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Comparison of Brillouin-Zone Integration Methods: Combined Linear and Quadratic Interpolation*

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A combined linear and quadratic interpolation method for Brillouin-zone integration is described. Comparisons of the combined method with previously introduced linear and quadratic approaches indicate that the combined scheme will require the least computer time in most cases. Calculations of the densities of states of phonons in copper and electrons in nickel are given as examples. Problems associated with critical points and the intersection of dispersion curves are also investigated numerically to a limited extent.

I. INTRODUCTION

In order to calculate many electronic properties of interest in solid-state physics, one is faced with integrations over the Brillouin zone (BZ) of functions of band energies and wave functions, e. g., electronic densities of states, magnetic susceptibilities, and dielectric-response functions. Such integrals also arise in many problems involving phonons, magnons, and other elementary excitations.

Two methods of carrying out these very complicated integrations have proved to be particularly useful. One is based on a linear-interpolation scheme introduced by Gilat and Raubenheimer[1](GR), whereas the other employs quadratic interpolation[2] as exemplified in the "Quad" scheme recently developed by Mueller *et al.*[3] We will not elaborate on the details of these two different approaches, since they are quite adequately described in the references cited. The GR scheme was originally developed for treating phonon systems, while Quad was developed later with applications to electronic systems as the primary consideration. It is possible to generalize the original GR method so that it too can be applied to electronic systems, and there is considerable interest at the present time in the relative merits of the two approaches for various systems.

In the course of using the original GR and Mueller *et al.* programs to do BZ integrals it became clear to us that a combination of these two approaches[4] might (i) give a single code which could be used for a variety of applications and (ii) reduce the total computer time required for most calculations. The purpose of this paper is to describe briefly our combined linear- and quadratic-interpolation procedure, which we shall refer to as CLQ, and to compare it with its two constituents taken independently.

II. LINEAR, QUADRATIC, AND COMBINED METHODS

A. GR Linear Scheme

The GR scheme was initially applied to the problem of calculating the phonon density of states from a given force-constant model. The method breaks up the irreducible segment of the BZ into very small cells in which the functions $f_i(\vec{k})$ involved in the integration are expanded to first order in the wave vector $\vec{k}$, i.e.,

$$f_i(\vec{k}) = f_i(\vec{k}_0) + (\vec{k} - \vec{k}_0) \cdot \nabla f_i(\vec{k})\big|_{\vec{k}=\vec{k}_0} \; ; \tag{1}$$

$\vec{k}_0$ is the wave vector at the center of the small cell. The resulting approximation to the integral inside each cell can then be evaluated exactly to give an analytic expression for the integral in terms of the $f_i(\vec{k}_0)$ and the gradients of $f_i(\vec{k})$ evaluated at $\vec{k}_0$. Finally, the results for each cell are summed to give the integral over the entire irreducible segment of the BZ. In principle, the size and hence the number of cells can be varied until convergence is reached. Since, by using group theory, the integral of any function over the entire BZ can be reduced to an integral over the irreducible segment, we, again in principle, can use the GR scheme to evaluate any integral of any combination of reasonably well-behaved functions over the full BZ.

Given the values of the functions and their gradients at the center of each cell, the evaluation of the integral in the GR scheme is very fast since all one does is evaluate an analytic function for each cell and then sum over all cells in the irreducible segment of the BZ. The calculation of the functions and their gradients, however, is another matter. Since the number of cells needed for convergence is rather large, the amount of time required to calculate $f_i(\vec{k}_0)$ and $\nabla f_i(\vec{k})$ at each $\vec{k}_0$ becomes very important. In particular, if band energies are needed, it would require many hours of computer time to generate from "first-principles" band-structure programs for the $E(\vec{k}_0)$ and $\nabla E(\vec{k})$ at enough $\vec{k}_0$ points to make the GR scheme converge. This fact alone suggests the desirability of combining the GR approach with some other interpolation procedure. For some cases, such as a Born–von Karman force-constant model for phonon systems with one or two atoms per unit cell, the entire calculation takes no more than a few minutes on the IBM 360/91.

