Evaluation of Brillouin-Zone Sums on the Cubic Lattices

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Simple prescriptions are given for the evaluation of Brillouin-zone sums on the cubic lattices for cases where the functions are known analytically and may have a singularity at the zone center. An octant of the zone is sampled by a weighted random distribution of points which can be readily adjusted to give a greater density of sampling points near the center of the zone. The prescriptions are tested by application to Watson's integrals whose integrands have a singularity at the zone center. An accuracy of 1 % is realized with a sample of 10 000 points in **k** space.

I. INTRODUCTION

Brillouin-zone sums arise in solid-state theories covering a very broad spectrum of phenomena because they are a direct consequence of the lattice periodicity. Since their evaluation generally requires use of some kind of numerical methods much progress has been achieved in recent years by the accessibility of high-speed digital computers. Despite this activity it is not clear what approach would be most suitable for a given problem. At first sight the literature seems to offer as many methods as applications; however, in some classes of problems there is a trend towards common techniques, a good example being the Gilat–Raubenheimer [1] methods used to evaluate the density of states for lattice and electronic spectra.

Realistic models used in lattice dynamics and bandstructure rarely provide an analytic dispersion function but rather require solving for the eigenvalues at a few selected points in the Brillouin zone, with perhaps some form of interpolation used to fill the gaps in economically. Naturally this aspect has had an influence on the development of methods used for evaluating Brillouin-zone sums as has the restricted goal of the density of states.

In a number of problems, particularly in theories of magnetic phenomena, there are, however, often realistic cases (often with a singularity of the function at the zone centre, $\mathbf{k} = 0$), where analytic dispersion formulas are available, and somewhat different considerations then apply. The motivation behind the present work was to facilitate the evaluation of that class of Brillouin-zone sums on the

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cubic lattices so that proper assessment of theories and their comparison with experiments can be undertaken. In doing so several important simplifications have been achieved and the final prescription is quite simple to implement on a computer.

As an example we show the equations [2] of the self-consistently renormalized spin wave approximation for a nearest-neighbor Heisenberg ferromagnet. The spin wave energies are renormalized by the factor

$$R(T) = 1 - (JS^2 Z \mathcal{N})^{-1} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} n_{\mathbf{k}} \tag{1}$$

in which $n_{\mathbf{k}}$ involves $R(T)$ through the function

$$n_{\mathbf{k}} = \{\exp[R(T)\beta\epsilon_{\mathbf{k}}] - 1\}^{-1}, \qquad \beta = 1/k_B T. \tag{2}$$

In (1) and (2),

$$\epsilon_{\mathbf{k}} = SJZ\omega_{\mathbf{k}}, \tag{3}$$

where

$$\omega_{\mathbf{k}} = 1 - \gamma_{\mathbf{k}}/\gamma_0 \tag{4}$$

with

$$\gamma_{\mathbf{k}} = \sum_{\delta}^{\text{n.n.}} e^{i\mathbf{k}\cdot\delta}, \tag{5}$$

δ being nearest-neighbor vectors.

Then the magnetization is given by

$$m = M(T)/M(0) = 1 - (S\mathcal{N})^{-1} \sum_{\mathbf{k}} n_{\mathbf{k}} \tag{6}$$

and the specific heat follows from the internal energy

$$U = \tfrac{1}{2}[1 + R(T)] \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} n_{\mathbf{k}}. \tag{7}$$

We note that (1) is self-consistent in $R(T)$ and might be solved iteratively. Similar effects occur for other types of magnetic ordering and for longer-ranged interactions: in the latter case the equations are more complicated, involving the replacement of (1) by several self-consistent renormalization factors [2].

