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The Fermi Surface of Zinc. Radio-Frequency Size Effect.

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THE FERMI SURFACE OF ZINC
RADIO-FREQUENCY SIZE EFFECT

A Dissertation

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in

The Department of Physics and Astronomy

by
Oscar Lucien Steenhaut
b.e.i., Rijksuniversiteit Gent, 1955
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ABSTRACT

The Fermi surface of zinc is determined from calipers obtained through rf size effect measurements. The 6- to 8-MHz rf measurements were performed at 1.2°K on high purity monocrystals of zinc approximately 0.5 mm in thickness. The Fermi surface was calipered using samples whose normals to the surfaces were parallel to one of the three principal symmetry directions $[0001]$, $[10\bar{1}0]$, and $[11\bar{2}0]$, with magnetic field rotations in the plane of the sample. Calipers are assigned to definite orbits on the first- and second-band hole surfaces and the third-band electron surface. The third-band electron "lens" is found to be smooth and round with a major diameter of $1.737 \text{ \AA}^{-1}$ and varying less than 0.5 pct. in the basal plane. The minor diameter has a caliper of $0.556 \text{ \AA}^{-1}$. Calipers are given for the first-band hole surface and the spin orbit induced gaps between the first and second bands are discussed. The second-band hole surface is discussed in detail with the assignment of 30 series of calipers to definite

orbits on this sheet of the Fermi surface. Both the first and second bands of holes are found to have considerably smaller cross sections than predicted by the single - orthogonalized - plane - wave construction. Detailed comparisons to a recent pseudopotential calculation of the energy bands and the Fermi surface are made. No calipers were observed that could be assigned to the third - band "stars" or the fourth - band electron "cigars".

Appendices describe the details of the field generator and the impedances measurement, together with a collection of all measured data and points on the FS obtained from Stark and Falicov.

I. INTRODUCTION

Ever since it has become known that most of the electrical conduction properties of a normal metal at low temperatures can be related to the topological peculiarities of the Fermi surface (FS) of the metal, the goal of many theoretical and experimental investigations has been to completely describe the FS for all normal metals.

The purpose of the investigation reported in this dissertation was to experimentally obtain extensive and detailed dimensions of the FS of zinc and to make comparisons with former reported experimental results and with a theoretical calculation of the FS by Stark and Falicov (SF).¹

Zinc is a divalent metal with a hcp lattice and the terminology introduced by Harrison² in describing the single OPW construction of the FS, as represented in Fig. 1, is used throughout this paper. The first zone hole surfaces around the H point are called the caps. The complicated, multiply connected hole surface of the

(b) second band

(a) first band

Fig. 1

(c) third band

(d) fourth band

Fig. 1

second zone is known as the monster. The third zone has a large section, centered around Γ , called the lens, small pockets at the K point are christened the needles and sheets centered on the HL line named stars. The fourth zone elements are completely enclosed within the stars and are known as cigars. As will be seen, the stars and cigars are above the Fermi level in Zn and consequently they were not observed in this experiment.

An early bandstructure calculation by Harrison³ indicated that the actual shape of the FS did not deviate appreciably from the single orthogonalized plane wave surface. Harrison's calculation was a pseudo-potential (PsP) calculation using a local first principles pseudo potential with the pseudo wave function subjected to the following additional condition: that

$$\frac{\int |\text{grad } \varphi_k|^2 d\tau}{(\varphi_k, \varphi_k)}$$

should be a minimum, this condition optimized smoothness. Electron-electron exchange and spin-orbit coupling were neglected and the effects of core screening were only partially dealt with. This calculation did not provide a definite conclusion concerning the stars and the cigars. A later calculation⁴ with a semi empirical pseudo potential but with the same approximations did not remove the uncertainty concerning the stars and cigars.

An improved PsP calculation was recently performed by Stark and Falicov,¹ in which a non-local empirical pseudo-potential was used. They adjusted a set of pseudo-potential coefficients to agree with the dHvA frequencies, in addition, spin-orbit coupling was explicitly included in the Hamiltonian. The energies were obtained from an n^{th} order ($18 \leq n \leq 32$) secular equation with the value of n being chosen to satisfy the group symmetry of each of the six major symmetry points and was used in the region of the Brillouin zone immediately surrounding these points. This calculation definitely did show that the stars and cigars were above the Fermi level. The secular equation was also solved along given directions for the Fermi level⁵. This procedure was done without the inclusion of spin-orbit coupling and the results are included for reference in Appendix C.

Attempts at experimental determination of the FS have been carried out by many methods, each having its own advantages and difficulties. Although none of the previous experiments gave a definitive description of the FS, certain aspects were delineated in each attempt. The most important experiments which have given information about the FS of zinc are listed here.

1.- The de Haas-van Alphen effect and allied effects (i.e. oscillations in electrical conductivity, acoustic attenuation, magneto-resistance, indeed oscillations

of every property of the metal with the magnetic field). In this class of experiments a characteristic frequency of oscillation is observed as the magnetic field is varied. This frequency measures A , an extremal cross-section area of the FS. The temperature and field dependence of the amplitude of the oscillations also give (in a complicated way) $\frac{dA}{dE}$ and information about scattering. Since an area is an integral over the surface, detailed aspects of the FS are inevitably ironed out.

Among the most carefully performed dHvA measurements are those by Joseph and Gordon.⁶ These authors were able to resolve six frequencies, giving rather accurate dimensions of the lens and establishing the general shape of the monster, they were unable however to discount entirely the existence of the stars and cigars.

Higgins et al.⁷ extended the dHvA measurements to higher fields. By using a very sensitive feedback torsion balance, they found seven more frequencies. From observing the angles of disappearance of some frequencies they concluded that the horizontal arms of the monster had to be much smaller than predicted by the single OPW FS. Two frequencies were tentatively assigned to the stars and cigars.

Further dHvA measurements on Zn were made by Higgins and Marcus,⁸ Lawson and Gordon,⁹ Thorsen et al.¹⁰, and

pressure dependent dHvA measurements were made by O'Sullivan and Schirber,¹¹ the frequencies formerly assigned to the stars and cigars were reassigned and the breakdown field between needles and monster was established at 2.2 kG.

Oscillations in magneto-resistance were analysed, among others by Stark¹² and by Schirber.¹³ From a very detailed analysis of the angular dependencies of the frequencies, Schirber was able to deduce the linear dimensions of the inside hole of the monster.

Oscillations in acoustic attenuation were reported by Myers and Boswell,¹⁴ but their analysis did not go beyond the results already obtained by Joseph and Gordon.

Oscillations in other properties were observed in Zn by many experimenters,¹⁵ none were analysed accurately enough to contribute to detailed knowledge of the Zn FS.

2.- The geometrical magneto-acoustic effect is the oscillatory change in attenuation of sound waves propagating in a sample subject to an increasing magnetic field. The oscillatory behaviour occurs when diameters of extremal orbits become equal to multiples of the sound wave length. This technique suffers from the problem of precisely measuring and resolving the frequencies and the resulting accuracy is generally poor. A few calipers were determined by Galkin and Koralyuk,¹⁶

and a detailed analysis with magnetic field variation in the $[10\bar{1}0]$ and $[11\bar{2}0]$ planes was published by Gibbons and Falicov,¹⁷ no estimates of accuracy were given but a comparison with other published values shows a maximum error of 5 pct. Calipers were erroneously assigned to the stars and cigars by these authors.

3.- Cyclotron resonance measurements allow a direct determination of $\frac{dA}{dE}$ which in conjunction with area measurements allow a complete determination of FS topology. Using thin samples and the Chaikin¹⁸ size effect linear extremal dimensions of the FS can be derived. Samples for these experiments, however, are not easy to prepare and the many frequencies simultaneous present are difficult to resolve. Very limited results were observed by Naberezhnykh and Mel'nik.¹⁹ A more detailed experiment was reported by Shaw et al.²⁰ in which measurements with the magnetic field in the three principal planes were made and then were able to assign cyclotron masses to all principal (except the needles) sheets of the FS, no frequencies were detected which could be attributed to star or cigar orbits.

4.- Many other effects give direct information about the FS and could in principle be used. We mention: the anomalous skin effect, related in a complicated way to the radius of curvature; positron-annihilation, which

in a simple interpretation could give the area of all sections of the FS; the Kohn effect, from which density of states could be derived. These effects are all difficult to measure and to interpret accurately. No results are reported as yet contributing directly to our knowledge of the FS of Zn.

5.- The radiofrequency size effect (RFSE), discovered by Ghanmacher,²¹ is the measurement of the discontinuities of rf surface impedance of a thin plate, when an extremal orbit size or its multiple just fits into the thickness. This measurement gives directly the linear dimensions of the FS. The method requires very pure, thin, strainfree samples but is otherwise easy to implement and gives very accurate results.