B. Quad Scheme

The Quad scheme was developed by Mueller *et al.* in an effort to overcome what they felt were some serious disadvantages of the GR approach when electronic systems were treated. One of these has already been mentioned in the preceding paragraph; another important one which we will discuss later has to do with the treatment of critical points. Instead of working entirely within the irreducible part of the BZ, they chose to work in a large cube called the "working volume," e.g., one-quarter of the BZ in a cubic lattice. This working volume was then subdivided into smaller ones. By using several ingenious mathematical devices they were able to set up a very fast method for obtaining analytic expressions for the $f_i(\vec{k})$ based on a quadratic-interpolation scheme in each of the small cubes. That is,

$$f_i(\vec{k}) = \sum_{j=1}^{10} A_{ij} C_j(\vec{k}) \; , \tag{2}$$

where the A_{ij} are the expansion coefficients for the small cube under consideration and the $C_j(\vec{k})$ represent linear combinations of products of k_x, k_y, k_z through second order. There are ten independent terms in the expansion and the A_{ij} are found by a least-squares fit to values of f_i at 27 points in a small cube.

Because of the quadratic terms and the fact that many cubes have points in common, only a relatively small number of fitting points are needed to set up quite accurate interpolation formulas. However, because of the quadratic terms in the expansion of the $f_i(\vec{k})$, Mueller *et al.* chose a Monte Carlo procedure for evaluating the integrals. This method requires a relatively large amount of computer time when compared with the analytical integration in the GR scheme. However, in most cases involving electronic systems, the time saved because of the need for fewer first-principles band energies greatly outweighs the increase in time due to the Monte Carlo integration.

C. Combination of GR and Quad

It should be apparent from the foregoing discussion that a combination of the two methods might possibly lead to a further reduction in computer time and provide a single flexible code which could be used for a wide variety of calculations. The most obvious thing to do in combining these schemes is to use quadratic interpolation to set up the analytic expressions for the $f_i(\vec{k})$ from which the gradients $\nabla f_i(\vec{k})$ can be calculated. Thus, we obtain from Eq. (2)

$$\nabla f_i(\vec{k}) = \sum_{j=1}^{10} A_{ij} \nabla C_i(\vec{k}) \; . \tag{3}$$

Since the $C_i(\vec{k})$ are known simple analytic functions of k_x, k_y, and k_z, the differentiation can be carried out readily and then programmed once and for all. With analytic expressions for $f_i(\vec{k})$ and $\nabla f_i(\vec{k})$ known, the fast GR integration can be used to evaluate the integrals instead of the relatively slow Monte Carlo procedure.

One final point should be made here about combining these schemes. Quad was originally set up to run over the small cubes which together make up the working volume. The GR scheme runs over the small cells which collectively make up the irreducible part of the BZ. Thus far, we have found that the fastest procedure is obtained by first setting up the quadratic-interpolation formulas only within those small Quad cubes which lie at least partially inside the irreducible sector of the BZ. We then subdivide these cubes into the smaller cells used in the GR scheme. Since the A_{ij} are known in this Quad cube, we can use the GR integration scheme to calculate the integral in that part of the Quad cube which lies inside the irreducible segment of the BZ and then move on to the next appropriately chosen Quad cube.

III. EXAMPLES AND COMPARISONS

For simplicity, we will use calculations of densities of states to illustrate the relative speed of the three methods outlined above. More specifically, we will consider calculations on phonons in copper and electrons in nickel. In all cases, the parameters which control the accuracy of each method also strongly influence the computer time, and so we will first give a brief discussion of these parameters.

