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The Magnetoacoustic Effect in Mercury.

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Submitted to the Graduate Faculty of the
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by
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ABSTRACT

Geometric resonances in the ultrasonic attenuation have been observed in high purity mercury single crystals with longitudinal sound waves propagated along five crystallographic directions at frequencies up to 165 MHz. Of the five, only data for the $(1\bar{1}0)$, (110) , and $(11\bar{2})$ directions are reported. The dominant resonance branches have been assigned to calipers of the second band electron lens-shaped surfaces with three major symmetry calipers being obtained. The remainder of the resonance branches have been assigned to orbits on the first band hole surface. Various breakthrough dimensions of the hole surface were determined from these orbits. The pseudopotential coefficients corresponding to the planes bounding the first Brillouin zone in mercury have been estimated by comparing the geometric resonance data with the results of a four pseudowave calculation neglecting spin orbit coupling.

I. INTRODUCTION

The Fermi surface of crystalline mercury has been studied both experimentally and theoretically by a number of investigators in the past few years. The de Haas van Alphen (dHvA) effect has yielded several extremal cross sectional areas¹; extremal calipers of a portion of the surface have been determined from preliminary magnetoacoustic data²; effective masses on the Fermi surface have been determined from an Azbel-Kaner cyclotron resonance experiment³; and information about the topology has been obtained from magnetoresistance measurements.^{4,5} The first theoretical determination of the band structure was a three plane wave pseudopotential calculation¹ based on the dHvA data. An empirical four parameter model⁵ based on magnetoresistance data was later presented and used as a starting point, along with the dHvA data, for an eight plane wave pseudopotential calculation including spin orbit coupling and constrained to satisfy the requirement of compensation.⁵ A detailed relativistic augmented plane wave (RAPW) calculation⁶ has been performed with the results yielding a surface topologically equivalent to that obtained from the plane wave calculations. All of these calculations yield a model in reasonable agreement with the above experiments with the following exceptions. The calculations predict cross sectional areas belonging to the second band electron surface much too large to be in agreement with the experimentally observed values. Also both pseudopotential and RAPW calculations fail to predict correctly the angular extent of the experimentally observed open orbits as seen from the

magnetoresistance data, whereas the four parameter model uniquely explains this angular range.

In the following sections the results of a detailed magnetoacoustic experiment are reported in an effort to gain a more precise knowledge of the Fermi surface of mercury. The details of a four pseudowave calculation of several cross sections of the Fermi surface of mercury are presented in Appendix A. The attenuation coefficient of a sound wave in the presence of a transverse magnetic field is calculated also in Appendix B. Results are obtained both for longitudinal waves and waves polarized perpendicular to the direction of propagation. The oscillatory behavior of the attenuation coefficient corresponding to geometric resonances is discussed. A relation is obtained for the caliper dimension, C , of the Fermi surface in terms of the period of the oscillations.

II. STRUCTURE

The structure of crystalline mercury has been discussed extensively by a number of authors^{1,3-6} and will only be summarized here along with the basic topological features of its Fermi surface.

Mercury is a divalent metal which crystallizes at approximately 223°K into a simple rhombohedral structure with one atom per unit cell. The rhombohedral structure can be considered as a distorted version of the more common face centered cubic structure where the distortion consists of stretching along the trigonal axis. A detailed discussion of the rhombohedral structure in general can be found in several textbooks.^{7,8}

The lattice parameters of mercury as well as other information pertaining to its crystal structure are listed in Table I. The first Brillouin zone with symmetry points and principal symmetry axes labeled is shown in Fig. 1. The first zone is composed of three distinct, inequivalent faces centered on X, T, and L, and perpendicular to the {110}, {111}, and {100} directions, respectively. The {100} faces are the largest and are closest to the zone center Γ . The hexagonal shaped {111} faces are about 1/2% further from Γ than the rectangular {110} faces.

Unlike most systems, the directions in the rhombohedral system are not generally normal to planes having the same index. The exceptions to this are the $\langle 111 \rangle$, $\langle 1\bar{1}0 \rangle$, and $\langle 11\bar{2} \rangle$ directions. All three $\langle 1\bar{1}0 \rangle$ and $\langle 11\bar{2} \rangle$ directions lie in the (111) plane. The $[1\bar{1}0]$ direction is parallel to the line joining T and W so that the (110) plane bisects the Brillouin zone along a line X-U-T-U-L. This plane and its two other

TABLE 1. Physical constants and crystallographic data for mercury at 5°K.

Symbol	Value	Definition
a_0^a	$2.9863\text{\AA}$	Real space lattice vector
g_0	$2.3002\text{\AA}^{-1}$	Reciprocal space lattice vector
α	$70^\circ 44.6'$	Real space rhombohedral angle
β^a	$104^\circ 21.7'$	Reciprocal space rhombohedral angle
Ω	$22.996\text{\AA}^3$	Volume of unit cell in real space
k_F	$1.3707\text{\AA}^{-1}$	Free electron Fermi radius
E_F	0.5261 Ry	Free electron Fermi energy
ρ	14.48 g/cm^3	Density
X-U	$0.6345\text{\AA}^{-1}$	See Fig. 1
T-U	$0.6254\text{\AA}^{-1}$	See Fig. 1
L-U	$1.0337\text{\AA}^{-1}$	See Fig. 1
T-W	$0.7220\text{\AA}^{-1}$	See Fig. 1
X-K	$0.3611\text{\AA}^{-1}$	See Fig. 1
Γ -L	$1.1500\text{\AA}^{-1}$	See Fig. 1
Γ -X	$1.4103\text{\AA}^{-1}$	See Fig. 1
Γ -T	$1.4144\text{\AA}^{-1}$	See Fig. 1
U-W	$0.3611\text{\AA}^{-1}$	See Fig. 1
L-W	$1.0951\text{\AA}^{-1}$	See Fig. 1
L-K	$0.8920\text{\AA}^{-1}$	See Fig. 1
$v_{1\bar{1}0}$	$1.70 \times 10^5 \text{ cm/sec}$	Longitudinal sound velocity in $(1\bar{1}0)$ direction
v_{110}	$2.35 \times 10^5 \text{ cm/sec}$	Longitudinal sound velocity in (110) direction
$v_{11\bar{2}}$	$1.72 \times 10^5 \text{ cm/sec}$	Longitudinal sound velocity in $(11\bar{2})$ direction
v_{111}	$2.55 \times 10^5 \text{ cm/sec}$	Longitudinal sound velocity in (111) direction
v_{100}	$2.11 \times 10^5 \text{ cm/sec}$	Longitudinal sound velocity in (100) direction

^aSource: C. S. Barrett, Acta Cryst. 10, 58 (1957).

Fig. 1

equivalents are the mirror planes in this system. The $[1\bar{1}0]$ direction is one of the three two-fold rotation axes, $[11\bar{2}]$ is parallel to the line joining T and U, and $[111]$ is parallel to the line Γ -T. Three other directions of interest are the (100) direction, parallel to Γ -L, the (110) direction, parallel to Γ -X, and the $[110]$ direction, parallel to Γ -U.

Previous experiments and calculations are in essential agreement with a Fermi surface consisting of a double convex, lens-shaped, second zone electron disc centered at L on each of the six {100} faces bounding the first zone and a multiply connected first zone hole surface. The electron lenses are due to an overlapping of Fermi spheres from adjacent zones along the line Γ -L. The first zone hole surface gives rise to a number of closed orbits along with several sets of open orbits. Experimental data and theoretical calculations indicate regions of contact between the Fermi sphere and the zone boundary at the points X and T in addition to L. This contact produces breakthrough regions, i.e., openings in the hole surface at these points. These openings allow for the existence of several additional closed orbits on the hole surface in addition to restricting the angular range of the open orbits.

III. EXPERIMENT

A. Sample Preparation

The samples used in this investigation were prepared from high purity (99.9999%) mercury obtained from the United Mineral and Chemical Company.⁹ Single crystals approximately 3mm in thickness with two smooth, flat, parallel surfaces were grown using a modified Bridgeman technique in the following manner. The sample mold, shown in Fig. 2, was first thoroughly cleaned with methyl alcohol making sure that all foreign matter was completely removed. The mold was then sandwiched between two previously cleaned microscope slides and clamped at both ends. The cavity of the mold was filled with reagent grade acetone and the high purity mercury immediately injected displacing the acetone in the circular part of the cavity. Care was taken to make sure that all bubbles were absent from the surfaces in contact with the microscope slides. The primary purpose of the acetone was to provide a film between the mercury surface and the glass in order to prevent the mercury from adhering to the glass. The mold, filled with the mercury, was then lowered into a dry ice-methyl alcohol bath at the rate of 3 inches per hour. Once the mercury was completely immersed in the bath, the mold was quickly removed, placed into a dish containing a similar bath of dry ice-methyl alcohol, carefully disassembled, and the mercury crystal removed and stored in liquid nitrogen.

Several single crystals were prepared in the previous manner, and six were chosen for investigation with the normal to the parallel surfaces

FRONT VIEW

END VIEW

Fig. 2

directed along the $(1\bar{1}0)$, (110) , $(11\bar{2})$, $[110]$, (111) , and (100) crystallographic directions, respectively. The orientation of each sample was determined to within $\pm 1^\circ$ using standard x-ray techniques. A thin stream of liquid nitrogen was directed over the crystal during the x-ray time to prevent the melting of the sample.

Prior to being x-rayed, each sample was electropolished in a solution of 1% by volume of perchloric acid and 99% methyl alcohol at dry ice temperatures.¹⁰ This served a twofold purpose in that any surface damage to the crystals was removed rendering better x-ray photographs, and it indicated whether or not the sample was a single crystal immediately since any grain boundaries were revealed. All samples were stored in liquid nitrogen between runs.

