Generalized Susceptibilities and Magnetic Properties of Some bcc Transition Metals*

W. E. EVENSON,† G. S. FLEMING, AND S. H. LIU
Institute for Atomic Research and Department of Physics, Iowa State University, Ames, Iowa 50010
(Received 23 September 1968)

Using the energy bands for tungsten calculated by Mattheiss, we have calculated the generalized susceptibilities $\chi(q)$ along ΓH for several bcc transition metals by appropriately adjusting the Fermi energies. The Fermi energies were chosen using Mattheiss's integrated density of states to have the proper number of electrons per atom to correspond to (a) the chromium series, (b) the vanadium series, and (c) europium. We have used procedures developed in our calculation of $\chi(q)$ for the heavy rare earths. The generalized susceptibility that corresponds to the chromium group has several small peaks and a prominent, narrow peak very near to H. The position of this prominent peak corresponds to the magnetic periodicity of chromium and to a Kohn anomaly observed in the Cr and Mo phonon spectra. The susceptibility for the vanadium group has a peak near the broad dip in the $[00q]L$ branch of the phonon spectrum of niobium. The susceptibility for europium has a peak near the magnetic wave vector for europium. The Fermi surface for Eu derived from this set of bands is quite similar to that calculated by Andersen and Loucks, and the susceptibility shows the important nesting across the tetracube and the superegg pieces of the Fermi surface.

INTRODUCTION

WE have calculated the generalized susceptibility function $\chi(q)$ for a number of transition metals with bcc structure. This is an extension of our earlier work on the relationship between the electronic structure and the magnetic ordering of heavy rare-earth metals.[1,2] We do not have the energy bands of the individual metals, but because of the close similarity of their electronic structure, we chose to use the energy bands of tungsten calculated by Mattheiss[3] and adjusted the Fermi energy of each metal to fit the number of conduction electrons per atom. Thus, we used $E_F=0.85$ Ry for Cr, Mo, and W; $E_F=0.74$ Ry for V, Nb, and Ta; and $E_F=0.58$ Ry for Eu. The numbers were obtained from the integrated density-of-states curve of Ref. 3 for 6, 5, and 2 electrons per atom, respectively. We chose the **q** vector along (001) because both Cr and Eu have periodic magnetic structure with wave vectors in this direction. The method of calculation is discussed in detail in Refs. 1 and 2. As in Ref. 1 we ignored the **k**, **k**+**q** dependence of the matrix element so the results are qualitatively instructive but quantitatively crude. In the following we discuss the Fermi surfaces and the generalized susceptibility functions for these three groups of metals and their physical implications.

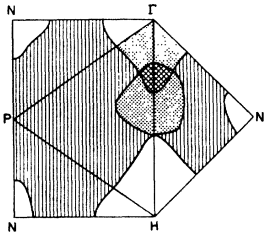

FIG. 1. Cross sections of the Fermi surface of Cr group metals.

Cr, Mo, AND W

The cross sections of the Fermi surface in symmetry planes are shown in Fig. 1 and the $\chi(q)$ curve for the wave vector $(0,0,q)$ is in Fig. 2. In Fig. 1 the flat pieces of the Fermi surface around Γ and H are shown, and it is understood that the nesting of these pieces is the cause of the antiferromagnetism of Cr.[4] On the susceptibility curve there are a number of small peaks and a narrow, prominent peak very near to H. If the average interaction between the electrons has the strength V, then the electron gas will go into a spin density wave state if $V\chi_{\max}\geq 1$.[5] Therefore, there exists a smallest value for V below which antiferromagnetism cannot occur.[6]

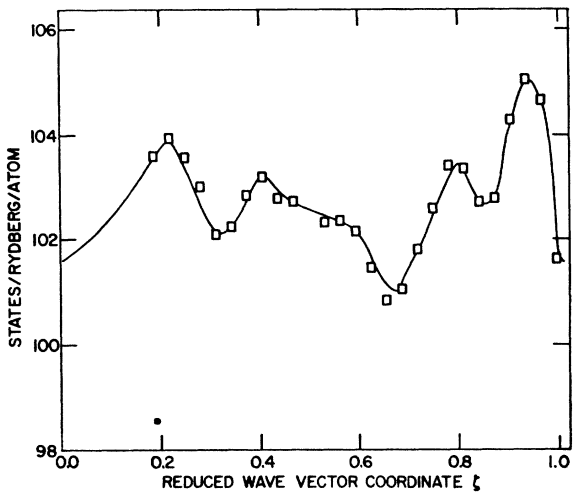

FIG. 2. Generalized susceptibility of Cr group metals along ΓH.

