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Non-recursive Chadi–Cohen integration over the Brillouin zone of cubic crystals

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ABSTRACT

We give closed-form non-recursive formulae for the Chadi–Cohen sets of special points associated with the bcc and fcc symmetries. The expressions are valid for arbitrary order n, which enters them as a parameter. This ameliorates the situation of the Chadi–Cohen method of integration over Brillouin zones, whose application to high-precision calculations has been severely limited by the difficulty of generating sets of special points of order higher than $n = 2$.

§1. INTRODUCTION

Most equations of solid-state theory describing macroscopic properties are expressed as integrals over the first Brillouin zone (BZ) of the $\mathbf{k}$ space. Quantitative results demand either simplified models that usually reduce the BZ to a sphere or numerical integration.

However, in those cases where determining the qualitative behaviour is not sufficient and precision is required, the standard methods of numerical integration may fail. Subintegral functions are normally sums of periodic functions with rather complex structure and the $\mathbf{k}$-space has to be discretized in a very high number of cells to achieve a reasonable accuracy. Rounding errors may contribute significantly to the total error. This problem is more than just a technical aspect because it affects a significant portion of the equations and methods that constitute the output of solid-state theory.

In an effort to consider the particularities of the BZ analytically, Baldereschi (1973) discovered the existence of a special point $\mathbf{k}_0$ in the BZ of cubic crystals, called by him the *mean value point*, which allows us to write the approximate expression

$$\frac{\Omega}{(2\pi)^3}\int_{\mathrm{BZ}} f(\mathbf{k})\,\mathrm{d}^3\mathbf{k} \approx f(\mathbf{k}_0), \tag{1}$$

where Ω is the volume of the primitive cell and $f(\mathbf{k})$ has cubic symmetry and the period of the reciprocal lattice. The error was surprisingly small in several calculations of charge density and energy of real systems.

Subsequently Chadi and Cohen (1973) developed a more elaborate method that consists essentially in determining a set of $\nu(n)$ special points $\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_{\nu(n)}$ in the irreducible BZ such that

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$$\frac{\Omega}{(2\pi)^3}\int_{BZ} f(\mathbf{k})\,d^3\mathbf{k} = \sum_{i=1}^{\nu(n)} \alpha_i f(\mathbf{k}_i) + \varepsilon_n, \tag{2}$$

where

$$\lim_{n\to\infty} \varepsilon_n = 0, \tag{3}$$

$n = 1, 2, \ldots$ determines the order of the approximation and the coefficients α_i do not depend on the function f but simply weight the number of points in the BZ that are equivalent to $\mathbf{k}_i$. The nth set has $\nu(n)$ points. The number n is related with the highest degree of vicinity in real space whose contribution is considered significant. The Chadi–Cohen sets of points are special because they optimize the speed at which the error ε_n goes to zero as n increases. They are generated recursively, starting from the set $n = 1$, which normally contains two points (Chadi and Cohen 1973).

Chadi and Cohen gave lists of their special points up to the order $n = 2$ for the cubic and hexagonal crystal symmetries, which are sufficient to establish the power of the method. However, accurate calculations for realistic systems may require a higher degree of approximation.

The convergence of the Chadi–Cohen method is extremely rapid. However, its application to high-precision calculations has been severely limited by the difficulty of generating sets of special points of order higher than $n = 2$. The recursive method established by Chadi and Cohen for determining the special points for each n is a rather involved procedure that becomes practicable only when the number of points $\nu(n)$ is small enough to examine them individually. Beyond $n = 3$ the procedure turns into too cumbersome a task.

MacGillivray and Scholl (1983) developed a computer program that generates the sets of special points for bcc and fcc lattices following a variant of the recursive procedure of Chadi and Cohen. However, the program was not able to reduce all equivalent points to a single representative point in the irreducible zone after each recursion step. This rapidly increases the number of points and lowers the associated weights α_i. The method again has a limit because the number of points become hardly manageable for orders higher than $n = 5$. MacGillivray and Scholl (1983) calculated in this way the lattice static Green functions of a number of cubic metals up to the order $n = 5$.