B. Experimental Details

Due to the high attenuation of ultrasound in mercury, a dual transducer, pulse transmission technique similar to that described by Kamm and Bohm¹¹ was employed to observe and record the geometric resonance signals. A block diagram of the experimental apparatus is shown in Fig. 3. The electronic equipment used was identical to that described by Coon et al.¹² with the addition of two wideband amplifiers cascaded in front of the receiver to provide additional gain. A Z-cut quartz delay rod¹³ was used to delay the received pulse for 5 μ sec in order to allow the receiver to recover sufficiently from the initial transmitter pulse which was capacitively coupled to the receiver. X-cut, gold plated, 1/4 inch diameter quartz transducers¹³ with a fundamental frequency of 15 MHz were excited at an odd harmonic of the fundamental to generate and receive longitudinal sound waves. The receiving

SPERRY PRODUCTS
ATTENUATION COMPARATOR
MODEL 56A001

Fig. 3

transducer was bonded to the delay rod with General Electric 7031 varnish and allowed to dry for approximately two days before each run. The technique and acoustic bonding agent used to bond the delay rod and generating transducer to the mercury crystal was critical and necessitates a detailed discussion.

It was necessary to be able to make both of the above bonds while preventing the mercury crystal from reaching or approaching its melting point. The normal bonding materials such as silicone oils, stopcock greases, and epoxies either solidify at high temperatures or refuse to adhere to the surface of the mercury at low temperatures. Numerous liquid hydrocarbon compounds were tried with the best results being obtained from a high purity mixture of 5 parts isopentane (2-methylbutane) and one part 3-methyl pentane (3 MP). Spectrographic grade isopentane and 3 MP were both obtained from the distillation of technical grade liquids.¹⁴ Both liquids were stored in separate air-tight containers to prevent evaporation with a small quantity of magnesium sulphate added to each container to remove any water that might have been absorbed. This removal of absorbed water was found to be a critical step in the bonding procedure as the bonds tended to crack at a few degrees above liquid helium temperatures if the water removal step had not been performed carefully. The liquids were mixed in the proper proportion immediately prior to use. The isopentane - 3 MP mixture remained a liquid down to liquid nitrogen temperatures although it became extremely viscous.

The above mixture was used successfully to simultaneously bond the 3.0 cm long, 1.2 cm diameter quartz delay rod and a 1/4 inch diameter quartz transducer to opposite sides of the mercury crystal.

The technique used was as follows. The mercury sample was placed on a flat piece of dry ice and both major surfaces cleaned with a cotton swab, being careful to remove all traces of alcohol or acetone from the surfaces. The delay rod was placed upright in a dish containing liquid nitrogen whose level was such that the upper three quarters of the delay rod was above the surface of the liquid. A small drop of the isopentane - 3 MP mixture was then placed on the upright face of the mercury crystal and the transducer applied. Immediately, another small drop of the mixture was placed on the upright surface of the delay rod and the sample then carefully lifted up and placed on the rod. The weight of the sample was sufficient to press out the bond quite thin. Liquid nitrogen was added until the whole assembly was submerged. The entire crystal assembly could then be handled and placed in the sample holder submerged in liquid nitrogen.

This bonding arrangement was found to be satisfactory in most cases yielding a strong transmission pulse down to liquid helium temperatures. In cases where either or both of the isopentane - 3 MP bonds fractured upon immersion in the liquid helium the sample holder containing the sample was lifted above the level of the liquid helium, allowed to warm up slightly, and then slowly lowered back into the liquid. In some instances this procedure had to be repeated several times before a satisfactory bond was obtained.

All data were taken at 1.2°K in order to reduce scattering due to thermal phonons. Since mercury is a superconductor at 1.2°K with a critical field of 360 G, it was necessary that the data be taken in magnetic fields in excess of this value. The magnetic field was set initially just below the critical value and swept such that H^{-1} was a

linear function of time, yielding geometric resonances periodic in time, thereby simplifying the data analysis.

The velocities of propagation of longitudinal sound waves along the various crystallographic axes were determined experimentally. They were measured at 1.2°K and are tabulated in Table I.

IV. THEORY AND DATA ANALYSIS

The general theory of magnetoacoustic attenuation in metals has been given by Cohen, Harrison, and Harrison¹⁵ and by Pippard.¹⁶ For the case of geometric resonances, it was found that the attenuation coefficient is periodic in the reciprocal of the magnetic field and that this period can be related to C , the k -space caliper of an electron orbit on the Fermi surface.

For the standard geometry in which the magnetic field $\vec{H}$ is rotated in a plane perpendicular to the direction of the sound propagation $\vec{q}$, the relation for the k -space caliper can be expressed as

$$C = \frac{\lambda e}{\hbar c \Delta(\frac{1}{H})} \quad (1)$$

where C is twice the "radial caliper" of the Fermi surface in the direction $\vec{q} \times \vec{H}$, λ is the sound wavelength, and $\Delta(\frac{1}{H})$ is the period of the oscillations in reciprocal field. The necessary condition for observing a series of geometric resonances is that $q\ell \gg 1$ and $\omega_c \tau > 1$, where q is the sound wave vector, ℓ is the electron mean free path, ω_c is the cyclotron frequency, and τ is the characteristic scattering time for the electrons. The condition $\omega_c \tau > 1$ requires that an electron complete at least one real space orbit before being scattered, while $q\ell \gg 1$ requires that the completed orbit encompass several sound wavelengths. In the case of mercury, this latter condition could be satisfied for quite reasonable ultrasonic frequencies.

The assumption is generally made that C measures the extremal projection of the Fermi surface in the direction $\vec{q} \times \vec{H}$. However, Pippard¹⁶⁻¹⁸ has indicated that a limited series of oscillations may arise from regions which are not extremal if these regions couple strongly to the sound wave.

As has been pointed out,¹⁹ extremal calipers can be uniquely converted into radius dimensions of the Fermi surface only if the given Fermi surface sheet has sufficient symmetry so that a set of extremal calipers measured on it for different directions of $\vec{H}$ all occur in a common plane about a common center. This occurs if a given sheet of the Fermi surface has both reflection symmetry in a plane perpendicular to $\vec{q}$ and inversion symmetry about some point in that plane.

It is advantageous at this point to briefly discuss the meanings of the terms extremal orbit and extremal caliper. An orbit is the intersection of the Fermi surface with a plane, $k_H = \text{constant}$, perpendicular to $\vec{H}$. The set of all possible calipers of the orbit may be obtained by measuring the normal distances between tangents to the orbit which are parallel to $\vec{q}$. An extremal orbit as used in geometric resonance refers to an orbit which has a caliper that remains stationary with respect to small changes in k_H . The caliper for which an orbit is extremal is referred to as an extremal caliper of the Fermi surface.

Throughout this paper a system of notation similar to that of Ref. 19 will be adopted. The measured calipers will be reduced to radii whenever allowed by symmetry and will be denoted by the symbol k with a superscript to identify the direction and a subscript to identify the particular surface. For example, $k_{\text{LENS}}^{L-\Gamma}$ refers to the radial caliper of the lens measured from L toward Γ . Calipers obtained from

orbits not having sufficient symmetry to permit a reduction to radii will be denoted by the symbol C with an equivalent notation. Radial calipers will hereafter be referred to as k-calipers while diametral calipers will be referred to as C-calipers, i.e., a C-caliper is twice a k-caliper where allowed by symmetry. It will be assumed that all calipers presented here are due to extremal orbits unless otherwise specified.

Experimental extremal calipers were calculated using Eq. (1). The periods, $\Delta(\frac{1}{H})$, were determined from the experimental data using a relation of the form

$$\frac{1}{H_n} = \Delta(\frac{1}{H})(n + \gamma) \quad , \quad (2)$$

where n is the resonance number, and γ is a phase factor which is a function of n for small n but rapidly approaches a constant value as n increases. Since the attenuation theoretically reaches a relative maximum at integral values of n and a relative minimum at half integral values, γ can be determined from a plot of $1/H_n$ vs n with the best straight line fit through these points extrapolated to $1/H_n = 0$.

For low magnetic fields such that the extremal dimension of an orbit is much longer than the wavelength λ , the resonances are strictly periodic in H^{-1} . This corresponds to the high phase region and occurs for large values of n . The low phase region occurs when the magnetic field is high enough such that λ is a significant fraction of the orbit diameter. The phase of the oscillations then shifts from its low field asymptotic value and the oscillations are no longer strictly periodic in H^{-1} . Deviations from the H^{-1} periodicity occurring in the

low phase region are thus easily detected.

A knowledge of the phase for large n is useful in identifying the oscillations and can yield information about the nature of the surfaces responsible for them. Theoretical considerations²⁰ indicate that $\gamma = 0.25$ for a circular cylinder and $\gamma = 0.375$ for a spherical surface. The data obtained for the lens surface of mercury yielded a value of $\gamma = 0.27 \pm 0.07$.

V. EXPERIMENTAL RESULTS AND DISCUSSION

A. Electron Surface

1. Results for $\vec{q}$ parallel to the $(1\bar{1}0)$ direction. Figure 4 presents a summary of all the C-calipers obtained from data in the $(1\bar{1}0)$ plane; $\vec{q}$ is in the $(1\bar{1}0)$ direction while θ measures the angle of the caliper direction from the trigonal axis. A total of ten distinct resonance branches were observed with each of the branches being designated with a Greek letter. Of these ten resonance branches, two, namely α_1 and α_2 , have been assigned to the second band electron surface.

