

Acoustic Kjeldaa Edge in Potassium*

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We investigate the propagation of shear acoustic waves in both a metal whose Fermi surface is spherical and one having a spin-density-wave ground state in a magnetic field parallel to the direction of sound propagation. In particular we study the nature of the Kjeldaa absorption edge for these two models with special emphasis on potassium at liquid-helium temperature. At sufficiently high frequency the position of the Kjeldaa edge of the spin-density-wave is substantially lower than for the free-electron model.

I. INTRODUCTION

THE optical anomaly of potassium discovered recently by Mayer and El Naby¹ has been discussed theoretically by several authors.²⁻⁴ In this paper we concern ourselves with Overhauser's suggestion⁴ that the optical anomaly in potassium can be accounted for by assuming that the ground state of this metal has a spin-density-wave⁵ (SDW). However, experiments on cyclotron resonance by Grimes and Kip⁶ and on the de Haas-van Alphen effect by Shoenberg and Stiles⁷ fail to show the anisotropy of the Fermi surface of potassium which is required by Overhauser's hypothesis. It is possible to reconcile these results if one assumes that the wave vector of the SDW orients itself parallel to an applied magnetic field. If this assumption is correct, de Haas-van Alphen measurements, which only provide a measure of the extremal cross-sectional area of the Fermi surface, would show no anisotropy in agreement with experiment. Overhauser and Rodriguez⁸ and McGroddy, Stanford, and Stern⁹ have studied the problem of propagation of helicon waves in potassium near the cyclotron edge. The conclusions of these works are the following. One finds that, in general, the comparison between theory and experiment cannot be based on the simple Doppler-shifted-frequency criterion, but rather that a detailed calculation of the surface impedance must be carried out to compare with the experimental results.¹⁰ One also finds that comparison of the

calculated surface impedance of potassium with experimental curves obtained by Taylor¹¹ give better agreement with the SDW model than with the free-electron model. The difference between the two models gives only a 4% shift in the position of the cyclotron edge and thus these experiments need not be regarded as providing conclusive evidence for the existence of a SDW ground state in potassium. The simple criterion is

$$\omega_c = qv_{\max}, \quad (1)$$

where v_{\max} is the maximum value of the component of the electron velocity along the direction of the magnetic field and q is the helicon wave number. Now for a SDW in potassium appropriate to an energy gap $G=0.62$ eV, which is necessary to account quantitatively for the optical anomaly, we have $v_{\max}=0.714 \times 10^8$ cm/sec while for the free-electron model $v_{\max}=v_F=0.864 \times 10^8$ cm/sec. (These calculations are done taking the lattice constant to be¹² $a=5.225$ Å.) If one now assumes that the wave vector \mathbf{q} of a helicon is not very sensitive to the particular electron model, then Eq. (1) shows that the shift in the cyclotron edge is $(\Delta B/B_e) \simeq (\Delta v_{\max}/v_{\max}) = 17\%$. In Refs. 8 and 9 it is proved that the assumption just made is, in general, incorrect. However, the detailed electronic model has little effect on the velocity of shear acoustic waves¹³ so that we can write $q=\omega/s$, ω and s being the angular frequency and the velocity of the acoustic waves. In this case Eq. (1) becomes

$$\omega_c = (\omega v_{\max}/s). \quad (2)$$

The study of the ultrasonic attenuation of shear waves in metals as a function of an applied magnetic field shows that there is an absorption edge at the magnetic field for which Eq. (2) is satisfied and a measurement of this field gives directly m^*v_{\max} where m^* is the cyclotron effective mass of the resonant electrons. The ultrasonic absorption edge was first discussed by Kjeldaa¹⁴ for the free-electron model. We shall call the onset of absorption as the magnetic field is lowered past its resonant value the Kjeldaa edge.

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¹ M. H. El Naby, Z. Physik **174**, 269 (1963); H. Mayer and M. H. El Naby, *ibid.* **174**, 280 (1963); **174**, 289 (1963).

² M. H. Cohen and J. C. Phillips, Phys. Rev. Letters **12**, 662 (1964).

³ M. H. Cohen, Phys. Rev. Letters **12**, 664 (1964).

