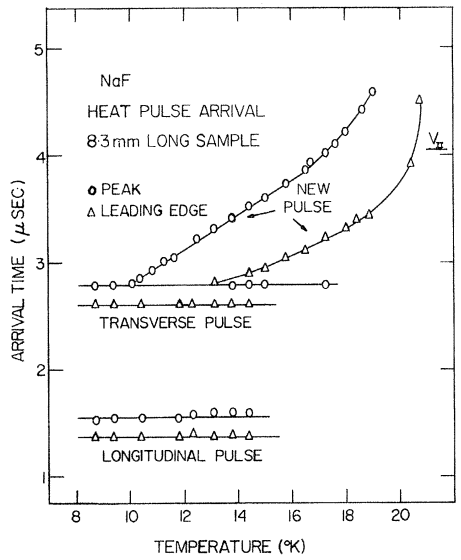

FIG. 3. Arrival times versus temperature for leading edges and peaks of longitudinal ballistic pulse, the transverse ballistic pulse, and the second pulse. V_{II} is the expected arrival time for fully developed second sound.

level off.

Thus, in spite of the fact that we have investigated second sound in a crystal of substantially higher purity, the behavior found in Ref. 1 is seen to continue to higher temperatures. This behavior is not predicted by current theories and is distinct from that seen so far in solid helium. Ackerman and Guyer[5] observed a gradual approach to a constant second-sound velocity with increasing temperature. If a leveling off is to be seen in NaF, it must occur much more abruptly since at 18°K the second-sound velocity is so close to the predicted value.[6] This difference between solid helium and NaF could be understood if the ratio of momentum-conserving to momentum-destroying processes (τ_N^{-1}/τ_R^{-1}) for NaF were significantly lower than that for solid helium. Alternatively, the behavior seen here and in Ref. 1 could be intrinsic to NaF.

We wish to express our thanks to Professor R. O. Pohl for many stimulating conversations, and to Mr. Rafael Gonzales for his assistance in the arduous purification program.

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ELECTRONIC PHASE SHIFTS AT THE FERMI SURFACE OF COPPER*

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The results of a phase-shift analysis of the Fermi surface of copper using the Korringa-Kohn-Rostoker method are reported. The values of the first four phase shifts and the Fermi energy differ from those obtained recently by Lee from an augmented-plane-wave calculation.

The augmented-plane-wave[1] (APW) and Korringa[2]-Kohn-Rostoker[3] (KKR) methods for band calculations have the feature that the single-particle potential does not enter explicitly into the computation of the dispersion curves when the muffin-tin approximation is used. The only relevant quantities are the partial-wave phase shifts η_l of the angular momentum components for scattering, at a particular energy, from the effective potential. Thus, as discussed in some detail by Segall and Ham,[4] it should be possible to treat the η_l's as parameters to be adjusted to obtain agreement between measured and computed Fermi-surface data. Since experience with alkali, noble, and transition metals has shown that only the first three or four phase shifts are important for the convergence of the KKR method, this approach appears to be both an attractive

and feasible technique for correlating experimentally obtained Fermi-surface dimensions. Such an approach also has added significance when one considers that the resulting phase shifts may correspond to single-particle, energy- and l-dependent potentials which include in some way both nonlocal exchange and correlation effects.

Recently, Lee[5] has published the results of a phase-shift analysis of the Fermi surface of copper using the APW formalism. He reports several sets of values of the first four phase shifts ($l=0, 1, 2, 3$) and the Fermi energy E_F, all of which apparently result in very good agreement between the calculated and measured areas of several high-symmetry de Haas–van Alphen orbits. However, he pointed out that the measured high-symmetry areas are not yet experimentally accurate enough to allow a choice of the "best" set and hence to estimate the Fermi energy. He therefore introduced three belly anisotropy parameters, D_1, D_2, and D_3, defined, for example in the case of D_1, by

$$D_1 = \text{area}\,[16^\circ \text{ from } \langle 100\rangle \text{ in (100) zone} - B_{100}],$$

in which B_{100} is the (100) belly orbit. The D's are rather sensitive to the $l=3$ phase shift and E_F and he used this fact to estimate the best set of phase shifts and E_F. He concluded that $E_F = 0.550 \pm 0.005$ Ry.

We have carried out a similar phase-shift analysis of copper with the KKR method. As far as we can ascertain, our approach differs from Lee's in only one other aspect, namely, we have relied on the condition $v_F = 1.0000 \pm 0.0001$ electrons/atom (v_F is the volume under the Fermi surface) to establish the Fermi energy, rather than on agreement between the measured and computed values of the D's. Most of our calculations were completed before Lee's work appeared and we were at first surprised, in light of the known similarities and well established accuracies of the APW and KKR methods, to find that we had arrived at a significantly different set of phase shifts and Fermi energy. We subsequently carried out calculations with Lee's values of these quantities and found results which differ noticeably from his. Since we have every reason to believe that our computational methods are as accurate as Lee's, we have tentatively concluded that Lee has probably overestimated the accuracy of some of his calculations due to not always carrying the APW method to the necessary convergence. However, his results, when compared with ours, do seem to make it clear that with the present experimental data and its accuracy no unique set of η_l's and E_F, if it exists, can be determined. We will return to these points after a brief explanation of the data shown in Table I, which compares the results of various calculations with the experimental values.

