The Calculation of Metallic Hall Constants: Topological Aspects and Applications to Copper

By JOHN R. KLAUDER

(Manuscript received March 30, 1961)

The theoretical prediction of the Hall constant in metals appropriate to high magnetic fields depends, in part, on a repeated computation of a specific topological invariant: Each of several parallel two-dimensional planes in crystal-momentum space must be analyzed to find, on a single sheet of the Fermi surface, the number of nonintersecting closed contours that surround an arbitrary point. This number is related to the effective sign of the charge of the "relevant" electronic carriers in the plane — carriers whose contribution to the Hall constant is based on their orbital area. Applications of the technique discussed in this paper have been made to the Pippard model for copper, and various carrier contours are illustrated that were found in the course of three calculations of the Hall constant in cases where the magnetic field direction lay along a principal crystallographic axis.

I. INTRODUCTION

When a current-carrying metallic sample is placed in a uniform magnetic field, a change in the resistance is generally observed. This phenomenon, known as *magnetoresistance*, is the basis for an important experimental technique for studying the band structure of metals. If a simple model is taken to represent a metal (i.e., an effective mass approximation, a constant relaxation time, etc.), then the expected change in resistance can be theoretically predicted. Even with a more realistic model, it is found that one experimentally observable feature can still be predicted, namely, the Hall constant. The analytical expression for the Hall constant [presented in (4)] is an integral over a family of parallel two-dimensional planes. For each plane the integrand is pro-

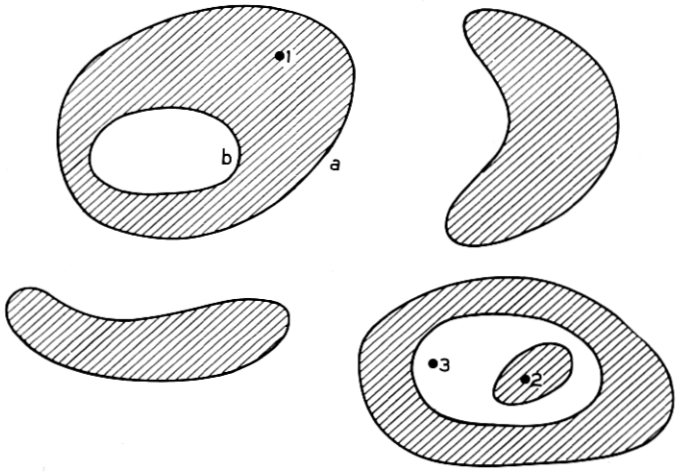

Fig. 1 — Several Fermi energy contours, shown in heavy lines, generated by the intersection of the plane P_z = constant with a hypothetical constant energy surface.

portional to the area of that part of the plane surrounded by an odd number of zero-contours of a function defined in that plane.

Prediction of this resistance parameter turns out in general to be a somewhat complicated analytical test, and this paper discusses some interesting aspects of a numerical method developed by the author to calculate the Hall constant. In part, the calculation procedure repeatedly requires a *topological* investigation to be carried out on a two-dimensional plane in order to evaluate a particular topological invariant associated with that plane.

Stripped of the particular physical problem which motivates the study, the essence of the topological inquiry is the following: Suppose there is a container with many pieces of string of varying lengths. The ends of each piece of string are tied together so that each piece forms a closed loop. As many loops of string as desired are placed on a table, subject only to the requirement that they do not touch one another; it should be emphasized that loops within loops are permitted (see Fig. 1 for a suitable example). Now, select a point on the table not on a string itself, and ask for the number of loops which surround that point (thus, for example, point 1 in Fig. 1 is surrounded by one loop, loop *a*). This is clearly a topological question, since the number of loops which surround a point is unaffected by an arbitrary displacement of each loop — a displacement which in addition does not permit any loop to pass through the point of investigation.

A simple pictorial model should help to clarify the role of topology in the calculation of the high-field Hall constant. Fig. 2 shows a hypothetical energy surface with cubic symmetry, composed of "spheres" and "cylinders." The intersection of this surface with each of a family of parallel planes defines the set of contours that are pertinent for the Hall constant calculation. For definiteness, consider those planes, two of which are illustrated in Fig. 2, perpendicular to the [001] axis. If the plane, like plane *a* in Fig. 2, cuts across the cylinders, then it is the area of the various cylindrical cross sections that contributes to the Hall constant calculation. However, for plane *b*, the second plane shown in Fig. 2, the contribution to the Hall constant is based on the planar area *outside* the spheres and cylinders, since now the regions in that plane surrounded by an odd number of contours lie outside the cylinders. Other planes are analyzed in a similar fashion.