⁴ A. W. Overhauser, Phys. Rev. Letters **13**, 190 (1964).

⁵ A. W. Overhauser, Phys. Rev. **128**, 1437 (1962).

⁶ C. C. Grimes and A. F. Kip, Phys. Rev. **132**, 1991 (1963).

⁷ D. Shoenberg and P. Stiles, Proc. Roy. Soc. (London) **A281**, 62 (1964).

⁸ A. W. Overhauser and S. Rodriguez, Phys. Rev. **141**, 431 (1966).

⁹ J. C. McGroddy, J. L. Stanford, and E. A. Stern, Phys. Rev. **141**, 437 (1966).

¹⁰ This result holds when $\omega_c\tau$, the product of the electron cyclotron frequency in the vicinity of the cyclotron edge and the electron relaxation time is less than about 40. If $\omega_c\tau$ exceeds this value, then the Doppler-shifted frequency condition is rather accurate.

¹¹ M. T. Taylor, Phys. Rev. Letters **12**, 497 (1964); Phys. Rev. **137**, A1145 (1965).

¹² C. S. Barrett, Acta Cryst. **9**, 671 (1956).

¹³ S. Rodriguez, Phys. Rev. **130**, 1778 (1963); J. J. Quinn and S. Rodriguez, *ibid.* **133**, A1589 (1964).

¹⁴ T. Kjeldaa, Jr., Phys. Rev. **113**, 1473 (1959).

In the present paper we discuss in some detail the difference, briefly discussed elsewhere¹⁵ between propagation of shear acoustic waves in a SDW metal and in a free-electron metal. Numerical applications are made to the case of potassium at liquid-helium temperatures.

II. THEORY FOR AN ELASTICALLY ISOTROPIC METAL

In this section we present an analysis of the propagation of shear acoustic waves in a metal and discuss the differences between two possible electronic structures. One model is that of free electrons already investigated by Kjeldaas and the other is the one in which the ground state of the metal possesses a SDW. We consider a metal in the presence of a magnetic field \mathbf{B}_0 which we choose parallel to the z axis of a Cartesian coordinate system. Now, the equation of motion of the lattice can be described by a displacement field $\xi(\mathbf{r}, t)$ whenever the wavelength of the acoustic waves is much longer than the lattice parameter. We shall consider here frequencies ν_0 of the order of 10^8 sec^{-1} so that the wavelength $\lambda \approx s/\nu_0 \approx 10^{-3} \text{ cm}$. Thus our assumption that $\lambda \gg a$ is well satisfied. The equation of motion of the lattice is obtained by considering the forces acting on the positive ions of the crystal arising from the other ions and the conduction electrons. This equation is

$$M \partial^2 \xi / \partial t^2 = C_l \nabla(\nabla \cdot \xi) - C_t \nabla \times (\nabla \times \xi) + ze \mathbf{E} + (ze/c) \mathbf{u} \times \mathbf{B}_0 + \mathbf{F}. \quad (3)$$

Here C_l and $C_t = Ms_0^2$ are elastic constants describing the interaction of the ion cores but excluding the long-range Coulomb repulsion. The quantity $\mathbf{u} = \partial \xi / \partial t$ is the velocity of the ions and \mathbf{F} is an average collision force on the ions arising from their interaction with the con-

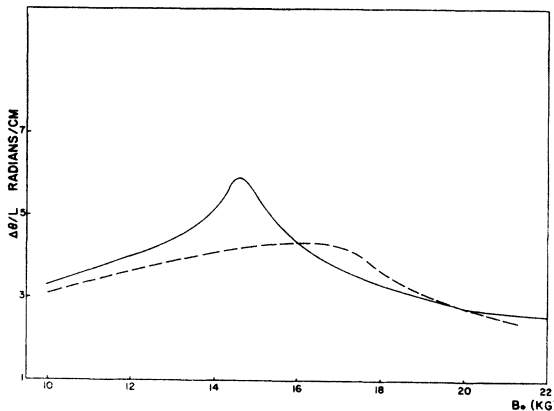


FIG. 1. Rotation of the plane of polarization per unit sample length as a function of applied magnetic field. The dashed curve corresponds to the free-electron model, the solid curve to the SDW model. These curves are appropriate to an acoustic frequency of 100 Mc/sec and a value of ql of about 50.