We report here the obtention of explicit non-recursive formulae for the Chadi–Cohen special points associated with the bcc and fcc cubic symmetries. The expressions are valid for arbitrary n, which enters them as a parameter. The explicit equations of the special points given here were obtained by incomplete induction. Then we used complete induction to demonstrate that the general equations for the n-dependent points satisfy the recursive definition given by Chadi and Cohen. To make sure that the set of points for each n is complete, that is no point or family of points is missing, we calculated simple integrals that can be analytically evaluated and performed a number of more elaborate calculations. The results for several values of n show strong convergence. We omit here the details of the inductive demonstration, which exhibits many branches and takes too much space. We give only a general description of it for the bcc lattice, which should be sufficient for those that may be interested in reproducing the technical steps.

Instead, we place emphasis on the practical results and on some examples of applications that illustrate the method, its accuracy and convergence. This means

that the article has a rather unusual structure because a sketch of the formal mathematical aspects is given at the end, after the examples for the applications.

In the past we applied our closed-form equations for the Chadi–Cohen sets to calculate the quantum diffusion of light species in several cubic metals (Rogan 1994, Lagos and Rogan 1995). We also calculated the static lattice Green functions of V, Nb, Ta, Ni, Pd, Pt and Cu, up to the order $n = 10$, and compared them with the data obtained by MacGillivray and Scholl *et al.* (1983), the agreement was very close. However, we never published these results.

In this report we intend to achieve the following:

(a) to provide explicit equations for the Chadi–Cohen sets of special points to any order n, valid for the bcc and fcc Bravais lattices;
(b) to show some straightforward applications that make apparent the rapid convergence of the method and give an idea of the errors associated with the succesive sets of points;
(c) to motivate other workers to search for non-recursive closed-form equations for the remaining crystal structures; our demonstration that the Chadi–Cohen sets of special points for the cubic lattices can be described this way suggests that the same may apply to other crystal symmetries.

§2. Bcc Bravais lattice

The Chadi–Cohen set of order n associated with bcc lattices, which we denote by $B^{(n)}$, is split into two subsets. In units of $2\pi/a$, where a is the lattice parameter, they are given by

$$B_1^{(n)} = \left\{ \frac{1}{2^{n+1}} (2i - 1, 2j - 1, 2\ell - 1) \right| \begin{array}{l} i = 1, 2, \ldots, 2^{n-1}; \\ j = 1, 2, \ldots, i; \\ \ell = 1, 2, \ldots, j \end{array} \right\}, \tag{4}$$

whose points are associated with the weights

$$\alpha(n; i, j, \ell) = \frac{3(1 - \delta_{ij}) + 3(1 - \delta_{j\ell}) + \delta_{i\ell}}{2 \times 8^{n-1}} \tag{5}$$

and

$$B_2^{(n)} = \left\{ \frac{1}{2^{n+1}} (2i - 1, 2j - 1, 2\ell - 1) \right| \begin{array}{l} i = 2^{n-1} + 1, 2^{n-1} + 2, \ldots, 2^n; \\ j = 1, 2, \ldots, 2^n + 1 - i; \\ \ell = 1, 2, \ldots, j \end{array} \right\}, \tag{6}$$

with the weights

$$\alpha(n; i,j,\ell) = \frac{3(1-\delta_{i+j,2^{n}+1}) + 3(1-\delta_{j\ell}) + \delta_{j\ell}\delta_{i+j,2^{n}+1}}{2\times 8^{n-1}}. \tag{7}$$

The total number of special points of $B^{(n)} = B_1^{(n)} \cup B_2^{(n)}$ is

$$|B^{(n)}| = \frac{2^{n-1}(2^{n-1}+1)(2^{n-1}+2)}{3}. \tag{8}$$

§ 3. Fcc Bravais lattice

The set $F^{(n)}$ of special points of order n for the fcc cubic lattice is more complex and was separated into seven subsets. They are

$$F_1^{(n)} = \left\{ \frac{1}{2^{n+1}}(2i-1, 2j-1, 2\ell-1) \middle| \begin{array}{l} i = 1,2,\ldots,2^{n-1}; \\ j = 1,2,\ldots,i; \\ \ell = 1,2,\ldots,j \end{array} \right\}, \tag{9}$$