The FS dimensions measured for this dissertation were obtained from RFSE measurements. Except for a few improvements which make the FS determinations more accurate, the experimental technique has been described in detail earlier.²² Briefly, the experiment consists of measuring the rf surface impedance of a thin slab of the sample as a function of magnetic field applied in the plane of the slab. Discontinuities in the surface impedance (R) are observed at values of the applied magnetic field which allow extremal electronic orbit sizes to span the sample thickness. Fermi surface

dimensions can then be obtained through the relation

$$k_c = 0.015194 Hd$$

where H is the value of the field at the discontinuity in gauss, d the thickness of the sample in mm, and k_c is an extremal distance across the FS in $\text{\AA}^{-1}$.

In the sections which follow, the important aspects of the experimental apparatus and procedure are described, the results presented, and a complete FS description obtained from these results is given. Finally, a comparison to the FS obtained by SF is made and a brief discussion of the line shapes is given.

Appendices describe the details of the field generator and the impedance measurement together with a collection of all measured data and points on the FS obtained from Stark and Falicov.

II. EXPERIMENTAL DETAILS

The samples on which the measurements in this experiment were performed were cut from a zone refined bar of Zn obtained from Cominco Products Incorporated (quoted purity: 99.9999 pct.). The 1 kg bar was etched in a 94 pct. HNO_3 and 6 pct. chromic acid solution which made the boundaries between several large monocrystals easily visible. One of these crystals was selected and cut from the bar by spark erosion. Samples to be used in the measurements were then oriented, cut and planed thin in the manner described in Ref. 22. In order to obtain strain free samples for field rotations in the (0001) plane, it was necessary to perform the spark erosion cutting and planing at temperatures above room temperature. This was accomplished by immersing the sample and goniometer in a small container of Primol 355 (Humble Oil and Refining Company) which was heated to 250°C with an immersion heater and, in addition, the bath was continuously stirred during the cutting procedure to avoid thermal gradients across the sample. Samples cut

and planed at 250°C showed no indication of strain on back reflection pictures after etching, whereas samples planed at room temperature always resulted in distorted x-ray spots.

After the cutting and thinning procedure was completed, the surfaces of the samples were cleaned and a small amount of residual surface strain due to the spark cutting was removed by dipping the samples in concentrated HNO_3 for 1 sec. An equally satisfactory procedure for preparing the surfaces was found to be to lap each surface on a microscope slide immersed in a 1 pct. solution of HNO_3 in alcohol. The finished samples were always checked to assure that the final orientation was correct and was always found to be within less than $\pm 1^{\circ}$ of the required orientation while exhibiting no discernable strain on the back reflection pictures.

The average thickness of each sample was determined by measuring the area of the face of the slab and weighing the sample in the manner described by JGF. The thickness determinations were made on large slabs from which the final sample was cut. The low temperature thickness used in calculating the k_c values was then determined using the thermal expansion data for Zn given by the National Bureau of Standards.²³ The sample holder and rf coil arrangement was the same as given in JGF and

all FS measurements were performed at 1.1°K obtained by pumping on the helium bath.

The electronic detection system and magnetic control used here were modified from that used by JGF to improve the accuracy with which the FS could be determined. A calculation of the RFSE line shape by Juras²⁴ shows that the point on the rather complicated line shape which gives the correct caliper value is the point of maximum slope preceding the first peak in the $\frac{dR}{dH}$ vs H curve. This point can be easily determined by recording $\frac{d^2R}{dH^2}$ vs H and the electronic detection system was modified for this purpose. The resulting detection circuitry is shown in Fig. 2. A harmonic generator is inserted in the reference signal side of the phase detector so that the system is tuned to twice the field modulation frequency. This arrangement is standard and allows $\frac{d^2R}{dH^2}$ to be plotted. The harmonic generator and rejection filter can be switched out of the circuit to record $\frac{dR}{dH}$ when desired.

In most FS determinations from RFSE measurements on high purity metals, highly stabilized and programmable magnetic fields in the range of 0 to 1000 G are required. A 4-inch diameter pole face iron core electromagnet with a 2 inch gap is used in this laboratory for these measurements and the field control system for this magnet was specially designed and built to make accurate RFSE

FIG. 2

measurements. The system allows the field to be set at any value between - 1000 G and + 1000 G and field sweeps of 2 up to 1000 G to be made starting from the preset field. Since magnetic field modulation at 50 Hz is used in the detection of the RFSE and high modulation amplitudes are not required, the field is modulated directly through the dc supply for the magnet.

The over-all reproducibility of this electronic system and sample thickness measuring technique is 0.5 pct. as determined by caliper values obtained for the same orbit on different samples.

III. EXPERIMENTAL RESULTS

Data were obtained for field rotations in three symmetry planes. Thus, samples were used having the normal to the face of the slab, $\underline{n}$, parallel to the $[0001]$, $[10\bar{1}0]$, and $[11\bar{2}0]$ axes. A general feature of all the data on Zn is that all of the RFSE lines are weaker than those previously observed in Cd^{22} even though the sample purity, state of strain, and the temperature dependence of the line intensity were approximately the same. In addition, many more broken orbits are observed in Zn than were observed in Cd and these type orbits depend on sharp corners of the FS in order to be detected. This may indicate that the FS is much sharper in Zn than in Cd.

All of the caliper values computed from the observed data are plotted in Fig. 4. The calipers which could be definitely assigned as being due to the addition of two orbits are not shown on this figure. The values given in Fig. 4 were determined through Eq. 1 from the field at which the first peak in the second derivative curve occurred. The values are reproducible to within ± 0.5 pct.

FIG. 3

between different samples and all of them can be assigned to orbits on the Zn FS.

The data for $\underline{n} \parallel [0001]$ were recorded by rotating the magnet in 1° steps over a 45° range that covered two axes, $[10\bar{1}0]$ and $[11\bar{2}0]$. Recorder traces obtained in this orientation for both first derivative and second derivative detection are shown in Fig. 3. The signal to noise ratio was always very poor for this orientation and degraded strongly when the sample was cycled between 4.2 and 300° K. This behaviour was observed on four different samples cut from different single crystals and was independent of sample size, rf frequency and method of surface preparation. In this orientation there was a strong field - dependent background signal extending over the entire field range investigated which added to the difficulty in observing the size effect peaks.

FIG. 4

IV. DATA ANALYSIS AND CALIPER ASSIGNMENT

Throughout this discussion the same definition of caliper is used as was defined by JGF. That is, an extremal caliper is defined as a vector quantity in k space which is in the direction of $\pm \underline{n} \times \underline{H}$ and has a magnitude equal to the length of the line segment formed by projecting an extremal orbit (in k space) onto a plane perpendicular to $\underline{n}$. Since the RFSE always obtains values of extremal calipers, the term caliper will be taken to mean extremal caliper throughout.

The Brillouin zone (BZ) for zinc is shown in Fig. 5 along with the zone dimensions for reference. The results of the calculation of SF show that there are only four sheets of the FS in Zn. The electron surfaces are in the third zone and in the repeated zone scheme form a large portion centered at the Γ point (lens) and an extremely small pocket at the K point (needles). The first band crosses the Fermi level near the H point (caps) and the second band gives rise to the complicated, multiply connected surface known as the "monster".

Zn

$$\Gamma A = 0.646106 \text{ \AA}^{-1}$$

$$\Gamma M = 1.36402 \text{ \AA}^{-1}$$

$$\Gamma K = 1.574919 \text{ \AA}^{-1}$$

	k_x	k_y	k_z
Γ	0	0	0
A	0	0	0.646106
K	1.574919	0	0
H	1.574919	0	0.646106
M	1.18128	0.682011	0
L	1.18128	0.682011	0.646106

FIG. 5

The single - orthogonal - plane - wave construction of the Zn FS predicts two additional sheets of the surface (third band stars and fourth band cigars), but the calculation of SF has shown these portions of the bands to be above the Fermi level and no data is presented here to contradict this conclusion.

A. Third Band Electrons

The assignment of caliper series u , α , and f in Fig. 4 to the third band lens was immediately obvious. In all three orientations the plane of the orbit giving rise to this caliper passes through the Γ point and all caliper values have their midpoint on Γ . The lens has a circular cross section in the Γ MK plane with a diameter of $1.737 \pm 0.0015 \text{ \AA}^{-1}$ with the error representing the maximum deviation found at all field directions and among four samples with $\underline{n} \parallel [0001]$.

From the data on the lens in the $\underline{n} \parallel [10\bar{1}0]$ and $\underline{n} \parallel [11\bar{2}0]$ orientations, series α and series f , it is seen that it is quite smooth and only slightly rounded on the edges. Since all of these caliper values lie in the Γ AHK and Γ ALM planes, respectively, the cross sectional areas of the lens in these planes could be calculated directly on an electronic computer. The results of these area calculations plus the area in the Γ KM plane

(area = $\pi k_c^2/4$) are presented in Table I and compared with direct measurements of the same areas by the de Haas - van Alphen (dHvA) effect. It is seen that the agreement for the Γ HK and the Γ ALM planes is particularly good and the Γ KM plane gives slightly more than 1 pct. difference. This is within our estimated error of 0.5 pct. for the caliper values which becomes 1 pct. for the areas.

