JOURNAL OF COMPUTATIONAL PHYSICS 10, 316–323 (1972)

Evaluation of Integrals over the Brillouin Zone by Houston's Method

S. P. SINGHAL

Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803

The weight factors for the Houston's method of integration are presented up to 16 terms. The results of Betts and Betts, Bhatia and Wyman contain a subtle error which is here pointed out and resolved.

I. INTRODUCTION

Integrals of the following type appear frequently in Solid State theory:

$$I = \int F(\mathbf{q})\, d^3q, \tag{1}$$

where $\mathbf{q}$ is a vector in the first Brillouin zone (IBZ) and the integration is taken over the entire volume of IBZ. The function F may be invariant under some or all operations of the cubic group O_h. A simple method for evaluating such integrals was given by Houston [1] in 1948.

Such integrals (using Houston's method) appear, for example, in the evaluation of Debye Temperatures [1–6], studies of specific heat [6, 7], thermal expansion coefficients [8] and phonon spectra [7, 9], comparison of de Haas–van Alphen data [10] with band structure calculations and in the study of solid state scattering [11].

Houston's method of evaluating the integral in (1) is based on expanding the function $F(\mathbf{q})$ in terms of the cubic harmonics of van der Lage and Bethe [12], i.e.,

$$F(q, \theta, \phi) = \sum_j a_j(q)\, K_j(\theta, \phi), \tag{2}$$

and the orthogonality of the K_j's

$$\int_0^{\pi} \int_0^{2\pi} K_j K_{j'} \sin\theta\, d\theta\, d\phi = 0, \qquad j \neq j'. \tag{3}$$

We find that

$$I = \frac{N_1}{K_1} \int dq\, q^2 a_1(q), \tag{4}$$

where K_1, the first cubic harmonic (often referred to as K_0) is a constant and N_1 is the normalization constant for K_1.

To obtain $a_1(q)$, one evaluates the quantity $F(\mathbf{q})$ in as many directions as the terms desired (for convergence) in the expansion on the right hand side of (2).

For other integrals where $F(\mathbf{q})$ is multiplied by a factor proportional to one of the cubic harmonics, we simply have moments of higher order and $a_1(q)$ is replaced by an appropriate $a_j(q)$ in (4).

In the theory of solid state scattering [11], one encounters integrals similar to (1) but $F(\mathbf{q})$ may not have the complete symmetry of the cubic group O_h. In such a case, we can use

$$F(\mathbf{q}) = \frac{1}{48} \sum_{\beta=1}^{48} F(\beta\mathbf{q}), \tag{5}$$

where β goes over the operations of the cubic group. The partial symmetry of $F(\mathbf{q})$ will reduce the β sum to a smaller number of terms (than the 48 shown above).

Houston [1] terminated the expansion in (2) with only three terms. That type of interpolation puts too much emphasis on the three directions used and the results are not accurate enough. To improve the accuracy, expansions have been made for 6 terms (Betts *et al.* [2]) and for 9 and 15 terms (Betts [3]). As we shall see later, these results contain subtle errors because all linearly independent combinations for a given l have not been included.

Since Houston's method replaces the IBZ by an equivalent sphere, there are errors introduced depending upon the discrepancy between the two. Corrections have been provided in terms of normalization factors [4, 5].

In this paper, we evaluate the coefficient $a_1(q)$ for different number of directions (up to 16) for cases where better accuracy is desired. For a face-centered cubic lattice, the results are applicable with a constant normalization. For other cases, one can use the normalization constants of Ganesan and Srinivasan [4] suitably adjusted.

2. General Theory

The cubic harmonics are suitable linear combinations of the spherical harmonics. There has been a considerable amount of work done [2, 10, 12–14] in evaluating these combinations, the most exhaustive being the work of Mueller and Priestley [10].

The cubic harmonics can be written as [10]

$$K_j = \sum_m a_{lm}^{(j)} c_{lm}, \tag{6}$$

where

$$c_{lm} = \frac{1}{\sqrt{2}} (Y_{lm} + Y_{l,-m}), \tag{6a}$$

$$c_{l0} = Y_{l0}, \tag{6b}$$

and $a_{lm}^{(j)}$ are the expansion coefficients. The value of l depends on j while m takes on values 0, 4, 8,..., $m_{\max}$. $m_{\max}$ is the largest integer divisible by 4 and is $\leqslant l$. The cubic harmonics thus defined are orthonormal over the unit sphere. The allowed values of l are even and $l = 4$ is the smallest value that gives rise to a combination with cubic symmetry (except $l = 0$ which gives a constant). The number of linearly independent combinations for a given l is given by the coefficient of $x^{l/2}$ in the expansion

$$[(1 - x^2)(1 - x^3)]^{-1} = 1 + x^2 + x^3 + x^4 + x^5 + 2x^6 + \cdots . \tag{7}$$