* Work was performed in the Ames Laboratory of the U. S. Atomic Energy Commission, contribution No. 2416.
† Danforth Foundation Fellow. Present address: Department of Physics, University of Pennsylvania, Philadelphia, Penna.
[1] W. E. Evenson and S. H. Liu, Phys. Rev. Letters **21**, 432 (1968).
[2] W. E. Evenson and S. H. Liu, Phys. Rev. **178**, 783 (1969).
[3] L. F. Mattheiss, Phys. Rev. **139**, A236 (1965).
[4] W. M. Lomer, Proc. Phys. Soc. (London) **80**, 489 (1962).
[5] P. A. Fedders and P. C. Martin, Phys. Rev. **143**, 245 (1966).
[6] S. H. Liu, Phys. Letters **27**, 493 (1968).

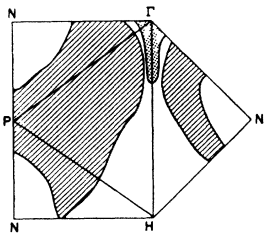

FIG. 3. Cross sections of the Fermi surface of V group metals.

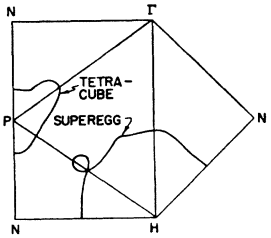

FIG. 5. Cross sections of the Fermi surface of Eu.

The interaction V is believed to arise from the exchange effect between spin-up and spin-down electrons in the d band. In Cr the exchange interaction is strong enough to stabilize the antiferromagnetic ground state. In Mo and W it appears that the exchange effect is not strong enough for antiferromagnetism to occur, presumably because of the wider d bands in these metals. In fact, these two metals are superconductors at very low temperatures.[7,8]

As pointed out in Ref. 1 the nesting anomaly should also appear in the phonon spectrum as a dip at the nesting wave vector. Indeed, such anomalies have been observed in Cr[9] and Mo.[10] The anomaly in W is less apparent.[11]

V, Nb, AND Ta

The Fermi surface cross sections and the generalized susceptibility curve are shown in Figs. 3 and 4, respectively. None of these metals is known to be antiferromagnetic so we can only correlate our results with their phonon spectra.[12,13] There are two peaks in the susceptibility curve, one near Γ and one near H. The latter corresponds quite well to the anomaly in the longitudinal branch of the phonon spectra of Nb and a Nb-rich Mo alloy.[14] The former has not been observed, probably because it is drastically suppressed by a wave-vector-dependent matrix element.

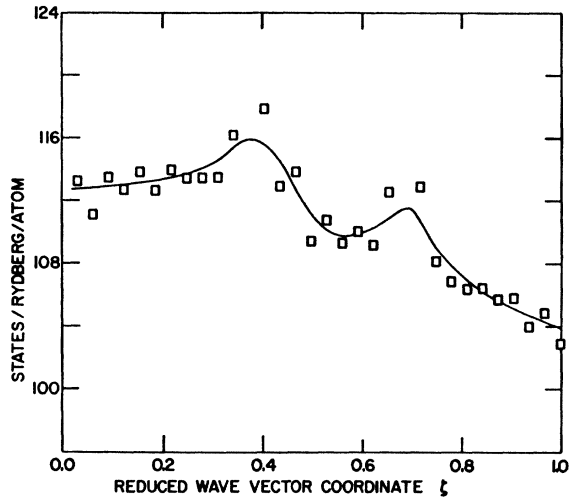

FIG. 4. Generalized susceptibility of V group metals along ΓH.