The resonances associated with the α_1 branch had the largest amplitude and have been assigned to calipers of a cross section of the second zone electron lens surface centered on the point L_1 in the $(1\bar{1}0)$ plane. The corresponding k-caliper data for α_1 is shown on a polar plot in Fig. 5, along with a projection of the Brillouin zone on the $(1\bar{1}0)$ plane with the free electron lenses sketched in for comparison. For notation purposes, the center of the lenses are denoted as L_1 , L_2 , and L_3 . The errors presented refer only to uncertainties in the determination of the periods. The extremal dimensions of the cross section centered on L_1 have been found to differ slightly from the values previously reported² due to a small misorientation of the crystal from which the original data were taken. The results of the present data indicate a value for the minimum radius, k_{LENS}^{L-I} , of $0.176 \pm 0.004 \text{ \AA}^{-1}$.

Fig. 4

Fig. 5

and a value for the maximum radius, $k_{\text{LENS}}^{\text{L-U}}$, of $0.538 \pm 0.010 \text{ \AA}^{-1}$, whereas the values reported initially were $k_{\text{LENS}}^{\text{L-}\Gamma} = 0.180 \text{ \AA}^{-1}$ and $k_{\text{LENS}}^{\text{L-U}} = 0.565 \text{ \AA}^{-1}$, respectively. Loucks²¹ has reported dimensions obtained from his RAPW calculation of $k_{\text{LENS}}^{\text{L-}\Gamma} = 0.215 \text{ \AA}^{-1}$ and $k_{\text{LENS}}^{\text{L-U}} = 0.540 \text{ \AA}^{-1}$, thus providing excellent agreement on the value of $k_{\text{LENS}}^{\text{L-U}}$. The cross sectional area of this section of the lens was determined graphically and found to be $0.299 \text{ \AA}^{-2}$ which is in good agreement with the value of $0.305 \text{ \AA}^{-2}$ determined by Brandt and Rayne from dHvA data. A comparison of the extremal areas of this cross section, along with the major and minor calipers as determined by different methods, is shown in Table II. This table includes the results of a 4 pseudowave (4 PW) calculation to be discussed later.

The C-calipers designated α_2 in Fig. 4 have been assigned to a projection of one of the electron lenses onto the $(1\bar{1}0)$ plane. This projection is shown centered on the point L_2 or L_3 on the zone projection in Fig. 5. Resonances corresponding to these calipers were observed over an interval of about 22° in the vicinity of the (001) direction. The C-calipers ranged from a value of $1.08 \pm 0.04 \text{ \AA}^{-1}$ to $1.20 \pm 0.02 \text{ \AA}^{-1}$ with considerable scatter in the data. The corresponding k-caliper values are also shown in polar plot in Fig. 5.

2. Results for $\vec{q}$ parallel to the (110) direction. Figure 6 shows a polar plot of the data for $\vec{q}$ in the (110) direction and $\vec{H}$ rotated in the (110) plane. A projection of the Brillouin zone onto the (110) plane with the free electron lenses sketched in for comparison is shown in the same figure. Only two distinct resonance branches were observed for this orientation as a result of the complete domination of the signal by resonances due to the lens. One branch was assigned to the projection of the lens centered on L_2 onto the (110) plane with the

TABLE II. Comparison of calipers and areas of lens
obtained by different methods in $(1\bar{1}0)$ plane.

Source	$k_{\text{LENS}}^{\text{L-}\Gamma} (\text{\AA}^{-1})$	$k_{\text{LENS}}^{\text{L-U}} (\text{\AA}^{-1})$	Area ($\text{\AA}^{-2}$)
Free electron	0.220	0.730	0.441
dHvA 3 PW ^a	0.204	0.600	0.344
8 PW ^b	0.22	0.64	0.423
RAPW ^c	0.215	0.540	0.354
dHvA			0.305
Present calculation	0.176	0.540	0.300
Present experiment	0.176	0.538	0.299

^aSee Ref. 1.

^bSee Ref. 5.

^cSee Ref. 21.

Fig. 6

remaining branch being assigned to a similar projection of the lenses centered on L_1 and L_3 . It should be noted that for perfect alignment of the sample, the projections of the surfaces centered on L_1 and L_3 should be identical if the lenses are surfaces of revolution about the Γ -L line.

With the magnetic field directed along the $[001]$ direction, the maximum caliper of the projection of the surface centered on L_2 was found to have a value of $c_{L_2}^{00} = 1.28 \pm 0.03 \text{ \AA}^{-1}$. This caliper corresponds to the remaining symmetry axis caliper not obtained from the $(\bar{1}\bar{1}0)$ data.

With the magnetic field in the $(\bar{1}\bar{1}0)$ direction, the minimum caliper of the projection of the lens centered on L_2 was found to be $c_{L_2}^{90} = 0.52 \pm 0.01 \text{ \AA}^{-1}$. A consistency check of this dimension can be made from a projection of the cross section of the lens obtained from the binary data onto a plane perpendicular to the (110) direction. Such a projection yielded a value $0.51 \pm 0.01 \text{ \AA}^{-1}$, which compares quite well with the above caliper.

The maximum dimension of the projection of the lenses centered on L_1 and L_3 was obtained with the magnetic field in the $(\bar{1}\bar{1}0)$ direction. The data indicate $c_{L_1}^{90} = c_{L_3}^{90} = 1.20 \pm 0.03 \text{ \AA}^{-1}$. The fact that $c_{L_2}^{00}$ differs slightly from $c_{L_1}^{90}$ and $c_{L_3}^{90}$ is evidence that the lenses are not exactly circular since a circular shape would imply that all three of these dimensions are equal. The minimum dimension c_{L_1, L_3}^{00} was obtained with the magnetic field in the $[001]$ direction. In this region the data split into two branches yielding two separate values for c_{L_1, L_3}^{00} . One set of data indicated a value of $0.81 \pm 0.02 \text{ \AA}^{-1}$, while the other set gave a value of $0.83 \pm 0.02 \text{ \AA}^{-1}$. This

split in the data can be attributed to a misalignment of the sample with the sound propagating about 1° off the (110) direction toward the $(\bar{1}10)$ direction.

3. Results for $\vec{q}$ parallel to the $(11\bar{2})$ direction. A total of five distinct resonance branches were obtained for $\vec{q}$ parallel to the $(11\bar{2})$ direction and $\vec{H}$ rotated in the $(11\bar{2})$ plane. The two primary branches are shown in a polar plot in Fig. 7 along with a projection of the Brillouin zone onto the $(11\bar{2})$ plane with the free electron lenses sketched in for comparison. One of these primary branches has been assigned to a projection of the lens centered on L_1 onto the $(11\bar{2})$ plane with the other primary branch being assigned to a similar projection of the lens centered on L_2 . Both of these projections should be symmetrical and should intersect at 0° and 90° in the polar representation of Fig. 7 if the crystal is properly oriented. There is no definite evidence of resonances corresponding to calipers of the projection of the third lens centered on L_3 . However, the orbits which should give rise to these resonances have a small radius of curvature over the region to be calipered. It has been pointed out²² that the amplitude of the geometric resonances should depend quite strongly on the radius of curvature of the orbit. Orbits with large radii of curvature should produce larger amplitude resonances than those with small radii of curvature. In light of this fact one expects the signals from the L_3 resonance to be weak.

The crystal from which the data in Fig. 7 was obtained was misoriented with the bisectrix plane rotated about 5 degrees about the trigonal axis. This misorientation is readily obvious from the data since the shapes and the areas of the projections of the two lenses,

Fig. 7

L_1 and L_2 , differ considerably. The experimental data indicate that the two projections intersect at polar angles of 20° and 88° instead of 0° and 90° . The minimum C-caliper dimension of the L_2 projection was found to be $0.69 \pm 0.01 \text{ \AA}^{-1}$, while the minimum dimension of the L_1 projection was found to be $0.50 \pm 0.01 \text{ \AA}^{-1}$. The crystal misalignment consequently accounts for a difference of roughly 39% in the minimum dimensions. In contrast, the maximum diametral dimensions of the two projections agree quite well with the L_2 projection having a dimension of $1.12 \pm 0.02 \text{ \AA}^{-1}$ and the L_1 projection having a dimension of $1.09 \pm 0.02 \text{ \AA}^{-1}$.

4. Results for $\vec{q}$ parallel to the (100), (111), and [110] directions.

In addition to the three orientations just discussed, an attempt was made to obtain data on the lens surfaces for $\vec{q}$ directed in the (100), (111), and [110] directions.

The (100) direction is most interesting since with $\vec{H}$ rotated in the (100) plane one should be able to obtain the main cross section of the lens cut by the (100) plane. However, due to the strong open orbit absorption that exists in this direction, the maximum frequency obtainable was 45 MHz, in which case only a maximum of about two oscillations were observed before the signal saturated. At higher frequencies the signal saturated with no resonances being observed. The lack of amplitude of the lens resonance in this plane could also be attributed to the large curvature of the orbits over the region to be calipered as was the case with the lens centered on L_3 in the (112) plane. Thus no additional information was obtained from this orientation.

An attempt was made to propagate the sound along the $[110]$ direction and obtain data for $\vec{H}$ in the $[110]$ plane. This direction is of interest because it would yield the symmetric cross section of the lens cut by the ΠW plane. This cross section forms, along with the two cross sections from the $(1\bar{1}0)$ and (100) planes, the set of three orthogonal cuts of the lens. A consistency check on the value of c_{L2}^{00} could have been made since with $\vec{q}$ parallel to $[110]$ and $\vec{H}$ parallel to $(11\bar{2})$, the caliper obtained from the lens should be identical to c_{L2}^{00} obtained from the (110) data. This attempt failed as the result of not being able to make a successful acoustic bond between the delay rod and the $[110]$ sample.

With $\vec{q}$ parallel to the (111) direction and $\vec{H}$ rotated in the (111) plane, resonances were observed which corresponded to calipers of the three identical elliptical cross sections of the electron lens. Since these three sections give rise to resonances all of about the same amplitude with two of the sections, and in some instances all three, having approximately the same caliper value, the additional information obtained from the present data was not of sufficient interest to be reported.