¹⁵ R. C. Alig, J. J. Quinn, and S. Rodriguez, Phys. Rev. Letters 14, 981 (1965).

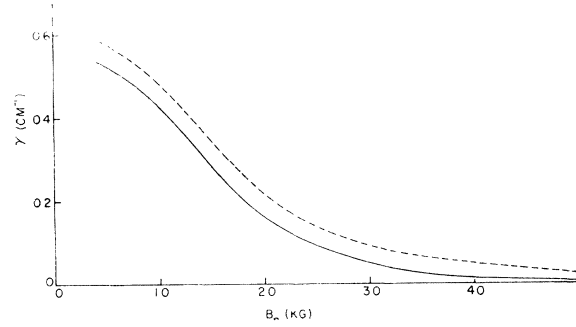


FIG. 2. The attenuation coefficient γ of the fast shear wave as a function of B_0 for an acoustic frequency of 10 Mc/sec and a value for ql of 2.

duction electrons. Simple considerations show that

$$\mathbf{F} = -(zm/n_0 e \tau)(\mathbf{j}_e + n_0 e \mathbf{u}),$$

where \mathbf{j}_e is the electron current density and n_0 the electron concentration, \mathbf{E} is the self-consistent electric field associated with the propagation of the wave and z the number of conduction electrons per atom. Equation (3) is applicable only if the system is elastically isotropic. In general, this is not the case but the results that we obtain are rigorously valid for propagation along symmetry directions for which the two polarizations for the shear waves have equal velocities. The case of an anisotropic metal is treated in Sec. III. Setting $\xi(\mathbf{r}, t) \propto \exp(i\omega t - i\mathbf{q} \cdot \mathbf{r})$ in Eq. (3) we find

$$(\omega^2 - s_0^2 q^2 \pm \omega \Omega_c) \xi_{\pm} = -(ze/M) E_{\pm} - F_{\pm}/M, \quad (4)$$

where $\xi_{\pm} = \xi_x \pm i \xi_y$, $E_{\pm} = E_x \pm i E_y$, and $\Omega_c = ze B_0 / M c$ is the cyclotron resonance frequency of the positive ions in the presence of the magnetic field B_0 . The relation between \mathbf{E} and ξ is obtained by solving Maxwell's equations together with the equation of motion of the electrons. The necessary relations are developed in some

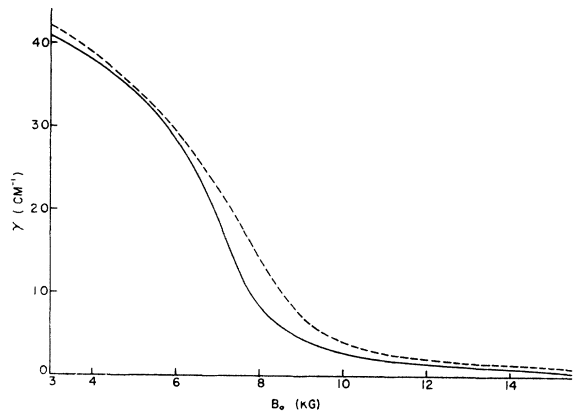


FIG. 3. The attenuation coefficient γ of the fast shear wave as a function of B_0 for an acoustic frequency of 50 Mc/sec and a value for ql of 10.

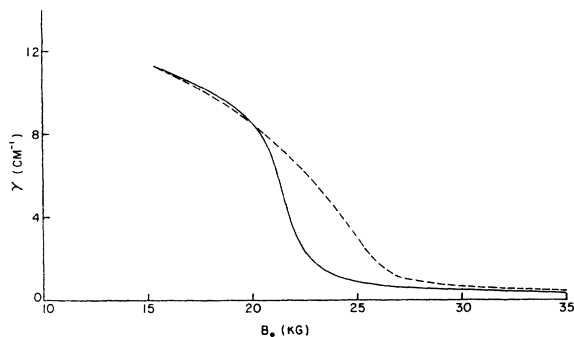


FIG. 4. The attenuation coefficient γ of the fast shear wave as a function of B_0 for an acoustic frequency of 150 Mc/sec and a value for ql of 30.