EUROPIUM

Europium has a helical magnetic structure with a periodicity of $3.5a$ just below the Néel temperature[15] (a=lattice parameter). The Fermi surface of Eu was previously calculated by Andersen and Loucks,[16] and they found a number of flat surfaces on what they call tetracube and superegg. The extremum dimension of the tetratube agrees very well with the magnetic-ordering wave vector. Our Fermi surface and susceptibility curve are shown in Figs. 5 and 6. The Fermi energy as found from the integrated density-of-states

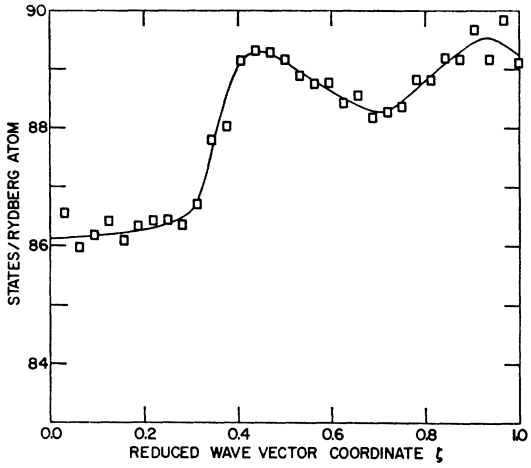

FIG. 6. Generalized susceptibility of Eu along ΓH.

[7] D. C. Rorer, D. G. Onn, and H. Meyer, Phys. Rev. **138**, A1661 (1965).
[8] J. W. Gibson and R. A. Hein, Phys. Rev. Letters **12**, 688 (1964); R. T. Johnson, O. E. Vilches, J. C. Wheatley, and S. Gygax, *ibid.* **16**, 101 (1966).
[9] H. B. Møller and A. R. Mackintosh, in *Inelastic Scattering of Neutrons* (International Atomic Energy Agency, Vienna, 1965), Vol. 1, p. 95.
[10] A. D. B. Woods and S. H. Chen, Solid State Commun. **2**, 233 (1964).
[11] S. H. Chen and B. M. Brockhouse, Solid State Commun. **2**, 73 (1964).
[12] Y. Nakagawa and A. D. B. Woods, Phys. Rev. Letters **11**, 271 (1963).
[13] A. D. B. Woods, in *Inelastic Scattering of Neutrons* (International Atomic Energy Agency, Vienna, 1965), Vol. 1, p. 87.
[14] A. D. B. Woods and B. M. Powell, Phys. Rev. Letters **15**, 778 (1965).
[15] G. P. Arnold, C. E. Olsen, and N. G. Nereson, J. Appl. Phys. Suppl. **33**, 1135 (1962); C. E. Olsen, N. G. Nereson, and G. P. Arnold, J. Appl. Phys. Suppl. **35**, 1031 (1964); N. G. Nereson, C. E. Olsen, and G. P. Arnold, Phys. Rev. **135**, A176 (1964).
[16] O. K. Andersen and T. L. Loucks, Phys. Rev. **167**, 551 (1968).

curve in Ref. 3 is 0.56 Ry for two electrons per atom. But we deliberately raised it to 0.58 Ry so that our Fermi surface would have a closer resemblance to that in Ref. 16. The piece centered around P corresponds to the tetratube. Notice that the arm along P to H is pinched off in our version. The piece centered around H corresponds to the superegg. The susceptibility curve shows two peaks at the diameters of these two surfaces. As in the case of hcp rare earths, we expect the peak at the smaller wave vector (tetratube) to dominate because of the effect of wave-vector dependence of the matrix elements.[2] Hence, our calculation lends support to the idea that the nesting between the opposite faces of the tetratube is responsible for the helical structure of Eu. The superegg nesting anomaly should best be observed in the phonon spectrum of Eu.

ACKNOWLEDGMENT

The authors wish to thank Dr. T. L. Loucks for his continued interest in our work and for his numerous helpful suggestions.