5. Summary of electron data. In summary, three major symmetry dimensions of the second zone electron lens have been determined experimentally. The values obtained are $k_{LENS}^{L-I} = 0.176 \pm 0.004 \text{ \AA}^{-1}$, $k_{LENS}^{L-U} = 0.538 \pm 0.010 \text{ \AA}^{-1}$, and $c_{L2}^{00} = 1.28 \pm 0.03 \text{ \AA}^{-1}$ or $k_{LENS}^{L-W} = 0.64 \pm 0.015 \text{ \AA}^{-1}$, respectively. The first two dimensions, along with intermediate calipers, give a cross sectional area in the $(1\bar{1}0)$ plane that agrees within 2% of the experimental dHVA data. The remaining dimension, c_{L2}^{00} , gives the maximum diameter of the lens along the L-W

line. The fact that the diameters of the lens along L-U and L-W, i.e., $2 k_{\text{LENS}}^{\text{L-U}}$ and $C_{L_2}^{00}$, differ by about 8% indicates that the lens is not a surface of revolution about the line Γ -L.

6. Pseudopotential coefficients. The pseudopotential coefficients corresponding to the planes bounding the first Brillouin zone in mercury have been estimated by comparing the geometric resonance data obtained from the lens with the results of a four pseudowave calculation neglecting spin orbit coupling. Further, there was no attempt to maintain compensation. Details of the calculation are presented in Appendix A.

The results of the calculation for the $(1\bar{1}0)$ cross section are shown in Fig. 8 compared to the data. It should be noted that the 4 PW method yields reasonable agreement with the data if the Fermi level is depressed to 0.505 Ry, about 4.0% below the free electron value. The dHvA area for the $(1\bar{1}0)$ cross section of the electron surface and that indicated by the present measurements are in excellent agreement, both with each other and the present 4 PW results.

Experimental and present theoretical results for both the electron and hole bands were compared at several points of interest in the zone and are summarized in Tables II, III, and IV. A survey of the results of the calculation shows general agreement with the topological features of the Fermi surface of mercury as suggested by other workers as well as by the present experiment; however, there remains need for improvement. Indeed, the present calculation is not presented as a substitute for a rigorous band calculation, but only as a method by which some of the available experimental data may be compared.

The 4 PW results, along with other existing calculations, will be compared to the data from the hole surface in the following section.

Fig. 8

TABLE III. Comparison of radii of openings in first zone hole surface.* Values are in $\text{\AA}^{-1}$.

Model	k_{IN}^{L-U}	k_{IN}^{X-U}	k_{IN}^{T-U}	k_{IN}^{T-W}	k_{IN}^{X-K}
RAPW ^a	0.948	0.117	0.117 [†]	0.117 [†]	0.115
HAA ^a	0.831	0.354	0.382 [†]	0.382 [†]	0.347
MAG V ^a	0.860	0.260	0.198 [†]	0.198 [†]	0.209
8 PW ^a	0.874	0.177	0.071 [†]	0.071 [†]	0.209
dHvA 3 PW ^a	0.897	0.299	0.324 [†]	0.324 [†]	0.182
Present calculation	0.870	0.300	0.270	0.340	0.185
Present experiment	0.90	0.30			

* For an explanation of notation see Figs. 10 and 11.

^a See Ref. 5.

[†] Circular approximation.

TABLE IV. Comparison of outside dimensions of the τ -section as measured from L, T, and X.* Values are given in $\text{\AA}^{-1}$.

Method	$k_{\text{OUT}}^{\text{L-U}}$	$k_{\text{OUT}}^{\text{T-U}}$	$k_{\text{OUT}}^{\text{X-U}}$	$k_{\text{OUT}}^{\text{T-W}}$
dHvA 3 PW ^a	1.16	0.78	0.765	0.935
Present calculation	1.18	0.79	0.79	1.00
Present experiment	1.14	0.77	0.765	0.90

*For an explanation of notation, see Figs. 10 and 11.

^aSee Ref. 1.

Further, the 4 PW calculation will allow some extrapolation of the experimental results to calipers not directly observed. The present theory is fit to the electron surface, as opposed to the method of earlier workers. Thus it is to be expected that the largest discrepancies between theory and experiment will be found for the smaller orbits on the hole surface such as the β orbits which will be discussed later. As will be evidenced in the next section, the larger hole surface calipers in general show better agreement between the present calculation and experiment than do those due to the smaller sections of the hole surface.

B. Hole Surface

1. Results for $\vec{q}$ parallel to the $(1\bar{1}0)$ direction. The resonance branches designated by β , ϵ_1 , ϵ_2 , δ , γ , μ_1 , μ_2 , and η shown in Fig. 4 have all been assigned to C-calipers associated with various orbits on the first zone hole surface. A representation of this surface along with the labeled orbits is shown in Fig. 9. Among the more interesting orbits from this set are those designated by ϵ_1 , ϵ_2 , δ , and η . The branch denoted by ϵ_1 has been assigned as the caliper of an orbit centered on L around the inside of the hole surface with $\vec{H}$ in the vicinity of the (001) direction. This orbit was observed over a range of about 6° and yielded a radial caliper that varied from $0.91 \pm 0.02\text{\AA}^{-1}$ to $1.03 \pm 0.02\text{\AA}^{-1}$. The branch denoted by ϵ_2 has been assigned to an orbit lying in the same plane as ϵ_1 , but moving on the outside of the hole surface and threading through the openings in the T faces. This orbit was observed over the same range as ϵ_1 and yielded a radial caliper that varied from $1.16 \pm 0.02\text{\AA}^{-1}$ to $1.18 \pm 0.02\text{\AA}^{-1}$.

Fig. 9

The η branch has been assigned to a hexagonal shaped orbit centered at T completely enclosing the T face which occurs when the magnetic field is directed in the vicinity of the trigonal axis. This orbit was observed over an angular range of about 12° on either side of the (111) direction and gave radial calipers that varied from a maximum of $0.83 \pm 0.02 \text{ \AA}^{-1}$ to a minimum value of $0.66 \pm 0.02 \text{ \AA}^{-1}$ with the field tilted 12° toward [001]. The radial caliper obtained with the field along the (111) direction was $0.77 \pm 0.02 \text{ \AA}^{-1}$.

The δ branch has been assigned to an orbit on the inside of the opening on the X face centered on the point X. This orbit was observed with the magnetic field in the vicinity of the (110) direction and was detectable over a range of approximately 8° on either side of the (110) direction giving a radial caliper of $0.30 \pm 0.01 \text{ \AA}^{-1}$ for this particular direction. The data obtained from these orbits are plotted in the $(1\bar{1}0)$ plane in Fig. 8 along with the α_1 data for comparison. Note that calipers obtained from ϵ_1 , ϵ_2 , η , and δ almost completely determine the cross section of the hole surface centered on U. This cross section corresponds to the area enclosed by the τ orbit of Brandt and Rayne. The cross section generated by the τ orbit will be referred to as the τ -section.

The results of the 4 PW calculation in the $(1\bar{1}0)$ plane based on the present data are shown in Fig. 8. As is evident, the fit to the lens section is extremely good with the extremal dimensions and enclosed area agreeing within experimental error. The fit to the τ -section is fairly good with the calculation lying for the most part slightly outside the experimental data. It should be noted that most of the experimental data assigned to the τ -section was taken from

orbits with rather large dimensions. Thus errors in determining the dimensions of these orbits imply large errors on the small scale of the τ -section. The area of the τ -section has been determined from the present calculation and found to be $0.132\text{\AA}^{-2}$. This is considerably smaller than the experimental dHvA area of $0.151\text{\AA}^{-2}$, but agrees with the RAPW calculation of $0.132\text{\AA}^{-2}$. The dHvA 3 PW calculation gives a value of $0.107\text{\AA}^{-2}$ while the 8 PW calculation yields a value of $0.151\text{\AA}^{-2}$ in agreement with the experimental dHvA data. It is to be noted that while the 8 PW calculation fits the dHvA experimental data for the τ -section, it is in disagreement with the corresponding experimental area for the (110) lens section by about 27%, giving a value of $0.423\text{\AA}^{-2}$ as compared to the experimental area of $0.305\text{\AA}^{-2}$. The present calculation gives good agreement for the area of the lens but is in disagreement with the measured dHvA area of the τ -section by about 15%.

There are several important dimensions that can be obtained from a knowledge of the τ -section. These include the width of the openings in the X, T, and L faces. Figure 10 indicates these dimensions along with the corresponding notation while the values are given in Table III. Data obtained from the δ orbit with the magnetic field in the (110) direction yield a value for the major dimension of the opening in the X face of $k_{\text{IN}}^{\text{X-U}} = 0.30 \pm 0.01\text{\AA}^{-1}$ which is precisely the same value obtained from the 4 PW calculation. The dimensions of the opening in the T face were determined exclusively from the 4 PW calculation since ultrasonic data could not be obtained for this direction. The lack of data from orbits from which the size of the opening could be determined was due to the fact that resonances from the lens and η orbits completely dominated the attenuation and consequently obscured

Fig. 10

weaker resonances. The calculation indicates a minimum value for the width of the opening of $k_{IN}^{T-U} = 0.27\text{\AA}^{-1}$ and a maximum width of $k_{IN}^{T-W} = 0.340\text{\AA}^{-1}$. A circular approximation to the opening has been made in the 8 PW calculation and gives a value of $k_{IN}^{T-U} = k_{IN}^{T-W} = 0.071\text{\AA}^{-1}$, while the dHVA 3 PW calculation gives a result of $0.324\text{\AA}^{-1}$ for the same dimension also in a circular approximation. The width of the opening in the L face should be measured directly from the ϵ_1 orbits. However, this opening can be better defined from the η orbit centered on T as is evident from Fig. 8. The data indicate a value of $k_{IN}^{L-U} = 0.90 \pm 0.02\text{\AA}^{-1}$ as compared to a calculated 4 PW value of $k_{IN}^{L-U} = 0.870\text{\AA}^{-1}$. A comparison of the various breakthrough dimensions on the hole surface as determined by different methods is given in Table III.