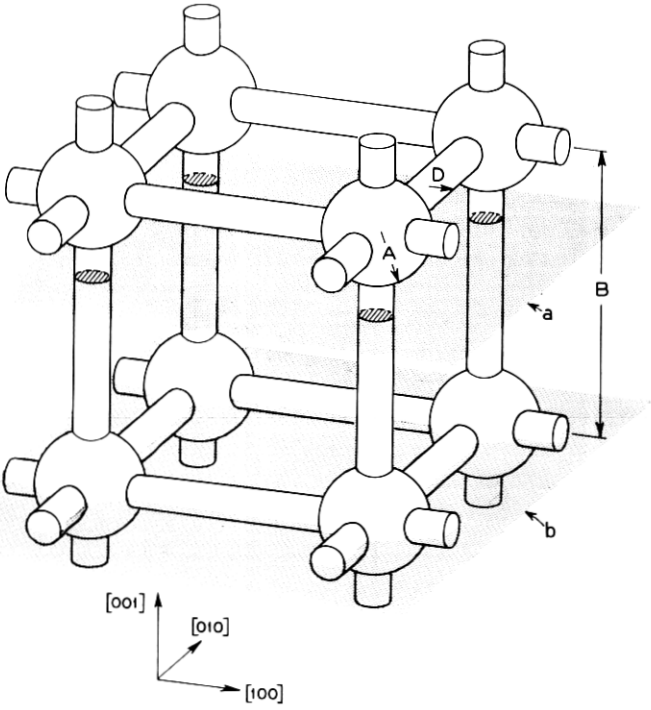

Fig. 2 — A portion of an ideal Fermi surface model of cubic symmetry composed of spheres of radius A and cylinders of radius D. The cube edge is of length B, and represents also the length of the cubic Brillouin zone, which is centered about each sphere. Two (001) planes, *a* and *b*, illustrate several different planar orbits.

In Section II, we define the customary resistance parameters in terms of the general resistance tensor that determines the electric field in terms of an applied current. The analytical expression for the high-field Hall constant is related to the direction of the magnetic field, the Fermi surface of the metal, and the symmetry of the crystal. In Section III those aspects of our calculation procedure that study the topology of nonintersecting planar contours are discussed in detail, and a logical procedure is developed, suitable for study with the aid of a digital computer, by which the "relevant" area may be ascertained in the most general case. In addition, a brief discussion is included of the significance of open contours, i.e., those contours that possess a net direction and never close upon themselves.

Section IV presents some of the numerical results obtained in the calculation of the Hall constant for copper. These results are based on the phenomenological model for copper that was proposed by Pippard.[1] Several figures are shown that depict orbits, both closed and open, computed for various charge carriers in planes transverse to the three axes [001], [011], and [111].

II. BACKGROUND AND ORIGIN OF THE PHYSICAL PROBLEM

In the most general situation, the relation between an applied current density (j_l) and the induced electric field (E_k) is described by a resistivity tensor (ρ_{kl}) according to the equation

$$E_k = \rho_{kl} j_l \,. \tag{1}$$

Here, and in what follows, all indices run from 1 to 3, and the summation convention is adopted. In the presence of a magnetic field (H_l), the tensor ρ_{kl} becomes a function of H_l, restricted by the Onsager relations so that $\rho_{kl}(-H_m) = \rho_{lk}(H_m)$. Two invariant expressions are commonly taken as descriptors of the resistivity tensor. The first is the resistivity ρ, defined by

$$\rho = \rho_{kl} n_k n_l \,, \tag{2}$$

a double summation involving the unit vector n_l which is in the direction of the current j_l. The second invariant parameter is the Hall constant R_H, defined by

$$R_H = \frac{\frac{1}{2}(\rho_{kl}\epsilon_{klm}H_m)}{H^2} \,, \tag{3}$$

where, as usual, $H^2 = H_l H_l$ and ϵ_{klm} is the three-index, completely antisymmetric tensor defined as $+1$ (or -1) whenever (klm) is an even (or odd) permutation of (123). Observe that the resistivity, (2), is

sensitive only to the symmetric part of the resistance tensor, while the Hall constant, (3), depends on the antisymmetric part of ρ_{kl}.

The theory developed by Lifshitz, Azbel, and Kaganov[2] and by Lifshitz and Peschanskii[3] treats conduction in a magnetic field in a very general way. The underlying picture of their theory is most easily visualized in crystal-momentum space, the dual space of the ordinary three-dimensional space in which the metallic lattice lies. At very low temperatures the motion of the charge carriers in a metal is confined to a unique energy surface, the Fermi surface; the carrier motion is also confined to lie in one of the planes in momentum space perpendicular to the direction of the magnetic field H_l. The periodicity of the lattice in physical space leads to a periodicity of the reciprocal lattice in momentum space, and the periodicity of the reciprocal lattice is imposed on the energy surfaces imbedded in momentum space.

If a closed segment of the Fermi surface is contained within a Brillouin zone, the fundamental zone of periodicity which we identify with the usual or "proximity" zone, then the orbits on which the charge carriers move are all *closed* contours, when studied for any direction of the magnetic field. If the region immediately within an orbit contains energies *less* than the Fermi energy E_f (a value which defines the Fermi surface), then that orbit is said to be "electron-like." Conversely, if the immediately interior region has energies *greater* than E_f, then the orbit is "hole-like."

When the Fermi surface encounters the boundary of the Brillouin zone, then the periodicity requirement can lead to a connected surface extending throughout the entire momentum space. For instance, the simple cubic model in Fig. 2 represents a connected Fermi surface composed of "spheres," each in a separate Brillouin zone, that are connected by "cylinders." On such an open surface, some orbits — open orbits — can have an infinite extension, never becoming closed. In particular, planar open orbits directed along the cylinders exist for the model illustrated in Fig. 2. Nevertheless, even for open Fermi surfaces, certain directions of the magnetic field (whose direction dictates the family of parallel planes on which the orbits lie) lead to all closed orbits; i.e., each orbit in every plane is closed, at least in some finite number of Brillouin zones. The fundamental property of all closed orbits characterizes the class of magnetic field directions for which the Hall constant R_H can be theoretically predicted. Under these circumstances, the analytical expression,[2,3]

$$R_H = \frac{h^3}{2ec}\left(\int dp_z \oint p_x \, dp_y\right)^{-1}, \tag{4}$$

defines R_H, where h is Planck's constant, $e > 0$ is the value of the electronic charge, and c is the speed of light. The integration over p_z represents a summation over the various momentum planes perpendicular to the magnetic field; now, and hereafter, the z direction is taken along the direction of the magnetic field. The domain of integration in (4) can be restricted to a single Brillouin zone, as will be discussed in Section 3.1.1. The contour integral extends around closed orbits in each $p_x p_y$ plane. If an orbit is electron-like, the contour integral in (4) is a positive number proportional to the area of the interior domain. On the other hand, if an orbit is hole-like, the contour integral in (4) is a *negative* number proportional to the area of the interior domain.

