3$; otherwise $\mu=6$

value of q depends on the order of approximation ν and on the lattice. In this context, the use of Eq. (2.9) yields, for a particular point,

$$\mathbf{k}_{(j)l}^{(\nu+1)}=\mathbf{k}_l^{(\nu)}+T_j\mathbf{k}_{\text{seed}}^{(\nu+1)}=(r',s',t')(2\pi/a)\ , \tag{4.1}$$

where r', s', and t' turn out to be rational numbers of the form $u/2^{q+1}$, $2^{q+1}>u>0$ and u is an odd integer. Each $\mathbf{k}_{(j)l}^{(\nu+1)}$ is necessarily in the first octant (or quadrant, for the square lattice), and one of three cases occurs: (i) The point belongs to the IBZ; (ii) the point belongs to the reducible Brillouin zone (RBZ) but not to the IBZ. Each (positive) coordinate (in units of $2\pi/a$) must be less than or equal to 1 for a point to be in the RBZ. For the bcc lattice, the sum of any two coordinates must, in addition, not exceed 1, and for the fcc lattice the sum of the three coordinates must, in addition, not exceed $\frac{3}{2}$. The point must be brought into the IBZ by one of the T operations; (iii) the point is outside the BZ; it must be brought into the RBZ by an appropriate translation and then into the IBZ by a rotation. The only operative translations here are "-1" on the two largest coordinates for the bcc lattice and "-1" on each coordinate for the fcc lattice. (No such translations are required for the SQ and sc lattices as the CC process generates no points outside the BZ for these cases.)

These operations yield the special points $\mathbf{k}_l^{(\nu+1)}$ given the special points $\mathbf{k}_l^{(\nu)}$. It is found that the CC points and their weighting factors can be written, for approximation order $\nu>1$ (for $\nu=1$ the points are given in Table I):

$$\mathbf{k}_l^{(\nu)}=(r,s,t)\frac{2\pi}{a}\frac{1}{2^\beta}\ , \tag{4.2}$$

$$\alpha_l^{(\nu)}=\mu/2^\gamma\ , \tag{4.3}$$

$$2^\lambda>r\geq s\geq t>0\ , \tag{4.4}$$

where r, s, and t are always positive odd integers, subject to the further restrictions that the sum of any pair is $\leq 2^\beta$ for the bcc lattice and that the sum of all three is $\leq 3(2^{\beta-1})$ for the fcc lattice; and β, γ, μ, and λ, given in Table II, all depend on the approximation order and on the lattice. The low-order points provided in CC (Ref. 1) for the three cubic lattices, and those given in Cunningham[7] for the square lattice, are consistent with these formulas.

V. THE EXTRAPOLATION

Starting at some order of approximation ν_1 with N_1 special points, one has an estimate f_{01} of f_0. The next orders $\nu_2,\nu_3,\ldots$, with $N_2,N_3,\ldots$, special points, provide the next approximations $f_{02},f_{03},\ldots$, of f_0. These successive approximations can be plotted[9] as a function of the inverse number of points, $(1/N)$, and extrapolated to $(1/N)\to 0$. We used a four-point extrapolation. The

TABLE III. Comparison of the direct and extrapolated methods in the evaluation of $F=(1/N)\sum_{\text{BZ}}f(\mathbf{k})$ with $f(\mathbf{k})=[1-\frac{1}{3}(c_x+c_y+c_z)]^{-1}$, where $c_l=\cos(k_l)$ $(l=x,y,z)$; the exact result (Ref. 4) is $F=1.516\,386\,059\,1\ldots$.

	Chadi-Cohen		Extrapolated Chadi-Cohen		
Order	F	Computer time (CPU sec)	Orders	F	Computer time (CPU sec)
1	1.294 12	0.005			
2	1.416 4	0.007			
3	1.464 06	0.011			
4	1.490 03	0.035	1,2,3,4	1.516 28	0.074
5	1.503 35	0.22	2,3,4,5	1.516 377	0.279
6	1.509 87	1.5	3,4,5,6	1.516 385 4	1.819
7	1.513 13	11.5	4,5,6,7	1.516 386 014	13.7
8	1.514 76	91.5			
9	1.515 57	727			

TABLE IV. Numerical evaluation of (6.1) without extrapolation for different CC orders and different choices of $|\mathbf{k}_0|$. The exact result (Ref. 11) is 3.198 663 937.... The value $\alpha=\frac{1}{8}$ is used.