The experimental results for the orbital areas shown in the last two columns of the table are taken from the work of O'Sullivan and Schirber[6] and Jan and Templeton[7] as indicated. B_{100} and B_{111} denote the areas of the (100) and (111) belly orbits, N_{111} the neck, D_{110} the dog's bone, and R_{100} the (100) rosette areas. The results for the anisotropy parameters are taken from Halse[8] and Joseph et al.[9] The column headed CDW (Cooke, Davis, Wood) shows the results of one of our KKR calculations along with the values of the η_l's and E_F we obtained. The columns labeled CDW-L1 and CDW-L2 show the results we obtained with our KKR programs from two sets of η_l's and E_F given by Lee, while the column labeled LR gives Lee's reported values. As mentioned earlier, all of the sets of η_l's and E_F given by Lee in his paper are supposed to result in the same values of the orbital areas, and these are shown in the LR column. These areas then should be appropriate to the sets of phase shifts shown in both the LR column and the CDW-L2 column. The D's shown in the LR column, however, are appropriate only to the values of the η_l's shown in that column and were taken from row (4) of Table IV in Ref. 5. These values of the η_l's were found using 30 APW. In testing the convergence of his APW calculation, Lee found that for $E_F = 0.55$ Ry the phase shifts changed from the values shown in the LR column to the values shown in the CDW-L2 column when he went from 30 to 60 APW (Ref. 5, Table VI). He apparently did not recalculate the D's for this new set of phase shifts, since he does not report values of the D's calculated with 60 APW.

It can be seen by comparing columns CDW-L2 and LR that the APW and KKR calculations give essentially the same values of the orbital areas (except perhaps B_{111}) when the phase shifts in CDW-L2 (60 APW) are used. It should be kept in mind that Lee's reported orbital areas are supposed to be valid for all of his reported η_l's. The D's of column LR were calculated with the phase shifts of that column using 30 APW, and they differ substantially from the D's in column CDW-L2. Using Lee's phase shifts from his

Table I. Comparison of various calculated and experimental quantities. The numbers in parentheses are the estimated errors in the last decimal places (± sign implied). The errors of the orbital areas are the same in all three CDW columns. The row and column labels are explained in the text.

	CDW	CDW-L1	CDW-L2	LR	EXP-1[a]	EXP-2[b]
B_{100}	.9808(2)	.9829	.9809	.9807(2)	.9810(10)	
B_{111}	.9504(2)	.9520	.9499	.9503(1)	.9510(10)	.9498(10)
N_{111}	.03564(6)	.03593	.03559	.03557(1)	.03561(4)	.03556(4)
D_{110}	.4103(4)	.4088	.4104	.4106(3)	.4112(5)	
R_{100}	.4018(4)	.4004	.4023	.4021(3)	.4027(5)	
D_1	-.00668	-.00696	-.00700	-.00647(10)	-.00645(10)	-.00669
D_2	-.00357	-.00374	-.00375	-.00349(6)	-.00342(10)	-.00332
D_3	.0205	.0201	.0201	.0203(5)	.0196(6)	-.0212
η_0	-.00717	.0581	.0574	.0581		
η_1	.09682	.1235	.1235	.1235		
η_2	-.13324	-.1150	-.1157	-.1150		
η_3	.00094	.0014	.0014	.0014		
E_F	.58794	.5500	.5500	.5500		
v_F	1.0000(1)	1.0026(1)	.9998(1)			

[a]Orbital areas from Ref. 6; D's from Ref. 8.
[b]Orbital areas from Ref. 7; D's from Ref. 9.

30-APW calculation, we found the results shown in CDW-L1, which again differ substantially from his reported values for the same phase shifts. The implication of the results of these calculations seems to be that, with a given set of four phase shifts and Fermi energy, approximately 60 APW are necessary to give results comparable to the KKR method. Because of this we feel that the accuracy of all of Lee's calculations in which only 30 APW were used can be questioned. This becomes particularly important when one remembers that Lee used the values of the D's from calculations with 30 APW to fix his value of the Fermi energy.

The overall agreement with experiment appears to be somewhat better for the set of phase shifts and Fermi energy given in the CDW column than for the sets given in the other columns. This is true, however, only when our KKR calculated values for the D's are introduced, but in light of the differences in the reported experimental values it is perhaps somewhat premature to put too much emphasis on these quantities. In fact, the value of v_F shown in column CDW-L2 very nearly meets our requirement that $v_F = 1.0000 \pm 0.0001$ electrons/atom and, had we not followed Lee in calculating the D's, we would be forced to admit that his values of the phase shifts and Fermi energy are as good as ours. Because of this and our own experience with other calculations not reported here, we tend to feel that a unique set of phase shifts and Fermi energy may not exist, or, at least, cannot be determined from the present experimental data.