After suitable scale factors are introduced it suffices to study a completely *geometrical* factor in the Hall constant, which we call G: Let $p_i \to P_i$, where the P_i represent appropriate dimensionless variables; then

$$G \equiv \int dP_z \oint P_x \, dP_y . \tag{5}$$

This integral is based only on (a) the *direction* of the magnetic field, which selects the z direction, (b) the several plane *surfaces*, fixed in crystal-momentum space, which define the Brillouin zone boundary, and (c) the Fermi *surface*, also fixed in crystal-momentum space, on which the orbits are constrained to lie. In many substances the Fermi surface is multisheeted in each Brillouin zone. In this case a "G" may be determined for each sheet independently according to (5); the true "G" is the sum of the various individual ones. For simplicity, we confine our further analysis to a Fermi surface with only one sheet.

III. STUDY OF THE GEOMETRICAL FACTOR IN THE HALL CONSTANT

3.1 *Computational Procedure*

3.1.1 *Domain of Integration and Subdivision of the Calculation*

The formal definition previously given[2,3] for (4) [or (5)] states that the integration domain covers all of momentum space (infinite in extent), but that the redundancy of the total number of Brillouin zones (also infinite) is to be divided out. The periodicity of the energy surface suggests that the numerical result obtained from an integration over this weighted infinite domain should be equal to the result of a momentum integration restricted to only one Brillouin zone. Indeed, if all the closed orbits lay within a single zone (as on a small sphere), then

the integration domain could readily be restricted to only one Brillouin zone.

However, when the Fermi surface is open, it is a common occurrence that all of the different closed orbits do *not* lie within a single zone. For example, for certain directions of the magnetic field, some of the larger orbits may close only after excursions through a number of different zones. It is the possibility that there may be some large orbits, which necessitates the seemingly redundant integration over a correspondingly larger domain of momentum space, so that within each P_z-plane, the true nature of the larger orbits, i.e., whether they are electron- or hole-like, may be ascertained directly.

If an independent determination of the nature of all the orbits — say, a "list" of their electron- or hole-like character — were already in hand, then G could be calculated by an integral over only one Brillouin zone. This limited integration would be valid because the "list" would already specify the true nature of any orbit for which only a *portion* of that orbit lay on a single plane within one Brillouin zone. It is this general scheme that we employ to limit the domain of integration to the customary first Brillouin zone centered about the point $P_x = P_y = P_z = 0$.

Must we examine every orbit in an arbitrary P_z-plane for our "list"? No, fortunately, as the following argument shows. In a fixed momentum plane, simultaneous electron- and hole-like orbits can exist on a single sheet of the Fermi surface only if one orbit type encloses another. Several different orbits are pictorially indicated in Fig. 1, separated by clear and shaded regions which represent, for example, energies above and below the Fermi energy. For the particular P_z-plane shown in Fig. 1, the geometrical factor G would acquire contributions from the entire area within the orbit marked a and also, with the opposite sign, the entire area interior to the orbit marked b. The net result consists in including, with a single sign, only the shaded area between the orbits a and b. This same line of reasoning applies to the remainder of the orbits in this plane, so that just the shaded area within the boundaries of the first Brillouin zone contributes to G. As a result only the "shaded area," or, as we shall call it hereafter, the "relevant area," corresponding to a *unique* sign of the energy relative to the Fermi energy, enters into the calculation of the Hall constant for each plane P_z = constant. Thus, to obtain the equivalent of a "list" of the orbits suitable for calculating G, it suffices to study just one point. If this point is surrounded by an odd (even) number of contours, then it is within (outside) the relevant area; all points whose energy E relative to the Fermi energy E_f is of the same (opposite) sign lie in the area relevant in calculating G.

3.1.2 *Certain Orbit Characteristics Determined by a Topological Study*

The relevant area in Fig. 1 is independent of whether the interior points have energies greater or less than the Fermi energy. Indeed, Fig. 1 graphically illustrates the following property: *Every point in the relevant area is enclosed by an odd number of closed orbits.* For example, point 1 is within a shaded region of Fig. 1 and is enclosed by one loop, and so on for points 2 and 3. Furthermore, this *characterization* of the points in the relevant area is invariant under any deformation of the contours such that no contour passes through the point under study. This invariance property is topological in nature, being independent of specific details of the orbit shapes.

In order to accurately determine the number of contours surrounding a given point, a portion of the plane P_z = constant must be "scanned" — a portion generally much larger than that lying in the first Brillouin zone. Orbits which surround a point can only be found if they are actually encountered in the investigation; however, the restriction to a finite region of investigation is not serious in practice.