CC order (No. of points in the order) \ $\|\mathbf{k}_0\|$	g_0	1.0388 0.0852	0.915 46 0.104 95	0.642 0.190	0.450 0.349
		Evaluation (No. of points in the $\|\mathbf{k}\|<\|\mathbf{k}_0\|$ region)			
4		3.198 27	3.198 921	3.197 3	3.197 15
(136)		(13)	(10)	(5)	(3)
5		3.198 56	3.198 793	3.199 4	3.199 36
(528)		(47)	(38)	(20)	(10)
6		3.198 45	3.198 709	3.198 9	3.198 97
(2080)		(182)	(146)	(72)	(35)
7		3.198 498	3.198 704	3.198 945	3.199 0
(8256)		(717)	(567)	(276)	(138)
8		3.198 493	3.198 700	3.198 958	3.199
(32 896)		(2844)	(2241)	(1091)	(542)

efficiencies of the direct and the extrapolated Chadi-Cohen method are compared, for a given $f(\mathbf{k})$ for the sc lattice, in Table III. This table shows that the extrapolated value quickly approaches the exact one to within a very small fraction of one percent. The computer times (Cyber 835 of Concordia University) are given for comparison purposes. A similar behavior was obtained for the SQ, bcc, and fcc lattices, confirming the feasibility of the extrapolation procedure.

VI. SUMMATION OF DIVERGING FUNCTIONS IN TWO DIMENSIONS

The following $\mathbf{k}$-space summation for the SQ lattice appears in a theory[10] for the calculation of the critical exponent η,

$$F=\frac{1}{N}\sum_{\mathbf{k}\in BZ}[1-\tfrac{1}{2}(\cos k_x+\cos k_y)]^{\alpha-1}\ , \tag{6.1}$$

where $0<\alpha<\frac{1}{2}$. The problem is that the closer any of the special points are to the origin (and in the CC process there are special points increasingly close to the origin in increasingly higher orders) the larger $f(\mathbf{k})$ becomes; this tends to destroy the convergence of the procedure. When the attempt is made to perform the calculation analytically for small $\mathbf{k}$ (with $|\mathbf{k}|<|\mathbf{k}_0|$ for some $|\mathbf{k}_0|$) and by the CC method for large $\mathbf{k}$, the CC method fails to converge due to the large discontinuity at $|\mathbf{k}_0|$.

One solution is to make use of a function $g(\mathbf{k})$, defined in terms of $f(\mathbf{k})$ and a constant g_0 by

$$g(\mathbf{k})=\begin{cases} g_0 & \text{for } |\mathbf{k}|\le|\mathbf{k}_0|, \\ f(\mathbf{k}) & \text{for } |\mathbf{k}|>|\mathbf{k}_0|, \end{cases}$$

and to write the integral in the following way:

$$\int_{BZ}f(\mathbf{k})d\mathbf{k}=\int_{|\mathbf{k}|<|\mathbf{k}_0|}f(\mathbf{k})d\mathbf{k}+\int_{BZ}g(\mathbf{k})d\mathbf{k} -\int_{|\mathbf{k}|<|\mathbf{k}_0|}g_0 d\mathbf{k}\ , \tag{6.2}$$

where the first and the third terms are to be evaluated analytically (the first by expanding $f(\mathbf{k})$ in a power series) and the second term is to be evaluated by the CC method. The choice $g_0=0$ corresponds to the failed attempt cited above.

While the best choice of $|\mathbf{k}_0|$ and g_0 will depend on the function $f(\mathbf{k})$, some guidelines for this choice may be given. It is desired to have $|\mathbf{k}_0|$ small enough so that the power series calculation will be accurate, and yet large enough so that the CC procedure applied to the second term will be able to sample the region $|\mathbf{k}|<|\mathbf{k}_0|$ sufficiently for good convergence. We have found that the optimum is obtained by having roughly ten percent of the special points lying in the $|\mathbf{k}<|\mathbf{k}_0|$ region.

Once $|\mathbf{k}_0|$ has been fixed, g_0 is chosen (so as to weaken substantially the jump discontinuity at $|\mathbf{k}_0|$) as an average of the function $f(\mathbf{k})$ over the general set of $\mathbf{k}$ vectors having magnitude $|\mathbf{k}_0|$. In Table IV we give the evaluation (without extrapolation) of (6.1) for $\alpha=\frac{1}{8}$.

VII. DISCUSSION AND CONCLUDING REMARKS

We have provided formulas that strictly produce the Chadi-Cohen points and their corresponding weighting factors to any order of approximation, for the three cubic lattices and for the square lattice. The question arises as to the existence of simple formulas for the CC process in other lattices. For the hcp lattice, the process described by CC is equivalent to the use of a formula. While there is no guarantee that a simple formula can be found for other lattices, our results indicate that this problem is worth investigating at least for single-parameter lattices. For a lattice described by more than one parameter, the ratio of the lattice constants may be crucial for the determination of the weighting factors.

The process described by CC has here been modified slightly in that the terms in (2.2) have been grouped according to the symmetry type of the points R_m, rather than according to the magnitude of the R_m. The enumerations according to these two groupings are the last two columns of Table V. We have found this grouping useful in the development of the present formulas.