Three other dimensions that can be determined from the experimental data are the outside calipers of the τ -section measured from the points X, T, and L. These calipers are denoted as k_{OUT}^{X-U} , k_{OUT}^{T-U} , and k_{OUT}^{L-U} as indicated in Fig. 10. The experimental results are tabulated in Table IV along with the corresponding 4 PW and dHVA 3 PW dimensions for comparison. The dimension k_{OUT}^{T-U} was determined directly from the η orbits while k_{OUT}^{X-U} was determined indirectly from the ϵ_1 orbits. The experimental determination of k_{OUT}^{L-U} utilizes the dimension c_{τ}^{L-U} as explained later in this text.

The calipers designated β have been assigned to orbits around the arms on the hole surface extending along the $\langle 100 \rangle$ directions as indicated in Fig. 9. Resonances corresponding to these calipers were observed over an angular range of about 18° and gave a value of $.065 \pm 0.010\text{\AA}^{-1}$. The minimum caliper should occur with the magnetic field directed along the $[100]$ direction, but unfortunately the β resonances

were obscured about 8° from this point. The dHvA 3 PW calculation indicates a minimum caliper in a circular approximation of approximately $0.04\text{\AA}^{-1}$ while the present calculation gives a value of $0.06\text{\AA}^{-1}$. It might be pointed out that dHvA type of oscillations have been observed in the acoustic attenuation with the magnetic field in the range of 7 to 12 kG in a separate oblique field experiment. These oscillations give areas assignable to the β orbits which agree with the data of Brandt and Rayne.

The calipers denoted by γ were assigned to an orbit that passes through the opening in the T face as illustrated in Fig. 9. Experimentally this orbit was observed over a range of approximately 40° giving C-calipers that varied from $0.38 \pm 0.04\text{\AA}^{-1}$ to $0.58 \pm 0.04\text{\AA}^{-1}$.

When the magnetic field is in the $(11\bar{2})$ direction, the γ orbit will be referred to as a τ' orbit in which case the height of the orbit denoted $C_{\tau'}^{(111)}$ in Fig. 11 was found to be $0.475 \pm 0.04\text{\AA}^{-1}$ as compared to the 4 PW value of $0.520\text{\AA}^{-1}$ and a dHvA 3 PW value of $0.420\text{\AA}^{-1}$.

The two remaining resonance branches in the $(1\bar{1}0)$ plane have been assigned to calipers associated with orbits μ_1 and μ_2 , with μ_1 being first proposed by Keeton and Loucks.⁸ μ_1 was observed over a range of approximately 30° with C-caliper values ranging from a minimum of $0.200 \pm 0.020\text{\AA}^{-1}$ to a maximum of $0.440 \pm 0.040\text{\AA}^{-1}$. With the magnetic field in the (001) direction the C-caliper obtained for the μ_1 orbit will closely match the diametral caliper of the τ -section along the L-U line. This dimension is denoted as C_{τ}^{L-U} ; and it can be seen from Fig. 10 that $k_{OUT}^{L-U} = k_{IN}^{L-U} + C_{\tau}^{L-U}$. The experimental data indicate a value of C_{τ}^{L-U} of $0.240 \pm 0.020\text{\AA}^{-1}$ as compared to the dHvA 3 PW value of $0.260\text{\AA}^{-1}$ and a value of $0.31\text{\AA}^{-1}$ obtained from the present 4 PW

Fig. 11

calculation. Using the values of C_T^{L-U} and k_{IN}^{L-U} determined experimentally, then $k_{OUT}^{L-U} = 1.14\text{\AA}^{-1}$ is obtained which is in reasonable agreement with the present calculated value of $1.18\text{\AA}^{-1}$. The resonance branch μ_2 has been assigned to a "bowtie orbit" as indicated in Fig. 9. This orbit was observed over an angular range of 10° with C-calipers ranging from $0.258 \pm 0.020\text{\AA}^{-1}$ to $0.166 \pm 0.020\text{\AA}^{-1}$.

The present calculation for the width of the openings in the T and X faces indicate that the $\vec{H} \parallel (1\bar{1}0)$ open orbit, first observed by Dishman and Rayne,⁵ can exist. It was impossible to detect any resonance due to this open orbit since the attenuation at fields corresponding to low integer values of the open orbit resonance was very high.

2. Results for $\vec{q}$ parallel to the $(11\bar{2})$ direction. Three resonance branches were observed in this direction which could be assigned to orbits on the hole surface. There was considerable evidence for the existence of the β orbits with the data indicating radial calipers that ranged from a minimum of $0.08 \pm 0.01\text{\AA}^{-1}$ to a maximum of $0.181 \pm 0.020\text{\AA}^{-1}$. With the magnetic field in the $(11\bar{2})$ plane, a direction was never assumed for which the minimum radial caliper of the β orbit could be obtained. As was pointed out earlier, the minimum radial caliper for this orbit should be approximately $0.06\text{\AA}^{-1}$.

With the magnetic field in the vicinity of the (111) direction there was strong evidence of the η orbit discussed previously. This orbit was observed over an interval of 10° and gave a radial caliper of $k_{OUT}^{T-W} = 0.90 \pm 0.02\text{\AA}^{-1}$ with $\vec{H}$ in the (111) direction. The dHvA 3 PW calculation gives $0.93\text{\AA}^{-1}$ while the present 4 PW calculation gives a value of $1.00\text{\AA}^{-1}$ for the same dimension.

The third resonance branch was observed with the magnetic field in the vicinity of the $(1\bar{1}0)$ direction yielding calipers in the region of the intersection of the L_1 and L_2 projections of Fig. 7. The data in this area were very difficult to analyze due to the complicated mixing of three or more periods. It was almost impossible to resolve more than one period with any accuracy. With the magnetic field in the region from 4° to approximately 16° from the $(1\bar{1}0)$ direction, the dominant resonance yielded C-caliper values that ranged from $1.02 \pm 0.02\text{\AA}^{\circ-1}$ to $1.20 \pm 0.03\text{\AA}^{\circ-1}$, too large to be associated with the L_1 or L_2 projections. It is possible that these calipers might be assigned to the open orbit that exists with the field in the $(1\bar{1}0)$ direction. Ideally, the caliper of the open orbit should give a value equivalent to $1/3$ the zone height or $0.943\text{\AA}^{\circ-1}$. However, it could be possible to obtain a larger value as a result of the misorientation of the crystal.

3. Summary of hole results. The primary information obtained from the various hole orbit calipers was a description of the π -section in the $(1\bar{1}0)$ plane along with several breakthrough dimensions on the hole surface. The data for the π -section is in general agreement with the results of a 4 PW calculation although the calculated area is still about 15% too small to agree with the experimental dHvA data. In order to fit the dHvA area of Brandt and Rayne, a breakthrough dimension in the T face much smaller than that predicted from the present 4 PW calculation is required. The 8 PW approach of Dishman and Rayne predicts such a dimension, i.e., $0.071\text{\AA}^{\circ-1}$. However, as discussed by Dishman and Rayne, a breakthrough dimension of this size in the T face is not compatible with their magnetoresistance open orbit data.

In view of this there is still need for a further determination, both experimentally and theoretically, of the τ cross section and in particular the dimension k_{IN}^{T-U} . The agreement between the remaining breakthrough dimensions determined experimentally from the hole orbits and those calculated using the 4 PW method is generally good wherever such comparisons can be made.

VI. CONCLUSION

The results of this investigation indicate that the Fermi surface of mercury consists of three electron lenses belonging to the second zone and a multiply connected first zone hole surface. This agrees with the model that has been previously proposed. The hole surface has been found to contact all faces of the Brillouin zone producing breakthrough regions or openings in the surface. The 4 PW calculation performed is in general agreement with the data obtained from both the electron and hole surface. It should be noted, however, that this calculation is not found to be superior to previous calculations. Rather, the primary consequence of performing the calculation is that it suggests no better fit to the available data for the Fermi surface can be obtained by choosing pseudopotential coefficients to fit only the electron data than was found by previous workers when they fit only the hole surface data. For example, the 4 PW calculation was fit to the experimental data on the second band electron surface and the resulting hole surface was also generated. Consequently, the fit to the electron surface was extremely good, but the agreement with the β and τ orbit data was not as satisfactory. The dHvA 3 PW and RAPW calculations which placed emphasis on fitting the dHvA data to the hole surface, in particular to the β orbit, both give essentially the same area for the τ -section which generally compares with that of the present data. These results, however, differ markedly from the dHvA data both for the τ -section and the electron surface. The 8 PW

calculation on the other hand fits the τ -section as well as the β -section to the dHvA data exactly, but in the process worsens the disagreement between the area of the electron section and the corresponding data as well as conflicting with the open orbit data.

It would appear therefore that there is need for further detailed band calculations to resolve the apparent discrepancies between the existing experimental and theoretical results.

APPENDIX A

A Discussion of the 4 PW Calculation

Recently Harrison²³ has pointed out that the Fermi surface of a number of metals can be calculated quite well in the nearly free electron approximation where the deviations from the free electron behavior can be expressed in terms of matrix elements between plane wave states of an effective pseudopotential in place of the real crystal potential. This method has been discussed extensively by Harrison and has been applied to a number of metals to give good agreement with experimental data. No attempt will be made here to justify why this method works or to present a detailed development of the theory, but rather emphasis will be placed on the mechanics of the calculation along with a brief introduction to the pseudopotential method. The reader is referred to the above reference for a more detailed discussion.