The class considered consists of single k-sums of high-symmetry functions that might be represented by

$$S = \frac{1}{\mathcal{N}} \sum_{\mathbf{k}} f_{\mathbf{k}}, \tag{8}$$

where the summation is over the $\mathcal{N}$ distinct $\mathbf{k}$ vectors of a crystal with $\mathcal{N}$ primitive cells. The domain of $\mathbf{k}$ is commonly chosen to be the first Brillouin zone or Wigner–Seitz cell of the reciprocal lattice. Many of the functions of interest have the full cubic symmetry O_h, so that the irreducible 1/48th portion of the zone (defined, e.g., by $k_z \leqslant k_y \leqslant k_x$) contains all the necessary information.

We exclude from present considerations all $\mathbf{q}$-dependent and multiple sums which do not decompose to single sums; these might be written, e.g., as

$$\frac{1}{\mathcal{N}} \sum_{\mathbf{k}} g_{\mathbf{k},\mathbf{q}} \quad \text{and} \quad \frac{1}{\mathcal{N}^2} \sum_{\mathbf{k},\mathbf{q}} h_{\mathbf{k},\mathbf{q}} .$$

While there are problems where these are important, they are more difficult than those represented by (8); Some aspects of our present approach could be used to deal with those situations if required.

Section II gives the theory behind the prescriptions and is based on the use of an octant of the first Brillouin zone which is randomly sampled to avoid the redundancy which would result if a regular grid of sampling points were used. Regular grids have to be restricted to the 1/48th irreducible section of this zone in order to avoid the redundancy problem, making resulting programming more tedious (especially for the f.c.c.). A simple transformation is employed to permit variation of the density of sampling points so that functions with a singular behavior at $\mathbf{k} = 0$ are readily accommodated.

Some time ago (in Loly [3]) a method was given for the b.c.c. lattice using a transformation of the 1/48th section (a tetrahedron). This incorporated an idea of Huggins [4] for the transformation of tetrahedral shapes into cubic regions and a density variation feature (by Loly) similar to that described in the present paper. The s.c. case could be treated in a very similar way but the extension to the f.c.c. case, where the 1/48th consists of a cluster of three tetrahedra, was not attractive and ultimately led us to the present octant scheme.

Section III details the transformation parameters for all the cubic lattices and Section IV discusses briefly two modes of implementation on a computer and the sampling procedure.

A test of the prescriptions is carried out in Section V using Watson's integrals [5]. These are appropriate for several reasons; they are known to high precision, their integrands have a difficult singularity at $\mathbf{k} = 0$ (similar to those occurring in thermodynamic functions) and they are the nucleus of a group of integrals which arise in many physical situations concerning lattice-bound systems. We demonstrate that an accuracy of 1 % or better can be achieved with a sample of 10 000 distinct points in $\mathbf{k}$ space.

Section VI is a discussion of the relationship of the present work with other methods which have been used in the literature.

II. THEORY

This will be dealt with as a series of steps:

(a)   Conversion of the sum to an integral in the standard manner [6]:

$$S = \frac{1}{\mathcal{N}} \sum_{\mathbf{k}} f_{\mathbf{k}} = \frac{V}{(2\pi)^3} \frac{1}{\mathcal{N}} \iiint_{\text{1stB.Z.}} d^3k \, f_{\mathbf{k}} \,, \tag{9}$$

where the volume of the crystal is given in terms of the number of primitive cells by

$$V = \epsilon \mathcal{N} a^3 \tag{10}$$

($\epsilon = 1$ for s.c.; $\epsilon = 1/2$ for b.c.c.; $\epsilon = 1/4$ for f.c.c.) in which "a" is the conventional lattice parameter.

(b)   Evaluation over the octant then requires a compensating factor of 8 so that

$$S = \frac{\epsilon}{\pi^3} \iiint_{\text{oct}} d^3(ka) f_{\mathbf{k}} \,. \tag{11}$$

(c)   We now employ transformations which permit compression of points toward $\mathbf{k} = 0$ (this set is not unique but is simple and works well in practice),

$$ak_x = A\alpha^l, \qquad ak_y = B\beta^m, \qquad ak_z = C\gamma^n, \tag{12}$$

where A, B, C limit the range of k_x, etc., and are given below in Section III for the various lattices. α, β, γ are then new coordinates which run independently from 0 to 1. l, m, n are the compression parameters ($l, m, n \geqslant 1$) which allow the density variation towards $\mathbf{k} = 0$.