The only work that has approached the present calculation by means of formulas has been that of Monkhorst

TABLE V. Distribution of sites around the origin in the bcc lattice.

$C_m=\frac{\lvert\mathbf{R}\rvert^2}{a^2}$	Number of sites	Typical points in units of $a/2$ (s,t,u)	Shell number	SPW number
0.75	8	(1,1,1)	1	1
1	6	(2,0,0)	2	2
2	12	(2,2,0)	3	3
2.75	24	(3,1,1)	4	4
3	8	(2,2,2)	5	5
4	6	(4,0,0)	6	6
4.75	24	(3,3,1)	7	7
5	24	(4,2,0)	8	8
6	24	(4,2,2)	9	9
6.75	32	(3,3,3), (5,1,1)	10	10,11
8	12	(4,4,0)	11	12
8.75	48	(5,3,1)	12	13
9	30	(4,4,2), (6,0,0)	13	14,15
10	24	(6,2,0)	14	16
10.75	24	(5,3,3)	15	17
11	24	(6,2,2)	16	18
12	8	(4,4,4)	17	19
12.75	48	(5,5,1), (7,1,1)	18	20,21
13	24	(6,4,0)	19	22
14	48	(6,4,2)	20	23
14.75	72	(5,5,3), (7,3,1)	21	24,25
16	6	(8,0,0)	22	26

and Pack;[3] they found a formula which, at stage 2^ν, appears to have all the Chadi-Cohen points of order ν. However, the fact that their special points are not confined even to the first BZ renders their process computationally lengthy.

We have also shown that the convergence of the Chadi-Cohen method can be substantially accelerated by combining these formulas with an extrapolation procedure, and have further indicated how this method can be adapted to the calculation of integrals over periodic functions with (integrable) singularities by roughly minimizing the jump discontinuity in a combined CC–analytical integration calculation. The ten percent rule of thumb for finding the optimum value of $|\mathbf{k}_0|$ was arrived at by plotting the locus of $\mathbf{k}$ satisfying $f(\mathbf{k})=$const for various values of the constant, choosing the value such that the locus is most circular, and designating $|\mathbf{k}_0|$ to be the (rough) radius of that circle. In finding g_0, it has been found sufficient to take a rough average, say over three points: $(k_x,k_y)=(|\mathbf{k}_0|,0)$, $(0,|\mathbf{k}_0|)$, $(|\mathbf{k}_0|/\sqrt{2},|\mathbf{k}_0|/\sqrt{2})$.

The validity of the formulas presented here is attested by the reproduction of the Watson[4] sums to the sixth decimal place, and of the extrapolated values of Table IV to five decimal places at a relatively low value of ν. A proof by induction is in the process of being constructed.

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APPENDIX

The expansion (2.2) applied to the bcc lattice gives, for some of the first few SPW (typical points R_m are given in Table V; the lattice constant a is taken equal to unity),

$$A_1(\mathbf{k})=8\cos\tfrac{1}{2}k_x\cos\tfrac{1}{2}k_y\cos\tfrac{1}{2}k_z\ ,$$

$$A_2(\mathbf{k})=2(\cos k_x+\cos k_y+\cos k_z)\ ,$$

$$A_6(\mathbf{k})=2(\cos 2k_x+\cos 2k_y+\cos 2k_z)\ ,$$

$$A_{10}(\mathbf{k})=8(\cos\tfrac{3}{2}k_x\cos\tfrac{3}{2}k_y\cos\tfrac{3}{2}k_z)\ ,$$

$$A_{11}(\mathbf{k})=8(\cos\tfrac{5}{2}k_x\cos\tfrac{1}{2}k_y\cos\tfrac{1}{2}k_z+\cos\tfrac{1}{2}k_x\cos\tfrac{5}{2}k_y\cos\tfrac{1}{2}k_z+\cos\tfrac{1}{2}k_x\cos\tfrac{1}{2}k_y\cos\tfrac{5}{2}k_z)\ ;$$

where $\mathbf{k}$ is in units of $2\pi/a$.

Following CC we choose, for the zero of the first SPW, A_1,

$$\mathbf{k}_{\text{seed}}^{(1)}=(1,1,1)\pi\ . \tag{A1}$$

The set $\mathbf{k}_l^{(1)}$ consists of only one point, namely $\mathbf{k}_{\text{seed}}^{(1)}$. This point will, in addition, cause all the $A_m(\mathbf{k})$ contributions in (2.5), generated by points $\mathbf{R}=\frac{1}{2}(R_x,R_y,R_z)$ with R_x, R_y, and R_z all odd, to vanish; that is, $A_m(\mathbf{k}_{\text{seed}}^{(1)})=0$ for $m=1$, 4, 7, 10, 11, 13, 17, 20, 21, . . . (an infinity of m's, in fact).