The conduction electron wave functions, ψ , satisfy the Schroedinger equation, i.e.,

$$\frac{-\hbar^2}{2m} \nabla^2 \psi + V(\vec{r})\psi = E\psi \quad , \quad (1)$$

where $V(\vec{r})$ is the periodic potential due to the ion cores and the self-consistent field of all the electrons. $V(\vec{r})$ is a rapidly varying function with a strong attractive part close to the ion cores. It is assumed that the core wavefunctions are the same as the isolated

ion although their energies are different. The conduction electron states ψ are orthogonal to the core states. It has been shown that this constraint forces the conduction electrons to sample $V(\vec{r})$ in a very special way which can be represented by a new wave equation which is identical to (1) but with an effective or pseudopotential, $V_{\text{eff}}(\vec{r})$, such that

$$\frac{-\hbar^2}{2m} \nabla^2 \Phi + V_{\text{eff}}(\vec{r}, \vec{k}) \Phi = E \Phi \quad (2)$$

This pseudopotential is much weaker than $V(\vec{r})$ and more smoothly varying. The pseudowave function Φ is a smooth function which does not include the typical atomic-core oscillations which insure that ψ is orthogonal to the core states. As a result, an expansion of Φ in plane waves converges rather rapidly. In general, $V_{\text{eff}}(\vec{r}, \vec{k})$ can be represented by a Fourier expansion, i.e.,

$$V_{\text{eff}}(\vec{r}, \vec{k}) = \sum_{\vec{G}_i} V_{\vec{G}_i}(\vec{k}) e^{i\vec{G}_i \cdot \vec{r}} \quad (3)$$

where the coefficients $V_{\vec{G}_i}$ are the pseudopotential coefficients and $\vec{G}_i$ is a reciprocal lattice vector. The pseudopotential coefficients are in general momentum dependent; however, in a local approximation, they may be treated as being independent of momentum. This expansion usually converges rapidly since the coefficients decrease in magnitude with increasing magnitude of the reciprocal lattice vector $\vec{G}_i$ and consequently can be truncated after a few terms.

The Hamiltonian for the system may be expressed as

$$H = \frac{p^2}{2m} + V_{\text{eff}}(\vec{r}) = H_0 + \sum_{\vec{G}_i} V_{\vec{G}_i} e^{i\vec{G}_i \cdot \vec{r}} \quad (4)$$

In order to determine the energy as a function of the wave vector k , it is necessary to diagonalize the matrix of H . If it is assumed that the pseudowave function Φ can be written as a linear combination of plane waves of the form

$$\Phi_k = \sum_{\vec{G}_j} a(k)_{\vec{k}+\vec{G}_j} e^{i(\vec{k}+\vec{G}_j) \cdot \vec{r}}, \quad (5)$$

then the secular equation can be written as

$$\sum_{\vec{G}_j} \{ [(k+\vec{G}_j)^2 - \lambda] \delta_{\vec{G}_i - \vec{G}_j} + U_{\vec{G}_i - \vec{G}_j} \} a_{k+\vec{G}_j} = 0. \quad (6)$$

The diagonal terms involve only the energy quadratic in the wave vector k , while the off-diagonal terms involve only the pseudopotential coefficients. The diagonal terms of the pseudopotential, U_0 , have been absorbed into λ .

The pseudopotential coefficients corresponding to the planes bounding the first Brillouin zone in mercury have been estimated by comparing the geometric resonance data obtained from the electron lens with the results of a calculation using first two pseudowaves to determine U_{100} and then using four pseudowaves to determine U_{111} and U_{110} . It should be pointed out that spin orbit coupling was neglected, and further, there was no attempt to maintain compensation. However, it appears that to first order, compensation was maintained. The

Fermi energy, λ , as well as the pseudopotential coefficients, were treated as adjustable parameters with the restriction that U_{111} and U_{110} would be equal as the magnitudes of the (111) and (110) reciprocal lattice vectors differ by less than 0.5%. It has been pointed out²⁵ that since the pseudopotential and its Fourier transform are continuous, then $U_{\vec{G}_i} = U_{\vec{G}_j}$ if $|\vec{G}_i| = |\vec{G}_j|$.

Since the data for the second band electron surface is the most reliable, the approach was to first seek agreement between the calculation and this data. The electron surface resembles a deformed lens centered on the point L; hence it was found convenient to start with only two pseudowaves in the (110) plane. Thus an initial value of U_{001} was obtained from a relation of the form

$$U_{100} = \frac{2k_1^2 (k_{\text{LENS}}^{L-\Gamma})^2}{(k_{\text{LENS}}^{L-U})^2 - (k_{\text{LENS}}^{L-\Gamma})^2} - \frac{(k_{\text{LENS}}^{L-U})^2 - (k_{\text{LENS}}^{L-\Gamma})^2}{2}$$

where $k_1 = \frac{1}{2}(100)$ and k_{LENS}^{L-U} and $k_{\text{LENS}}^{L-\Gamma}$ are the experimental values for the electron lens calipers. The Fermi energy, λ , was then calculated from the expression

$$\lambda = k_1^2 + (k_{\text{LENS}}^{L-\Gamma})^2 + [4(k_1 k_{\text{LENS}}^{L-\Gamma})^2 + U_{100}^2]^{1/2}.$$

The value of U_{100} was then varied and λ recalculated for each variation. It was thus determined that λ varied very slowly, on the order of 0.1%, as U_{100} was varied by approximately 10%. For each pair of values for U_{001} and λ , $k_{\text{LENS}}^{L-\Gamma}$ was held fixed and the value of k_{LENS}^{L-U} was recalculated, and restrictions placed on

the maximum and minimum values of U_{001} such that the calculated value of k_{LENS}^{L-U} remained within $\pm 1\%$ of the experimentally determined value.

The calculation was then extended to four pseudowaves about the point L in the Γ LW plane which allowed the best values for U_{110} and U_{111} to be determined as well as the final value for the Fermi energy which was consistent with the second band data. The calculation was performed by selecting the four plane wave states which had the lowest free electron energies when restricted to regions near the point of interest. In this case, the calculation was done along the line L-W with the plane wave states corresponding to k values of $k_1 = \frac{1}{2}(001)$, $k_2 = k_1 + (00\bar{1})$, $k_3 = k_1 + (010)$, and $k_4 = k_1 + (\bar{1}0\bar{1})$. This necessitated solving a 4×4 determinant which was done on an IBM 7040 digital computer. The final values obtained for the pseudopotential coefficients are $V_{110} = V_{111} = 0.0616$ Ry and $V_{100} = -0.0546$ Ry. These values are in reasonable agreement with the work of Animalu and Heine²⁶ and are compared with their results in Fig. 12. The results of Brandt and Rayne are also shown for comparison.

Once the pseudopotential coefficients were known, the calculation was extended to obtain profiles of sections of the Fermi surface in planes of interest. Again the four plane wave states which had the lowest free electron energies when restricted to regions near the point of interest were selected. The secular determinant was constructed from (6) and a search was performed at a fixed Fermi energy for those values of k which caused the determinant to vanish. The results were subsequently plotted to give profiles of the portion of the Fermi surface under investigation. This procedure was found to be convenient in that calipers not along symmetry lines

Fig. 12

could be as easily determined as those along lines of high symmetry, and a comparison of dHvA areas could also be accomplished.

A plot of nine different cross sections of the τ -section centered on U in the $(1\bar{1}0)$ plane is shown in Fig. 13 with the corresponding values of λ , V_{100} , and V_{110} indicated. For comparison purposes, the experimental data points are indicated. As has already been indicated, the best fit to the experimental data was for a value of $V_{110} = 0.0616$ Ry and $\lambda = 0.505$ Ry.

$$\lambda = .5033$$

$$V_{100} = -.0520$$

$$V_{110} = .0616$$

$$\lambda = .5038$$

$$V_{100} = -.0532$$

$$V_{110} = .0616$$

$$\lambda = .5050$$

$$V_{100} = -.0546$$

$$V_{110} = .0616$$

$$\lambda = .5033$$

$$V_{100} = -.0520$$

$$V_{110} = .0644$$

$$\lambda = .5038$$

$$V_{100} = -.0532$$

$$V_{110} = .0644$$

$$\lambda = .5050$$

$$V_{100} = -.0546$$

$$V_{110} = .0644$$

$$\lambda = .5033$$

$$V_{100} = -.0520$$

$$V_{110} = .0672$$

$$\lambda = .5038$$

$$V_{100} = -.0532$$

$$V_{110} = .0672$$

$$\lambda = .5050$$

$$V_{100} = -.0546$$

$$V_{110} = .0672$$

Fig. 13

APPENDIX B

Calculation of the Attenuation Coefficient

in Transverse Magnetic Fields

In the following discussion a semiclassical approach to the calculation of the attenuation coefficient of a sound wave in the presence of a transverse magnetic field is carried out following a method due to Sievert.²⁷ This method yields the attenuation coefficient in a direct manner as the result of the solution of the wave equation for a sound wave propagating in a metal. Extensive use is also made of several results of the calculation of the attenuation coefficient by Cohen, Harrison and Harrison (CHH).¹⁵

Consider as a model for a metal a free electron gas consisting of N_0 electrons per unit volume moving through a uniform background of positive ions of the same particle density. A sound wave is introduced into the system which causes the ions to be moved in a periodic fashion over a macroscopically small region of the metal. This motion of the ions causes an electric field to be produced which will then act as a perturbation on the free electron gas. It is this interaction with the free electrons that gives rise to the attenuation of the sound wave by the electron gas. As will be shown, the attenuation is governed principally by the conductivity of the electron gas and accounts for the dependence of the attenuation coefficient upon the magnetic field.