The first case of "degeneracy" appears when $l = 12$. There must be two combinations formed from $l = 12$. Since such a choice is not unique, when one terminates the expansion (2), it must be such that all independent combinations for a given l are used. This fact is overlooked by Betts *et al.* [2] and Betts [3]. Table I gives the corresponding values of j and l (for l up to 30). For a given l, one must use the largest value of j shown to invert (2).

(A) *Evaluation of a_j's*

To evaluate the coefficients $a_j(q)$ in (2) for a given value of q (magnitude of $\mathbf{q}$), we rewrite (2) omitting the q dependence (for n terms)

$$F(\theta, \phi) = \sum_{j=1}^{n} a_j K_j(\theta, \phi). \tag{8}$$

To evaluate a_j's, we choose n directions θ_s, ϕ_s for $s = 1, 2,..., n$ and define the matrices Q and $\mathscr{F}$ such that

$$Q_{ij} = K_j(\theta_i, \phi_i) \tag{9a}$$

and

$$\mathscr{F}_i = F(\theta_i, \phi_i), \tag{9b}$$

such that (8) becomes a matrix equation

$$\mathscr{F}_i = \sum_{j=1}^{n} Q_{ij} a_j, \qquad i = 1, 2,..., n, \tag{10a}$$

TABLE I

Values of l and m for K_j ($j = 1$ to 27) and the suggested directions up to $j = 16$.

j	l	m	Suggested direction[a]
1	0	0	⟨100⟩
2	4	0, 4	⟨110⟩
3	6	0, 4	⟨111⟩
4	8	0, 4, 8	⟨321⟩
5	10	0, 4, 8	⟨831⟩
6	12	0, 4, 8, 12	⟨210⟩
7	12	0, 4, 8, 12	⟨211⟩
8	14	0, 4, 8, 12	⟨441⟩
9	16	0, 4, 8, 12, 16	⟨741⟩
10	16	0, 4, 8, 12, 16	⟨411⟩
11	18	0, 4, 8, 12, 16	⟨221⟩
12	18	0, 4, 8, 12, 16	⟨410⟩
13	20	0, 4, 8, 12, 16, 20	⟨732⟩
14	20	0, 4, 8, 12, 16, 20	⟨651⟩
15	22	0, 4, 8, 12, 16, 20	⟨821⟩
16	22	0, 4, 8, 12, 16, 20	⟨543⟩
17	24	0, 4, 8, 12, 16, 20, 24	
18	24	0, 4, 8, 12, 16, 20, 24	
19	24	0, 4, 8, 12, 16, 20, 24	
20	26	0, 4, 8, 12, 16, 20, 24	
21	26	0, 4, 8, 12, 16, 20, 24	
22	28	0, 4, 8, 12, 16, 20, 24, 28	
23	28	0, 4, 8, 12, 16, 20, 24, 28	
24	28	0, 4, 8, 12, 16, 20, 24, 28	
25	30	0, 4, 8, 12, 16, 20, 24, 28	
26	30	0, 4, 8, 12, 16, 20, 24, 28	
27	30	0, 4, 8, 12, 16, 20, 24, 28	

[a] Given only up to 16 terms. Minimum number of terms desirable in terminating the expansion in (2) is three.

with the solution

$$a_j = \sum_{i=1}^{n} (Q^{-1})_{ji} \mathscr{F}_i , \qquad j = 1, 2,..., n. \tag{10b}$$

Due to cubic symmetry, the directions in the unit sphere are equivalent to those in the 1/48th segment with the bounding interior planes $k_z = 0$, $k_x = k_y$ and $k_y = k_z$. We should choose the directions (θ_i , ϕ_i) in such a way that they are distributed evenly as far as possible over this segment (or any other equivalent segment) and are such that the evaluation of the integrand is simple. The three directions often used are (100), (110) and (111). For larger n, the suggested directions (based purely on distribution in this segment) are given in Table I and roughly shown as planar projections in Fig. 1.