detail in Ref. 13. The result is

$$E_{\pm} = (mi\omega/\epsilon\tau)[(G_{\pm}-1)/(G_{\pm}-i\beta)]\xi_{\pm}, \quad (5)$$

where

$$\sigma_0 G_{\pm} = \sigma_{\pm} = \sigma_{xx} \mp i\sigma_{xy}, \quad (6)$$

and

$$\beta = c^2 q^2 / 4\pi\omega\sigma_0. \quad (7)$$

In Eqs. (5)–(7) σ_0 is the dc electrical conductivity and σ_{xx} and σ_{xy} are components of the magneto-conductivity tensor.¹⁶ We have made the assumption that the Fermi surface possesses rotational symmetry about the z axis so that $\sigma_{xx} = \sigma_{yy}$, $\sigma_{xy} = -\sigma_{yx}$, while $\sigma_{xz} = \sigma_{yz} = 0$. Equation (4) can now be rewritten in the form

$$(\omega^2 - s_0^2 q^2 \pm \omega\Omega_c)(\omega G_{\pm} - i\omega_0\beta_0) = (zmi\omega/M\tau)(\omega - i\beta_0\omega_0)(1 - G_{\pm}). \quad (8)$$

For convenience we have used $\omega_0 = s_0 q$ and β_0

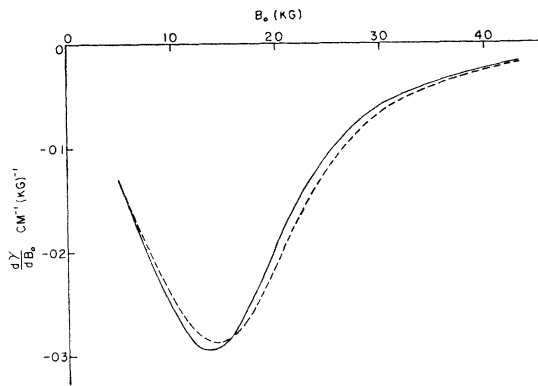


FIG. 5. Plot of $d\gamma/dB_0$ versus B_0 for the conditions given in Fig. 2.

¹⁶ The components of the magnetoconductivity tensors appropriate to the propagation of circularly polarized waves are given by

$$\sigma_{\pm} = \frac{e^2 m \tau}{4\pi^2 \hbar^2} \int dk_x \frac{v_x^2}{1 + i(\omega\tau \mp \omega_c\tau - qv_x\tau)},$$

where v_x and v_z are the components of the velocity of an electron on the Fermi surface perpendicular and parallel to \mathbf{B}_0 , respectively.

We have used $E(\mathbf{k}) = \hbar^2 k^2 / 2m$ for the free-electron-model calculations. For the calculations using the SDW model we have used

$E(\mathbf{k}) = \hbar^2 k^2 / 2m + \mu(\frac{1}{2}Q - |k_x|) - [\mu^2(\frac{1}{2}Q - |k_x|)^2 + \frac{1}{4}G^2]^{1/2}$, where $\mu = \hbar^2 Q / 2m$, Q is the wave vector of the SDW, $|k_x|$ denotes the magnitude of k_x , and G is the energy gap due to the SDW.

$= (c^2 q^2 / 4\pi\omega_0\sigma_0) = (c^2 q / 4\pi s_0\sigma_0)$. Solutions of Eq. (8) give us the dispersion formulas $\omega = \omega(q, B_0)$. Now we could solve Eq. (8) for $q = q_1 - iq_2$ as a function of ω but we prefer to consider q as real and solve for $\omega = \omega_1 + i\omega_2$ as functions of q and B_0 . Both procedures can be used since the velocity of sound changes very little from its value s_0 in the absence of the electron interactions and because $q_2 \ll q_1$. Since we are only interested in the attenuation as a function of B_0 we have calculated changes in $\omega_1 + i\omega_2$ as a function of B_0 for fixed q . The coefficient of attenuation γ is given by

