

## A General Strategy for Brillouin Zone Sampling and Integration

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A systematic approach to the tetrahedron method of Brillouin zone partition is proposed. This approach has advantages over existing techniques and is more generally applicable.

### 1. INTRODUCTION

Many calculations in solid-state Physics require as a first step the selection of a set of points within a Brillouin zone. For example, a commonly used means of obtaining a density of states distribution is to generate a mesh of points in  $K$ -space, evaluate the model Hamiltonian at these points, and display the results in a histogram. This technique, known as "root sampling," is considered by some to be superseded now by various methods which are reviewed by Gilat [1]. However, its simplicity ensures its continuing appearance in the literature.

A common feature of all the later methods is the partition of the zone, or the irreducible part of the zone, into small volumes or microzones. The mesh of microzones may be cubic, or consist of rectangular or triangular prisms [2–5]; integration or other operations may be performed analytically by extrapolation or interpolation of suitable functions within these small cells [6–10]. These methods have been applied to cubic, hexagonal, tetragonal, and trigonal systems.

A slightly different approach has been developed in which the Brillouin zone is divided into tetrahedral cells [11–13]. Several advantages are claimed for this method, critically discussed by Gilat and Bharatiya [14].

In general one may propose several criteria to be met by any method of partitioning a Brillouin zone, whether one wishes complete microzones to use as integration cells or merely points from each to form a root sampling mesh. These criteria are:

- (1) that the zone be completely filled;
- (2) that the spread of cells be uniform;
- (3) that the method of selection be straightforward and applicable to as many systems as possible.

For some purposes it is also desirable to avoid symmetry points, and edges and bounding planes of the Brillouin zone or its irreducible segment [1].

In this paper an improvement of the tetrahedron method of zone partition is proposed: it will be shown that the approach outlined satisfies the above criteria at least as well as methods in current use, while being more generally and easily applicable.

## 2. METHOD

The irreducible part of a Brillouin zone (IRBZ) of any symmetry can be divided up initially into a few large tetrahedral sections. For example the IRBZ of the face-centered cubic system may be split into three parts, the tetrahedra with vertices at  $\Gamma$ LKW,  $\Gamma$ LWU, and  $\Gamma$ XWU—in the notation of Kunc [15]. The simple cubic IRBZ is a tetrahedron in any case, while systems of low symmetry would require division into more than three sections.

It is now convenient to state two well-known theorems, which are used later.

**THEOREM 1.** *The volume  $V$  of a tetrahedron ABCD with vertices at the points defined by the vectors  $\mathbf{A}$ ,  $\mathbf{B}$ ,  $\mathbf{C}$ , and  $\mathbf{D}$  is given by [16]*

$$V = \frac{1}{6}[(\mathbf{A} \cdot \mathbf{B} \times \mathbf{C}) - (\mathbf{A} \cdot \mathbf{B} \times \mathbf{D}) + (\mathbf{A} \cdot \mathbf{C} \times \mathbf{D}) - (\mathbf{B} \cdot \mathbf{C} \times \mathbf{D})]. \quad (1)$$

**THEOREM 2.** *Any point  $\mathbf{P}$  lying on the surface of or contained within a tetrahedron ABCD is expressible as [17]*

$$\mathbf{P} = x_1\mathbf{A} + x_2\mathbf{B} + x_3\mathbf{C} + x_4\mathbf{D}, \quad (2)$$

where

$$x_1 + x_2 + x_3 + x_4 = 1$$

and

$$0 \leq x_i \leq 1, \quad i = 1, \dots, 4.$$

In particular the centroid  $\mathbf{K}_c$  is given by

$$\mathbf{K}_c = \frac{1}{4}(\mathbf{A} + \mathbf{B} + \mathbf{C} + \mathbf{D}). \quad (3)$$

Since  $\mathbf{K}_c$  is the center of weight of the tetrahedron, an integral  $I$  of a function  $f(\mathbf{K})$  which is linear in  $\mathbf{K}$ , taken over the volume of  $K$ -space contained in ABCD, is given exactly by

$$I = \iiint f(\mathbf{K}) d\tau = Vf(\mathbf{K}_c), \quad (4)$$

where  $d\tau$  is a volume element in  $K$ -space and  $V$  is the volume of ABCD. This

illustrates a sense in which  $K_c$  is the best single sampling point for the tetrahedral volume.