An expression is now sought for the attenuation coefficient of a sound wave propagating in a metal in a transverse magnetic field. A coordinate system is chosen such that $\vec{H} = H\vec{z}$ and $\vec{q} = q\vec{x}$, i.e., the sound wave is propagated in the x direction. The wave equation for sound propagation in the metal is given by

$$\frac{\partial^2 \vec{S}}{\partial t^2} - v_s^2 \frac{\partial^2 \vec{S}}{\partial x^2} = \frac{\vec{F}}{N_0 M} \quad (1)$$

where M is the ionic mass, $\vec{F}$ is the force per unit volume acting on the ions, N_0 is the ionic density, v_s is the velocity of sound before the interactions with the conduction electrons are included, and $\vec{S}$ is the ionic displacement field. The velocity field of the sound wave, $\vec{u}(\vec{r}, t)$ is assumed to have the dependence

$$\vec{u}(\vec{r}, t) \propto \exp\{i[(q + iA)x - \omega t]\} \quad (2)$$

where iA is the deviation of the wave number from $q = \frac{\omega}{v_s}$ induced by the interaction with the electrons. A can be regarded as the attenuation coefficient. From (2) it is evident that

$$\vec{S} = \frac{i\vec{u}}{\omega} \quad , \quad (3)$$

and (1) can be written as

$$[-i\omega + i\left(\frac{v_s^2}{\omega}\right)(q + iA)^2]\vec{u} = \frac{\vec{F}}{N_0 M} \quad (4)$$

The force $\vec{F}$ on the system, neglecting the deformation potential,

is given by

$$\vec{F} = N_0 |e| (\vec{E} + \frac{1}{c} \vec{u} \times \vec{H}) + \vec{F}_c \quad (5)$$

where $\vec{E}$ is the self-consistent electric field, $\vec{H}$ is the external magnetic field, and $\vec{F}_c$ is the force per unit volume which feeds energy coherently from the electrons back into the ion system. This force arises from the fact that the average electron velocity $\langle \vec{v}_e \rangle$ differs from that of the ions, $\vec{u}$. The electrons collide with the ions, and momentum is transferred from the electrons to the ion system. The net force exerted by the electrons on a unit volume of the positive charge is given by

$$\vec{F}_c = \left(\frac{N_0 m}{\tau} \right) (\langle \vec{v}_e \rangle - \vec{u}) \quad (6)$$

Here τ is the relaxation time or the characteristic scattering time for the electrons and m is the mass of the electron. The average velocity of the electrons is given by

$$\langle \vec{v}_e \rangle = \frac{-\vec{j}_e}{N_0 |e|} \quad (7)$$

where $\vec{j}_e$ is the electron current density. The total current density, $\vec{j}$, of the system is the sum of the electronic current density and a current $N_0 |e| \vec{u}$ due to the background of positive ions,

$$\vec{j} = \vec{j}_e + N_0 |e| \vec{u} \quad (8)$$

The total current is related to the self-consistent electric field,

$\vec{E}$, by Maxwell's equation and may be expressed as

$$E_1 = \left(\frac{4\pi}{i\omega}\right) j_1 \quad (9)$$

$$E_2 = \frac{\left(\frac{4\pi}{i\omega}\right) \left(\frac{v_s}{c}\right)^2}{1 - \left(\frac{v_s}{c}\right)^2} j_2 \quad (10)$$

The subscripts 1 and 2 refer to components parallel and perpendicular to the direction of propagation, i.e., the x and y directions, respectively. Thus the total current may be written as

$$\vec{j} = -\sigma_0 \hat{B} \cdot \vec{E} \quad (11)$$

where for $\vec{H} = H\vec{z}$ and $\vec{q} = q\vec{x}$,

$$\hat{B} = \begin{pmatrix} -i\gamma & 0 \\ 0 & i\beta \end{pmatrix} \quad (12)$$

with

$$\gamma = \beta \left(\frac{v_s}{c}\right)^2 \quad \text{and} \quad \beta = \frac{\omega c^2}{4\pi\sigma_0 v_s^2} \quad (13), (14)$$

and σ_0 is the dc conductivity given by

$$\sigma_0 = \frac{N_0 e^2 \tau}{m} \quad (15)$$

It should be noted that the quantity $\left(\frac{v_s}{c}\right)^2$ in the denominator of (10) was neglected as being small in comparison to unity. The electronic current density, $\vec{j}_e$, has been determined by CHH as the result of

solving the Boltzmann transport equation in the relaxation time approximation. Their result is

$$\vec{J}_e = \sigma_0 \hat{\sigma}' \cdot (\vec{E} - \frac{m\vec{u}}{e\tau}) \quad (16)$$

where

$$\hat{\sigma}' = (\hat{1} - \hat{R})^{-1} \cdot \hat{\sigma}/\sigma_0 \quad (17)$$

and $\hat{R}$ is a tensor whose components are given by

$$R_{ij} = R_i \delta_{1j} \quad (18)$$

The vector $\vec{R}$ and the conductivity tensor $\hat{\sigma}$ are given as follows:

$$\vec{R} = \frac{\partial \epsilon_f^0}{3N_0 \tau v_s} \int \vec{v} K(\vec{v}) \left(\frac{\partial f_0}{\partial \epsilon} \right) d\vec{v} \quad (19)$$

and

$$\hat{\sigma} = \int e\vec{v} \cdot J(\vec{v}) \left(\frac{\partial f_0}{\partial \epsilon} \right) d\vec{v} \quad (20)$$

where

$$(J(\vec{v}), K(\vec{v})) = \int_{-\infty}^t (-e\vec{v}', 1) \exp\{i[\vec{q} \cdot (\vec{r}' - \vec{r}) - \omega(t' - t) - \frac{(t-t')}{\tau}]\} dt' \quad (21)$$

ϵ_f^0 in Eq. (19) is the Fermi energy, and f_0 in both expressions is

the Fermi-Dirac distribution function. The self-consistent electric field $\vec{E}$ should be related linearly to $\vec{u}$, i.e.,

$$\vec{E} = \hat{W} \cdot \frac{N_0 e}{\sigma_0} \vec{u} \quad . \quad (22)$$

An explicit expression for $\hat{W}$ may be obtained by combining (8), (11), (16), and (17) to yield

$$\hat{W} = -[\hat{\sigma}' + \hat{B}]^{-1}[\hat{1} - \hat{\sigma}'] \quad (23)$$

Now using (7), (8), (11), and (22) in (5) and (6), the force $\vec{F}$ becomes

$$\vec{F} = \frac{N_0^2 e^2}{\sigma_0} [\hat{1} + \hat{B}] \cdot \hat{W} \cdot \vec{u} + \frac{N_0 e}{c} \vec{u} \times \vec{H} \quad . \quad (24)$$

Using (23), the term $[\hat{1} + \hat{B}] \cdot \hat{W}$ may be written as

$$[\hat{1} + \hat{B}] \cdot \hat{W} = -[(\hat{1} + \hat{B}) \cdot (\hat{\sigma}' + \hat{B})^{-1}(\hat{1} + \hat{B}) - (\hat{1} + \hat{B})] \quad . \quad (25)$$

Now define

$$\hat{S} = -[\hat{1} + \hat{B}] \cdot \hat{W} = (\hat{1} + \hat{B})[(\hat{\sigma}' + \hat{B})^{-1} \cdot (\hat{1} + \hat{B}) - 1] \quad .$$

Consequently, (24) becomes

$$\vec{F} = -\left(\frac{N_0^2 e^2}{\sigma_0}\right) \hat{S} \cdot \vec{u} + \frac{N_0 e}{c} \vec{u} \times \vec{H} \quad . \quad (27)$$

Substituting this expression for $\vec{F}$ into (4) and neglecting terms quadratic in A , one gets

$$\frac{1}{2} \left(\frac{mv_f}{mv_s} \right) \left[\hat{S} \cdot \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} - \omega_c \tau \begin{pmatrix} u_2 \\ -u_1 \end{pmatrix} \right] = A \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \quad (28)$$

where $\omega_c = \frac{eH}{mc}$ and the mean free path ℓ is given by $\ell = v_F \tau$. If one defines

$$\hat{G} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad (29)$$

then (28) can be written as

$$\frac{1}{2} \left(\frac{mv_F}{Mv_s \ell} \right) [\hat{S} - \omega_c \tau \hat{G}] \cdot \vec{u} = A \vec{u} \quad (30)$$

Letting

$$\hat{D} = \frac{1}{2} \left(\frac{mv_F}{Mv_s \ell} \right) [\hat{S} - \omega_c \tau \hat{G}] \quad (31)$$

Eq. (30) can be expressed as

$$\hat{D} \cdot \vec{u} = A \vec{u} \quad (32)$$

which is an eigenvalue equation for the complex attenuation coefficient

A. The secular determinant is

$$\begin{pmatrix} D_{11} - A & D_{12} \\ D_{21} & D_{22} - A \end{pmatrix} = 0 \quad (33)$$

Solving for the eigenvalues yields

$$A_{\pm} = \frac{D_{11} + D_{22}}{2} \pm \frac{(D_{11} - D_{22})}{2} \left[1 - \frac{4D_{12}D_{21}}{(D_{11} - D_{22})^2} \right]^{1/2} \quad (34)$$