In the selection of a logical procedure to find the number of contours enclosing a particular point, simplicity is certainly a desirable feature. One very simple means of counting the contours (modulo 2, which is all that is necessary here) would seem to be the following: Pick a point not on a contour (i.e., $E \neq E_f$) and, starting there, investigate the energy values for a large sequence of closely spaced points all lying in a straight line. If an odd (even) number of crossings of the Fermi energy is found, the original point lies inside (outside) the relevant area. This intuitive procedure is, unfortunately, not always correct. Fig. 3 illustrates a set of contours in a fixed plane and shows three possible paths that could be used to determine the topology using the preceding scheme. Both paths 1 and 2 encounter three contours, and both emanate from shaded regions, i.e., relevant regions, as would be predicted by the above rule. However, path 3 illustrates the difficulty with this technique. In this example, the path ends inside a "sand-trap," and only two contours are encountered. Thus, we would erroneously conclude that the initial point did not lie within the relevant area. Clearly, a more sophisticated procedure of investigation is required that avoids the possibility of ending in a "sand-trap" by skirting around it.

Several alternate schemes of investigation come to mind which have the desired property of skirting around "sand-traps." In each of these an original test point is selected, and a series of points lying in some preselected straight line are tested for the crossing of a Fermi surface contour. If a contour is encountered, the *contour* is then followed, by

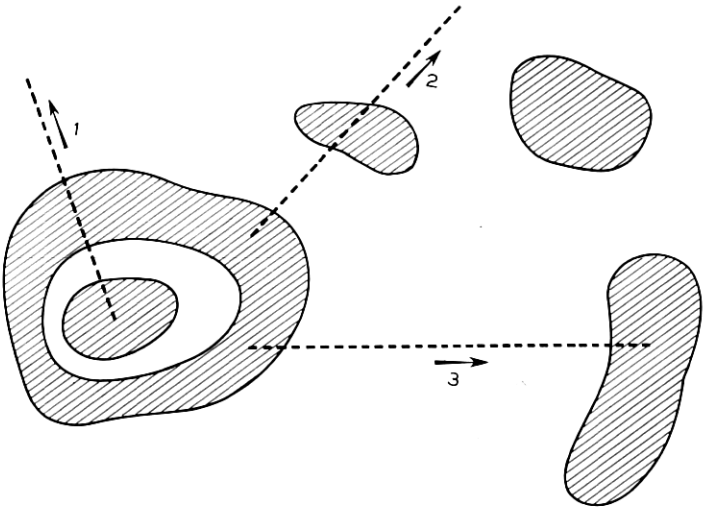

Fig. 3 — Fermi energy contours in a plane of fixed P_z. Three different paths, directed as shown, are tested in an attempt to determine where the shaded or "relevant" area lies.

always turning (with no loss of generality) initially to the left. The schemes differ in how far the contour is followed before the path leaves it.

One suggestive scheme has the path leave the contour as soon as it can proceed, without crossing the contour itself, in a radial direction whose origin is the original test point. A simple study reveals several fallacies in this scheme. Another scheme, of slightly greater complexity, has the path follow the contour until an extension of the original straight line of investigation is first encountered. At this point the path leaves the contour and continues in the original direction searching for a new contour. This scheme is likewise not foolproof in general, and must be abandoned. Among the contours it fails to analyze correctly is one shaped like the letter G if the test point is below the "hook" and the direction to be followed is upwards. Of course, in the general case, the location of the original point and the direction of inquiry are quite arbitrary, relative to the position and orientation of the contours to be studied.

The method of investigation illustrated in Fig. 4, although still more complicated, leads to an accurate count of the orbits surrounding any point. When a contour is encountered in the present scheme, that contour is followed *completely* until the point is reached at which the contour

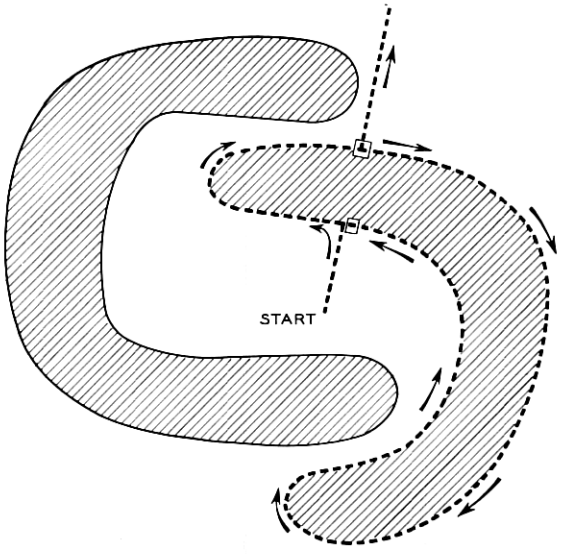

Fig. 4 — A satisfactory means of investigating an arbitrary layout of contours to establish the number of orbits which surround any point. It is applied here to a plane of fixed P_z that contains two distinct contours.

was originally engaged. While the entire contour is being examined, the number of points on the contour are counted that lie along a line which is an extension of the original line of investigation. Whether this number is odd or even determines whether that contour does or does not surround the original test point.* After the contour is completed, the path jumps to the furthest of these points, and then proceeds radially again along the original direction searching for a new contour to study. If a new contour is found, it is studied in completely the same fashion. Fig. 4 schematically illustrates the steps in a complete study of one contour by the present technique: the quest for the contour, the entire tracing of the contour, and the subsequent leaving in the original direction to continue the topological investigation. This investigation procedure is the one employed in the topological study of the various P_z-planes in calculating the geometrical part of the Hall constant by (5). A straightforward numerical integration, not discussed here, was used to determine the appropriate area in each plane that contributes to G.