(d)   The Jacobian of this transformation is

$$J(\alpha, \beta, \gamma) = ABClmn\alpha^{l-1}\beta^{m-1}\gamma^{n-1} \tag{13}$$

so that

$$\iiint_{\text{oct}} d^3(ka) f_{\mathbf{k}} = \iiint_{\text{oct}} d\alpha \, d\beta \, d\gamma \, J(\alpha, \beta, \gamma) f(\alpha, \beta, \gamma). \tag{14}$$

(e)   We may remove the restrictions on α, β, γ in (14) by writing

$$\iiint_{\text{oct}} d\alpha \, d\beta \, d\gamma \cdots = \int_0^1 \int_0^1 \int_0^1 d\alpha \, d\beta \, d\gamma \, P(\alpha, \beta, \gamma) \cdots, \tag{15}$$

where $P(\alpha, \beta, \gamma)$ acts as a projection function

$$P(\alpha, \beta, \gamma) = \begin{cases} 1 & \text{if} \quad (\alpha, \beta, \gamma) \subset \text{octant} \\ 0 & \text{otherwise.} \end{cases} \tag{16}$$

(f)   Now we use the idea that an integral is equal to the average of a set of uniformly chosen samples of the function in the limit of a large set of samples

$$\int_0^1 f(x)\, dx = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^n f_i\,, \tag{17}$$

where i labels a value of x in the range of $0 \leqslant x \leqslant 1$ which is chosen in a uniform way. This can be achieved in several ways [see Section IV (iii)].

(g)   For our problem this means that

$$\int_0^1 \int_0^1 \int_0^1 d\alpha\, d\beta\, d\gamma\, J(\alpha, \beta, \gamma) f(\alpha, \beta, \gamma)\, P(\alpha, \beta, \gamma) \approx \frac{1}{N} \sum_{i=1}^M J_i f_i\,, \tag{18}$$

where N is the total number of points used to sample the α, β, γ cube and i labels the M samples which correspond to points in the octant. ($N \geqslant M$ and $M = 10^4$ leads to an accuracy of better than 1% as will be shown later in Section V.)

(h)   Adding all these steps together, we have

$$S \approx \sum_{i=1}^M W_i f_i\,, \tag{19}$$

where

$$W_i = \delta lmn\alpha^{l-1}\beta^{m-1}\gamma^{n-1}/N \tag{20}$$

and

$$\delta = \epsilon ABC/\pi^3. \tag{21}$$

(i)   In most of our applications it is appropriate to set $l = m = n = c$, whence