PHYSICAL REVIEW VOLUME 178, NUMBER 3 15 FEBRUARY 1969

Landau-Level Widths, Effective Masses, and Magnetic-Interaction Effects in Lead*

R. A. PHILLIPS AND A. V. GOLD†
Institute for Atomic Research and Department of Physics, Iowa State University, Ames, Iowa 50010

(Received 28 June 1968; revised manuscript received 15 November 1968)

The amplitudes of the de Haas–van Alphen effect in lead have been studied in detail using large impulsive magnetic fields and employing a narrow-band filtering system. Crystals of high purity were grown, cut, and mounted in a manner which was essentially strain-free, and the Dingle broadening temperatures T_D for many of these crystals were found to be less than 0.1°K, corresponding to Landau-level widths of less than 1% of the level spacing $\hbar\omega_c$ in a field of about 10^5 G. These findings strongly suggest that the large level widths ($T_D \approx 1$–2°K) frequently reported in the past for many pure metals arise from destruction of phase coherence by dislocations. Accurate effective mass values have been determined for the extremal orbits at symmetry directions, and these results are compared with the data obtained directly from cyclotron resonance. The temperature dependences of the amplitudes for the harmonic and combination tones provide yet further detailed evidence for the correctness of Shoenberg's proposal that the Lifshitz-Kosevich theory must be modified when the magnetic interaction between conduction electrons is important. The absolute amplitudes of the fundamental oscillations are compared with the theoretical predictions, and the harmonic content is also discussed.

I. INTRODUCTION

IN studies of the de Haas–van Alphen (dHvA) oscillations in metals,[1,2] the major emphasis has usually been on the orientation dependence of the frequencies F which are directly related to extremal cross-sectional areas $\mathcal{A}_0$ of the Fermi surface. On the other hand, it is well known that studies of the amplitudes and waveforms of the oscillations can yield additional information about the conduction electrons in metals, in particular the cyclotron effective masses m^*, the effective widths $k_B T_D$ of the Landau levels, and magnetic-interaction effects, but careful amplitude studies have been made for only a few metals so far. This paper is concerned with a detailed analysis of the temperature and field dependences of the dHvA amplitudes in lead, as well as with a comparison of the absolute values of the amplitudes and the harmonic content with the predictions of the basic Lifshitz-Kosevich (LK) theory.[3] In order to make a careful comparison of this kind it is necessary to know the shape of the Fermi surface in some detail, and we have chosen lead for this study since the shape of its Fermi surface is now well understood.[4]

One of the main objectives of this research was to make a comparison of the m^* values from the dHvA

* Work was performed in the Ames Laboratory of the U. S. Atomic Energy Commission, contribution No. 2346. This paper is based in part on a Ph.D. thesis submitted by R. A. Phillips to Iowa State University, Ames, Iowa, 1967 (unpublished); see Ref. 26.

† Alfred P. Sloan Fellow. Now at Department of Physics, University of British Columbia, Vancouver 8, Canada.

[1] D. Shoenberg, in *Progress in Low Temperature Physics*, edited by C. J. Gorter (North-Holland Publishing Co., Amsterdam, 1957), Vol. II, pp. 226–265.

[2] D. Shoenberg, in *Proceedings of the Ninth International Conference on Low-Temperature Physics, Columbus, Ohio*, edited by J. G. Daunt *et al.* (Plenum Press, Inc., New York, 1965), pp. 665–676.

[3] I. M. Lifshitz and A. M. Kosevich, Zh. Eksperim. i Teor. Fiz. **29**, 730 (1955) [English transl.: Soviet Phys.—JETP **2**, 636 (1956)].

[4] J. R. Anderson and A. V. Gold, Phys. Rev. **139**, A1459 (1965). The frequency values reported in this reference were subject to a systematic error (4–6%) due to a dynamic instability in the electronics which escaped detection under normal calibration procedures.

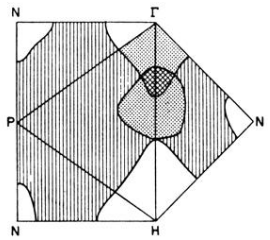

FIG. 1. Cross sections of the Fermi surface of Cr group metals.

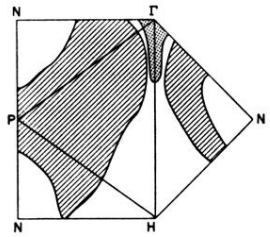

FIG. 3. Cross sections of the Fermi surface of V group metals.