* The more lengthy procedure of summing the polar angle variations along the contour can and has been used. This method can provide an exact count of the number of contours surrounding the original point, rather than an exact count modulo 2 provided by the method discussed in the text.

3.2 *Additional Features of a Calculation Encountered in Practice*

It was pointed out in Section II that the Hall constant cannot be theoretically predicted on the basis of (5) for magnetic fields which lead to a sizable, or nonnegligible, number of open orbits. However, this does not mean that open orbits will not be encountered in practical calculations of the Hall constant. On the contrary, open orbits may be present for one of several reasons. For example, all the magnetic field directions which support open orbits may not be known *a priori* for a phenomenological Fermi surface; only by trial and error can all such directions be discovered.

Another reason why open orbits may be encountered is based on the fact that numerical computations on digital machines can never be made with absolute precision. In particular, in the technique employed, a path of investigation is said to follow a contour so long as the value of the energy E satisfies the relation $| E - E_f | < \epsilon$, where ϵ is a small, nonzero number ($\epsilon \approx 10^{-4} E_f$), fixed by the gradient of the energy function and by practical computation requirements. It is entirely possible that two closed orbits which come close to each other cannot (computationally) be distinguished from a single connected orbit if the energy values satisfy $| E - E_f | < \epsilon$ along some path that connects the contours. If a sequence of closely spaced closed orbits exists, an error may be repeatedly or even unpredictably made, so that the path of investigation does not close. While the likelihood of errors being made decreases as ϵ is made smaller, a proviso must be made for encountering either one of two types of "open" contours: (a) valid open orbits for which the path proceeds through momentum space along an open contour possessing a net directivity, or (b) "lost" open orbits, which may or may not indicate the presence of true open contours, for which the path of investigation gets lost and wanders rather aimlessly throughout momentum space. The first type of open orbit, i.e., a valid open orbit, is detected to a high accuracy by placing an upper bound on the radial distance from the test point that the path travels in momentum space; the second type, i.e., a "lost" open orbit, is sensed by an upper bound on the number of individual points of investigation that can be made along any single contour. Whether an open orbit declared "valid" is truly open or just part of an exceedingly extended closed orbit is not too important, since the magnetic field is, after all, finite, and greatly extended closed orbits become indistinguishable from open orbits whenever the orbit circumference c divided by the mean free scattering length l is comparable with the magnetic field strength, suitably normalized.

Such considerations can in fact act as a guide in selecting the upper bounds placed on the path's excursion.

The presence of open contours generated by "tunnelling through an energy barrier" (i.e., along a path such that $|E - E_f| < \epsilon$) is not necessarily an academic case when ϵ is small. There is a small but very important class of magnetic field directions that lead to both closed and open orbits, but to the latter only on a set of P_z-planes of measure zero. The hypothetical connected Fermi surface illustrated in Fig. 2 is one for which sets of open orbits of measure zero exist when the magnetic field is along the principal crystalline axis [001], or equivalently along either the [010] or [100] directions.

Even in the presence of an infinitesimal number of open orbits, the geometrical part of the Hall constant is still theoretically predicted according to (5), since the contribution from those few P_z-planes is negligible. In fact, those magnetic field directions that lead to a negligible number of open orbits are often among the most interesting, for they are axes that possess high symmetry. When a Hall calculation is carried out for such a direction and one of the few open orbits is encountered (in one of the two ways discussed above), that entire P_z-plane is disregarded; no investigation of the size of the relevant area is or even can be made. Since the open orbits are ideally of zero measure, they should be encountered in the computation on at most a few of the large number of parallel planes studied that are perpendicular to the magnetic field. An open orbit of this kind, ideally belonging to a set of measure zero, will be illustrated in the next section.

Finally, there is some additional information that can be found from a knowledge of the extent and of the directions of the open orbits themselves. This additional information pertains to the expected behavior of the other magnetoresistance parameter, the resistivity ρ defined in (2). Generally speaking, it follows from theory[2,3] that, on the one hand, the resistivity saturates in a high magnetic field for those magnetic field directions which lead to all closed orbits, and, on the other hand, the resistivity continues to increase as H^2 for those magnetic field directions which possess a nontrivial set of open orbits, all of which lead off in the same net direction. Thus, to predict qualitatively the resistivity behavior for various magnetic field directions, it suffices to study the geometrical shape of the Fermi surface in order to see for which directions of the magnetic field open orbits are permitted.

Conversely, the analysis of high-field resistivity data gained from measurements on high-purity metal single crystals is one of the best means available to gain information regarding the topology of the Fermi

surface, and even to provide some quantitative limitations on the shape of the Fermi surface. Therefore, a valuable auxiliary feature of a general procedure to calculate the Hall constant is the ability to shed some light on the expected resistivity behavior of a particular Fermi surface model by displaying the open orbits that are encountered for an arbitrary magnetic field direction. Preliminary discussions of the interpretation of the observed resistivity behavior for copper have been given elsewhere,[4,5,6,7] and an extensive paper is in preparation in collaboration with J. E. Kunzler that will discuss magnetoresistance measurements and their explanation in some detail.

IV. APPLICATION TO METALS: COPPER

In this section we present some of the results of Hall constant analyses for a particular model of the Fermi surface of copper. Copper, or any of the noble metals, is particularly attractive for a discussion of the present type, since it involves a Fermi surface with only one "sheet"; the essential ingredients needed to discuss more complex metals are present without any unnecessary complications.