$$W_i = \delta c^3(\alpha\beta\gamma)^{c-1}/N. \tag{22}$$

III. Transformations

Simple Cubic Lattice

We use the positive octant shown in Fig. 1(a) for which

$$ak_x = \pi\alpha^l, \tag{23}$$

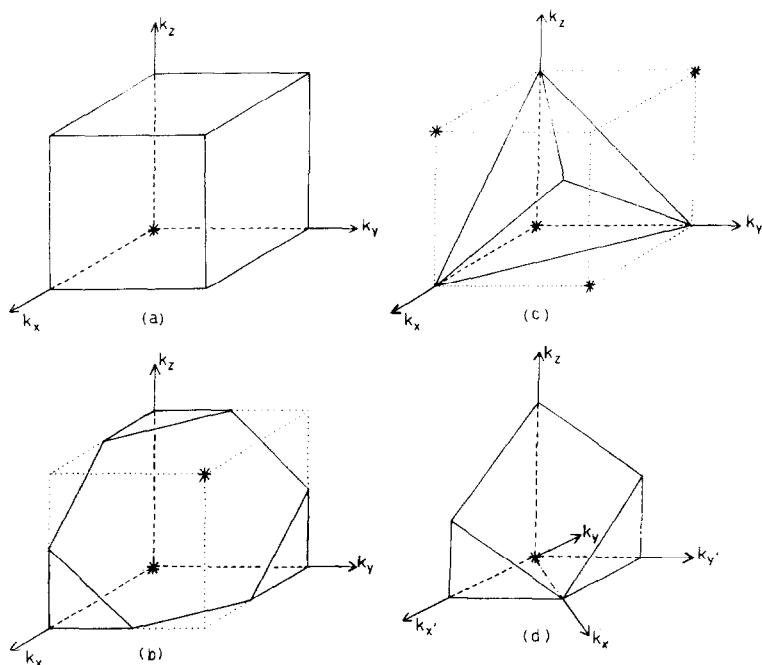etc., or $A = B = C = \pi$, hence $\delta = 1$, and also $N = M$.

FIG. 1. Octants of the first Brillouin zone of the cubic lattices, (a) s.c., (b) f.c.c., (c) b.c.c. (symmetric), (d) b.c.c. (asymmetric).

Face-Centered Cubic Lattice

This uses the positive octant shown in Fig. 1(b) for which

$$ak_x = 2\pi\alpha^l,$$

etc., or $A = B = C = 2\pi$, hence $\delta = 2$, but $N > M$ because of the condition for the octant that

$$k_x + k_y + k_z \leqslant 3\pi/a \tag{24}$$

[for $c = 1$, $M/N = 1/2$; $c = 2$, $M/N \approx 0.825$ (see Fig. 2 for a larger range of c)].

Body-Centered Cubic Lattice

Here there are two possibilities; the positive octant which is symmetrical and a more efficient "asymmetrical" one.

BCC Symmetric.   This is shown in Fig. 1(c) and requires that

$$ak_x = 2\pi\alpha^l,$$

etc., or $A = B = C = 2\pi$, hence $\delta = 4$, but restricted by the 3 conditions,

$$k_x + k_y \leqslant 2\pi/a, \qquad k_x + k_z \leqslant 2\pi/a, \qquad k_y + k_z \leqslant 2\pi/a \qquad (25)$$

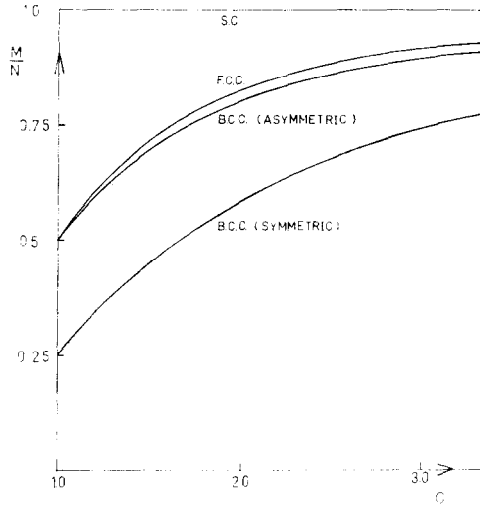[for $c = 1$, $M/N = 1/4$; $c = 2$, $M/N \approx 0.585$ (see Fig. 2)].

FIG. 2.   Efficiency factor as a function of the compression.

BCC Asymmetric.   Shown in Fig. 1(d), the octant is within the rectanguloid rotated $45°$ about the z axis from the symmetrical case and in the positive octant described by

$$k_x' = \sqrt{2}\,(k_x + k_y), \qquad k_y' = \sqrt{2}\,(k_y - k_x), \qquad k_z' = k_z.$$

For this case we have

$$ak_x' = \pi\sqrt{2}\,\alpha^l, \qquad ak_y' = \pi\sqrt{2}\,\beta^m, \qquad ak_z = 2\pi\gamma^n$$

or $A = B = \pi\sqrt{2}$, $C = 2\pi$, hence $\delta = 2$ with just one restriction that

$$(k_x'/\sqrt{2}) + (k_y'/\sqrt{2}) + k_z \leqslant 2\pi/a \qquad (26)$$

[for $c = 1$, $M/N = 1/2$; $c = 2$, $M/N \approx 0.805$ (see Fig. 2)].