The second portion of the third - band electron surface is the needle located at the K point. No calipers for the needles were observed in the present investigation. This, however, is not surprising because the expected field for observing the needles is between 1 and 10 G for the sample thicknesses used. In this field range, there is an extremely steep background slope in the traces which could not be entirely removed even when recording $\frac{d^4R}{dH^4}$. In addition, the iron magnet used demagnetizes inhomogeniously giving rise to a very inhomogenous field below 15 G. A search for the needles was performed on one of the $n \parallel [11\bar{2}0]$ samples, but the results were not considered reliable.

B. Second Band Hole Surface

There are two methods by which the second zone hole surface (monster) in Zn can be described. First, the

TABLE I. Comparison of measured cross sectional areas of the "lens" in zinc. All areas measured in $\text{\AA}^{-2}$.

Plane	Γ_{KM}	Γ_{AHK}	Γ_{ALM}
Thorsen, Valby and Joseph ^a	2.39	-----	-----
Stark ^b	2.34	0.693	0.693
Present Investigation	2.37	0.692	0.689

^a See Ref. 10.

^b R. W. Stark, private communication and to be published.

attitude can be taken that the monster is a single surface described by a ring centered at the Γ point with branches extending toward the corner of the zone. Second, because of inversion symmetry through Γ one can consider it as a set of two trifoliate posts per BZ centered along the KH line in the repeated zone scheme and connected together in the Γ ALM planes. In both of these descriptions the surface is multiply connected in the $[0001]$ direction. The first of these approaches is the one always taken in beryllium since this surface is not connected in the $[0001]$ direction, the second is usually taken in cadmium since this surface is not connected in the Γ ALM planes, and these two cases represent the extremes of divalent hexagonal metals. The Zn surface is connected both in the $[0001]$ direction and in the Γ ALM planes, thus a combination of these two approaches is taken here. The surface will be considered to be a ring entirely contained in one BZ but, because of the connections, the repeated zone scheme will be required to assign some of the calipers and some of the calipers will be degenerate because of the inversion symmetry through the Γ point. In Fig. 6 the solid line cross section is the ring surface in the Γ MK plane (the connection regions in the Γ AML planes are called the "arms"), the cross-hatched triangular sections are in the AHL plane ("neck"),

and the shaded portions are the extremities of the surface between these two planes (i.e., the shadow of the surface projected onto the Γ MK plane).

Because of the lack of inversion symmetry for each trifoliate part of the surface, the monster has no central calipers for $\underline{n} \parallel [0001]$ or $\underline{n} \parallel [10\bar{1}0]$ except for those orbits which include the Γ point in their plane. That is, there are no series of calipers that have a common fixed point on a symmetry point or line in the BZ for these orientations other than those traversing the complete connected ring.

There are several different type extremal calipers that can give rise to an RFSE peak: (1) calipers due to orbits having a true maximal or minimal extent in the $\underline{n} \times \underline{H}$ direction, (2) calipers due to truncated orbits which are orbits in planes perpendicular to $\underline{H}$ that increase in extent until they reach a point on the surface at which they no longer exist in the same form (these calipers are still classified as extremal calipers even though they are not extremal in the same sense as in case 1 and case 3), and (3) calipers due to broken orbits which are obtained between turning points on an orbit. Orbits of the above types can be either open or closed.

Open orbits existing on the monster with $\underline{H}$ in the (0001) plane have their extremities perpendicular to

[0001] in the AHL and Γ MK planes. Thus open orbits on the monster caliper the difference in extent of the surface in these two planes. These orbits have a shape similar to the cross section of the monster given by the points from the calculation of SF and labeled O_1 in Fig. 7. The projection of the monster on the Γ AHK plane was obtained from the $\underline{n} \parallel [10\bar{1}0]$ data and is shown in Fig. 7. The heavy lines indicate the portions of the surface lying in the Γ AHK plane and the lighter lines are the extremities of the surface between adjacent Γ AHK planes projected onto a Γ AHK plane. The principal calipers obtained with $\underline{n} \parallel [11\bar{2}0]$ are central in the sense that the corresponding orbits are symmetrical relative to either the Γ K or AH lines. Non-central calipers are obtained from truncated orbits for this orientation. The projection of the extremities of the monster onto the Γ ALM plane is shown in Fig. 8.

As a starting point for the assignment of calipers to the FS, the points on the FS obtained from the pseudopotential calculation of SF were plotted and then modifications were made to give a completely self-consistent result with extremal calipers in all directions fitting the data. The calculated points used here are from the non-local pseudopotential calculation, but without spin-orbit coupling (SOC) included. As will be

FIG. 6

seen, this only causes a measurable discrepancy near the K point and on the neck and arms of the monster. The calculated points are shown in Figs. 6 and 7 as large open circles.

Series z was easily identified as being produced by a dogbone-shaped orbit connecting two non-adjacent diagonal arms. This series of calipers determines the outline of the extremities of the monster between the Γ KM and the AHL planes projected onto the Γ KM plane. Further calipering of these extremities is obtained from the x series which is a minimum caliper due to a closed orbit. Since neither of these two calipers is central, the outline was constructed self-consistently until at each angle both of the measured caliper series were extremal and of the correct value. Series y is due to the open orbit in the [0001] direction and was found to fit the calculated values to within 1 pct. This cross section is further confirmed by the n caliper due to an orbit around the inside ring of the monster for $\underline{H} \parallel [0001]$ and $\underline{n} \parallel [10\bar{1}0]$ which also fits the distance from Γ to the monster in the Γ KM plane to better than 1 pct.

Series w for $\underline{n} \parallel [0001]$ is due to an orbit around the connecting arm. The signal due to this caliper was very weak. Since it is a small value, it is observed at

FIG. 7

low fields where the background slope is steep and was only observable when recording $\frac{d^2R}{dH^2}$ because of the reduction of the background. The calipers obtained from this series are slightly smaller than those predicted by SF. This is again confirmed by the θ series for $\underline{H} \parallel [0001]$ and $\underline{n} \parallel [11\bar{2}0]$ which is due to the inside monster orbit and is slightly larger than calculated.

Several other calipers were observed for $\underline{H} \parallel [0001]$ and $\underline{n} \parallel [10\bar{1}0]$ or $\underline{n} \parallel [11\bar{2}0]$ which give information about the surface in the Γ KM and AHL planes. Series ρ , π , h and k caliper between the points on the surface in the Γ KM plane nearest the K point of the BZ. All of these calipers arise from orbits around the outside ring of the monster. Only one of them, however, is due to a complete orbit, π ; the remainder arise from broken orbits at the sharp turning points. It is found that these calipers consistently give about 1 pct. smaller values than predicted by SF meaning probably that these corners near K are slightly rounded by the SOC.

Since most of the calipers obtained for $\underline{n} \parallel [10\bar{1}0]$ are non-central, the projection of the surface on the Γ AHK plane (Fig. 7) was constructed self-consistently starting with one outline from the calculation of SF. Series n corresponds to central orbits around the inside ring of the monster and gives calipers which reproduce

the SF outline over a small angular range near the Γ MK plane. The orbits giving rise to the n series break into orbits giving rise to the l series of calipers when the angle between $\underline{H}$ and [0001] becomes larger than 3° . The orbit giving the l series is a dogbone-shaped closed orbit passing across the arms and through the openings near the K point until $\underline{H}$ is directed greater than 11° from [0001]. After 11° the l caliper is obtained from the turning points on a more extended orbit. This assignment is verified by the fact that at 11° the line shape giving the l series changes drastically. Since the plane of this orbit always passes through the Γ ALM mirror plane, it could be plotted with its midpoint on the Γ M line, giving part of the outline labeled O_2 in Fig. 7 directly. The remainder of outline O_2 was constructed from a self-consistent fitting of series b which arises from a broken orbit around the neck. This portion of O_2 can only be tentatively drawn since there is not a second series of calipers with which to check the self-consistent fitting procedure for uniqueness.

The outline indicated as O_3 on Fig. 7 was constructed self-consistently from five different caliper series. The two-zone orbit giving series j and the neck orbit giving series d both have one caliper point on the SF outline (O_1) and the other caliper point on O_3 .

Caliper series O arises from a rather complicated orbit extending across two arms (and therefore non-central on the Γ M line) and through two openings near the K points close to the caliper points. Series c is due to a truncated orbit and extends from the top of the opening near K to O_3 . Series e calipers between the O_2 and O_3 outline and confirms both of their constructions. The O_2 outline is constructed such that every measured caliper in these five series is extremal and has the correct magnitude at each angle. This completes the definitely assigned outline of the monster projection onto the Γ AHK plane except for points near the K-point and along outline O_1' for which no calipers are obtained.

From the angular ranges of series l, e, and h the extent of the opening along the KH line can be deduced. Series e disappears sharply when they no longer pass through this opening and the h and l series undergo a change in intensity and line shape as they change from closed to broken orbits. All of these series give a distance of $0.130 \pm 0.005 \text{ \AA}^{-1}$ for the distance from the K point to the point where the second band crosses the HK line of the BZ. The value of $0.135 \text{ \AA}^{-1}$ for this distance that was found by Schirber¹³ is in excellent agreement with the present determination.