$$F_2^{(n)} = \left\{ \frac{1}{2^{n+1}}(2i-1, 2j-1, 2\ell-1) \middle| \begin{array}{l} i = 2^{n-1}+2, 2^{n-1}+4,\ldots,2^{n}; \\ j = 1,2,\ldots,3\times 2^{n-2} - \dfrac{i}{2}; \\ \ell = 1,2,\ldots,j \end{array} \right\}, \tag{10}$$

$$F_3^{(n)} = \left\{ \frac{1}{2^{n+1}}(2i-1, 2j-1, 2\ell-1) \middle| \begin{array}{l} i = 2^{n-1}+2, 2^{n-1}+4,\ldots,3\times 2^{n-2}; \\ j = 3\times 2^{n-2} - \dfrac{i}{2} + 1, 3\times 2^{n-2} - \dfrac{i}{2} + 2,\ldots,i; \\ \ell = 1,2,\ldots,3\times 2^{n-1} + 1 - i - j \end{array} \right\}, \tag{11}$$

$$F_4^{(n)} = \left\{ \frac{1}{2^{n+1}}(2i-1, 2j-1, 2\ell-1) \middle| \begin{array}{l} i = 3\times 2^{n-2} + 2, 3\times 2^{n-2} + 4,\ldots,2^{n}; \\ j = 3\times 2^{n-2} - \dfrac{i}{2} + 1, 3\times 2^{n-2} - \dfrac{i}{2} + 2,\ldots,3\times 2^{n-1} - i; \\ \ell = 1,2,\ldots,3\times 2^{n-1} + 1 - i - j \end{array} \right\}, \tag{12}$$

$$F_5^{(n)} = \left\{ \frac{1}{2^{n+1}} (2i - 1, 2j - 1, 2\ell - 1) \middle| \right.$$
$$i = 2^{n-1} + 1, 2^{n-1} + 3, \ldots, 2^n - 1;$$
$$j = 1, 2, \ldots, 3 \times 2^{n-2} - \frac{i-1}{2};$$
$$\left. \ell = 1, 2, \ldots, j \right\}, \tag{13}$$

$$F_6^{(n)} = \left\{ \frac{1}{2^{n+1}} (2i - 1, 2j - 1, 2\ell - 1) \middle| \right.$$
$$i = 2^{n-1} + 1, 2^{n-1} + 3, \ldots, 3 \times 2^{n-2} - 1;$$
$$j = 3 \times 2^{n-2} - \frac{i-1}{2} + 1, 3 \times 2^{n-2} - \frac{i-1}{2} + 2, \ldots, i;$$
$$\left. \ell = 1, 2, \ldots, 3 \times 2^{n-1} + 1 - i - j \right\} \tag{14}$$

and

$$F_7^{(n)} = \left\{ \frac{1}{2^{n+1}} (2i - 1, 2j - 1, 2\ell - 1) \middle| \right.$$
$$i = 3 \times 2^{n-2} + 1, 3 \times 2^{n-2} + 3, \ldots, 2^n - 1;$$
$$j = 3 \times 2^{n-2} - \frac{i-1}{2} + 1, 3 \times 2^{n-2} - \frac{i-1}{2} + 2, \ldots, 3 \times 2^{n-1} - i;$$
$$\left. \ell = 1, 2, \ldots, 3 \times 2^{n-1} + 1 - i - j \right\}. \tag{15}$$

The relative weights are given by

$$\alpha(n; i, j, \ell) = \frac{3(1 - \delta_{ij}) + 3(1 - \delta_{j\ell}) + \delta_{i\ell}}{4 \times 8^{n-1}} \tag{16}$$

and the total number of points of $F^{(n)} = \bigcup_{\mu=1}^{7} F_\mu^{(n)}$ is

$$|F^{(n)}| = \frac{2^{n-1}(2^n + 1)(2^{n-1} + 1)}{3}. \tag{17}$$

These relations for fcc lattices are valid for any n and can be blindly applied for $n > 2$. However, care must be taken in the well known cases $n = 1$ and $n = 2$. In both situations the definitions of the intervals for the indices i, j, ℓ in some of the subsets determine fractional, negative or null values for them. The rule is just to discard anomalous indices.