Equation (2) expresses the geometrical equivalence of all tetrahedra; they are related by simple linear transformations. For this reason if it is necessary to improve the sampling of a volume of  $K$ -space it is desirable to do so without using cells of different geometry. The initial tetrahedra should be subdivided into smaller tetrahedra.

Although there are many ways of arranging this subdivision, arguments due to Gilat [1] and Lehmann and Taut [13] suggest that the accuracy associated with a given mesh is related to the dimensions of the microzones. Thus in order to reduce inaccuracies the maximum length from the center of each cell to its edges should be made as small as possible.

To achieve this with the minimum of computation the following scheme is proposed: a tetrahedron  $ABCD$  will in general have one side longest, which may readily be found. Suppose this to be  $AB$ . Then, as Fig. 1 shows, the original tetrahedron may be split into two by taking as vertices the sets

$$A, X, C, D \quad \text{and} \quad B, X, C, D, \quad \text{where } X = \frac{1}{2}(A + B). \quad (5)$$

It follows from Eq. (1) that the two new tetrahedra each have one-half of the volume of the original. The centroids of the new cells are given by Eq. (2), where  $x_1, \dots, x_4$  are quickly found. This is the most efficient way of reducing the sampling cell dimensions in one step.

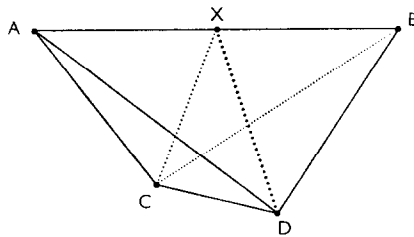


FIG. 1. Point  $X$  is the midpoint of side  $AB$ . The tetrahedra  $AXCD$  and  $BXCD$  have half the volume of  $ABCD$ .

If the procedure is repeated a total of  $n$  times, the original tetrahedron will have been divided into  $2^n$  cells of similar geometry, evenly spaced and of equal volume. The set of centroids of these cells may be taken as the mesh on which to sample the section of the zone represented by the original tetrahedron. Where the IRBZ was divided initially into several sections of differing volume, in general the statistical weights of points in different sections will not be the same—there will be as many different weights as initial sections—but because of the possibility of adjustment by repeated division by 2 these weights need not differ by more than a factor of  $2^{1/2}$ . Thus the contributions and inaccuracies from cells in different sections may be kept comparable. The weights are easily found, using Eq. (1).

The method outlined above differs from the schemes used by Lehmann and Taut [13], who either divided the IRBZ first into cubes and then subdivided these into tetrahedra, or set up a mesh of tetrahedra of arbitrary shape. Because they did not choose cells with minimized dimensions, highest accuracy will not be attained. Further, their first scheme applies only to cubic zones, while the second is not a general prescription and would require modification and justification for each different system.

Chen [21] has proposed a novel system for Brillouin zone integration which requires the initial partition of the IRBZ into tetrahedra and then constructs a mesh of points inside each of these sections. This mesh is so constructed that it is possible to interpolate over each entire section rather than over just one microzone, or a small cluster of microzones, as in previous schemes. The mesh is not intended to constitute a set of points to be used for root sampling or in conjunction with other existing integration procedures. In fact it would be particularly inappropriate in that respect since weighting factors would vary not only between interior and surface points, but in general throughout the volume of each segment. Although a comparison of different zone integration methods is beyond the scope of this paper, it is noted that the bisection-based algorithm suggested here may find an application in Chen's approach at a later stage. That is, he suggests that increase in accuracy may be achieved by subdividing the thin tetrahedra used in his ray integration into microtetrahedra, and subsequently using the original tetrahedron integration results. The subdivision could be done systematically using the method described above.

### 3. COMPARISON WITH A CUBIC MESH

The purpose of this section is to test how well the above method of partition satisfies the conditions stipulated in the Introduction, and also to provide an illustrative numerical example. Although different methods of integration have been compared before, it does not appear that the question of the adequacy of a set of sampling points in the IRBZ has previously been studied. Since no logical system of constructing a tetrahedral mesh has been suggested, and it seems of little value to construct random samples, a comparison is made here between integrals over the simple cubic IRBZ using a cubic mesh with 1140 points, centered on the origin, and a mesh of 1024 tetrahedra. In each case a linear approximation was used, in that the calculated integral  $F(p)$  was found by

$$F(p) = \sum_i g(p, \mathbf{K}_i) \tau_i / V, \quad (6)$$

where  $\mathbf{K}_i$  = centroid of the  $i$ th tetrahedral cell or cubic cell,  $\tau_i$  = weighting factor of  $i$ th cell,  $V$  = total volume of IRBZ, and the summation runs over all cells in the IRBZ.