The projection of the surface onto the Γ ALM plane

is shown in Fig. 6 and it was much easier to construct than the other two because most of the calipers pass through the Γ AHK mirror plane and are therefore central calipers. Caliper series ν is readily assigned as being due to an orbit on one section of the monster passing through the opening near K and out over the body. This series is observed over a 68° range and almost completely determines the outline of this portion of the surface labeled O_1' in Fig. 8. The β series is due to a two zone orbit and calipers the same outline as the ν series. The second portion of the outline, O_2' , is obtained from caliper series γ , the neck orbit, ω , a two zone orbit β and δ , a broken orbit on the neck. In each of these cases the lines are observed over the full angular range allowed by this construction and disappear at other angles.

The two zone σ orbit caliper is due to a broken orbit and calipers between the two outlines, O_1' and O_2' . The η orbit is a broken orbit around the neck and the ϵ orbit is a broken orbit from the arms to the sharp turning point near the KH line. Neither of these calipers gives any new information about the outline. The dogbone orbit arising when $\underline{H}$ is near the $[10\bar{1}0]$ axis does not have an extremal caliper in these directions and is not observed. However, extremal calipers are observed from

two parts of this orbit. Series k and k' are due to broken portions of the dogbone orbit which do give an extremal caliper for the field near $[10\bar{1}0]$. The line shape is very complicated in this field region for these orientations, but the two peaks giving the k and k' calipers can be determined. Series τ can be fit on a non-central truncated orbit around the arms.

The remainder of the calipers obtained in this orientation arise from either complete or broken orbits around the ring network for H near $[0001]$. The θ series is due to the complete orbit around the inside of the monster and gives the outline of the arms in the ΓML plane. As was stated earlier, the arm cross section is found to be slightly smaller than calculated by SF without spin orbit coupling. The π and ρ series are the complete and broken parts of the orbit around the outside of the monster giving the distance between the extremities of the openings near the K points.

C. First - Band Hole Surface

The first - band hole surface (cap) consists of two surfaces per BZ centered at the H point. Except for the connectivity in the KM direction of the monster, the caps have the same symmetry properties as the monster. All of

FIG. 8

the calipers for this surface can be assigned by considering only one of the two surfaces.

Series a and b have been assigned to the caps and the cross sections obtained are shown in Fig. 9. Due to poor signal to noise ratios for $\underline{n} \parallel [0001]$, no calipers were obtained for the caps for $\underline{H}$ rotated in the basal plane. As in the case of the second-zone surface, the calipers obtained for the cap with $\underline{n} \parallel [11\bar{2}0]$ do not all lie in a plane, and the outline for the Γ AML plane is not a true cross section of the cap, but a profile or projection of the extremities onto the plane. In order to construct the cross section of the cap in the Γ AHK plane, the points shown as circles in Fig. 9 were plotted from SP. Then the calipers were put on the outline self-consistently until at each angle an extremal caliper was obtained.

Estimates of the gap between the first and second band caused by spin-orbit coupling in the AHL plane can be made from the calipers obtained for the cap and the neck of the monster. The difference in the calipers for $\underline{H} \parallel [0001]$ and $\underline{n} \parallel [10\bar{1}0]$ gives the sum of the gaps along the AH line and the LH line. This difference is a maximum of $0.005 \pm 0.001 \text{ \AA}^{-1}$. The RFSE lines from the cap and neck orbits overlap with $\underline{H} \parallel [0001]$ with the separation between peaks only 0.6 G at 60 G, thus causing the large

$\Gamma A H K$ Plane $\Gamma A L M$ Plane

FIG. 9

uncertainty in this value. In the $\underline{n} \parallel [11\bar{2}0]$ data the gap is $0.009 \pm 0.0005 \text{ \AA}^{-1}$ for the projection onto the ΓALM plane. Although the plane in which these caliper values lie is not determined, it should be a close approximation to twice the gap along the HL line showing that the gap along the AH line is probably less than $0.001 \text{ \AA}^{-1}$.

V. CONCLUSIONS

The experimental numbers obtained in this experiment show very good agreement with the non-local pseudopotential calculation of Stark and Falicov¹ without the inclusion of spin-orbit coupling. Where disagreement greater than 1 pct. occurs is at points where the spin-orbit coupling would have the greatest effect. Some of the results of both the theoretical numbers and the calculated points are given in Table II. It can be seen that except near the H point and along the Γ M line the agreement is excellent, and the inclusion of spin-orbit coupling into the theory would shift calculated values to be in better agreement.

The overall reproducibility from sample to sample of the caliper values reported here is ± 0.5 pct. This level of reproducibility is only achieved when accurate average thickness values are obtained by weighing and the proper point on the rather complex line shapes is chosen. The FS of Zn appears to be very sharp, without a great

TABLE II. Dimensions of the FS of Zn. All dimensions in $\text{\AA}^{-1}$

	Expt.	Theory ^a
Third - zone lens		
From Γ in ΓA direction	0.278	
From Γ in ΓK direction	0.869	0.863 ^b
From Γ in ΓM direction	0.869	0.863
Second - zone holes		
From Γ in ΓK direction to inside ring	0.978	0.974
near K point	1.547	1.558
From Γ in ΓM direction	1.026	1.018
From A in AH direction	1.467	1.459
Across neck in AH direction	0.282	0.267
Across neck in HL direction	0.285	0.269
Across arms in ΓA direction	~ 0.08	
Across arms in ΓM direction	~ 0.08	0.0866
From K on KH line	0.130	
First - zone holes		
Across in AH direction	0.277	0.267
Across in HL direction	0.276	0.269

^a Values obtained from SF without spin-orbit coupling included.

^b Obtained from area data of Stark (private communication) to which the SF calculation was fit exactly and using an assumed circular orbit.

deal of rounding due to the lattice potential or spin-orbit coupling, as evidenced by the large number of turning point or broken orbits observed here.

No calipers which could be assigned to the third-band needed were observed. This is due to the experimental apparatus used, and under proper conditions of low homogenous applied field and thin (~ 0.2 mm) samples, they should be readily observable.

Finally, it is noted that the detailed overall shape of an RFSE line is strongly dependent on the shape of the orbit giving rise to that line. In the case of the lens orbit where the shape is known, the agreement between the observed lines and the line shape given by Juras is good. The point on the complicated line shapes at which the caliper values are calculated does not, however, seem to vary between different line shapes. That is, if one always chooses the first peak in the second derivative of the line, consistent caliper values are obtained.

APPENDIX A

Details of the Magnet Supply

In RFSE measurements on high purity metals, highly stabilized and programable magnetic fields in the range of 0 to 1000 G are required. A 4 inch diameter pole face electromagnet with a 2 inch gap has been used in this laboratory for these measurements,²² and the field control system for this magnet is described here. The system allows the field to be set at any value between -1000 G and +1000 G and fields sweeps of 2 up to 1000 G to be made starting from the preset field. Since magnetic field modulation at 40 Hz is used in the detection of the RFSE, a provision is included to modulate the field directly through the power amplifier.

A block diagram of the entire control circuitry is shown in Fig. 10. A highly stabilized Wien bridge oscillator operating at 6700 Hz drives a power amplifier which in turn provides a signal for the remainder of the circuit. The power amplifier has an output of 7.5 V rms and

FIG. 10

directly drives the bridge circuit and two phase-shifting networks. In the bridge circuit, shown in Fig. 11 and described in detail later, a voltage is generated which drives the Hall probe at a constant current of 150 mA rms. The Hall probe output is then proportional to the applied field. A divider network within the bridge provides a reference voltage to which the Hall probe output is compared and their difference is fed to the error amplifier. The error amplifier is a double-tuned, low-noise, high-gain amplifier (voltage gain approximately 5000). The output of this amplifier is fed into phase sensitive detector A. This detector derives its reference from phase A and provides the control signal for the dc power amplifier. A second system of phase shifter and phase sensitive detector, which is driven by a signal from the bridge circuit proportional to the field, provides a dc voltage to an x - y recorder or field indicator.

The principal component in accurately making the field measurement and producing the sweep is the bridge comparator circuit, which is shown in Fig. 11. The bridge circuit is a resistive Wheatstone bridge which keeps a constant resistance between points A and B. The center arm of this bridge is the high input impedance transformer T_1 (input impedance 0.8 M Ω). The input impedance of this transformer is high with respect to the

FIG. 11

impedance of the bridge arms, and the current through it can be neglected. The field is set by potentiometer P_2 which unbalances the bridge. The field is swept by a motor drive on P_1 , and the range of the sweep is determined by the fixed unbalance caused by R_7 through R_{22} . Capacitors C_1 through C_5 adjust the output phase of T_1 and T_2 .