It remains to be seen just how useful the method of phase-shift analysis may ultimately prove to be. In any case, it seems apparent already that the numerical calculations can be carried out with great accuracy. Therefore, any further refinement of the present experimental data, especially values of the anisotropy parameters, will be helpful for future work of this type.

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PHASE TRANSITION IN A COMPRESSIBLE ISING FERROMAGNET

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Within the droplet model for the Ising spin system it is shown that the magnetic specific heat C_p and the susceptibility χ_p for constant vanishing pressure and magnetic field remain finite in a compressible lattice as the critical point T_c is approached from below. This regularization of C_p and χ_p is caused by the long-range indirect spin-spin interaction, which is a consequence of the dependence of the exchange integral on the lattice spacing.

It was pointed out by Fisher[1] that constrained "hidden" variables (e.g., impurity density, elastic degrees of freedom) renormalize the critical exponents of a system undergoing a second-order phase transition. In this note we examine the effect of elasticity on the nature of the Curie point in an Ising ferromagnet with a compressible harmonic lattice. The hidden variables in this case are the deviations $u_\mu{}^m$ ($m = 1, \cdots, N$; $\mu = x, y, z$) of the mth atom from its rest position $\vec{R}^m$. The $\vec{R}^m$ are determined from the minimum of the lattice potential energy. A spin variable $\sigma^m = \pm 1$ is attached to the mth atom. External mechanical forces $\vec{K}^m$ enter the Hamiltonian via a term $-\vec{u}^m \cdot \vec{K}^m$ (summation over repeated indices is implied). If the thermal averages $\langle \vec{u}^m \rangle$ are constrained by prescribing a strain tensor $\epsilon_{\mu\nu} = \epsilon\delta_{\mu\nu}$, where $\langle u_\mu{}^m \rangle = \epsilon_{\mu\nu} R_\nu{}^m$, then, according to Fisher's theory, one expects that the specific heat C_v for constant ϵ (i.e., for constant volume V) remains finite at the Curie point, displaying a cusp-shaped maximum at T_c. The magnetic susceptibility χ_v at constant V should still diverge, but also has a renormalized exponent. The basic hypothesis made in the theory is that for constant forces $\vec{K}^m$, C_K and χ_K behave "ideally", as in a rigid lattice.[2] For example, it is assumed that $C_K \propto (T_c - T)^{-\alpha'}$ for $T \to T_c - 0 \equiv T_c{}^-$, with $\alpha' \approx \frac{1}{16}$, as is obtained from exact series expansion methods.[3]

In contrast to this hypothesis we find that C_K and χ_K remain finite in the compressible Ising ferromagnet as $T \to T_c{}^-$. Specifically, we start from an Ising model for spins on a simple cubic lattice, with an exchange integral acting only between nearest-neighbor (nn) spins and depending on the distance between them. For simplicity we consider only the case[4] $\vec{K}^m = 0$. In the Hamiltonian $H = H_L + H_S + H_{SL}$, H_L describes harmonic phonons, H_S the Ising spin system, and H_{SL} is the spin-lattice interaction, which is obtained by expanding the exchange integral in powers of $\vec{u}^m$ and keeping only the linear terms:

$$H_{SL} = -u_\mu{}^m (\nabla_\mu{}^m J^{mn}) \sigma^m \sigma^n \equiv -u_\mu{}^m F_\mu{}^m, \tag{1}$$

with $J^{mn} = J(|\vec{R}^m - \vec{R}^n|) = J(a) > 0$. The coupling term (1) can be transformed into an indirect spin-spin interaction with the help of the unitary transformation $A\vec{u}^m A^\dagger = \vec{u}^m + \vec{v}^m$, where $v_\mu{}^m = -D_{\mu\nu}{}^{mn} F_\nu{}^n$. The $D_{\mu\nu}{}^{mn}$ is the static one-phonon Green function of the lattice, described by H_L, and may be expressed in terms of the frequencies $\omega_j(\vec{q})$ and polarization vectors $\vec{e}^j(q)$ of the normal modes with wave vector $\vec{q}$, polarization index $j = 1, 2, 3$:

$$D_{\mu\nu}{}^{mn} = -\sum_j \int \frac{d\vec{q}}{(2\pi)^3} \frac{e_\mu{}^j(\vec{q}) e_\nu{}^j(\vec{q})}{\rho \omega_j{}^2(\vec{q})} e^{i\vec{q}(\vec{R}^m - \vec{R}^n)}, \tag{2}$$

where ρ denotes the mass density. The unitary transformation changes the form of the Hamiltonian into $H_A = H_L + H_S + H_S'$, where

$$H_S' = \tfrac{1}{2} F_\mu{}^m D_{\mu\nu}{}^{mn} F_\nu{}^n. \tag{3}$$

In H_A the spin system is formally decoupled from the lattice. $H_S + H_S' = H_S{}^{\text{eff}}$ can be considered as an effective Hamiltonian for spins on a rigid lattice in the (temperature-independent) configura-