Copper has a face-centered cubic space lattice whose cube edge is 3.61 angstroms long. It follows that the reciprocal lattice in crystal-momentum space is body-centered cubic. The Brillouin zone that is characteristic of this lattice is an octahedron, truncated by a cube at the six vertices. If we make use of the cubic symmetry, then two inequivalent planes suffice to define the Brillouin zone boundary: one face perpendicular to the [111] axis — this face forms one of the eight surfaces of the octahedron; and three equivalent faces perpendicular respectively to the [100], [010], and [001] axes — these faces truncate the octahedron.

Because copper has only one valence electron, the region within the first zone that is also contained within the Fermi surface must equal one-half the total volume of the first Brillouin zone. Subject to this volume requirement, the confining surface may, in principle, be arbitrarily deformed. Suppose, as an extreme, the Fermi surface assumes the free-electron spherical shape. It is readily deduced from the volume constraint that this sphere does not intersect the boundary of the Brillouin zone, although it does come close to the octahedral faces. In this case the Fermi surface would consist of a number of disconnected spheres, each lying completely within a separate zone of periodicity. Only electron-like orbits would exist; no hole-like or open orbits would be present. Consequently, the Hall constant would depend on the sum of all the electron-like areas, i.e., it would depend simply on the volume within the Fermi surface. The observed Hall constant would be the same for

any orientation of the magnetic field, and by (5), $G \equiv G_{\text{free}} = \frac{1}{2}$, expressed in units in which the volume of the Brillouin zone is unity. Such a state of affairs would be present if the conduction electrons were free and felt no perturbing influence from the lattice.

In real copper the electrons are, of course, not free, and the Fermi energy surface deviates from a simple sphere. Pippard[1] in 1957 was the first investigator to successfully derive a phenomenological, nonspherical Fermi surface for copper. Speaking picturesquely, the surface he found from anomalous skin effect measurements possesses "arms" or "necks", which extend outward from the Fermi surface, that actually contact the hexagonal Brillouin zone faces associated with the ⟨111⟩ directions, i.e., the [111] and equivalent directions. Each area of contact is about 10 per cent of the area of one of the hexagonal zone faces. The Fermi surface of copper therefore consists of a sequence of sphere-like "bodies" situated on a body-centered lattice that are completely interconnected by "arms" which lie along ⟨111⟩ directions.

An "arm" along one of the ⟨111⟩ directions supports open orbits whose net direction is along the same ⟨111⟩ direction. However, in copper (and surely in various other metals) the shape of the "bodies" and "arms" is such as to provide support for open orbits along additional directions. The origin of the support for additional open orbits is straightforward and is discussed elsewhere.[8] Resistivity measurements bear out in detail the presence of the primary open orbits along ⟨111⟩ directions, as well as additional open orbits that the ⟨111⟩ "arms" support,[7] principally in the ⟨100⟩ and ⟨110⟩ directions.

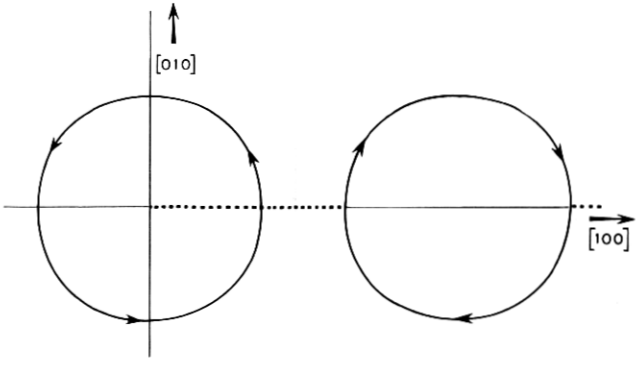

Fig. 5 — Contours on the Pippard Fermi surface in the $P_z = 0$ plane transverse to the [001] axis. The topological path of investigation proceeded along the dotted line and around the contours in the direction of the arrows. This plane was determined to be electron-like since at the initial point $E < E_f$.

The periodic energy surface determined by Pippard has been expressed to an accuracy of 1 per cent by Garcia-Moliner[9] in terms of a three-parameter Fourier series. His analytical expression has been employed in calculations on IBM 704 and 7090 computers to study the Hall constant for various directions of the magnetic field, based on the procedure developed in this paper. In these calculations, electron-like, hole-like, and open orbits were all encountered. Some of the contours that are present when the magnetic field is along either a ⟨100⟩, ⟨110⟩, or ⟨111⟩ type direction are shown in Figs. 5 through 9. In these figures the path of investigation is explicitly exhibited by which the relevant area was determined according to the procedure indicated in Fig. 4: The dotted line denotes that part of the path, always proceeding to the right, for which contours are being sought. The heavy line or lines represent the part of the path on which, in the direction indicated by the arrows, a contour on the Fermi surface is being followed.

Figs. 5 through 7 represent the behavior in three parallel (001) planes,

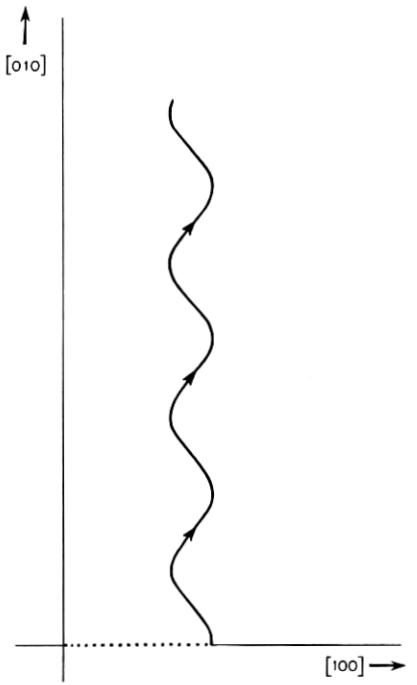

Fig. 6 — An open contour on the Pippard Fermi surface in the $P_z = 0.585$ [if center to (001) face of Brillouin zone $\equiv 1$] plane transverse to the [001] axis.