The zero field voltage and the temperature dependent parameter of the Hall probe have been compensated for by the network consisting of P_3 , P_4 , R_1 , R_2 , S_1 , and S_2 in Fig. 11. Potentiometers P_3 and P_4 and the resistor R_2 cause the temperature independent zero field voltage to be less than $1 \mu\text{V}$. Both the resistance and Hall coefficient of the probe are temperature dependent and must be compensated to give a temperature independent Hall voltage. Compensation for the probe resistance is necessary since a change in the resistance of the probe causes a change in the drive current. The network consisting of R_1 , S_1 , and S_2 compensates for both effects. The choice of values for these components depends critically on the Hall probe used. In the present application, a Model BH-200 Bell Hall Pack²⁵ was used and has the following approximate characteristics: Hall coefficient, $\gamma_{1B} = 0.085 \text{ V A/kG}$ at 25°C with a temperature coefficient of $k_H = -0.08 \text{ pct}/^\circ\text{C}$; Hall probe drive resistance, $R_0 = 1.65 \Omega$ with a temperature coefficient of

$\alpha_H = +0.15 \text{ pct}/^\circ\text{C}$. The sensitor S_1 has a resistance of 47Ω at 25°C with $\alpha_1 = 0.7 \text{ pct}/^\circ\text{C}$ and the thermistor S_2 has a resistance of 100Ω at 25°C with $\alpha_2 = -3.9 \text{ pct}/^\circ\text{C}$.

The values used in the temperature compensating network shown in Fig. 11 were derived under the assumption that the temperature coefficients were linear and small so that only terms of first order needed to be retained. For the combination of R_1 and S_2 the first order expression for the parallel resistance is

$$R_e = \frac{R_1 S_2}{R_1 + S_2} = \frac{R_1 S_{20} (1 - \alpha_2 \Delta t)}{R_1 + S_{20} (1 - \alpha_2 \Delta t)},$$

or

$$R_e = \frac{R_1 S_{20}}{R_1 + S_{20}} \left[1 - \frac{R_1 \alpha_2 \Delta t}{R_1 + S_{20}} \right].$$

Putting

$$x = \frac{R_1}{R_1 + S_{20}},$$

the sum of the probe resistance, R_H and R_e can be written in the following form:

$$R_s = R_H + R_e = R_{H0} (1 + \alpha_H \Delta t) + x S_{20} (1 - x \alpha_2 \Delta t)$$

or

$$R_s = (R_{Ho} + x S_{20}) \left[1 - \left(\frac{x^2 \alpha_2 S_{20} - R_{Ho} \alpha_H}{x S_{20} + R_{Ho}} \right) \Delta t \right] .$$

The coefficient of the temperature change here must be adjusted to compensate for the decrease in sensitivity of the Hall probe with temperature. Thus, the following condition must be met :

$$k_H = \frac{x^2 \alpha_2 S_{20} - R_{Ho} \alpha_H}{x S_{20} + R_{Ho}} .$$

This may be solved for x (keeping only the positive root)

$$x = \frac{k_H}{2 \alpha_2} + \left[\left(\frac{k_H}{2 \alpha_2} \right)^2 + \frac{R_{Ho}}{S_{20}} \frac{\alpha_H + k_H}{\alpha_2} \right]^{\frac{1}{2}} ,$$

and R_1 may be found

$$R_1 = \frac{x}{1 - x} S_{20} .$$

The total resistance of the network then becomes :

$$\frac{1}{R_t} = \frac{1}{(R_{Ho} + x S_{2o})(1 - k_H \Delta t)} + \frac{1}{S_{1o}(1 + \alpha_1 \Delta t)} .$$

Upon expanding this

$$R_t = \frac{1 + k_H \Delta t}{(R_{Ho} + x S_{2o})} + \frac{1 - \alpha_1 \Delta t}{S_{1o}} .$$

Thus, the entire network resistance, R_t , becomes temperature independent if

$$\frac{k_H}{R_{Ho} + x S_{2o}} = \frac{\alpha_1}{S_{1o}} .$$

From this condition the value of S_{1o} can be found

$$S_{1o} = (R_{Ho} + x S_{2o}) \frac{\alpha_1}{k_H} .$$

Putting the fixed values in the equations gives the value of x as 0.042 which in turn determines R_1 to be 4.2 Ω .

The choice of R_1 is critical for optimum temperature independence of the entire network and the value of 4.2Ω derived above gives a starting point from which the optimum value could be determined. Table III gives the percentage changes in Hall voltage at constant field for a temperature change of 25°C . It is seen from this table that the choice of $R_1 = 3.5 \Omega$ gives an over-all temperature dependence of the Hall voltage between 25° and 50°C of less than $-0.0012 \text{ pct } ^\circ\text{C}$ which is an improvement by a factor of 50 over the uncompensated case. Above 60°C the quality of the compensation scheme decreases rapidly but remains better than the uncompensated case. In addition, when R_1 was chosen to be 3.5Ω there was not a measurable change in resistance between points C and D in the circuit for the 25°C temperature change. This is necessary to keep the calibration of the bridge and comparator circuit independent of temperature. The two temperature dependent elements, S_1 and S_2 , and the Hall probe were mounted on a copper plate and potted in epoxy to make a single unit for the field control.

The phase - sensitive detector circuit is shown in Fig. 12. This circuit does not require the use of a transformer and is easy to adjust for symmetry. There is, furthermore, no need of feeding it with a square wave reference. The transistors T_1 and T_2 are a combination

TABLE III. Percentage changes in Hall voltage for various values of R_1 in the circuit shown in Fig. 11 for a 25°C change in temperature.

R_1	$\frac{\Delta V}{V}$
3.1 Ω	- 0.8 pct.
3.3 Ω	- 0.2 pct.
3.5 Ω	- 0.03 pct.
4.0 Ω	+ 0.6 pct.
4.2 Ω	+ 0.8 pct.
Uncompensated	- 1.5 pct.

FIG. 12

giving a very low output impedance (40Ω) and are fed respectively by the error signal and the reference signal. The phase sensitive detector is shown inside the dotted square and functions as follows: The diode D_1 will prevent point B from becoming positive with respect to point A at any time. The diode D_2 will prevent point C from becoming negative with respect to ground. The short conduction times of the diodes will give rise to a charge distribution across the condensers C_e and C_r , such that at point A a DC potential V_{20} will be present on which the AC error signal $V_2 \sin(\omega t + \varphi)$ is superposed. At B V_{10} and the reference signal $V_1 \sin \omega t$ is present. From the conditions stated above we may write

$$V_B - V_A \leq 0 \rightarrow V_{10} + V_1 \sin \omega t - V_{20} - V_2 \sin(\omega t + \varphi) \leq 0$$

$$V_C \geq 0 \rightarrow \frac{1}{2} \left[V_{10} + V_1 \sin \omega t + V_{20} + V_2 \sin(\omega t + \varphi) \right] \geq 0$$

Taking the equalities, the following result is obtained

$$V_{10} - V_{20} = (V_1^2 + V_2^2 - 2 V_1 V_2 \cos \varphi)^{\frac{1}{2}}$$

$$V_{10} + V_{20} = - (V_1^2 + V_2^2 + 2 V_1 V_2 \cos \varphi)^{\frac{1}{2}}$$

from which :

$$V_{10} = (V_1^2 + V_2^2 - 2 V_1 V_2 \cos \varphi)^{\frac{1}{2}} - (V_1^2 + V_2^2 + 2 V_1 V_2 \cos \varphi)^{\frac{1}{2}}$$

It is clear from this expression that for $\varphi = 0$ $V_{10} = V_2$ and for $\varphi = \pm \frac{\pi}{2}$, $V_{10} = 0$. If, furthermore, $V_1 \gg V_2$ the following first order expression is easily obtained :

$$V_{10} = V_2 \cos \varphi .$$

The time constant for detection is given by the product of $C_e R_3$ and in the present case is 0.5 sec giving rise to an equivalent noise bandwidth of the order of 2 Hz. The resultant DC correction voltage is obtained at point B, with the reference being filtered out by $R_4 C_4$. The field effect transistor T_3 allows a DC level shift. Potentiometer P_1 adjusts the balance and potentiometer P_2 adjusts the output level. The zener diode D_3 fixes the voltage of the FET such that the working point is independent of temperature.

The DC power amplifier is shown in Fig. 13 and is unusual in design since it has a class B output stage using complementary pair transistors. It also has the advantage of being able to deliver full power with either plus or minus polarity. Transistors T_1 , T_2 , T_3 , and T_8 form a conventional differential amplifier. The emitter follower T_2 is inserted as an additional current amplifier which allows T_1 to operate at low current values, minimizing drift and noise. Potentiometer P_1 can be adjusted to compensate for differences in emitter-base voltage drift between T_{1a} and T_{1b} . The emitter-base sensistor resistor at T_8 is mounted on the heat sink with T_1 and has the correct temperature coefficient of resistance to compensate for temperature dependent variations once the drift balance P_1 has been set. The voltage feedback is through R_1 and R_2 , and C_1 and C_2 shape the loop response for stability. The differential amplifier is connected directly to a two stage complementary emitter follower. This emitter follower combination gives the power amplification with good efficiency. The diodes D_3 set the quiescent current, and potentiometers P_1 and P_2 allow adjustment of this current to 100 mA in each section, resulting in a smooth crossover through zero output. The use of four diodes on each side mounted on the same heat sink as the emitter followers makes the

Fig. 13

quiescent current practically independent of temperature and gives an improvement in balance over the use of a resistor. The diodes D_1 and D_2 protect T_6 and T_7 from voltage surges from the high inductance of the magnet during rapid field changes.