Figures 1(b) and 1(c) show the circumscribing cubes for the f.c.c. and b.c.c. (symmetric) cases where asterisks denote $\mathbf{k} = 0$ type points of neighboring Wigner–Seitz cells. Figure 1(d) shows the analogous situation for the other choice of octant for the b.c.c. case.

IV. IMPLEMENTATION

This depends on several factors—the nature of the problem in which the Brillouin-zone sum occurs, the type of function involved, the accuracy required and the amount of fast storage available. Some guidelines can be given in two fairly distinct categories which we now consider.

(i) "One-Shot" Type

Here one requires only one summation over $\mathbf{k}$ (for a given c) but might require a very large number of points—e.g., to evaluate a special constant to high precision, or to find the density of states.

In this case the coordinates and weighting factor can be used as soon as generated and no storage problems occur.

(ii) Repetitive Type

Now many $\mathbf{k}$ sums may be needed (e.g., in iteratively solving an integral equation) and it is important to use fast storage for the weighting factor and coordinate information since they will be used many times and their regeneration is uneconomic. (Often coordinates themselves need not be stored but rather compact information like the dispersion law is appropriate.)

Typically we use 10^4 sample points with $c = 2$ and find results generally better than 1% accuracy. Thus in the repetitive mode the minimum storage needed is 10^4 values of W and 10^4 values of the dispersion law—the total of $20\,K$ is a reasonable amount in terms of modern computers. A discussion of random sampling and an analysis of these procedures with Watson's integrals as test functions is given below. In Fig. 2 we show the ratio M/N as a function of compression for the cases with cutoff. M/N may be regarded as an efficiency factor counting what proportion of the generated points fall in the octant. Figure 2 was obtained by using a random sampling stream [$B(2, 3, 5)$ discussed below] rather than an analytic result which was considered extremely difficult to perform.

(iii) Sampling Procedure

The cube spanned by α, β, γ can be sampled in several ways that tend to uniformity for large samples. Simplest is a grid of equally spaced points—we have

not used this because we did not want to emphasize the boundary in a finite sample and also to prevent any possibility of picking up spurious effects [7] (see Section VI).

A random set of points would seem appropriate—in practice one uses pseudo-random numbers generated by an algorithm. We used the IBM 360 RANDU Generator which is of the common multiplicative congruential or power residue type (machine specific)—with an odd integer IJ as a trigger it will produce a set of numbers distributed between 0 and 1. We shall denote such a stream as $A(IJ)$.

In addition, another sampling system was used with somewhat better results—basically because it approaches uniformity faster than the random numbers [8]. It is based on the Diophantine approximation—essentially one takes an integer with a noninteger square root, e.g., 2, 3, 5, 6,..., and uses the fractional part of this root as a starting value x (obviously $0 < x < 1$). The required numbers are then given by the fractional parts of nx, where n is an integer—we use $n == 1, 2, 3, 4,...$. We label streams of sampling points obtained this way by the integers used for each coordinate, e.g., $B(2, 3, 5)$. It is advisable to use double precision for their generation on 360 series computers, since the word length in single precision can result in duplication because of the relatively small cycle then obtained.

We might at this point note a simple test which can be used as a check on these procedures:

$$\frac{1}{\mathscr{N}} \sum_{\mathbf{k}} 1 = 1, \qquad \text{for any compression.} \tag{27}$$

V. Watson's Integrals on the Cubic Lattices

These are defined by

$$W = \frac{1}{\mathscr{N}} \sum_{\mathbf{k}} (\omega_{\mathbf{k}})^{-1} \tag{28}$$

in which $\omega_{\mathbf{k}}$ was defined in (4). Watson's integrals are related to the generalized Watson integral [9], $1/\mathscr{N} \sum_{\mathbf{k}} n_{\mathbf{k}}$, with $n_{\mathbf{k}}$ defined by (2), because the integrand of (28) is proportional to the high-temperature limit of $n_{\mathbf{k}}$ and has the same $\mathbf{k} \to 0$ singularity problem.