The accuracy of the GR scheme depends on a parameter K which ultimately determines the number and magnitude of the small cells into which the irreducible segment is divided. As we have used the GR programs, the distance from Γ to X of the BZ for an fcc lattice is subdivided into $4K$ equal intervals. It has been our experience from previous calculations that setting $K=9$ is sufficient to guarantee very good convergence, and so we have used this value in the present calculations. Although in practice the GR method, like the other two, represents the density of states by a histogram, the computational time is not very sensitive to the histogram parameters. This is a result of the analytic integration which makes the GR approach, in principle, not a histogram method.

The accuracy of the Quad scheme depends on two parameters. One of these is the mesh size M defined so that M^3 gives the number of small cubes in the working volume. The mesh size will determine the accuracy of the quadratic interpolation. The second parameter N_r gives the number of randomly distributed $\vec{k}$ vectors which are used in each small cube; it therefore controls the statistical accuracy of the Monte Carlo integration. The running time of the Quad scheme is a very sensitive function of N_r. Mueller *et al.* estimate that 1% statistical accuracy requires an average of 10^4 samplings per histogram box. In fact, if we have interpreted their statements correctly, they indicate that N_r can be obtained from the relationship

$$N_b M^3 N_r = 10^4 N_h \,. \tag{4}$$

Here N_b is the number of bands and N_h the number of histogram boxes. Consistent with this statistical accuracy, it was felt that a value of 10–13 for M should give acceptable fitting accuracy even around critical points. If N_b and M are held fixed, an increase in N_h implies an increase in N_r and hence in the Quad running time which is necessary to retain about 1% statistical accuracy.

An important factor to be considered here is that it is, in general, not necessary to increase N_h beyond a certain value. For example, if the error inherent in the calculation of the electron or phonon energy fitting points from a given potential or model is ϵ, then we can keep

$$N_h < \Delta E/\epsilon \,, \tag{5}$$

where ΔE is the electron- or phonon-energy bandwidth. For the case of nickel, which we will present later on, the first-principles band energies are generally accurate to within several milli-electron-volts (larger inaccuracies do occur at a few points) and the bandwidth is about 1 Ry. Thus, for this case, a realistic upper bound for N_h is about 1800. For convenience and as an aid in making direct comparisons between the three schemes, we have used 1800 histogram bins in almost all of the calculations discussed here.

The accuracy of the CLQ scheme depends on the same mesh parameter M used in Quad and the K parameter used in the GR integration. For simplicity, we generally choose K as an integer multiple of M and, in fact, we have found that for $M=10$, $K=M$ is usually sufficient. Thus, since we keep $M=10$ in all of the calculations discussed herein, we have $K=10$ for the CLQ scheme compared with $K=9$ for the GR scheme. Because the combined approach utilizes the GR analytic integration, it is quite insensitive to the histogram parameters.

The first example we give is a calculation of the phonon density of states for copper based on a Born–von Karman force-constant model.[5] The results for the Quad, GR, and CLQ schemes are given in Fig. 1. The curves were not exactly superimposed because they are essentially indistinguishable from one another except for small differences in the region A–B shown on the figure. The differences which are observable are evidently due to