The error voltage from the field measuring circuitry is inserted at point E, and a modulation signal can be inserted at point M. By controlling only one side of the difference amplifier, larger control signals are required but the stability of the entire servo loop is increased. A 700 mV signal at either point E or M will produce 1.5 A out into a 40 Ω load. After a 30 minute warmup period the long term stability of this amplifier with constant error signal in is 5 mA hr at an output power of 40 W. Higher power outputs than the 200 W maximum of this circuit can easily be obtained by using this circuit to drive a series of balanced emitter follower stages. A diagram of the entire system is shown in Fig. 14.

Fig. 14

APPENDIX B.

Experimental Calipers for Zinc Obtained Using the Radio - Frequency Size Effect.

Four samples (#1, #2, #3, #4) with $\underline{n} \parallel [0001]$ were used, their room temperature thickness and conversion formulas were respectively :

#1	0.5764 mm	$k_c = 0.00861175 H (\text{\AA}^{-1})$
#2	0.3493 mm	$k_c = 0.00530922 H (\text{\AA}^{-1})$
#3	0.3099 mm	$k_c = 0.00470966 H (\text{\AA}^{-1})$
#4	0.4025 mm	$k_c = 0.00601280 H (\text{\AA}^{-1})$

Two samples (#5, #6) with $\underline{n} \parallel [12\bar{1}0]$ were used, their room temperature thickness and conversion formulas were respectively :

#5	0.3363 mm	$k_c = 0.00510138 H (\text{\AA}^{-1})$
#6	0.1961 mm	$k_c = 0.00358581 H (\text{\AA}^{-1})$

One sample (#7) with $\underline{n} \parallel [10\bar{1}0]$ was used, its room temperature thickness and conversion formula was :

#7	0.2471 mm	$k_c = 0.00459466 H (\text{\AA}^{-1})$
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TABLE IV. Caliper values obtained from sample #3
 The magnetic field was rotated in the (0001) plane.

Angular Direction of Magnetic Field	k_c ($\text{\AA}^{-1}$)	
	x	y
[11 $\bar{2}$ 0]		
0.5		0.486
1.5	0.332	0.484
2.5		0.486
3.5	0.329	0.486
4.5		0.486
5.5	0.327	0.486
6.5		0.488
7.5	0.318	0.492
8.5		0.492
9.5	0.309	0.493
10.5	0.304	0.495
11.5	0.292	0.495
12.5	0.283	0.497
13.5	0.285	0.500
14.5	0.278	0.501
15.5	0.276	0.504
16.5	0.276	0.504
17.5	0.275	0.513
18.5	0.274	0.513
19.5	0.269	0.523
20.5	0.269	0.522
21.5	0.269	0.528
22.5	0.269	0.538

TABLE IV continued

Angular Direction of Magnetic Field	k_c ($\text{\AA}^{-1}$)	
	x	y
23.5	0.265	0.534
24.5	0.265	0.540
25.5	0.264	0.552
26.5	0.264	0.557
27.5	0.264	0.563
28.5	0.265	0.575
29.5	0.265	0.581
$[10\bar{1}0]$		

TABLE V. Caliper values obtained from samples #2 and #3.

The magnetic field was rotated in the (0001) plane.

Angular Direction of Magnetic Field	$k_c (\text{\AA}^{-1})$		
	w^a	z^a	z^b
[11 $\bar{2}$ 0]		1.667	1.663
1		1.668	
2	0.103	1.668	1.667
3		1.675	1.680
4	0.104	1.679	1.681
5		1.683	1.687
6	0.106	1.695	
7		1.702	1.697
8			1.719
9			
10			1.768

^a Sample #2

^b Sample #3

TABLE VI. Caliper values obtained from sample #5.
The magnetic field was rotated in the $(11\bar{2}0)$ plane.

Angular Direction of Magnetic Field		k_c ($\text{\AA}^{-1}$)		
η	ϕ	γ	ψ	
[0001]				
0.3	0.148	0.256	0.296	
1.7	0.148	0.255	0.249	
3.7	0.148	0.256	0.296	
5.7	0.148	0.257	0.299	0.902
7.7	0.152	0.259	0.303	0.839
9.7	0.152	0.261	0.306	0.794
11.7	0.155	0.265	0.313	0.762
13.7	0.155	0.266	0.319	0.733
15.7		0.269	0.323	0.713
17.7		0.271	0.333	0.695
19.7	0.159	0.277	0.342	0.677
21.7	0.158	0.278	0.353	0.661
23.7	0.160	0.281	0.364	0.646
25.7	0.162	0.284	0.376	0.634
27.7	0.167	0.281	0.392	0.628
29.7	0.168	0.283	0.408	0.618
31.7		0.283	0.426	0.615
33.7	0.175	0.285	0.450	0.610
35.7	0.183	0.285	0.477	0.606
37.7	0.188	0.291	0.510	0.606
39.7	0.191	0.293	0.556	0.602
41.7	0.196	0.298	0.604	0.604
43.7	0.204	0.301	0.664	0.606

TABLE VI continued

Angular Direction of Magnetic Field	k_c ($\text{\AA}^{-1}$)			
	η	ξ	γ	ν
45.7	0.203	0.309	0.759	0.611
47.7	0.221	0.312		0.615
49.7	0.232	0.317		0.619
51.7		0.324		0.630
53.7		0.335		0.639
55.7	0.265	0.345		0.644
57.7	0.279	0.354		0.665
59.7	0.300	0.364		0.682
61.7	0.310	0.380		
63.7	0.345	0.394		
65.7	0.373	0.404		
67.7	0.392	0.409		
69.7	0.428	0.439		
71.7		0.458		
73.7		0.484		

TABLE VII. Caliper values obtained from sample #5.
The magnetic field was rotated in the $(11\bar{2}0)$ plane.

Angular Direction of Magnetic Field	k_c ($\text{\AA}^{-1}$)				
	δ	ϵ	i	x'	x
[0001]					
27.7	0.335	0.308			
29.7	0.346	0.312			
31.7	0.350	0.312			
33.7	0.357	0.317	0.250		
35.7	0.365	0.319	0.249		
37.7	0.372	0.326	0.247		
39.7	0.385	0.335	0.245		
41.7	0.396	0.344	0.242		
43.7	0.413	0.357	0.243		
45.7	0.426	0.372	0.239		
47.7	0.453	0.385			
49.7	0.491	0.399		0.197	
51.7	0.553	0.419	0.236	0.201	
53.7	0.574	0.443	0.237	0.201	
55.7		0.475		0.199	
57.7		0.513		0.201	
59.7		0.556		0.201	
61.7		0.596		0.202	
63.7		0.633		0.205	
65.7				0.205	
67.7				0.210	
69.7				0.212	
71.7				0.213	

TABLE VII continued

Angular Direction of Magnetic Field	k_c ($\text{\AA}^{-1}$)				
	δ	ϵ	i	κ'	κ
73.7				0.220	
75.7				0.222	
77.7				0.228	0.418
79.7				0.230	0.424
81.7				0.238	0.357
83.7				0.245	0.338
85.7				0.253	0.320
87.7				0.261	0.305
89.7				0.267	0.300

TABLE VIII. Caliper values obtained from sample #6.

The magnetic field was rotated in the $(11\bar{2}0)$ plane.

Angular Direction of Magnetic Field	κ_c ($\text{\AA}^{-1}$)		
	ρ	θ	π
[0001]		1.920	2.688
1	1.323		2.696
2		1.936	
2.5	1.326		2.704
4.5	1.333		
7.5	1.340		
	ω		
	<u>52.5</u>		
	54.5		
	56.5		
	58.5		
	60.5		
	62.5		
	64.5		
	66.5	<u>1.881</u>	
	68.5	1.891	
	70.5	1.914	
	72.5	1.94	
	74.5	1.889	
	76.5	1.880	
	78.5	1.873	
	80.5	1.870	
	82	1.86	
	83	1.76	
			σ
			<u>2.16</u>

TABLE IX. "Lens" caliper values obtained from sample # 6.

The magnetic field was rotated in the $(11\bar{2}0)$ plane.

Angular Direction of Magnetic Field	k_c ($\text{\AA}^{-1}$)
[0001]	
0.5	1.747
1	1.738
2.5	1.700
4.2	1.646
5.5	1.588
7.5	1.500
9.5	1.423
11.5	1.364
13.5	1.289
14.5	1.243
15.5	1.225
17.5	1.168
18.5	1.140
19.5	1.111
21.5	1.062
24.5	0.996
29.5	0.912
34.5	0.835
39.5	0.772
76.5	0.558
81.5	0.552
85.5	0.547
90	0.541

TABLE X. Caliper values obtained from sample # 7.
The magnetic field was rotated in the $(10\bar{1}0)$ plane.

