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FIELD-INDUCED CHANGES IN THE BAND STRUCTURE AND FERMI SURFACE OF NICKEL*

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The de Haas–van Alphen effect has been studies in spherically shaped crystals of nickel. The unusual angular variations in the frequencies arising from the X_5 hole pockets can be accounted for in terms of an interpolation scheme which includes the effect of spin-orbit coupling. The sizes of the hole pockets depend markedly on the axis of spin quantization, i.e., on the direction of the applied magnetic field.

A self-consistent calculation of the ferromagnetic band structure of nickel was recently carried out[1] incorporating correlation effects through the use of an intra-atomic Coulomb interaction. This calculation was based on a simple interpolation scheme for paramagnetic transition metals and made use of several parameters obtained from first-principles augmented-plane-wave band calculations; use was also made of the experimentally determined magneton number as well as other experimental information such as the size of the [111] "neck" in the copperlike sheet of the Fermi surface as determined by the low-frequency de Haas–van Alphen oscillations of Joseph and Thorsen.[2] The limited nature of this experimental information coupled with the uncertainties inherent in the first-principles band structure prevented an exact determination of the position of some of the energy bands near the Fermi surface, and as a consequence the size, shape, and even the existence of a number of small hole pockets in the Fermi surface could not be accurately ascertained. In this paper we wish to present the results of further studies of the de Haas–van Alphen effect in spherical samples of nickel and to discuss the relevance of these results to the band structure. Excellent agreement with experiment is found when the original interpolation scheme[1] is modified by readjusting certain parameters[3] and by including the effects of spin-orbit coupling; this interaction leads to variations in the band structure (and in the Fermi surface) which

depend on the orientation of the applied magnetic field.

A new set of de Haas–van Alphen oscillations, with frequencies somewhat higher than those originally reported by Joseph and Thorsen,[2] was first detected in impulsive-field experiments on hollow nickel whiskers[4]; however, these whisker results were rather meager and the data were not very reliable on account of the nonuniform demagnetizing field created by the awkward shape of the samples. In this work we have used carefully polished spherical specimens to study these new oscillations in some detail; low-frequency (~40 Hz) modulation techniques were used in conjunction with a 63-kG Varian superconducting magnet, and the sample temperature was usually close to 1.1°K. The samples were prepared by hand-lapping "rough" spheres which had been spark cut from a rod of zone-refined material[5] with a resistance ratio $R_{300°K}/R_{4.2°K} = 980$ (as measured in the presence of the earth's magnetic field), and their departures from perfect sphericity of only a few parts in 10^5 ensured a high degree of uniformity in the magnetic induction. The angular variation of the frequencies were obtained by Stark's "overmodulation" variation[6] of the Shoeberg-Stiles technique in which the sample is rotated in a constant applied field, supplemented by absolute frequency determinations from conventional field sweeps. The frequency variations in the $(1\bar{1}0)$ and (001) planes are shown in Fig. 1. In the meantime Tsui and Stark[7] have published the results of similar experiments which were carried out on rod-shaped samples, and it is very gratifying to find good agreement between the results of our independent investigations with radically different sample geometries.[8]