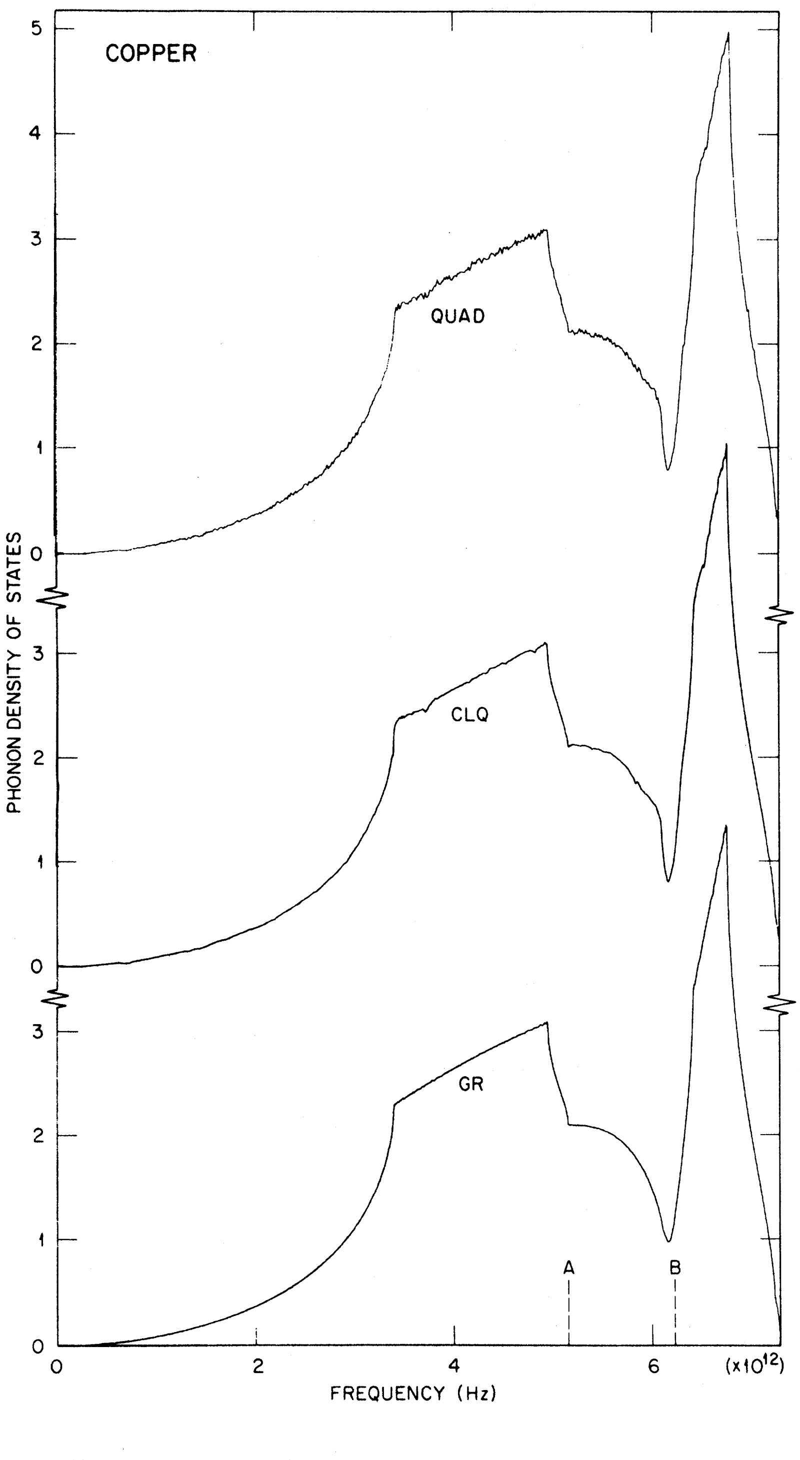

FIG. 1. Computer plot of phonon density of states for copper obtained from GR with $K=9$, CLQ with $M=10$, and Quad with $M=10$, $N_r=1500$. The frequency range is divided into 1800 intervals in each case.

the different methods of fitting the energies in the three approaches. The GR scheme works entirely with linear interpolation. In the Quad and CLQ schemes we use a force-constant model to obtain the energies at the fitting points for the quadratic interpolation. We then use these quadratic expansions to generate the input to the linear-interpolation formulas in the small cells of the GR method. As we increase the number of Quad cubes in the working volume (by putting $M=13$), we find that the small differences are reduced even further and that the Quad and CLQ results approach the results given by the GR scheme. The statistical noise on the Quad curve is obvious. It gives an idea of the order of magnitude of the error introduced into the calculation by the Monte Carlo integration.

TABLE I. Comparison of CPU times to compute the phonon density of states of copper.

Program	Time in sec[a]
CLQ	18.4
GR	45.14
Quad	200.59

[a] IBM 360/91.