Angular Direction of Magnetic Field	k_c ($\text{\AA}^{-1}$)				
	a	b	n	g	h
[0001]			1.956		
1	0.277	0.244	1.959		0.817
3	0.277	0.242			0.784
5	0.278	0.242	<u>e</u>		0.791
7	0.277	0.239			0.790
9	0.278	0.240	0.731		0.796
11	0.276	0.241	0.700		0.799
13	0.277	0.241	0.669		0.804
15	0.276	0.241	0.645	1.042	0.810
17	0.276	0.243	0.617	0.996	0.816
19	0.275	0.243	0.602		0.820
21	0.276	0.243	0.588	0.946	0.828
23	0.275	0.243	0.573	0.922	0.838
25	0.277	0.248	0.562	0.913	0.849
27	0.278	0.249	0.554	0.899	0.859
29	0.280	0.251	0.547	0.899	0.869
31	0.281	0.254	0.539	0.884	
33	0.284	0.258	0.532		
35	0.287	0.260	0.530	0.879	
37	0.290	0.265	0.525	0.875	
39	0.291	0.268	0.524	0.875	
40	0.294	0.272			
41	0.296	0.275	0.523	0.870	
43	0.304	0.282	0.524	0.875	
45	0.307	0.288	0.525	0.876	

TABLE X continued

Angular Direction of Magnetic Field	k_c ($\text{\AA}^{-1}$)				
	a	b	e	g	j
47	0.309	0.294	0.525	0.878	
49	0.314	0.301	0.531	0.884	1.830
50					1.825
51	0.324	0.311	0.534	0.886	1.816
52					1.811
54	0.336	0.324	0.543	0.899	1.806
57	0.341	0.361	0.557		1.814
59			0.570	0.932	
61	0.360	0.387	0.581		
64	0.375	0.420		0.976	1.827
67	0.392	0.473	0.635	1.030	
69	0.411		0.659	1.051	1.894
				<u><u>8</u></u>	
71	0.425	0.501	0.694	0.743	
73	0.440	0.554	0.733	0.651	
74					1.997
75	0.466		0.784	0.678	
77	0.491		0.812	0.698	
79	0.523		0.841	0.733	2.175
81	0.562		0.889	0.778	2.292
83	0.612		0.937		
84					2.544
85	0.672		0.998		
87			1.099		

TABLE XI. Caliper values obtained from sample # 7.
The magnetic field was rotated in the $(10\bar{1}0)$ plane.

Angular Direction of Magnetic Field		k_c ($\text{\AA}^{-1}$)			
		c	d	k	l
[0001]				1.569	
1	0.473			1.568	
2				1.571	
3	0.458	0.283		1.569	1.783
4				1.574	1.757
5	0.445	0.284		1.574	1.736
5.5					1.723
6					1.720
7	0.431	0.285			1.698
8				1.593	1.691
9	0.419	0.287		1.596	
11	0.410	0.290			1.680
13	0.399	0.292			
15	0.394	0.297			1.621 1.689
17	0.386	0.301			1.581 1.706
19	0.380	0.308	i	1.556	
21	0.375	0.313	-----		
23	0.372	0.322	1.107	1.519	
25	0.368	0.330	1.107		
27	0.363	0.342	1.114		
29	0.353	0.353	1.120	1.500	
31	0.340	0.363	1.130		
33	0.344	0.385	1.147		
34				1.512	

TABLE XI continued

Angular Direction of Magnetic Field	k_c ($\text{\AA}^{-1}$)				
	c	d	i	o	l
35	0.344	0.404	1.166		
36				1.532	
37	0.344	0.431	1.185		
39	0.342	0.459	1.221		
40	0.344	0.477			
41	0.346	0.493	1.243		
43	0.346				
45	0.348				
47	0.353				
49	0.353				
51	0.359				
54	0.363				

TABLE XII. "Lens" caliper values obtained from sample # 7.

The magnetic field was rotated in the $(10\bar{1}0)$ plane.

Angular Direction of Magnetic Field	$k_c (\text{\AA}^{-1})$	Angular Direction of Magnetic Field	$k_c (\text{\AA}^{-1})$
[0001]	1.744		
1	1.732	41	0.773
2	1.699	43	0.755
3	1.665	45	0.734
4	1.634	47	0.716
5	1.596	49	0.699
5.5	1.575	51	0.683
6	1.560	54	0.663
8	1.482	57	0.644
9	1.445	59	0.635
11	1.379	61	0.610
15	1.255	64	0.610
17	1.196	67	0.596
19	1.153	69	0.591
21	1.100	71	0.584
23	1.051	73	0.580
25	1.014	75	0.575
27	0.976	77	0.570
29	0.939	79	0.526
31	0.908	81	0.562
33	0.875	83	0.562
35	0.821	85	0.560
37	0.821	87	0.558
39	0.801	89	0.556

TABLE XIII. "Lens" diameters obtained from
samples with $\underline{n} \parallel [0001]$.

Sample	Diameter.
# 1	$1.7390 \text{ \AA}^{-1}$
# 2	$1.7353 \text{ \AA}^{-1}$
# 3	$1.7359 \text{ \AA}^{-1}$
# 4	$1.7372 \text{ \AA}^{-1}$

APPENDIX C.

The Stark - Falicov Pseudo - Potential Calculation.

In this appendix a brief discussion and outline of the particular features of the pseudo - potential calculation performed by Stark - Falicov is given.

In the single electron approximation it is assumed that the electrons move in an attractive self-consistent crystal-potential. The Schrödinger equation then has the form :

$$\left[T + V(\underline{r}) \right] \psi_{\underline{k}}(\underline{r}) = E_{\underline{k}} \psi_{\underline{k}}(\underline{r})$$

where T the kinetic energy operator $= \frac{\hbar^2}{2m} \Delta$, $V(\underline{r})$ the self-consistent potential, $E_{\underline{k}}$ the energy eigenvalue, $\underline{k}$ the collection of quantumnumbers characterizing the state, $\psi_{\underline{k}}$ the wave function of the electron in the state $\underline{k}$. Following Kleinmann and Phillips,²⁶ the wave function is written :

$$\psi_{\underline{k}}(\underline{r}) = \varphi_{\underline{k}}(\underline{r}) - \sum_{t,i} |t, \underline{R}_i\rangle \langle t, \underline{R}_i| \varphi_{\underline{k}}$$

where $|t, \underline{R}_i\rangle$ is the wave function of a core electron with quantumnumbers t associated with an atom at the site $\underline{R}_i$. Since $|t, \underline{R}_i\rangle$ satisfies the Schrödinger equation, the following equivalent equation is found in $\varphi_{\underline{k}}$ upon using this form of $\psi_{\underline{k}}$ in the wave equation

$$\left[T + V(\underline{r}) + V_R \right] \varphi_{\underline{k}} = E_{\underline{k}} \varphi_{\underline{k}}$$

where

$$V_R \varphi_{\underline{k}} = \sum_{t,i} (E_{\underline{k}} - E_t) |t, \underline{R}_i\rangle \langle t, \underline{R}_i| \varphi_{\underline{k}}$$

The operator V_R has the character of a repulsive potential which cancels most of V . The electron may consequently be thought as moving in a smooth pseudo-potential $V_{\text{eff}} = V + V_R$. Stark and Falicov choose their pseudo-potential as follows

$$V_{\text{eff}} = V_L + V_N + W_{\text{so}}$$

where V_L is a local potential, V_N a non-local potential

and W_{so} the spin-orbit interaction. The local potential was then expressed as follows :

$$V_L = \sum_{i,h} V_L(\underline{G}_h) e^{i \underline{G}_h \cdot (\underline{r} - \underline{R}_i)}$$

where the $V_L(\underline{G}_h)$ were fitted to experiment and were taken to be non-zero for the following reciprocal lattice vectors in the hexagonal notation of $(h, k, \overline{h+k}, l)$

$$\begin{aligned} V_L(0002) &= 0.0140 \text{ Ry} & V_L(10\bar{1}0) &= 0.0150 \text{ Ry} \\ V_L(10\bar{1}1) &= 0.0345 \text{ Ry} & V_L(10\bar{1}2) &= 0.0200 \text{ Ry} \end{aligned}$$

The non-local potential was given the following form

$$V_N = \sum_{t,i} V_d |t, \underline{R}_i\rangle \langle t, \underline{R}_i|$$

where V_d is also fitted to experiment and given as 3.15 Ry. The index t runs over all the states of the last occupied d shell in the core and the wave functions $|t, \underline{R}_i\rangle$ are the Hartree-Fock-Slater atomic functions as given by Herman and Skillman²⁷ and centered at the atomic sites $\underline{R}_i$.

The spin-orbit term was given the truncated Weiss²⁸ form :

$$W_{so}(\underline{k} s, \underline{k} + \underline{G} s') = i \lambda_p (\underline{k} + \underline{G}) \times \underline{k} \cdot \underline{\sigma}_{ss'},$$

where $\underline{\sigma}_{ss'}$, are ss' components of the Pauli matrices. The coefficient λ_p was chosen to be 0.005. The value of this coefficient was not obtained from experiment, but rather, it was inferred from a similar calculation on cadmium. Experimentally the spin-orbit splitting is smaller in Zinc than in Cadmium and cannot be observed in the dHVA experiment when the field is high and magnetic breakdown is occurring.