$$\gamma = 2\omega_2 / s_0. \quad (9)$$

The experimental conditions are such that ω is kept constant so that we should solve Eq. (8) for $q_1 - iq_2$. It is, however, more convenient to do what we have done. The results are, of course, the same because of the fact that $q_2 \ll q_1$. In Fig. 1 of Ref. 15 we have displayed the attenuation coefficient γ as a function of the magnetic induction B_0 for acoustic waves of 100 Mc/sec for both the free-electron and SDW models. We have taken τ , the electron collision time, such that $\omega_c\tau$ at 18 kG is 50 and the velocity of sound $s_0 = 1.74 \times 10^5$ cm/sec. Figure 2 of that work shows $d\gamma/dB_0$ as a function of B_0 under the same conditions. The difference in the velocities of the right- and left-circularly polarized components of a linearly polarized shear wave gives rise to a rotation of the plane of polarization of the sound wave given by

$$\Delta\theta/L = \Delta\omega_1 / 2s_0, \quad (10)$$

where $\Delta\omega_1$ is the difference in the real parts of the frequencies of the two circular polarizations and L is the length of the sample. The order of magnitude for a magnetic field of about 15 kG turns out to be of a few radians per cm of path. Figure 1 in the present paper shows a graph of $\Delta\theta/L$ versus B_0 . The values of γ and $d\gamma/dB_0$ for shorter mean free paths are similar but the peak in $d\gamma/dB_0$ and the absorption edge are less pronounced in the latter case.¹⁷ We have also investigated

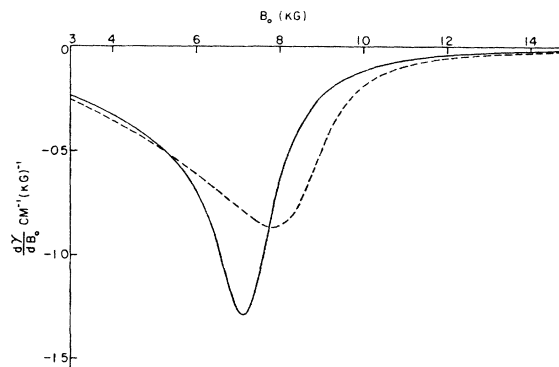


FIG. 6. Plot of $d\gamma/dB_0$ versus B_0 for the conditions given in Fig. 3.

¹⁷ Values of $\omega_c\tau$ of 5, 10, 25, 100, and 250 have been used in the numerical calculations. The results show that the minimum of $d\gamma/dB_0$ is shifted slightly to lower magnetic fields as the mean free path l is decreased but the width of the line decreases rapidly with increasing τ .

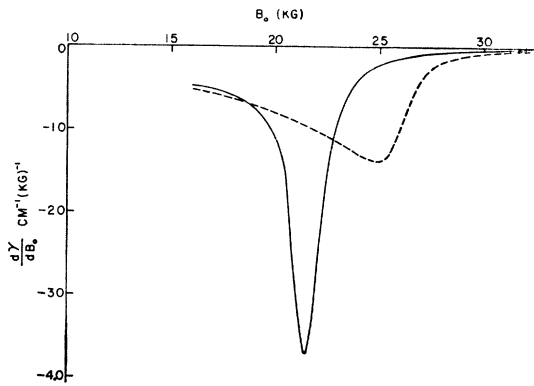


FIG. 7. Plot of $d\gamma/dB_0$ versus B_0 for the conditions given in Fig. 4.

propagation at frequencies lower than 100 Mc/sec and obtained again similar results.

III. THEORY FOR AN ELASTICALLY ANISOTROPIC SOLID

In this section we consider the situation in which the metal possesses a Fermi surface which has rotational symmetry about the z axis as before, but now we assume that the solid is elastically anisotropic. We make the further assumption that when a wave propagates parallel to the z axis, the acoustic waves can be classified into purely longitudinal and purely transverse modes. In the case of shear waves the elastic force on each ion arising from the short-range ion core interactions is of the form

$$\mathbf{S} \cdot \xi,$$

where \mathbf{S} is a 2×2 tensor operating on vectors $\xi = (\xi_x, \xi_y)$ in a plane perpendicular to the z axis. We choose the x and y axes in such a way that \mathbf{S} is diagonal. Then we can write, instead of Eq. (3) the following relation for ξ_{\pm} , the displacements appropriate to circular polarization,

$$-M\omega^2 \xi_{\pm} = -\frac{1}{2} M s_x^2 q^2 (\xi_+ + \xi_-) \mp \frac{1}{2} M s_y^2 q^2 (\xi_+ - \xi_-) + ze E_{\pm} \pm (zewB_0/c) \xi_{\pm} + F_{\pm}. \quad (11)$$