In the case of the tetrahedral mesh  $\tau_i$  is simply the volume of the cell, that is,  $V/1024$ , for every cell. The volume of each cubic cell is equal to  $6V/18^3$ , but  $\tau_i$  also has to take into account overfilling of the zone since cells at the edge of the zone project

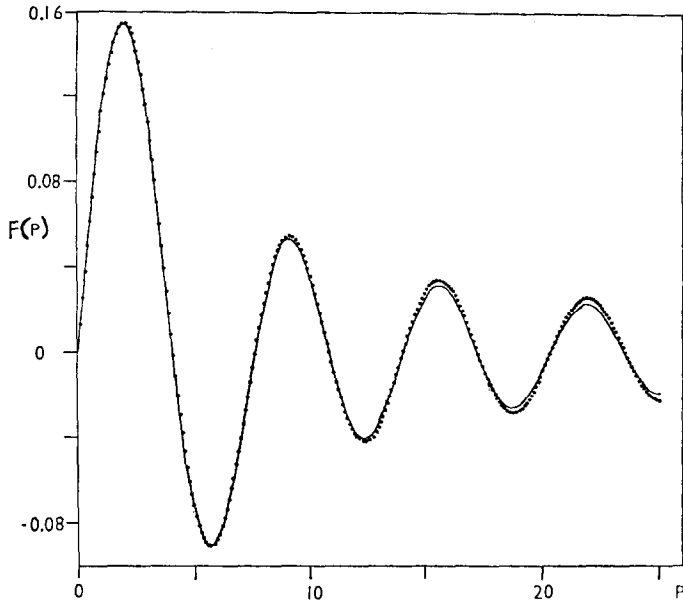


FIG. 2.  $F(p)$  is the integral of  $\sin(pk_x)$  over the simple cubic IRBZ. The solid curve gives the exact values. The points show the results of a linear approximation using a mesh of 1024 tetrahedra.

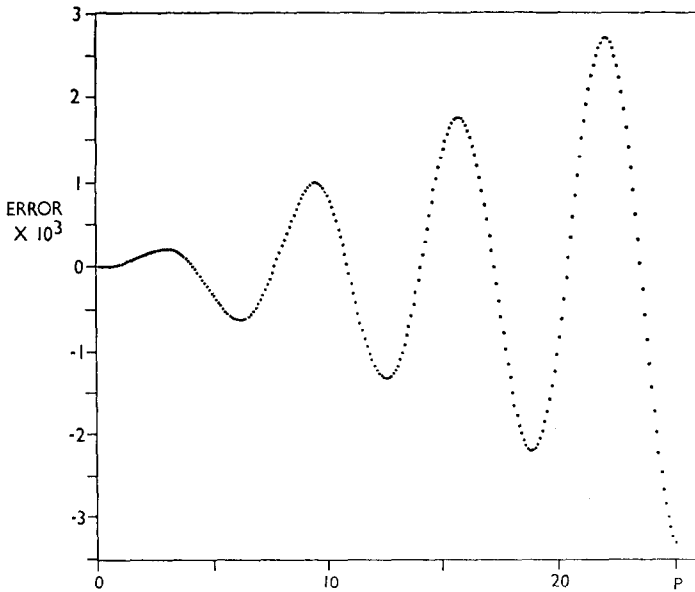


FIG. 3. The error plotted is the difference between the exact and calculated values of  $F(p)$  in Fig. 2.

beyond it. Thus several additional weighting factors for differently positioned cells, ranging from 1 to  $1/48$ , have to be calculated.

The simple cubic IRBZ is congruent to a tetrahedron with vertices at (000), (010), (110), and (111), with axes ( $K_x$ ,  $K_y$ ,  $K_z$ ). The function chosen for integration over this volume was  $\sin(pK_x)$ , which oscillates increasingly rapidly over the zone as  $p$  increases, so that the accuracy of the linear approximation inherent in Eq. (6) will decrease. This should provide a reasonable test of the assertion that the bisection method minimizes the dimensions of the microzones, and so reduces the effects of the quadratic and higher-order terms ignored in the calculation.