The GR and the CLQ results show no statistical noise since they both were obtained on the basis of the GR analytic-integration techniques outlined above.

A comparison of the running times of the three computer programs is given in Table I. The figures listed represent the total amount of time required to do the entire calculation, that is, to obtain fitting points, set up interpolation formulas, do the integration, etc. The combined scheme CLQ is apparently about 2.5 times faster than the GR scheme and about 11 times faster than Quad for this calculation. We might mention here that we have reprogrammed part of the original version of the Quad scheme to increase its speed. We might also remind the reader at this point that the relative time factors we quote are dependent on the details of the calculation. In fact, any absolute comparison of running times is difficult to make for several reasons which we shall mention in Sec. IV.

The second example we give concerns a calculation of the electronic density of states for nickel. We did not attempt to use the GR scheme here because it would have taken many hours of computer time to generate the first-principles energies and gradients at enough k_0 points to give us the desired accuracy. The quadratic-interpolation scheme with $M = 10$, however, requires knowledge of first-principles energies at only 916 select points in the irreducible segment of the BZ. These fitting energies were generated by the Korringa-Kohn-Rostoker (KKR) band-structure method.[6] The results of calculations based on six up-spin and six down-spin bands ($N_b = 12$) obtained from a given ferromagnetic nickel potential are shown in Fig. 2 for the Quad and CLQ schemes, respectively. Again the curves are slightly displaced from one another because the only differences which occur are very minor ones in the heights of several of the smaller peaks. A comparison of the running times for the Quad and CLQ schemes for the nickel calculation is shown in Table II. These figures do not include the time required to generate the points used to set up the quadratic fits of the energy which, of course, were the same for the two schemes. Again, taking these numbers at face value, the CLQ scheme is about

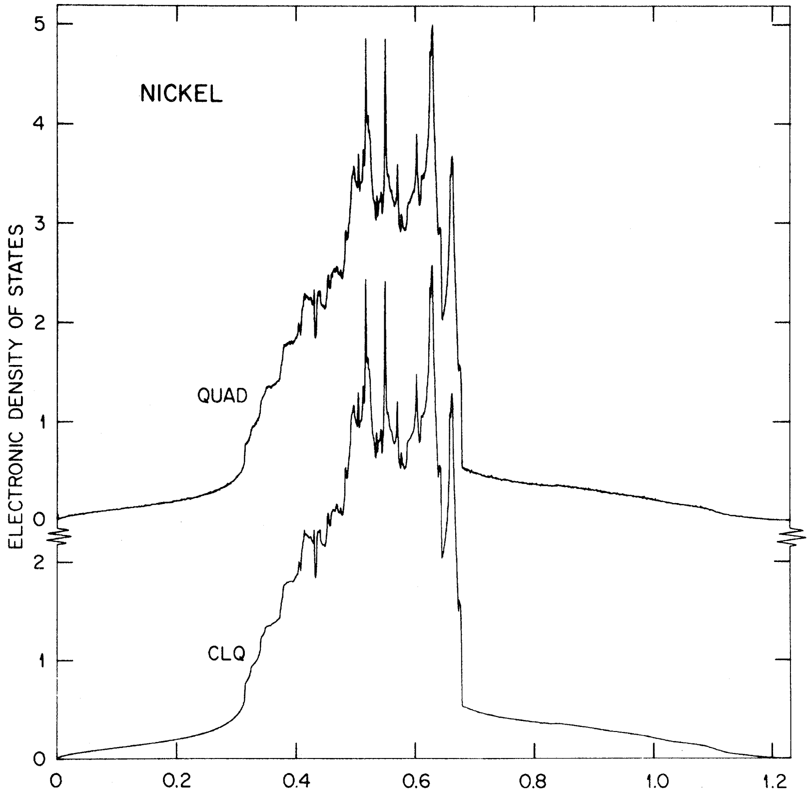

FIG. 2. Computer plot of electronic density of states for nickel obtained from CLQ with $M=10$ and Quad with $M=10$, $N_r=1500$. The energy range is divided into 1800 intervals in each case.