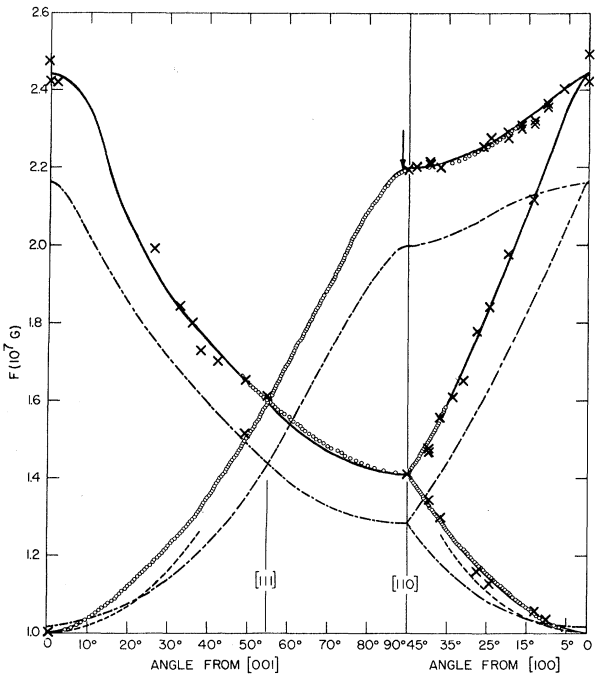

FIG. 1. Orientation dependence of the de Haas–van Alphen frequencies arising from the hole pockets at X, in the $(1\bar{1}0)$ and (001) planes. Open circles, changes in frequency from rotations at constant field; crosses, absolute frequency determinations from field sweeps. Frequency values in 10^7 G at symmetry directions are the following: [100], 1.00 ± 0.01 and 2.44 ± 0.04; [111], 1.59 ± 0.02; [110], 2.19 ± 0.02 and 1.41 ± 0.02 (the quoted uncertainties are on the conservative side and ample allowance has been made for possible errors associated with irreproducible "image effects"). Solid curves: frequency variations from interpolation model with $\bar{\xi} = 0.0075$ Ry; dot-dashed curves: frequency variations from same model, but with $\bar{\xi} = 0$; dashed curves: $1/\cos\theta$ variations for cylindrical Fermi surfaces in ΓX directions.

Full details of our experimental apparatus, sample preparation, etc., are given elsewhere,[9] but some comments concerning the demagnetizing field are in order here. Since the demagnetizing factor for our spheres is exactly $\frac{1}{3}$, it should be possible to determine the saturation magnetization $4\pi M_S$ from the periodicity of the oscillations (cf. Ref. 4), and we have indeed been able to determine $4\pi M_S$ with a standard deviation of as little as 0.2% from a least-squares analysis of the data obtained from any given field sweep. Unfortunately the results were found to fluctuate from day to day by as much as 5%, and it is felt that these relatively large fluctuations are due to irreproducible "image effects" associated with the presence of a ferromagnetic specimen in the field of the superconducting magnet. (No significant irreproducibilities were found when the field was monitored by an nmr probe in the absence of a ferromagnetic sample.) We have adopted the value $4\pi M_S = 6.39$ kG, about which our determinations are grouped, and it is satisfactory that this value is in good agreement with Danan's absolute measurement [10] when it is corrected for the 3.2% difference between room temperature and helium temperatures.[11]

The angular variations of the frequencies shown in Fig. 1 are consistent with a symme-

try-related set of small closed sheets of the Fermi surface associated with the equivalent points X of the Brillouin zone. Two distinct sets of hole pockets, associated with the levels X_5 and X_2 for minority-spin electrons, are predicted by the band calculation of Ref. 1, whereas only one set is implied by the experimental results. The observed set has been related to the X_5 level since this level must remain above the Fermi level in order to maintain agreement with the observed magneton number; on the other hand, only a slight adjustment of the parameters in the calculation could depress the X_2 level below the Fermi level,[3] thereby eliminating the second set of hole pockets. Early attempts to interpret the observed frequency anisotropy were hampered by the observation that the smallest extremal area, which corresponds to the lowest branch near [001] and [100] in Fig. 1, increases faster than the $1/\cos\theta$ dependence expected from a cylindrical Fermi surface with its axis along one of these directions (dashed curve). Any simple closed surface which gives rise to such a rapid frequency variation would be expected to be hyperboloidal in form in the vicinity of the relevant extremal area and, being closed, we would expect each such surface to have at least two distinct extremal areas normal to [001], i.e., as for a dumb-bell–shaped surface; however, this conclusion is at variance with the fact that only one frequency is observed for each surface at [001]. It might be possible to account for the rapid angular variation of the lowest branch by supposing the hole pockets to resemble highly fluted ellipsoids; however, no such fluting is evident in the results of the band calculation,[1] and we shall see that the experimental variations can be explained in a natural way when the band calculation is modified by taking spin-orbit coupling into account.