Figure 2 shows the results for the tetrahedral mesh compared with the exact theoretical values; the approximate values are a good fit for small  $p$ , becoming worse as  $p$  increases. This is more clearly shown in Fig. 3, which plots the error as a function of  $p$ . Interestingly the results for the cubic mesh are similar, but the fit is rather less good (see Figs. 4 and 5). Figures 3 and 5 show that the errors with the cubic mesh are some 20% larger, in spite of the greater number of points used in the computation.

Clearly the above calculations are a very crude form of zone integration, using a fairly simple function. However, the interest is not in comparing different methods of zone integration but in testing two sets of samples of  $K$ -space, such as might be used subsequently for integration but also might be used for root sampling. Difficulties in making a comparison are already clear from the unequal number of points used in each case: it is felt that a complex calculation using a less straightforward function would only confuse the interpretation more.

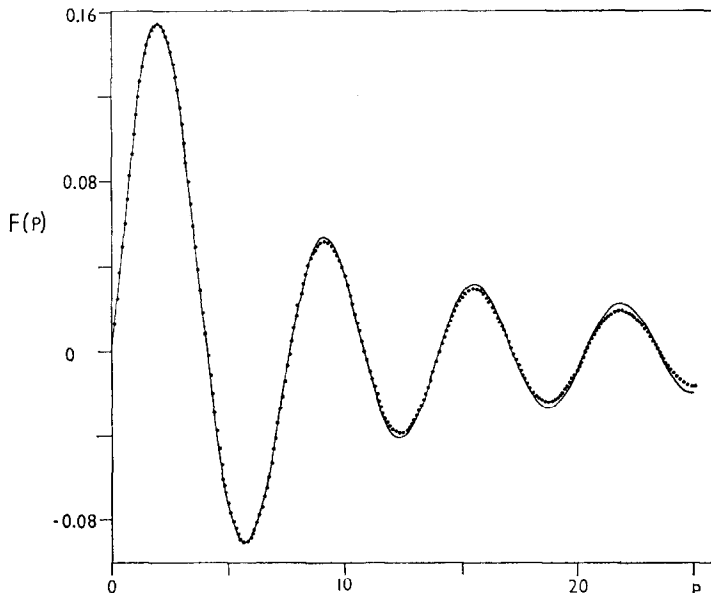


FIG. 4.  $F(p)$  is the integral of  $\sin(pK_x)$  over the simple cubic IRBZ again, but the points represent values calculated using a cubic mesh with 1140 points. The solid curve gives the theoretical behavior.

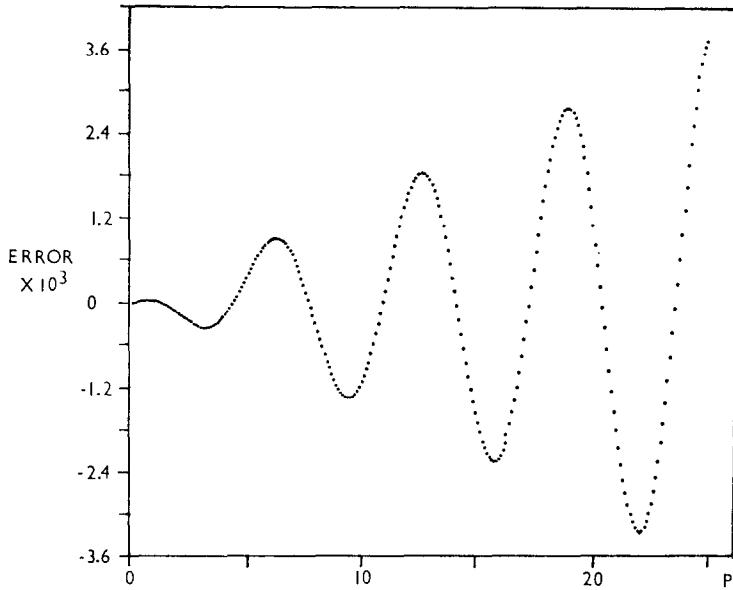


FIG. 5. The differences between the correct and the approximated values of Fig. 4 are shown. Comparing with Fig. 3, apart from a sign change the two methods yield similar results, but the errors due to the cubic mesh are greater than those due to the tetrahedral mesh.