The term $\frac{4D_{12}D_{21}}{(D_{11}-D_{22})^2}$ arises from a mixing of the longitudinal and transverse modes of vibration. This term has been calculated²⁷ both for the case of simple circular orbits and open orbits. In both cases the real and imaginary parts were no greater than 10^{-3} for the magnetic fields of interest. Consequently, this term may be neglected in (34). Thus

$$A_{\pm} \approx \frac{D_{11}+D_{22}}{2} \pm \frac{(D_{11}-D_{22})}{2} \quad (35)$$

for the case of a pure longitudinal mode in the 1 direction, $D_{21} = 0$, and

$$A_{+} = D_{11} \quad (36)$$

The ordinary attenuation coefficient α may be defined as

$$\alpha = \text{Re } A_{+} = \text{Re } D_{11} \quad (37)$$

From (31)

$$D_{11} = \frac{mv_F}{Mv_s \ell} [S_{11} - \omega \tau G_{11}] \quad (38)$$

But from (29), $G_{11} = 0$

$$D_{11} = \frac{1}{2} \frac{mv_F}{Mv_s \ell} S_{11} \quad (39)$$

from which (37) becomes

$$\alpha = \frac{1}{2} \frac{mv_F}{Mv_s \ell} \text{Re}(S_{11}) \quad (40)$$

From (26)

$$S_{11} = (\hat{1} + \hat{B})_{11} [(\hat{\sigma}' + \hat{B})_{11}^{-1}] (1 + B_{11}) - (1 + B_{11}) \quad (41)$$

or

$$\text{Re}(S_{11}) = \text{Re}(1 + B_{11})^2 [(\hat{\sigma}' + \hat{B})_{11}^{-1}] - 1 \quad (42)$$

since $\text{Re } B_{11} = 0$. Thus

$$\alpha = \frac{1}{2} \frac{mv_F}{Mv_s \ell} \{ \text{Re}(1 + B_{11})^2 [(\hat{\sigma}' + \hat{B})_{11}^{-1}] - 1 \}$$

for longitudinal waves

$$|B_{11}| = \gamma = \beta \left(\frac{v_s}{c} \right)^2 \quad (44)$$

Since β is typically of the order 10^{-5} for metals and $\frac{v_s}{c}$ of the order 10^{-5} , then $|B_{11}|$ may be neglected for all practical purposes. Therefore,

$$\alpha_L = \frac{1}{2} \frac{mv_F}{Mv_s \ell} \text{Re}\{(\hat{\sigma}' + \hat{B})_{11}^{-1}\} - 1 \quad (45)$$

This may be written in terms of $\hat{\sigma}'$ as

$$\alpha_L = \frac{1}{2} \frac{mv_F}{Mv_s \ell} \text{Re}\left\{ \frac{\sigma'_{22} + i\beta}{\sigma'_{11}(\sigma'_{22} + i\beta) + (\sigma'_{12})^2} \right\} - 1 \quad (46)$$

where use has been made of the fact that

$$\sigma'_{12} = -\sigma'_{21} \quad (47)$$

The magnetic field dependence of the attenuation is implicit in the expressions for the σ 's in (46). They have been calculated by CHH and are as follows:

$$\sigma'_{11} = \frac{-3i\omega\tau(1-i\omega\tau)[1-g_0(X)]}{q^2\ell^2[1-i\omega\tau-g_0(X)]} \quad (48)$$

$$\sigma'_{12} = -\sigma'_{21} = \frac{-3i\omega\tau g'_0(X)}{2q\ell[1-i\omega\tau-g_0(X)]} \quad (49)$$

$$\sigma'_{22} = \frac{3}{1-i\omega\tau} \left(s_0 + \frac{\left[\frac{g'_0(X)}{2} \right]^2}{1-i\omega\tau-g_0(X)} \right) \quad (50)$$

where

$$g_0(X) = \int_0^{\pi/2} J_0^2(X \sin\theta) \sin\theta \, d\theta \quad (51)$$

$$g'_0(X) = \left(\frac{d}{dX} \right) g_0(X) \quad (52)$$

$$s_0(X) = \int_0^{\pi/2} [J'_0(X \sin\theta)]^2 \sin^3\theta \, d\theta \quad (53)$$

and

$$X = \frac{qv_F}{\omega_c} = \frac{v_F}{v_s} \frac{\omega}{\omega_c} = qR$$

θ is the polar angle in $\vec{v}$ space. The expression for the σ 's were calculated under the assumption that the sound wavelength is the order

of the classical orbit radius, i.e., $X \sim 1$. Also, the assumption was made that

$$|\omega_c \tau / (1 - i\omega\tau)|^2 \gg 1 \quad . \quad (54)$$

When the expressions for the σ 's are substituted into (46), the attenuation coefficient α_ℓ may be written as

$$\alpha_\ell \propto \frac{q^2 \ell^2}{3(1 + \omega^2 \tau^2)} \left(\frac{1}{\frac{(g'_0)^2}{1 - g_0 + \frac{2}{s_0}}} - 1 \right) \quad . \quad (55)$$

The field dependent part which is included within the brackets above has been calculated by CHH and the results are shown in Fig. 14. Note that the abscissa is proportional to the reciprocal of the magnetic field while the ordinate exhibits strong oscillation with maxima and minima occurring whenever $g'_0(X)$ vanishes.

For pure transverse propagation we obtain from (34)

$$A_- = D_{22} \quad (56)$$

or

$$\alpha_t = \text{Re } D_{22} \propto \text{Re } S_{22} \quad (57)$$

and in a manner similar to that used for determining α_ℓ we find that

$$\alpha_t \propto \left[\frac{1}{3 \left[\frac{s_0 + (g'_0/2)^2}{1 - g_0} \right]} - 1 \right] \quad . \quad (58)$$

Fig. 14

As for the longitudinal case, this expression has been evaluated by CHH and a plot is given in Fig. 15.

It should be noted that in both Fig. 14 and Fig. 15 only the field dependent factor contained in the brackets of (55) and (58) has been plotted. Both these factors are independent of parameters associated with the material provided that $\omega_c \tau \gg 1$, $q\ell \gg 1$, and $\beta \ll 1$. Thus both the attenuation coefficients for longitudinal and transverse polarized sound waves exhibit oscillatory behavior as a function of the reciprocal of the magnetic field. These geometric resonances in the attenuation are associated with the Bessel functions in the conductivity tensor.

The geometric resonances can be understood in simple physical terms for transverse waves polarized perpendicular to the magnetic field at low frequencies. If the frequency of the sound wave is low, the electrons are able to follow the ionic motion in a manner such as to neutralize the electric field almost completely and cause the total current of the system to vanish, that is, $\vec{j} \approx 0$. From (8) then

$$\vec{j}_e = -N_0 e \vec{u} \quad . \quad (59)$$

Energy is transferred from the sound wave to the electron system at a rate $\vec{j}_e \cdot \vec{E}$. The attenuation coefficient is given by²⁸

$$\alpha = \frac{\text{Re}[\vec{j}_e^* \cdot \vec{E}]}{M u^* u c_s} \quad . \quad (60)$$

Fig. 15

Since the electron current response is fixed from (59), the system is one of constant current and the electric field may be written as

$$\vec{E} = \hat{\rho}(q, H) \cdot \vec{j}_e \quad (61)$$

Therefore (60) can be written as

$$\alpha = \frac{\text{Re}\{\vec{j}_e^* \hat{\rho}(q, H) \cdot \vec{j}_e\}}{M u^* u c_s} \quad (62)$$

Using (59), the previous expression can be expressed as

$$\alpha \propto \hat{\rho}(q, H) \quad (63)$$

or schematically

$$\alpha \propto \frac{1}{\hat{\sigma}(q, H)} \quad (64)$$

Thus the attenuation coefficient is inversely proportional to the conductivity. Assuming that the sample is pure enough and that the temperature of the sample kept sufficiently low to reduce the number of thermal phonons which scatter the electrons, then the electrons in the metallic sample are able to execute simple closed orbits in a plane perpendicular to the magnetic field. These are illustrated in Fig. 16 where the vertical arrows correspond to the self-consistent electric field associated with the lattice wave. The magnetic field is into the page and the sound is propagated in the x direction. For H_1 the electron is alternately accelerated and decelerated by the

Fig. 16

electric field as it traverses its orbit. Thus there is no net increase in the velocity of the electron per cycle. This corresponds to a small current response, a low conductivity and hence a high attenuation. For H_2 , the component of the field in the direction of the electron motion is negative and the electron's velocity increases with each passage. This corresponds to a significant increase in the current response, a large conductivity and hence a low attenuation. The attenuation thus passes through an extrema whenever the orbit diameter encompasses an integral or half integral number of sound wavelengths.

The information derived from the period of these oscillations is obtained in the following manner. In $\vec{k}$ space we have

$$\vec{k} = \frac{e}{\hbar c} \vec{r} \times \vec{H} \quad . \quad (65)$$

The orbit of the electron in k-space is the same as the path in real space except that it is multiplied by the factor $\frac{eH}{\hbar c}$ and rotated 90° about H. This is indicated in Fig. 15. The radius in real space is then given by

$$r_x = \frac{\hbar c}{eH} k_y \quad . \quad (66)$$

Now consider what happens if we examine this expression at two adjacent maxima in the attenuation. At the field value H_n , we have enclosed n wavelengths of sound.

$$n\lambda = 2r_x = \frac{2\hbar c}{e H_n} k_y \quad (67)$$

while at a lower value of the field H_{n+1} we have spanned one additional wavelength. Thus

$$(n+1)\lambda = 2r_x = \frac{2\hbar c}{e H_{n+1}} k_y \quad (68)$$

Subtracting these two equations we get

$$2k_y = \frac{\lambda e}{\hbar c \Delta(\frac{1}{H})} \quad (69)$$

where

$$\Delta(\frac{1}{H}) = \frac{1}{H_{n+1}} - \frac{1}{H_n} \quad (70)$$

Thus, from a knowledge of the frequency of the sound wave, the velocity of sound, and the period of the oscillations of the attenuation coefficient, the diameter, $2k_y$ of the orbit in k-space can be determined.

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