It was pointed out in Ref. 1 that the spin-orbit interaction can be easily incorporated into the interpolation scheme, and in doing so, it is of course natural to choose the axis of spin quantization along the direction of the magnetization vector. The matrix elements of the spin-orbit interaction will therefore depend on the polar and azimuthal angles of the magnetization in the manner indicated by Abate and Asdente.[12] The spin-orbit interaction has striking effects on the hole pockets at X, causing them to vary in size and shape as the applied-field direction (and thus the direction of the magnetization) is changed. This point is illustrated in Figs. 2(a) and 2(b), which show the minority-spin energy bands near the various X points when the field is along the [001] direction. In Fig. 2(a) the minority spin bands interact with themselves and are split by an amount approximately equal to $\bar{\xi}$, whereas in Fig. 2(b) the interaction is between bands of opposite spin and is reduced by the ferromagnetic splitting which is several times larger than $\bar{\xi}$. Thus the two hole pockets along the field direction will be smaller in all dimensions than the four hole pockets perpendicular to the magnetization. As the external field (and thus the magnetization) is rotated, say from [001] to [010], the spin-orbit interaction will cause the hole pockets to change size until it is the two hole pockets at the X points $(2\pi/a) \times(0,\pm,0)$ which are the smallest. As a consequence, the lowest frequency branch observed near [001] and [100] in Fig. 1 can appear to arise from a hyperboloidal surface because the relevant hole pockets are actually increasing in size as the field is being rotated. This effect is important, despite the smallness of the spin-orbit interaction in nickel, because the dimensions of the hole pockets are also very small and therefore rather sensitive to the magnitude of this minute splitting.

We have calculated the variation of the de Hass–van Alphen frequencies for the hole pockets using the band structure shown by the solid curves in Fig. 2, in which the spin-orbit parameter was taken to be $\bar{\xi}=0.0075$ Ry. This value of $\bar{\xi}$ has been chosen to maximize agree-

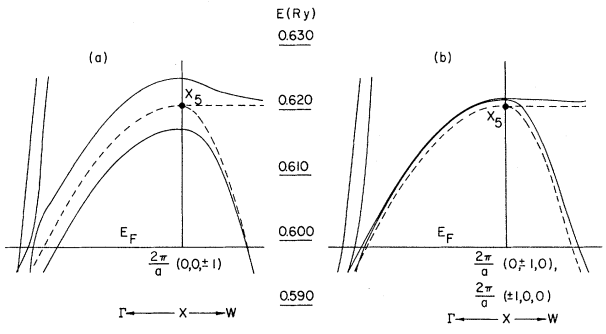

FIG. 2. Large-scale drawings showing the effect of spin-orbit coupling on the energy bands for minority-spin electrons near the various points X; the magnetization vector is parallel to [001]. Solid Curves: $\bar{\xi}=0.0075$ Ry; dashed curves: $\bar{\xi}=0$.

ment with the experimental frequencies and it is about 35% larger than the atomic value of 0.0055 Ry. This is similar to the situation in lead[13] in which the Fermi-surface data indicated a spin-orbit parameter about 50% larger than in the atomic case. The computed variations of the frequencies are shown in Fig. 1 by the solid curves, which are virtually indistinguishable from the experimental points. By way of comparison, the dot-dashed curves in Fig. 1 illustrate what would happen if we were to set $\bar{\xi}=0$, but it should be understood that a better $\bar{\xi}=0$ representation of the experimental results can be achieved by readjusting the other parameters. When this is done, the calculated curves are akin to those from the geometrical model of Tsui and Stark[7] and for this reason we do not present them here; they cannot account for the abnormally rapid variation of the lowest branch near [100] and [001] in Fig. 1. In Table I we list the dimensions of the hole pockets as predicted by the interpolation scheme; the pockets are equivalent only when the field is along $\{111\}$.

In the present experiments[9] no evidence was found of the minority-spin hole pockets at L predicted by the band structure of Ref. 1. This tends to support the reordering of the bands at L suggested by Krinchik and Canshina,[14] and this reordering has been incorporated into the ferromagnetic band structure upon which the present calculations are based.[3] Data predicted by this band structure for the large electron orbits (which have not yet been experimentally observed) are presented in Table II. The actual calculation of the de Haas–van Alphen frequencies expected from these large surfaces is complicated by the necessity for incorporating the full spin-orbit interaction in a basis which includes plane waves as well as d bands.

Table I. Distances from X to the surface of the hole pocket in units of $2\pi/a$, where $a=3.5166$ Å [T. Heumann, Naturwiss. 32, 296 (1944)].