TABLE I

Moments of the Single Cubic IRBZ Computed with a Cubic Mesh, and with a Tetrahedral Mesh

Function computed	Percentage error		
	Cubic mesh	Tetrahedral mesh	True value
Volume	$<10^{-6}$	$<10^{-6}$	1/6
$\overline{K_x}$	$<10^{-6}$	$<10^{-6}$	1/2
$\overline{K_x^2}$	+0.10	-0.14	3/10
$\overline{K_x K_y}$	+0.07	$-6 \times 10^{-4}$	2/5
$\overline{K_x^3}$	+0.22	-0.31	1/5
$\overline{K_x^2 K_y}$	+0.17	-0.12	1/4
$\overline{K_x K_y K_z}$	$-8 \times 10^{-6}$	$<10^{-6}$	1/8
$\overline{K_x^4}$	+0.37	-0.52	1/7
$\overline{K_x^3 K_y}$	+0.30	-0.29	6/35
$\overline{K_x^2 K_y^2}$	+0.32	-0.17	3/14
$\overline{K_x^2 K_y K_z}$	+0.10	-0.10	6/70

As a further test several moments of the form  $\overline{K_x^l K_y^m K_z^n}$ , where  $l, m, n$  are integers, have been calculated over the same region. These functions are relevant to the various levels of interpolation used in approximating functions over sections of Brillouin zones. Where a linear approach is used, as in the example above, errors arise from the neglect of terms where  $l + m + n \geq 2$ . With a quadratic interpolation, cubic and higher terms would contribute. In every case the resulting errors will be smaller for a better conditioned mesh, with microzones of lesser dimension. The percentage errors accruing are given in Table I, together with the theoretical values. As may be expected, results are best for lowest-order moments. In this test the results of each method are similar, but again it is stressed that more points were needed using the cubic mesh to get the same level of accuracy, thus involving more computing effort and time.

Although the number of points doubles at each bisection of the tetrahedral cells, the increase in accuracy is not so rapid. Calculating the set of moments listed in Table I with only 512 points gives errors 1.6 times larger on average compared to the values listed for 1024 tetrahedral cells. For 256 points the errors are 2.4 times greater. This is as expected from the above discussion since although the volume of each microzone is reduced to one-half at each step, each new tetrahedron is still bounded by three of the sides of the original cell, unreduced in length. Thus the decrease at each step in the average dimension of a microzone is not as great as one-half.

#### 4. SUMMARY

Sampling using a cubic mesh is a well-established method. The last section has examined errors that may arise in using it to evaluate integrals of quite simple functions in a Brillouin zone, and it is found by comparison that the method proposed in this paper can give similar results with less computing effort. This is achieved by eliminating the need for the inclusion of many points on the edges of the zone which have low statistical weight. The same consideration will apply to those systems where meshes of rectangular and triangular prisms have been used. Moreover the possibility of programming error is reduced since one does not require calculation of different weighting factors for cells which are in the same segment of the zone; factors for different segments follow arithmetically from the coordinates of the symmetry points of the zone, using Eq. (1).

The total computing time in any application will depend on the particular calculation to be performed at each representative point, and the number of such points, but it may be of interest to know the time required initially to set up the sampling mesh. In the present study, a FORTRAN program on an IBM 360/44 system took 1.7, 3.5, and 6.8 sec of CPU time to establish 256, 512, and 1024 points inside the simple cubic IRBZ using the tetrahedral method. The bisection algorithm finds the longest cell dimension at each step. The time required for this means that setup time using a cubic mesh is much shorter, even when the time for finding the weights is included. For



example, cubic meshes of 286, 560, and 1140 points, suitably weighted, required 0.06, 0.14, and 0.28 sec of CPU. Thus for very short calculations if a cubic mesh can be used, it may give faster results. For longer calculations, this saving in time will be outweighed by the fewer points required by the tetrahedral mesh.

The method can be used with the existing sophisticated techniques worked out for tetrahedral meshes [13, 14, 18–20]. Its advantages over previous alternative methods are its increased accuracy for the same computing effort, and its simplicity and generality of application.

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