For $n = 1$ the first subset $F_1^{(1)}$ has no problem. In $F_4^{(1)}$, only the upper limits $i = 2$ and $j = \ell = 1$ must be taken into account. All indices in the other subsets are fractional and are thus discarded. For $n = 2$ the subsets $F_1^{(2)}$, $F_2^{(2)}$ and $F_5^{(2)}$ have no problem and $F_3^{(2)} = F_6^{(2)} = \phi$ show anomalous indices. Only the upper limits $i = 4$ and $i = 3$ are regular in $F_4^{(2)}$ and $F_7^{(2)}$, respectively. No anomaly occurs for larger values of n.

§4. Simple and more elaborate applications

To illustrate how the proposed scheme works we apply it to evaluate two integrals, over the BZ of the bcc and fcc lattices, whose exact results are known. They are

$$I_B = \frac{\Omega}{(2\pi)^3}\int_{\mathrm{BZ\,bcc}} k^2\,\mathrm{d}^3k = \frac{3}{8}\left(\frac{2\pi}{a}\right)^2 \qquad (18\,a)$$

and

$$I_F = \frac{\Omega}{(2\pi)^3}\int_{\mathrm{BZ\,fcc}} k^2\,\mathrm{d}^3k = \frac{19}{32}\left(\frac{2\pi}{a}\right)^2 \qquad (18\,b)$$

respectively. Because of the numerical rounding error, which increases with increasing n, we determined that the total error has a minimum for about $n = 6$ when simple precision is used. Using double precision the error decreases monotonically even for $n = 10$. Table 1 shows the values obtained with double precision for I_B and I_F for different values of n, together with the relative error.

Tables 2 and 3 illustrate the results of more elaborate calculations. Columns B show our results for the static lattice Green functions calculated for the cubic metals V, Nb, Ta, Ni, Pd and Pt. Columns A show the values obtained previously by MacGillivray and Scholl (1983). The apparent agreement contributes to corroborate these previous calculations.

The calculation of Green functions involve integration over the BZ of complex functions depending on the dispersion relations $\omega_{\mathbf{k}\mu}$ of the crystal modes, where $\mathbf{k}$ and μ are the wave-vector and branch index respectively (MacGillivray and Sholl 1983). The frequencies $\omega_{\mathbf{k}\mu}$ and polarization vectors of the modes at each point of the BZ were calculated from the force constants obtained from neutron inelastic scattering experiments, together with the corresponding models for the crystal dynamics. In general we used the same model employed to analyse the neutron data by the authors of each experiment (Birgeneau *et al.* 1963, Woods 1964, Collela and Batterman 1970, Miiller and Brockhouse 1971, Dutton *et al.* 1972, Powell *et al.* 1977).

Table 1. Values of the integrals I_B and I_F obtained from the successive Chadi–Cohen sets of special points.

n	$\lvert B^{(n)}\rvert$	I_B (units of $(2\pi/a)^2$)	Error (%)	$\lvert F^{(n)}\rvert$	I_F (units of $(2\pi/a)^2$)	Error (%)
1	2	0.437 500 00	16.666 67	2	0.562 500 00	5.263 16
2	8	0.390 625 00	4.166 67	10	0.585 937 50	1.315 79
3	40	0.378 906 25	1.041 67	60	0.591 796 88	0.328 95
4	240	0.375 976 56	0.260 42	408	0.593 261 72	0.082 24
5	1 632	0.375 244 14	0.065 10	2 992	0.593 627 93	0.020 56
6	11 968	0.375 061 04	0.016 28	22 880	0.593 719 48	0.005 14
7	91 520	0.375 015 26	0.004 07	178 880	0.593 742 37	0.001 29
8	715 520	0.375 003 82	0.001 02	1 414 528	0.593 748 09	0.000 32
9	5 658 112	0.375 000 95	0.000 25	112 504 32	0.593 749 52	0.000 08
10	45 001 728	0.375 000 24	0.000 06	89 740 800	0.593 749 88	0.000 02

Table 2. Static lattice Green functions of some bcc metals. Columns A and B show the results of MacGillivray and Scholl and our results respectively.