TABLE II. Comparison of CPU times to compute the electronic density of states of nickel.

Program	Time in sec [a]
CLQ	30.32
Quad	342.28

[a] IBM 360/91.

a factor of 11 faster than the Quad scheme. Although the programs do not lend themselves to a quantitative step-by-step comparison of the times involved, the following seems clear. For any one energy band, the time required by the CLQ scheme for the evaluation of the energy and gradients at each k point and for the subsequent GR analytic integration is greater than the simple evaluation of an energy required by Quad. However, the difference in time from this source is more than compensated for by the greatly increased number of k points (randomly generated) which must be considered to obtain a given accuracy with Quad.

IV. DISCUSSION AND CONCLUSIONS

We discuss the copper results first. It should be apparent from a careful study of Fig. 1 that the times shown in Table I must be interpreted with caution. We were seeking 1% statistical accuracy from Quad when working with $M = 10$ and 1800 histogram bins. It can be seen that the result already approximates the GR curve quite well, with the major differences coming in the A–B region. To test the convergence further we carried out a CLQ calculation with $M = 13$ which should substantially improve the quadratic-fitting procedure. The resulting curve was practically indistinguishable from the GR result in Fig. 1 except near the point B where there were still some minor differences. If the statistical noise is ignored, we expect the Quad scheme to give almost exactly the same result and so it would appear that the Quad and CLQ curves would eventually become very nearly identical to the GR curve. This illustrates the importance of both statistical and fitting accuracy in the Quad scheme and suggests that if the accuracy of the three methods could be made strictly comparable the time factors in Table I would change.

One might argue that 1800 histogram bins are really not needed for the copper calculation because of the relatively slowly varying density of states (compared with electrons in nickel, for example). We have carried out a Quad calculation with $M = 10$ and 180 histogram bins. The number of Monte Carlo samplings for 1% accuracy was thus reduced by an order of magnitude compared with the number used to obtain the Quad curve in Fig. 1. The density-of-states curve differed little in gross features from those shown in Fig. 1 but it had become rather lumpy in places due to the statistical noise and the relatively large bin width. In fact, without more refined curves for comparison, some of the statistical noise might easily be misinterpreted, although the calculation would probably be quite useful for many purposes. The time required for this calculation was about 72 sec on the IBM 360/91.

Comparison of the curves in Fig. 1 appears to provide information on two other points of interest. The first of these has to do with the question of how well the GR scheme can handle critical points. Mueller *et al.* state that no linear-interpolation scheme can accurately treat critical points. For the relatively simple critical-point structure observed in copper, however, it would seem that the GR scheme does very well indeed. The other, somewhat related, point has to do with the problem of band crossing, which has been discussed briefly by Gilat and Herman[7] and more extensively by Janak [Ref. 4(b)]. It is easy to see that the ordering of frequencies or energies into bands may sometimes produce cusps, ridges, etc., in the dispersion surfaces. One might expect that the Quad and CLQ schemes, as they now stand, would have trouble fitting these accurately. That this is indeed the case seems to be borne out by the behavior of the curves of Fig. 1 in the region A–B and our results for the CLQ calculation with $M = 13$. A glance at the dispersion curves for copper in Ref. 5 shows that ordering the bands in increasing frequency produces cusps exactly in the region of 6.2×10^{12} Hz where the deviations of the GR and Quad results from each other are greatest. As the mesh size in the CLQ scheme is increased to 13, the deviations are substantially reduced and those that still occur do so in a much narrower region around 6.2×10^{12} Hz.