Watson [5] evaluated these integrals using analytic reduction to Elliptic integrals for the three cubic lattices. For small $\mathbf{k}$, $(\omega_{\mathbf{k}})^{-1} \sim k^{-2}$, but the integral does converge since the volume of integration goes as $k^2 \, dk$.

Let us note at this point a further check on the results that is afforded by

$$\frac{1}{\mathscr{N}} \sum_{\mathbf{k}} \omega_{\mathbf{k}} == 1. \tag{29}$$

All the results will be given for a sample size of 10^4 points in the region of integration.

In evaluating the l.h.s. of (27) the value obtained, NORM, will not be exactly unity, mainly because of the finite sample size [unless $c = 1$ when all the W_i's of (22) are the same] and partly due to rounding errors if single-precision arithmetic is used. Attempts at other integrals will not result in the correct values either, and one might try to compensate for that part of the error associated with the W_i's by dividing the raw results by NORM—thereby arranging for (27) to be satisfied. However, since there is some value in the raw result we average it with the compensated value to arrive at a renormalization factor

$$R = \frac{1}{2}\left\{\frac{1}{\text{NORM}} + 1\right\}. \tag{30}$$

In the graphical results that follow we give both the raw results and the result of applying this somewhat *ad hoc* renormalization.
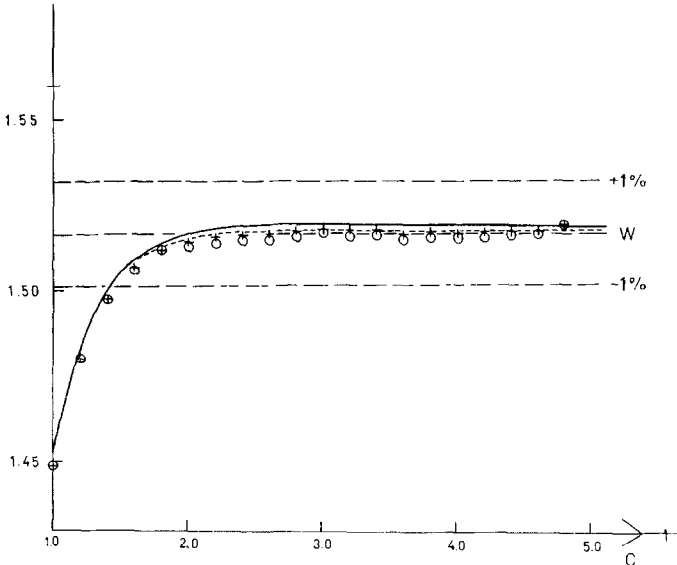

FIG. 3.   Single precision vs double precision for the $B(2, 3, 5)$ stream on s.c. lattice. Raw results are given by solid curve and $+$; renormalized results are given by broken curves and 0.

In Fig. 3 we show the effect of using single precision instead of double precision for the $B(2, 3, 5)$ stream. The single-precision results show a fluctuation about the double-precision results which are sufficiently smooth to be drawn as a continuous

curve. We estimate the effects of rounding errors to be about $1/3\%$ on average which is quite acceptable for many applications.