		Green function (10^{-2} m N^{-1})					
		V		Nb		Ta	
$2l/a$	ij	A	B	A	B	A	B
(0, 0, 0)	11, 22, 33	1.523	1.569	1.399	1.573	1.065	1.063
(1, 1, 1)	11, 22, 33	0.468	0.490	0.507	0.587	0.339	0.337
	23, 13, 12	0.084	0.088	0.070	0.077	0.070	0.070
(2, 0, 0)	11	0.432	0.451	0.511	0.631	0.259	0.258
	22, 33	0.335	0.353	0.384	0.427	0.257	0.256
(2, 2, 0)	11, 22	0.329	0.343	0.354	0.400	0.228	0.227
	33	0.208	0.221	0.251	0.231	0.157	0.156
	12	0.050	0.051	0.053	0.062	0.052	0.052
(3, 1, 1)	11	0.304	0.317	0.315	0.421	0.197	0.195
	22, 33	0.220	0.232	0.241	0.232	0.156	0.154
	23	−0.004	−0.003	0.0003	−0.001	0.002	0.002
	13, 12	0.032	0.034	0.034	0.041	0.024	0.024
(2, 2, 2)	11, 22, 33	0.241	0.247	0.258	0.266	0.178	0.177
	23, 13, 12	0.040	0.046	0.030	0.032	0.041	0.041
(4, 0, 0)	11	0.242	0.253	0.315	0.340	0.140	0.138
	22, 33	0.173	0.185	0.184	0.185	0.116	0.115
(3, 3, 1)	11, 22	0.206	0.211	0.229	0.235	0.146	0.144
	33	0.144	0.152	0.167	0.150	0.114	0.112
	23, 13	0.006	0.015	0.009	0.005	0.009	0.009
	12	0.044	0.038	0.041	0.050	0.041	0.041
(4, 2, 0)	11	0.233	0.240	0.271	0.309	0.147	0.146
	22	0.178	0.189	0.194	0.188	0.123	0.122
	33	0.150	0.158	0.162	0.146	0.108	0.107
	12	0.039	0.037	0.038	0.051	0.031	0.031
(4, 2, 2)	11	0.203	0.211	0.230	0.251	0.136	0.134
	22, 33	0.148	0.154	0.163	0.150	0.108	0.107
	23	0.010	0.014	0.008	0.003	0.009	0.009
	13, 12	0.025	0.028	0.026	0.027	0.023	0.023

§ 5. The formal demonstrations

As was mentioned in the introduction, the special points were first obtained by incomplete induction and then proven by complete induction. Applying the Chadi–Cohen recursive procedure to the sets of order $n = 1, 2$ and 3 one can gain experience on the structure of the next set and on how this structure evolves when the recursion procedure is iterated. The task is quite involved because the recursion rule does not ensure that the resulting points are in the irreducible part of the BZ. The reduction to the irreducible zone by adding a vector of the reciprocal lattice determines the coefficients α_i and the several families of points. The goal of this process is to identify the families that remain stable for successive iterations. This can be recognized by testing that the application of the Chadi–Cohen recursion procedure to any representative of a family gives a point of the same family in the next set. This way, it is not necessary to derive the whole Chadi–Cohen set of next order for testing that the families of points are stable, which is quite fortunate for $n = 3$.

Table 3. Static lattice Green functions of some fcc metals. Columns A and B show the results of MacGillivray and Scholl and our results respectively.