Because s_x and s_y have different values, the two circular polarizations are coupled by a term proportional to $(s_x^2 - s_y^2)$. This results in normal modes, which in the presence of the dc magnetic field are elliptically polarized. By proceeding in a manner analogous to the treatment in Sec. II, Eq. (11) can be put in the form

$$\omega^2 \xi_{\pm} - \frac{1}{2} q^2 (s_{\pm}^2 \xi_{\pm} + s_{\mp}^2 \xi_{\mp}) \pm \omega \Omega_c \xi_{\pm} - (zmi\omega/M\tau) [(1 - G_{\pm})(1 - i\beta)/(G_{\pm} - i\beta)] \xi_{\pm} = 0. \quad (12)$$

In this equation, the symbol s_{\pm}^2 stands for $s_x^2 \pm s_y^2$. We have carried out a numerical calculation of the velocity and attenuation of the acoustic normal modes of the system represented by Eq. (12). More specifically we have studied shear waves propagating along the $[110]$ direction in potassium. The values of s_x and s_y , de-

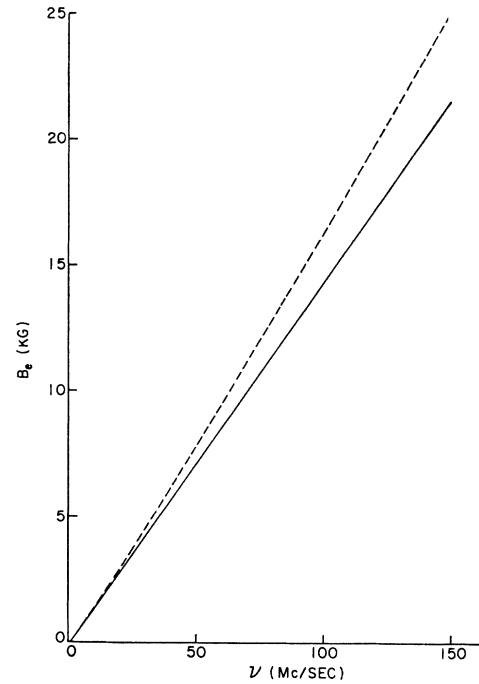


FIG. 8. Position of the experimental edge B_e for the fast shear wave (i.e., position of the minimum of $d\gamma/dB_0$) as a function of frequency for a potassium sample having $ql = 10$ at 50 Mc/sec.

termined from the measurements of the low-temperature elastic constants given by Marquardt and Trivisonno¹⁸ are 1.78×10^5 cm/sec and 0.646×10^5 cm/sec,

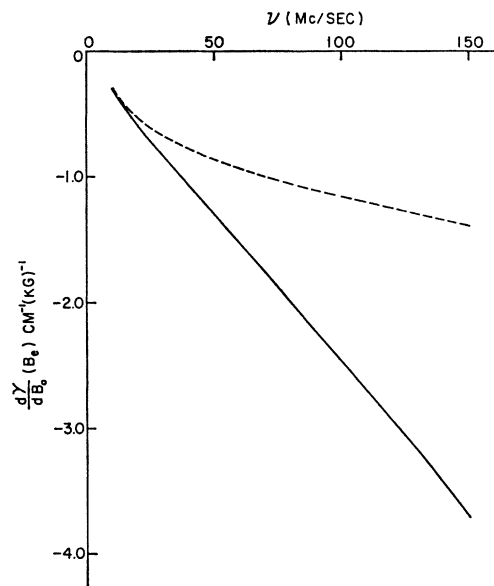


FIG. 9. The magnitude of $d\gamma/dB_0$ at the edge as a function of frequency for a sample having $ql = 10$ at 50 Mc/sec.