Field direction	Location of pockets	$k_{X\Gamma}$	k_{XW}	k_{XU}
[001]	$(0,0,\pm1)$	0.195	0.100	0.094
	$(0,\pm1,0)$, $(\pm1,0,0)$	0.220	0.112	0.108
[111]	$(0,0,\pm1)$, $(0,\pm1,0)$, $(\pm1,0,0)$	0.208	0.107	0.098
[110]	$(0,0,\pm1)$	0.219	0.109	0.103
	$(0,\pm1,0)$, $(\pm1,0,0)$	0.205	0.106	0.102
$\bar{\xi}=0$		0.215	0.102	0.095

Table II. Data for the large electron surface predicted by the band structure of Fig. 2. These dimensions are essentially unaffected by the weak spin-orbit interaction; the unit of length is $2\pi/a$ as in Table I.

	Majority 6th band	Minority 6th band	Minority 5th band
$k_{\Gamma X}$	0.77	0.75	0.77
$k_{\Gamma L}$	(necks)	0.71	0.71
$k_{\Gamma K}$	0.58	0.52	0.95
Area $\perp$[001]	1.33	1.12	2.24

This interaction will affect not only bands of a given spin but may be expected to remove the accidental degeneracies between bands of opposite spin and cause a blurring of the usual distinction between majority- and minority-spin Fermi surfaces. An electron passing through one of these regions in k space is expected to have a certain probability of undergoing magnetic breakdown or of suffering a change in spin and moving on to what was initially another sheet of the Fermi surface. These regions of "spin-dependent magnetic breakdown" occur at least twice for each of the large electron orbits for most field orientations, and we are thus tempted to speculate that herein may lie the reason for the unobservably small amplitudes of the de Haas–van Alphen effect associated with these orbits. However, quantitative estimates of the reduction in amplitude must await the results of further calculations of the spin-orbit splittings and of the details of the switching probabilities.

We are indebted to Dr. W. A. Reed for the gift of the zone-refined nickel, and to Dr. H. Ehrenreich, Dr. S. H. Liu, and Mr. W. Furey for helpful discussions.

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INELASTIC ELECTRON SCATTERING FROM LEVELS AT 19.5-MeV EXCITATION IN C^{12}

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An apparently good fit of the summed transverse and longitudinal form factors to the total measured form factor for inelastic electron scattering to the 19-Mev levels of C^{12} appears less good when the two components are distinguished. Evidence for the $T=1$, $J=1^-$ and $T=1, J=2^-$ states seems clearly established, but the longitudinal form factor indicates that another level is contributing.

A recently published study[1] of the inelastic scattering of electrons by C^{12} with excitation of levels at 19.5 MeV attributes the major portion of the cross section to a single-particle dipole transition leading to a $T=1, J=1^-$ state. The assignment is based on the similarity of the observed cross section, for scattering at forward angles only, with the total cross section calculated for a particle-hole model of the nucleus.[2] This theoretical cross section, however, is the sum of longitudinal and transverse contributions, so that agreement with experiment can only be considered to support the theory if the predicted proportions of the two components are observed. That electron-scattering experiments enable the experimenter to separate these two components by measurement is well established.[3] As the measurements of Ref. 1 were carefully confined to forward scattering angles, no experimental separation could be attempted.

There is also evidence[4-6] for the excitation of a 2^- state at 19.2 MeV, which is interpreted as a particle-hole state[7] or as a collective spin-isospin state,[8] dubbed the magnetic quadrupole giant resonance. Unfortunately, there is no region of overlap in momentum transfer for the cross sections of Ref. 1, 4, and 6 which would permit application of the forward-backward method to separate longitudinal and transverse components.

This method can be applied, however, for one value of momentum transfer by use of a measurement made at Orsay.[9] The Orsay cross section was measured for an incident energy of 198 MeV, at a scattering angle of 135°, and gave a differential cross section of $(7 \pm 2) \times 10^{-33}$ cm^2/sr for the 19-MeV complex. At the corresponding value of momentum transfer of 368 MeV/c (equivalent to 1.86 F^{-1}), the cross section of Ref. 1 for an incident energy of 550 MeV and a scattering angle of 40° is stated to lie between limits of 4×10^{-32} cm^2/sr and 1.7×10^{-32} cm^2/sr. These limits are established