The two curves for nickel given in Fig. 2 are virtually indistinguishable except for the statistical noise on the Quad curve. The relative times shown in Table II can be significantly altered by any change in the number of random samplings used in the Quad scheme. Our use of 1800 histogram bins was dictated by considerations which we have already mentioned in Sec. III. According to Eq. (4) a statistical accuracy of 1% for 12 bands and $M = 10$ requires 1500 samplings per Quad cell or 1.8×10^7 for the entire working volume and this was the number we used to obtain the time shown in Table II. We tried cutting this number down first to 1000 and then to 500 while keeping N_h, the number of histogram bins, fixed at 1800. The former number gave results which could hardly be distinguished from the Quad curve of Fig. 2, but with the latter number quite pronounced differences began to show up. This suggests to us that for this case Eq. (4) may tend to overestimate the number of random points (N_r) needed for a given N_h in order to achieve

1% statistical accuracy. This is important because the Quad running time depends more or less linearly on N_r once M is fixed. With 1000 points per cell the Quad time is 236 sec, which is still almost an order of magnitude greater than the CLQ time. One of the nice features about the CLQ scheme is that it is so fast that the parameter controlling the number of linear-interpolation points is not very critical. Our nickel results also have some bearing on the question of how well the GR scheme can treat critical points. It should be recalled from our description of the Quad and the CLQ schemes that both approaches are based on the same quadratic-interpolation fit of the first-principles band structure. In the CLQ scheme we make an additional linear interpolation of this quadratic fit in order to use the GR integration technique. Thus, if there is any inherent difficulty in using the linear-interpolation method, it doesn't show up on the scale we are using here for this particular calculation. This was also found to be true for five other nickel potentials that we considered.

The nickel calculations presented here do not permit us to say very much about the problem of band crossings. In this connection, the reader should keep in mind that the least-squares quadratic fitting of the first-principles energies may lead to new, slightly modified, dispersion curves in which the cusps, ridges, etc., arising from degeneracies are deemphasized. Thus, it is quite possible that some of the very fine structure on the curves in Fig. 2 may be spurious. We are somewhat reassured by an rms error of about 10^{-3} Ry, which indicates close agreement between the first-principles energies and the least squares fit to them for the vast majority of the 916 points in k space. We found, in substantial agreement with Janak, that the maximum fitting error was somewhat less than 10^{-2} Ry, but we also found that the number of points and bands where errors of this order of magnitude occurred was extremely small. Furthermore, these large errors did indeed correlate with band-crossing points and dropped rapidly with increasing distance away from them.

We can summarize our experience with the three schemes as follows. The most serious drawback of the GR scheme is the very large number of "exact" calculations which are needed in order to justify linear interpolation. This may not be critical for many phonon problems but for electronic calculations it is such a limiting factor that one is almost compelled to couple the GR scheme with some other interpolation procedure. The Monte Carlo integration appears to be the major shortcoming of the Quad scheme and the CLQ scheme eliminates this difficulty very effectively. We have not yet uncovered any evidence that the GR or CLQ schemes cannot handle standard critical points adequately. There is some evidence that quadratic interpolation may have minor problems in fitting cusps, ridges, etc., in the dispersion surfaces caused by band ordering. We suspect the same problems will arise with the GR scheme if it is really necessary or desirable to order the bands by energy. It may be possible to find ways around the difficulty and perhaps its importance should not be overemphasized at this time. The CLQ scheme combines the best features of the GR and Quad schemes. It has a particularly significant advantage in running time over the Quad scheme whenever a great many random samplings are necessary in Quad.

Finally, we would like to point out that the degree of accuracy we have been considering in this paper is really not necessary for many problems. We have found both the Quad and CLQ schemes extremely useful for calculating phonon Green's functions for use in defect problems, e.g., perturbed projected densities of states, infrared side bands, Raman scattering, etc. In many of these cases the experimental information is not yet detailed enough to demand high accuracy in the calculations and so the computer time required by Quad can be kept reasonably modest. Nevertheless, we have now gone over entirely to our CLQ method for these problems because they involve numerous computations of the relevant Green's functions and any reduction in computer time via the integration procedure is important. For example, by going from Quad with marginally acceptable accuracy to a highly accurate CLQ scheme, we were able to reduce the time for a typical calculation from about 5 to about 2 min on the IBM 360/91. Because these calculations involve more than just the BZ integration, the above times do not represent a meaningful comparison between the Quad and CLQ schemes; they do illustrate, however, that a substantial saving in computer time can be obtained over an extended series of calculations. For another problem on which we have worked, the integrals over the BZ involved fermion-occupation functions at zero temperature. In this case we required rather high accuracy and again found that the CLQ scheme is faster than Quad alone. We suspect that this will prove to be true in almost all applications and particularly so whenever high accuracy is needed.