Figure 4 gives the results of further streams for the s.c. In this graph and the others which follow we have used double-precision results in order to understand the variations which are not due to rounding effects. From Figs. 3 and 4 we see that, except for small c, the values obtained lie within 1% error limits for $A(4321)$, $B(2, 3, 5)$ and $B(11, 12, 13)$ with the renormalized values closer to the correct value over a wider range of the compression factor. Results for $A(21)$ and $A(55)$ are not as good.
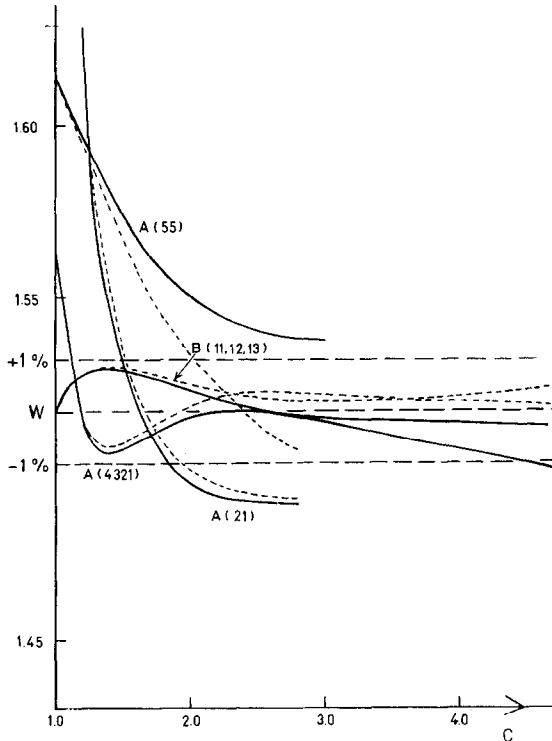

FIG. 4.   Further streams for s.c. lattice.

We can understand the small c behavior quite readily—since $c = 1$ is a uniform distribution in $\mathbf{k}$ space there are not many sampling points in the important small $\mathbf{k}$ region—the resulting error can easily account for the results shown in the graphs. Moderate compression, say, $c = 2$–3, will put more points in the small $\mathbf{k}$ region and give better results; this is demonstrated adequately in the numerical results. Very high compression will only treat properly the region very close to $\mathbf{k} = 0$, resulting in errors for the bulk of the contributions.

Figure 5 shows what happens for the b.c.c. (asymmetric) and f.c.c. cases. The results are not as smooth as for the s.c. case and this may be understood as due to the changing character of the sample of points as c is varied because of the cutoff plane which only retains those points in the α, β, γ cube which lie in the octant. Some of this will be reflected in NORM so it is not surprising that the renormalization achieves some smoothing.
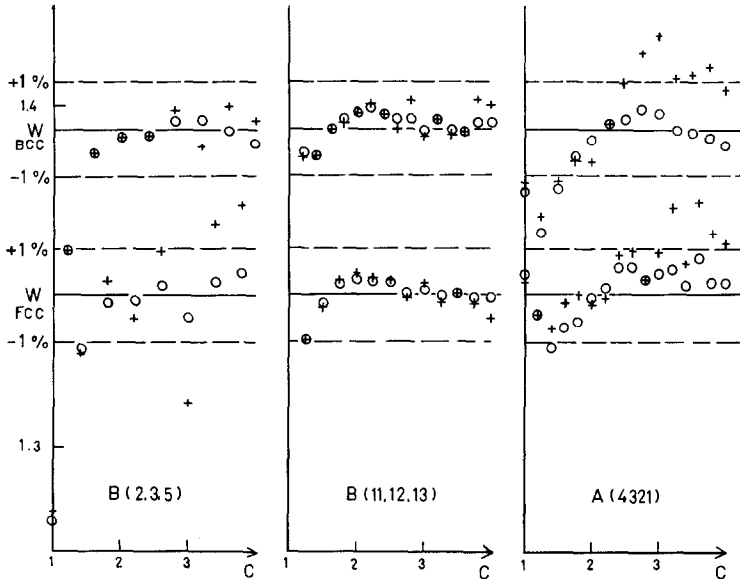

FIG. 5.   Results of 3 streams for b.c.c. and f.c.c. lattices.

The symmetric version of the b.c.c. gives similar results to the asymmetrical version and is not given in detail since it is less efficient.