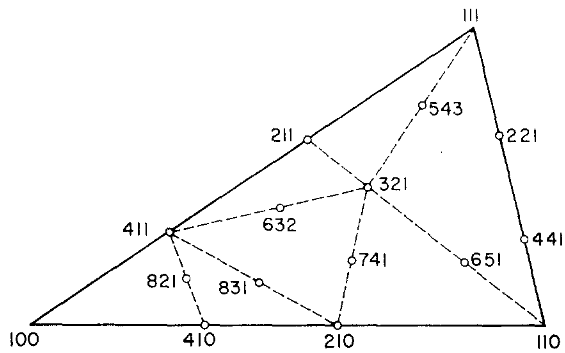

FIG. 1. Planar projections of the suggested directions.

Table II gives the values of $(Q^{-1})_{ji}$ for the case of $n = 5$. Since K_1 is a constant (equal to $1/(4\pi)^{1/2}$), the integral in (1) becomes

$$I = (4\pi)^{1/2} \int dq\, q^2 \left(\sum_{i=1}^{n} (Q^{-1})_{1i}\, \mathscr{F}_i(q) \right). \tag{11}$$

TABLE II

The coefficients $(Q^{-1})_{ji}$ for the five-term expansion and the corresponding directions

j	Directions for diff i	⟨100⟩ 1	⟨110⟩ 2	⟨111⟩ 3	⟨321⟩ 4	⟨831⟩ 5
1		0.23353051	0.32877823	0.31545227	1.56319692	1.10394979
2		0.47199890	−0.19855325	−0.45511268	−0.98577917	1.16744620
3		0.34336476	−0.95782087	0.50765313	0.43792425	−0.33112127
4		0.45743050	0.66009805	0.27188482	−0.69197970	−0.69743367
5		0.23224970	−0.32204923	−0.38440648	1.15943840	−0.68523240

For cases of n up to 16, a_1 is given below in Eqs. (12a)–(12i) using the suggested directions:

$$a_1^{(3)} = (1.012831)\, F(100) + (1.620529)\, F(110) + (0.911548)\, F(111), \tag{12a}$$

$$a_1^{(4)} = (0.607698)\, F(100) - (0.190062)\, F(110) - (0.303849)\, F(111) + (3.431121)\, F(321), \tag{12b}$$

$$a_1^{(5)} = (0.233531)\,F(100) + (0.328778)\,F(110) + (0.315452)\,F(111) + (1.563197)\,F(321) + (1.103950)\,F(831), \tag{12c}$$

$$a_1^{(7)} = (0.213058)\,F(100) + (0.370902)\,F(110) + (0.323287)\,F(111) + (1.534489)\,F(321) + (1.233336)\,F(831) - (0.124902)\,F(210) - (0.0052625)\,F(211), \tag{12d}$$

$$a_1^{(8)} = (0.221613)\,F(100) + (0.110091)\,F(110) + (0.294637)\,F(111) + (0.635562)\,F(321) + (1.083847)\,F(831) + (0.137543)\,F(210) + (0.474521)\,F(211) + (0.587092)\,F(441), \tag{12e}$$

$$a_1^{(10)} = (0.189198)\,F(100) + (0.562487)\,F(110) + (0.277915)\,F(111) + (2.498654)\,F(321) - (0.442905)\,F(831) + (1.743576)\,F(210) - (0.230456)\,F(211) - (0.354493)\,F(441) - (1.642709)\,F(741) + (0.943639)\,F(411), \tag{12f}$$

$$a_1^{(12)} = (0.138472)\,F(100) + (0.351457)\,F(110) + (0.234507)\,F(111) + (1.246640)\,F(321) - (0.230632)\,F(831) + (0.875489)\,F(210) + (0.184069)\,F(211) - (0.0332286)\,F(441) - (0.341204)\,F(741) + (0.679635)\,F(411) + (0.225170)\,F(221) + (0.214534)\,F(410), \tag{12g}$$

$$a_1^{(14)} = (0.127178)\,F(100) + (0.110069)\,F(110) + (0.174104)\,F(111) - (0.0146192)\,F(321) + (0.550694)\,F(831) - (0.345529)\,F(210) + (0.627955)\,F(211) - (0.0248196)\,F(441) + (1.066374)\,F(741) + (0.310125)\,F(411) + (0.520343)\,F(221) + (0.258138)\,F(410) - (0.167635)\,F(732) + (0.352530)\,F(651), \tag{12h}$$