ACKNOWLEDGMENTS

We would like particularly to thank F. M. Mueller for supplying us with a copy of his Quad programs and a preprint of the work in Ref. 3. We also wish to acknowledge the interest and encouragement of G. Gilat and F. Herman as well as a preprint of the work in Ref. 7. The coopera-

tion of H. L. Davis in generating the first-principles band energies for nickel has been invaluable.

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[1] G. Gilat and L. J. Raubenheimer, Phys. Rev. 144, 390 (1966).

[2] As far as we have been able to ascertain, Brust [Phys. Rev. 139, A489 (1965)] was the first to employ quadratic interpolation extensively for BZ integration.

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[4] The idea of combining various interpolation schemes is, of course, not new. A combined linear-quadratic approach very similar in spirit to the one we use here was introduced by Janak; however, we were unaware of his work at the time we amalgamated the GR and Quad schemes. Descriptions of Janak's work are given in (a) J. F. Janak, Phys. Letters 28A, 570 (1969); (b) J. F. Janak, in *Computational Methods in Band Theory*, edited by P. M. Marcus, J. F. Janak, and A. R. Williams (Plenum, New York, 1971), p. 323.

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Microwave Transmission Spectroscopy of Copper and Silver

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This paper describes a set of microwave transmission experiments carried out at a frequency of 35 GHz and a temperature of 4.2 K, in the presence of a dc magnetic field applied normal to the plane of the sample. Strong resonant bursts of transmission are observed in samples thin compared with the mean free path and these are shown to be a new form of cyclotron resonance, not of the Azbel-Kaner type. These resonances are called "cyclotron phase resonances," because they occur when many propagating electrons arrive at the second surface of the sample with the same microwave phase. This resonant effect arises where there is a large region of constant mass on the Fermi surface. In thick samples, a high-frequency version of the Gantmakher-Kaner oscillation is observed. A mechanism is proposed, to explain the propagation in thick samples, which is concerned with the "topological effectiveness" of the electron orbits. A measurement of the microwave phase of the oscillation is used to determine the Fermi velocity by a time-of-flight technique.

I. INTRODUCTION

A thick slab of metal is generally thought of as nontransparent to microwave-frequency electromagnetic radiation when its thickness is much greater than the skin depth δ. However, there are conditions under which an electromagnetic wave initiated at one surface may be detected at the second. Various mechanisms which are known to exist for such effects include conduction-electron propagation (anomalous-field penetration),[1] plasma-wave propagation,[2] spin diffusion,[3] spin-wave propagation,[4] and antiresonance transparency[5] in magnetic metals. Other possible mechanisms would presumably include helicon waves (or Alfvén waves) at high fields and phonons in superconductors.

This paper discusses both experimentally and theoretically some aspects of the mechanism of electromagnetic-wave propagation associated with conduction electrons of long mean free path, at microwave frequencies, and in the geometry of a dc magnetic field normal to the plane of the surface of the specimen. Generically, the phenomena we shall be studying would be classified as types of anomalous-field penetration,[1] by which it is meant that the dynamics of transmission is dominated by the trajectories of individual electrons in the magnetic field rather than by the collective aspects of the self-consistent fields to which the motion of these electrons give rise. However, the specific aspects of anomalous-field penetration which will concern us here have only recently been observed and understood,[6, 7] and the present work is a full exposition of the ideas and observations of our earlier commu-