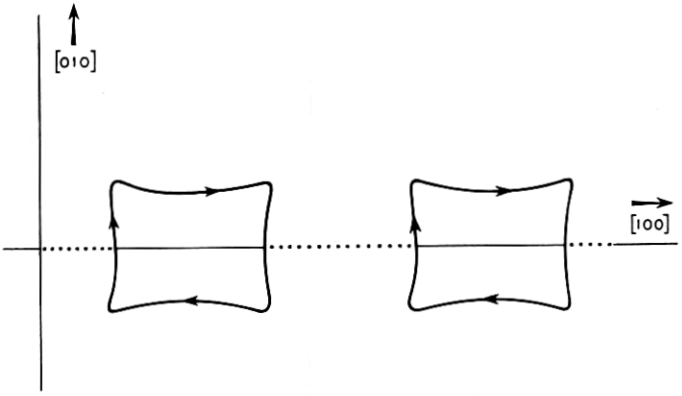

Fig. 7 — Contours on the Pippard Fermi surface in the $P_z = 0.575$ plane transverse to the [001] axis. This plane was determined to be hole-like since at the initial point $E < E_f$.

the first at $P_z = 0$, which shows the contours of electron-like behavior around the "belly" of the Fermi surface. Fig. 6 shows an open orbit, ideally belonging to a set of measure zero, located on the (001) plane at $P_z = 0.585$, where for present purposes the distance to the (001) face of the Brillouin zone boundary is taken as unity. Just a short distance below this plane, at $P_z = 0.575$, the carrier behavior is quite different, being hole-like; the Fermi surface contours for this plane are shown in Fig. 7.

In Fig. 8, hole-like contours are illustrated that lie in the $P_z = 0$ plane when the magnetic field is along the [011] axis. Oscillations in gold and silver of similar so-called "dog-bone" orbits have been observed in de Haas-van Alphen experiments.[10]

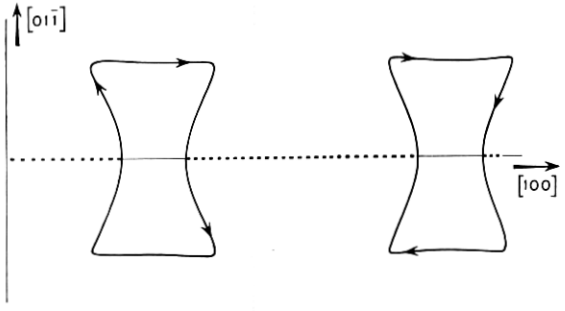

Fig. 8 — Contours ("dog-bone" orbits) on the Pippard Fermi surface in the $P_z = 0$ plane transverse to the [011] axis. This plane was determined to be hole-like since at the initial point $E < E_f$.

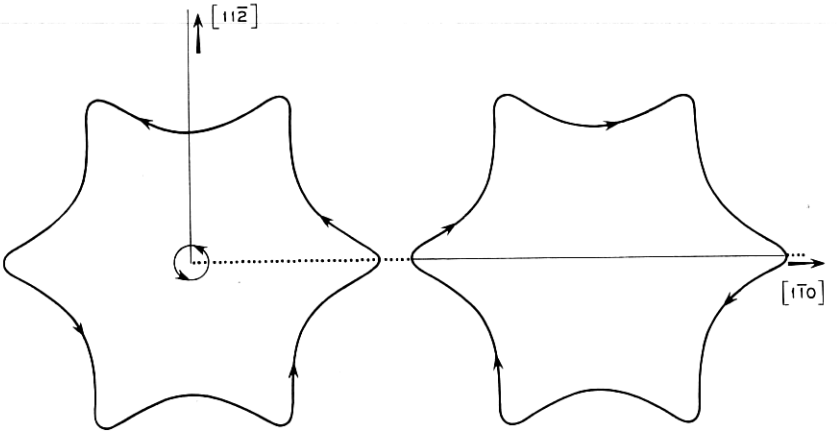

Fig. 9 — Contours on the Pippard Fermi surface in the $P_z = 0.866$ plane transverse to the [111] axis, which is tangent to one of the hexagonal faces of the Brillouin zone. This plane was determined to be hole-like, since at the initial point $E < E_f$.

Fig. 9 shows the contours found when the magnetic field was in the [111] direction and the particular plane of investigation lay on the surface of the Brillouin zone, i.e., $P_z = \frac{1}{2}\sqrt{3} \cong 0.866$, expressed in the same units as above. The small contour represents a cross section of one of the "necks" which connects the sphere-like "bodies." However, the large hole-like contour, which surrounds the small one, determines the behavior in the plane for purposes of the Hall constant calculation. An investigation of the contours that terminated before the first big contour had been reached would have given an erroneous result, although it would have covered all of the area within the first Brillouin zone.