and

$$a_1^{(16)} = (0.101332)\,F(100) + (0.191861)\,F(110) + (0.109811)\,F(111) + (0.326929)\,F(321) + (0.0450450)\,F(831) + (0.0395619)\,F(210) + (0.342493)\,F(211) + (0.255739)\,F(441) + (0.783543)\,F(741) + (0.603400)\,F(411) + (0.216117)\,F(221) + (0.605269)\,F(410) + (0.0208283)\,F(732) - (0.0269079)\,F(651) - (0.378570)\,F(821) + (0.308456)\,F(543), \tag{12i}$$

where $a_1^{(n)}$ is the n-term approximation for a_1 and $F(klm)$ is the value of the function $F(\mathbf{q})$ in the direction (k, l, m). The coefficients for $a_j (j > 1)$ for the above cases are available from the author.

3. Conclusions

It is found that Houston's method is useful in evaluating integrals over the Brillouin zone. It reduces the integral over the sphere (solid angles 0 to 4π) to a sum of a few terms, when the integrand has the cubic symmetry. In cases where the integrand has only partial symmetry, two sums must be performed, one over the operators of the cubic group and the other for evaluating a_1.

One specific case where this method has been used by the present author [11] is the study of an interstitial in silicon. We encounter integrals over the Brillouin Zone of quantities that do not possess the cubic symmetry. The integrand is of the type

$$I = \int g(\mathbf{k})\, d^3k, \tag{13}$$

where

$$g(\beta\mathbf{k}) = g(\mathbf{k}) \tag{13a}$$

for β's satisfying

$$\beta\mathbf{k} = \mathbf{k}. \tag{13b}$$

The above method is used by symmetrizing the integrand, i.e.,

$$I = \frac{1}{48} \int \left(\sum_{\beta=1}^{48} g(\beta\mathbf{k}) \right) d^3k \tag{14}$$

$$= \frac{\sqrt{4\pi}}{48} \int k^2\, dk \sum_{i=1}^{n} (Q^{-1})_{1i} \sum_{\beta=1}^{48} g(k\beta\hat{k}_i). \tag{14a}$$

The sum over β can now be reduced to the operations of the factor group O_h/(group of $\hat{k}_i$). The k integral can then be done by other techniques (Gaussian method, for example).

It is noted that for certain values of l, there are more than one independent combinations with the cubic symmetry. The first such case appears for $l = 12$. Thus to include properly all the terms of that order in our expansion (2), we must include all K_j's with the same l. Consequently, the results derived by Betts *et al.* [2] and Betts [3] for 6, 9 and 15 terms are incorrect. We give the results for the correct number of terms, up to 16 term expansions.

For those who would like to use either different directions than those suggested here or a larger number of terms in the expansion, the author will supply the computer program on request.

The computer time in evaluating a typical integral with say 16 terms, is a few seconds on IBM-360-65.

Acknowledgments

The author would like to thank A. K. Rajagopal and J. Callaway for many helpful discussions.

REFERENCES

1. W. V. HOUSTON, *Rev. Mod. Phys.* **20** (1948), 161.
2. D. D. BETTS, A. B. BHATIA, AND MAX WYMAN, *Phys. Rev.* **104** (1956), 37.
3. D. D. BETTS, *Canad. J. Phys.* **39** (1961), 233.
4. S. GANESAN AND R. SRINIVASAN, *Canad. J. Phys.* **40** (1962), 1153.
5. S. GANESAN AND R. SRINIVASAN, *Indian J. Pure Appl. Phys.* **1** (1963), 282.
6. S. GANESAN AND R. SRINIVASAN, *Proc. Nat. Inst. of Sci. (India)* **29** (1963), 389.
7. S. GANESAN AND R. SRINIVASAN, *Canad. J. Phys.* **40** (1962), 74.
8. S. GANESAN AND R. SRINIVASAN, *Canad. J. Phys.* **40** (1962), 91.
9. A. K. RAJAGOPAL AND R. SRINIVASAN, *Z. Phys.* **158** (1960), 471.
10. F. M. MUELLER AND M. G. PRIESTLEY, *Phys. Rev.* **148** (1966), 638.
11. S. P. SINGHAL, *Phys. Rev. B* 4 (1971), 2497.
12. F. C. VON DER LAGE AND H. A. BETHE, *Phys. Rev.* **71** (1947), 612.
13. D. G. BELL, *Rev. Mod. Phys.* **26** (1954), 311.
14. S. L. ALTMANN AND A. P. CRACKNELL, *Rev. Mod. Phys.* **37** (1965), 19.