The pseudo wave function $\varphi_{\underline{k}}$ was then expanded in plane waves with the number of plane waves varying between 18 and 32 depending on the symmetry of the point in $\underline{k}$ space. These plane waves were of the form :

$$\varphi_{\underline{k},s} = \sum_{\underline{G}} \alpha_{\underline{G}}(\underline{k}) |\underline{k} + \underline{G}, s\rangle$$

where

$$|\underline{k} + \underline{G}, s\rangle = \frac{1}{\sqrt{\Omega}} e^{i(\underline{k} + \underline{G}) \cdot \underline{r}} |s\rangle$$

The pseudo wave equation then becomes :

$$\left(-\frac{\hbar^2}{2m} \Delta + V_L + V_N + W_{so}\right) \sum_{\underline{G}} \alpha_{\underline{G}}(\underline{k}) |\underline{k} + \underline{G}, s\rangle =$$

$$E_{\underline{k}} \sum_{\underline{G}} \alpha_{\underline{G}}(\underline{k}) |\underline{k} + \underline{G}, s\rangle$$

This equation is multiplied to the left with some $\langle s', \underline{k} + \underline{G}' |$, where $\underline{G}'$ takes all values $\underline{G}$. A system of equations in the coefficients $\alpha_{\underline{G}}(\underline{k})$ is obtained. The matrix of this system has the following elements :

$$\langle s', \underline{k} + \underline{G}' | -\frac{\hbar^2}{2m} \Delta + V_L + V_N + W_{so} | \underline{k} + \underline{G}, s \rangle$$

Replacing $\underline{k} + \underline{G}$ by the equivalent $\underline{k}$ and denoting by $\underline{k}'$, a wave vector differing from $\underline{k}$ by a reciprocal lattice vector $\underline{G}'$, the following expressions are obtained for the components of the matrix element

$$\begin{aligned} \langle s', \underline{k}' | -\frac{\hbar^2}{2m} \Delta | \underline{k}, s \rangle &= \frac{1}{\Omega} \int e^{-i \underline{k}' \cdot \underline{r}} \left(-\frac{\hbar^2}{2m} \Delta\right) e^{i \underline{k} \cdot \underline{r}} d\tau \delta_{ss'}, \\ &= \frac{\hbar^2 k^2}{2m} \delta_{\underline{k}\underline{k}'} \delta_{ss'}, \end{aligned}$$

$$\begin{aligned}
\langle s' \underline{k}' | V_L | \underline{k} s \rangle &= \sum_{i, n} \frac{1}{\Omega} \int e^{-i \underline{k}' \cdot \underline{r}} V_L(\underline{G}_n) e^{i \underline{G}_n (\underline{r} - \underline{R}_i)} \\
&\quad e^{i \underline{k} \cdot \underline{r}} d\tau \delta_{ss'}, \\
&= S(\underline{G}_n) V_L(\underline{G}_n) \delta_{\underline{k} - \underline{k}', \underline{G}_n} \delta_{ss'},
\end{aligned}$$

where $S(\underline{G}_n)$ the so called structure factor for the hcp lattice, which can be calculated from the knowledge of the positions of the atoms in the unit cell

$$S(\underline{G}_n) = \frac{1}{N_i} \sum_i e^{-i \underline{G}_n \cdot \underline{R}_i} = \cos 2\pi \left(\frac{n+2k}{6} + \frac{1}{4} \right)$$

$$\langle s' \underline{k}' | V_N | \underline{k} s \rangle = \sum_{t, i} \langle s' \underline{k}' | t, \underline{R}_i \rangle \langle t, \underline{R}_i | \underline{k} s \rangle$$

the functional dependence of the wavefunctions $|t, \underline{R}_i\rangle$ is of the form $|r - \underline{R}_i|$:

$$\begin{aligned}
\langle s' \underline{k}' | V_N | \underline{k} s \rangle &= \sum_{t, i} \frac{1}{\Omega} \int e^{-i \underline{k}' \cdot \underline{r}} \psi_t(|r - \underline{R}_i|) d\tau \\
&\quad \int e^{i \underline{k} \cdot \underline{r}} \psi_t^*(|r - \underline{R}_i|) d\tau \delta_{ss'},
\end{aligned}$$

$$\langle s' \underline{k}' | V_N | \underline{k} s \rangle = \sum_i e^{-(\underline{k}-\underline{k}') \cdot \underline{R}_i} \sum_t \frac{1}{\Omega} \left| \int e^{-i \underline{k}' \cdot (\underline{r} - \underline{R}_i)} \psi_t(|\underline{r} - \underline{R}_i|) d\tau \right|^2 \delta_{ss'},$$

again the structure appears, and the integral can be evaluated by numerical methods ($\underline{r} - \underline{R}_i$ is a dummy variable). There results :

$$\langle s' \underline{k}' | V_N | \underline{k} s \rangle = \delta_{\underline{k} - \underline{k}', G_h} \delta_{ss'} S(G_h) V_{N\underline{k}\underline{k}'},$$

$$\langle s' \underline{k}' | W_{so} | \underline{k} s \rangle = \delta_{\underline{k} - \underline{k}', G_h} W_{so, \underline{k}s \underline{k}'s'}$$

Diagonalisation of the matrix for a given $\underline{k}$ produces the corresponding energy, and when this is done for different values of $\underline{k}$ the bandstructure is obtained.

By evaluating these energy vs $\underline{k}$ curves in different directions at the Fermi energy, the points on the Fermi Surface are obtained. They are given in the following table.

TABLE XIV. Calculated Points on the Fermi Surface.

k_x ($\text{\AA}^{-1}$)	k_y ($\text{\AA}^{-1}$)	k_z ($\text{\AA}^{-1}$)
1.567920	0.000000	0.000000
1.401062	0.110170	0.000000
1.448871	0.075968	0.000000
1.358180	0.142672	0.000000
1.283701	0.203330	0.000000
1.219834	0.259273	0.000000
1.163332	0.311627	0.000000
1.112111	0.361320	0.000000
1.065442	0.408942	0.000000
1.022546	0.455245	0.000000
0.984560	0.501723	0.000000
0.952245	0.549728	0.000000
0.877221	0.506456	0.000000
0.900271	0.458643	0.000000
0.917666	0.408562	0.000000
0.931080	0.35735	0.000000
0.94204	0.30613	0.000000
0.950923	0.25473	0.000000
0.95791	0.20352	0.000000
0.96339	0.152502	0.000000
0.96736	0.101668	0.000000
0.96963	0.050834	0.000000
0.97387	0.000000	0.000000

TABLE XIV continued

k_x ($\text{\AA}^{-1}$)	k_y ($\text{\AA}^{-1}$)	k_z ($\text{\AA}^{-1}$)
0.99287	0.00000	0.037795
1.03312	0.00000	0.07559
1.07470	0.00000	0.113385
1.11476	0.00000	0.151180
1.15293	0.00000	0.18897
1.18903	0.00000	0.22677
1.2232	0.00000	0.26456
1.25611	0.00000	0.30236
1.28654	0.00000	0.340155
1.31488	0.00000	0.37795
1.34153	0.00000	0.41574
1.36610	0.00000	0.45354
1.38877	0.00000	0.491335
1.40950	0.00000	0.52913
1.4284	0.00000	0.566925
1.4458	0.00000	0.604472
1.46304	0.00000	0.64610
1.57548	0.00000	0.113385
1.5805	0.00000	0.151180
1.5647	0.01757	0.22677
1.5645	0.00000	0.22677
1.5596	0.00000	0.26456
1.55449	0.00000	0.30226
1.5480	0.00000	0.34015
1.5407	0.00000	0.37795

TABLE XIV continued

k_x ($\text{\AA}^{-1}$)	k_y ($\text{\AA}^{-1}$)	k_z ($\text{\AA}^{-1}$)
1.5327	0.00000	0.41574
1.52389	0.00000	0.45354
1.51406	0.00000	0.49133
1.5032	0.00000	0.52913
1.4915	0.00000	0.56692
1.47873	0.00000	0.60472
1.46304	0.00000	0.64610
1.46304	0.00000	0.64610
1.46323	- 0.01474	0.64610
1.46380	- 0.029669	0.64610
1.46474	- 0.04554	0.64610
1.46644	- 0.06273	0.64610
1.46909	- 0.08107	0.64610
1.47400	- 0.10091	0.64610
1.48251	- 0.12018	0.64610
1.49706	- 0.13473	0.64610

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VITA

Oscar L. Steenhaut was born in Brasschaat Belgium on January 23, 1933. His secondary education was completed at the Hogere Technische School, Aalst. In 1950 he enrolled at the University of Ghent where he received the degree of Civil Engineer in 1955. He was in the service from 1955 to 1957 and was employed from 1957 to 1960 as a maintenance engineer by SABENA, Belgian Airlines. From 1960 to date he was a staff member of the Technical Institute for Nuclear Industries, Brussels. In July 1960 he married the former Julia Van Holsbeeck. From 1963 to 1964 he enrolled at Louisiana State University and received the Master of Science degree in Electrical Engineering in 1964. He enrolled at the same University in 1967 and is presently a candidate for the degree of Doctor of Philosophy.

EXAMINATION AND THESIS REPORT

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Major Field: Physics

Title of Thesis: The Fermi Surface of Zinc: Radio-Frequency Size Effect

Approved:

Ray E. Goodrich
Major Professor and Chairman

Wm. Goodrich
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Date of Examination:

January 9, 1970