		Green function (10^{-2} m N^{-1})							
		Ni		Pa		Pt		Cu	
$2l/a$	ij	A	B	A	B	A	B	A	B
(0, 0, 0)	11, 22, 33	1.112	1.111	1.371	1.340	1.068	1.068	1.616	1.614
(1, 1, 0)	11, 22	0.328	0.327	0.488	0.474	0.367	0.370	0.508	0.506
	33	0.264	0.263	0.406	0.397	0.284	0.283	0.412	0.410
	12	0.114	0.114	0.156	0.156	0.120	0.121	0.180	0.180
(2, 0, 0)	11	0.177	0.176	0.273	0.255	0.222	0.224	0.258	0.257
	22, 33	0.177	0.176	0.293	0.286	0.204	0.205	0.285	0.283
(2, 1, 1)	11	0.184	0.183	0.279	0.267	0.215	0.217	0.284	0.282
	22, 33	0.165	0.164	0.253	0.243	0.172	0.171	0.259	0.257
	23	0.021	0.021	0.048	0.053	0.037	0.039	0.040	0.040
	13, 12	0.039	0.039	0.071	0.072	0.049	0.047	0.066	0.066
(2, 2, 0)	11, 22	0.173	0.172	0.248	0.238	0.176	0.175	0.267	0.265
	33	0.133	0.132	0.188	0.175	0.120	0.118	0.203	0.201
	12	0.062	0.062	0.092	0.086	0.059	0.061	0.106	0.106
(3, 1, 0)	11	0.124	0.123	0.179	0.171	0.154	0.153	0.176	0.175
	22	0.123	0.122	0.188	0.181	0.129	0.128	0.193	0.191
	33	0.117	0.115	0.170	0.161	0.115	0.115	0.180	0.178
	12	0.019	0.019	0.035	0.032	0.023	0.023	0.033	0.033
(2, 2, 2)	11, 22, 33	0.125	0.124	0.197	0.192	0.142	0.141	0.197	0.195
	23, 13, 12	0.030	0.030	0.065	0.065	0.038	0.035	0.053	0.053
(3, 2, 1)	11	0.123	0.122	0.185	0.178	0.141	0.142	0.189	0.187
	22	0.116	0.115	0.178	0.171	0.122	0.120	0.184	0.182
	33	0.103	0.102	0.148	0.141	0.101	0.101	0.159	0.157
	23	0.014	0.014	0.030	0.030	0.018	0.018	0.026	0.026
	13	0.018	0.018	0.033	0.032	0.019	0.018	0.030	0.030
	12	0.034	0.034	0.058	0.055	0.036	0.037	0.059	0.059
(4, 0, 0)	11	0.093	0.092	0.128	0.129	0.121	0.123	0.124	0.123
	22, 33	0.094	0.093	0.140	0.133	0.096	0.095	0.148	0.146

After identifying the points, their weights α_i and analytic expressions valid for $n = 1$, 2 and 3, and testing family stability for $N = 4$, complete induction is used to demonstrate that the results hold for any n. Although the general idea is simple, its realization involves many cases whose detailed description would take too much space.

Consider, for instance, the set of equations (4)–(8) for the bcc lattice. They give the correct set of points for $n = 1$. Hence it remains to show that the application of the Chadi–Cohen original algorithm to the sets $B_1^{(n)}$ and $B_2^{(n)}$ gives $B_1^{(n+1)}$ and $B_2^{(n+1)}$, consistently with equations (4) and (5). That is, adding the eighth vectors

$$\left(\pm\frac{1}{2^{m+2}}, \pm\frac{1}{2^{m+2}}, \pm\frac{1}{2^{m+2}}\right) \tag{19}$$

to each vector of the sets given by equations (4) and (5), and then reducing the resulting vectors to the irreducible zone, one obtains the same equations (4) and (5) with n replaced by $n + 1$.

To accomplish this program it is convenient to split each set $B_1^{(n)}$ and $B_2^{(n)}$ into subsets of vectors that have the same weight factor α_i. There are four such subsets in each set. The task demands some time and patience. Although the closed-form equations determining the Chadi–Cohen set of points for the fcc lattice seem more involved than those for the bcc symmetry, their proofs are of similar length.

§6. Final remarks

With the formulae given above the computer subroutine for Chadi–Cohen integration becomes very short and rapid. However, the method has inherent limitations. As the density of points is not uniform it may be inaccurate if the subintegral function has a sharp step that separates the BZ into two sectors. In these cases the method gives values that are influenced by the number of special points in the two sectors. The same applies for functions whose integral is dominated by sharp maxima. This way, the method is not accurate in electronic calculations involving the Fermi distribution at low temperatures. Any simple s-band calculation serves to illustrate the point. At $T \approx 0$ the dependence on n of the results show steps and may converge to wrong values.

The method gives excellent accuracy for functions that vary smoothly, even if they exhibit complex structure.

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