In the planes transverse to either one of the two types of symmetry directions, ⟨100⟩ or ⟨111⟩, closed orbits of both electron- and hole-like character exist in different planes, this being possible because, by rotational symmetry, only a finite (hence negligible) number of intermediate planes can occur that contain open orbits. This is not the case for copper if the magnetic field lies along a ⟨110⟩ direction, and the analysis of this particular direction requires an individual study, which will be given presently. For the former two symmetry directions the predicted and observed[11] values of the geometrical factor G — divided by the free-electron value G_f — are tabulated along with the Hall constant R_H in Table I. The ratio G/G_f measures the effective number of metallic electrons that are contributed per atom. The observed Hall voltage is very sensitive to field orientation in the neighborhood of the ⟨111⟩ direction,[11] and accounts for the increased experimental uncertainty. This extreme

sensitivity with orientation can be readily understood: It is due to the rapid transformation of hole-like regions similar to that illustrated in Fig. 9 into electron-like regions as the magnetic field orientation deviates from a <111> axis.

When the magnetic field is in, say, the [011] direction the Fermi surface of copper supports not only planes of hole-like or electron-like behavior separated by a finite number of planes with open orbits, but also a small yet nontrivial band of planes that support [100]-directed open orbits. In principle, these open orbits are broken into very large but nevertheless closed orbits if the magnetic field is reoriented very near to the [011] direction with a slight component along the [100] direction. If the angle of deviation from the [011] direction is small, then only an an extremely small number of any new open orbits could have been introduced. Consequently, it appears quite permissible to treat the Hall constant in the immediate neighborhood of a <110> direction as numerically significant *if* the magnetoresistance exhibits a point of saturation in the proximity of the <110> axis, which indicates that at some point open orbits were actually absent experimentally, *and* if the measured Hall voltage is a smooth function of the magnetic field orientation in that vicinity. The experimental results support both of the requirements in question: The magnetoresistance shows a point of saturation near the <110> axes,* and the Hall voltage shows a broad flat peak in the neighborhood of the <110> directions.[7,11] Thus this Hall measurement is significant, and it was used to obtain the observed Hall constant for the <110> directions shown in Table I. The theoretically calculated value for Table I was computed by assuming that the magnetic field was along the [011] axis, so as to determine the principal contribution, including that from the hole-like regions. The band of planes with open orbits, which was actually detected, was then reinterpreted as a band of planes having electron-like behavior, the behavior each of these planes would acquire if the magnetic field were tilted ever so slightly in the [100] direction.

The precision of the various Hall constant predictions is estimated at 1 to 2 per cent. Better agreement with the experimental Hall constants can be obtained if a Fermi surface model is used whose "arms" or "necks" are increased in diameter. With fatter "arms," more hole-like planes, such as in Figs. 7 and 8, will be present for fields along <100> and <110> axes, and, as a consequence, higher Hall constants would be predicted. It is interesting that the results of de Haas-van Alphen measurements[10]

* See Ref. 7, especially Fig. 1b, which shows the saturation behavior near to an [011] axis.

TABLE I—A COMPARISON BETWEEN THE PREDICTED AND OBSERVED HALL CONSTANT FOR THREE INEQUIVALENT FIELD ORIENTATIONS IN COPPER

Magnetic Field Directions	Predicted*		Observed†	
	G/G_{free}	R_H‡	G/G_{free}	R_H‡
⟨100⟩	.71	10.3	0.59	12.6 ± .5
⟨110⟩	.72	10.2	0.65	11.4 ± .5
⟨111⟩	.32	22.7	0.37	20.0 ± 5.0

* Based on the Garcia-Moliner[9] expression of the Pippard Fermi surface of copper.
† Based on the data of Kunzler and Klauder.[11]
‡ The numbers in this column when multiplied by 10^{-12} represent the Hall constant expressed in volt-cm/abamp gauss.

also suggest that a more realistic copper Fermi surface would have fatter "arms" than the Pippard model.

V. ACKNOWLEDGMENTS

It is a pleasure to thank C. Herring for bringing this problem to my attention and for his interest in this work. Many valuable conversations with J. E. Kunzler are greatly appreciated, and a critical reading of the manuscript by E. I. Blount is acknowledged. The author wishes to thank Miss B. Cetlin for her advice and encouragement.

REFERENCES

1. Pippard, A. B., Phil. Trans. Roy. Soc., **A250,** 1957, p. 325.
2. Lifshitz, I., Azbel, M., and Kaganov, M., J. Exptl. Theoret. Phys. (U.S.S.R.), **31,** 1956, p. 31; Soviet Phys. J.E.T.P., **4,** 1957, p. 41.
3. Lifshitz, I., and Peschanskii, V., J. Exptl. Theoret. Phys. (U.S.S.R.), **35,** 1958, p. 1251; Soviet Phys. J.E.T.P., **8,** 1959, p. 875ff.
4. Kunzler, J. E., and Klauder, J. R., Bull. Am. Phys. Soc., **5,** 1960, p. 150.
5. Alekseevskii, N., and Gaidukov, Y., J. Exptl. Theoret. Phys. (U.S.S.R.), **36,** 1959, p. 447; Soviet Phys. J.E.T.P., **9,** 1959, p. 311.
6. Priestley, M. G., Phil. Mag., **5,** 1960, p. 111.
7. Klauder, J. R., and Kunzler, J. E., *Proceedings of the International Conference on Fermi Surfaces*, John Wiley & Sons, New York, 1961.
8. Klauder, J. R., and Kunzler, J. E., J. Phys. Chem. Solids, **18,** 1961 p. 256.
9. Garcia-Moliner, F., Phil. Mag., **3,** 1958, p. 207.
10. Schoenberg, D., Phil. Mag., **5,** 1960, p. 105.
11. Kunzler, J. E., and Klauder, J. R., Phil. Mag., in press.