We might also note that in Fig. 5 a given stream behaves similarly for the b.c c. and f.c.c. cases, but that from Figs. 3 and 4 the corresponding streams used in the s.c. case have a somewhat different character.

VI. DISCUSSION

It will be clear from the nature of our approach that the dispersion formula employed can be quite complicated (e.g., including many-neighbor interactions). Moreover, for problems which do not yield an analytic dispersion law an interpolation scheme could be used to obtain the large number of required eigenvalues economically. The accuracy may be improved by using larger numbers of sampling

points but will be limited by increased computer time; the error for a sample of N points going as $(1/\sqrt{N})$ [10].

In a few special cases it is possible to achieve a much higher accuracy by analytic reduction of the triple integral. The classic example would be Watson's work but more recent work by Flax and Raich [10] in connection with generalized Watson's integrals is another example. The drawback here is that each function has to be treated separately and the algebraic manipulations become complex in the general case. (In this connection see the commentary by Loly [11] on Flax and Raich's approach.)

One feature of the analytical-reduction approach deserves some attention in the present content. This is the use for *all* the cubic lattices of a cubic region of integration in **k** space. This is trivial for the s.c., but is obtained in the other cases by consideration of octants from adjacent Wigner–Seitz cells (2 for the f.c.c. and 4 for the b.c.c.). The diagrams of Fig. (1b and 1c) show clearly the region concerned, the asterisks showing the centers of the various Wigner–Seitz cells. One might think these cubic regions even more convenient to use than our truncated octant approach. However for integrals of functions singular at the zone center we have not been able to find a simple way of achieving the density variation feature of the truncated octant scheme. Nevertheless if the object were the density of states, where a uniform density in **k** space is often acceptable, the combination of the random sampling approach with the cubic shapes would suggest a much simplified approach for the b.c.c. and the f.c.c. Elsewhere Buchheit and Loly [12] have demonstrated this with the case of spin waves in an f.c.c. magnetic structure with first- and second-neighbor exchange. It has recently come to our attention that the QUAD [13] method does this together with an interpolation scheme.

The density-of-states approach may be used when $f_\mathbf{k}$ can be expressed as $f(\phi_\mathbf{k})$ if the density of states of $\phi_\mathbf{k}$ is either known or easy to evaluate. For cubic lattices and nearest-neighbor dispersion laws Jellitto [14] has recently provided accurate tabulations. However, in general the calculation of the density of states is a difficult task.

Before this work various kinds of numerical integration were used and it is appropriate to show how we have improved on those procedures. First of all there is the convenience of the truncated cubic shape over the irreducible 1/48th from the programming point of view (see comments in the Introduction). In order to avoid the redundancy problem it was then necessary to use random sampling instead of the regular grids that are used in much of the literature. In the density-of-states connection, Brust [7] has shown how spurious oscillations can result from rows of sampling points lying near energy surfaces and advocated random sampling in 1/48th's to overcome that problem [10]. When a regular grid is used with the irreducible 1/48th, it is not unusual to find that the contribution from grid points which lie on its boundaries (corners, edges, or faces) are weighted according to the

number of 1/48th's to which they contribute [7]. It is clear, however, that for a high density of sampling points these boundary points give a negligible contribution to the integral and even for a relatively low density of sampling points they are best avoided lest they distort the integral. In random sampling it is highly unlikely that a point will lie on the surface of a volume so the problem is avoided. (Mueller [15] has discussed this point in a recent review.) In our work we have also found a simple way of varying the density of sampling points in a manner that helps evaluate integrals of functions which have zone center singularities. An application of these techniques to evaluate integrals arising in the self-consistently renormalized spin wave approximation has been made for all cubic lattices and for all interesting spin magnitudes [2].

In conclusion we feel that the task of evaluating many Brillouin-zone sums has been simplified to the extent that we doubt if it is appropriate to provide explicit program details because the techniques may be so readily implemented in part or in whole.

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