The next SPW to examine is $A_2(\mathbf{k})$ which leads to

$$\mathbf{k}_{\text{seed}}^{(2)}=(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})\pi\ ; \tag{A2}$$

which will remove from Eq. (2.5) all $A_m(\mathbf{k})$ generated by points $\mathbf{R}$ having coordinates that are all odd multiples of 2 (in units of $\frac{1}{2}$); that is, for $m=2, 3, 5, 8, 9, 16, 18, 23, \ldots$.

A_3, A_4, and A_5 having been removed, one next examines $A_6(\mathbf{k})$ which has as a zero the point

$$\mathbf{k}_{\text{seed}}^{(3)}=(\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4})\pi \ ; \tag{A3}$$

$\mathbf{k}_{\text{seed}}^{(3)}$ will remove contributions to (2.5) by all $A_m(\mathbf{k})$ generated by points $\mathbf{R}$ with all coordinates equal to an odd multiple of 4 (in units of $\frac{1}{2}$); i.e., for $m=6$, (8 and 9 have already been removed at order 2), 12, 19, 22, ...

So far, all SPW up to $m=25$ have been removed from (2.5); $A_{26}(\mathbf{k})$ (not A_{28} as stated in CC) has as a zero the point

$$k_{\text{seed}}^{(4)}=(\tfrac{1}{8},\tfrac{1}{8},\tfrac{1}{8})\pi \ . \tag{A4}$$

Inserting (A1) and (A2) into (2.9) (with $\nu=2$) will clearly generate $\mathbf{k}$-space points with coordinates $\frac{1}{2}$ or $\frac{3}{2}$ (in units of π). Some of these points will be outside the IBZ and even outside the first BZ. Bringing them into the IBZ, one orders the coordinates such that $\mathbf{k}_x \geq \mathbf{k}_y \geq \mathbf{k}_z$ all of which, in units of $\pi/4$, will be odd positive integers. This operation leads to only two distinct $\mathbf{k}_l^{(2)}$:

$$\mathbf{k}_1^{(2)}=(3,1,1)\pi/4, \quad \alpha_1^{(2)}=\tfrac{1}{2} \ , \tag{A5a}$$

$$\mathbf{k}_2^{(2)}=(1,1,1)\pi/4, \quad \alpha_2^{(2)}=\tfrac{1}{2} \ . \tag{A5b}$$

Inserting (A3) and (A5) into (2.9) (with $\nu=3$), the $\mathbf{k}_l^{\nu-1}$ of (2.9) being given by (A5) and the $\mathbf{k}_{\text{seed}}^{\nu}$ by (A3), points are generated in $\mathbf{k}$ space with odd coordinates (in units of $\pi/8$) which, when brought back into the IBZ, are

$$\mathbf{k}_1^{(3)}=(1,1,1)\pi/8, \quad \alpha_1^{(3)}=\tfrac{1}{16} \ , \tag{A6a}$$

$$\mathbf{k}_2^{(3)}=(3,1,1)\pi/8, \quad \alpha_2^{(3)}=\tfrac{3}{16} \ , \tag{A6b}$$

$$\mathbf{k}_3^{(3)}=(3,3,1)\pi/8, \quad \alpha_3^{(3)}=\tfrac{3}{16} \ , \tag{A6c}$$

$$\mathbf{k}_4^{(3)}=(3,3,3)\pi/8, \quad \alpha_4^{(3)}=\tfrac{1}{16} \ , \tag{A6d}$$

$$\mathbf{k}_5^{(3)}=(5,1,1)\pi/8, \quad \alpha_5^{(3)}=\tfrac{3}{16} \ , \tag{A6e}$$

$$\mathbf{k}_6^{(3)}=(5,3,1)\pi/8, \quad \alpha_6^{(3)}=\tfrac{3}{16} \ , \tag{A6f}$$

$$\mathbf{k}_7^{(3)}=(5,3,3)\pi/8, \quad \alpha_7^{(3)}=\tfrac{1}{16} \ , \tag{A6g}$$

$$\mathbf{k}_8^{(3)}=(7,1,1)\pi/8, \quad \alpha_8^{(3)}=\tfrac{1}{16} \ . \tag{A6h}$$

The weighting factors are in sixteenths because each of Eqs. (A5) generates eight points. The final weighting factors depend on how many of the three coordinates are equal and whether the points lie on the surface of or inside the BZ (e.g., $\mathbf{k}_7^{(3)}$ lies on the surface of the BZ, while $\mathbf{k}_3^{(3)}$ lies inside the BZ). The bcc lattice formulas (4.2), (4.3), and (4.4) are now apparent.

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