¹⁸ W. R. Marquardt and J. Trivisonno, J. Phys. Chem. Solids 26, 273 (1965).

respectively. We shall refer to these modes as the fast and slow shear waves, respectively.

To facilitate comparison with experiment we define B_e , the experimentally determined position of the edge, as the position of the minimum of $d\gamma/dB_0$. In Figs. 2, 3, and 4 we display the attenuation coefficient γ as a function of B_0 for frequencies of 10, 50, and 150 Mc/sec and a value of τ corresponding to $ql=10$ at 50 Mc/sec for the fast shear wave. In Figs. 5, 6, and 7 we plot $d\gamma/dB_0$ as a function of B_0 for the same cases. In each of these figures two graphs are displayed. The dashed line is appropriate to the free-electron model, the solid one to the SDW model. Figure 8 shows the position of the edge B_e as a function of frequency $\nu=\omega/2\pi$ for both models and the same value of τ as given above. It

should be noted that at low frequencies the values of B_e do not differ by much. Finally, in Fig. 9, the magnitude of $d\gamma/dB_0$ at the edge is plotted as a function of frequency.¹⁹

The [110] direction in potassium was selected in our discussion because the large difference in the velocities of the fast and slow shear modes permits considerable simplification in the interpretation of experimental results. The behavior in this case is in contrast to the results for the elastically isotropic solid where care had to be exercised to measure both the apparent attenuation and the rotation of the plane of polarization.

¹⁹ Similar calculations have been carried out for the slow shear mode but, since the results are rather similar, we do not display them here.

New Inversion Scheme for Obtaining Fermi-Surface Radii from de Haas-van Alphen Areas

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The existing solution to this problem has not been useful in practice. We have found a new and much simpler method based on an expansion of both the area and of the radius squared in appropriate spherical harmonics. The integral equation between these objects yields the simple result

$$a_L^m = b_L^m \pi P_L(0),$$

where $P_L(0)$ is the Legendre function of order L and a_L^m and b_L^m are the coefficients of expansion.

MEASUREMENT of the periodic variation of the magnetic susceptibility of pure metals at low temperatures gives detailed information about the Fermi surfaces of these materials. This de Haas-van Alphen effect has long been used as an experimental tool for finding the Fermi surface extremal cross-sectional areas. Recent improvements in experimental technique now yield results accurate to a few parts in 10^4 . We have developed a simple method which, while maintaining mathematical exactness and high experimental accuracy, converts the extremal-area measurements into Fermi-surface radii. The conversion of extremal areas to radii is a purely geometrical problem. By an elegant piece of differential geometry, Lifshitz and Pogorelov¹ (LP) found a formal solution and gave sufficient conditions for the inversion to be unique: These are that the surface be closed, have a center of inversion symmetry, and have a unique radius vector from that center. Their technique depends on a complete knowledge of the extremal area, $A(\theta, \varphi)$. This is impracticable experimentally, so that the technique has never been applied

successfully. There is also a mathematical difficulty because one is required to evaluate a principal-value integral of the data, a necessarily discontinuous function.

These two requirements are so stringent that, in practice, accurate data have been fitted by trial and error. The method of expansion in spherical harmonics outlined below needs only a small number of independent data points, performs the principal value integral implicitly, and automatically provides a least-squares fit to the data. It also provides a prescription for finding orientations of the external field which determine the Fermi surface most efficiently, and avoids duplication of effort.

We shall write the equatorial area, $\sigma(\hat{\xi})$, as the integral of the square of the radius over the unit sphere,

$$\sigma(\hat{\xi}) = \frac{1}{2} \int \rho^2(\hat{\epsilon}) \delta(\hat{\epsilon} \cdot \hat{\xi}) d\Omega(\hat{\epsilon}), \quad (1)$$

where $\hat{\xi}$ and $\hat{\epsilon}$ are unit vectors. This equation, first considered by LP, compactly states the formal problem. The Dirac delta function selects those directions of $\rho^2(\hat{\epsilon})$, the square of the radius vector, perpendicular to $\hat{\xi}$, the magnetic field direction. Thus, the surface integral

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¹ I. M. Lifshitz and A. V. Pogorelov; Dokl. Akad. Nauk SSSR 96, 1143 (1954).