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[10]The electric field F was determined experimentally to be 0.95×10^4 V/cm in Ref. 8. However f is also proportional to μ^{*-2}, where μ^* is the reduced mass of the electron-hole pair. The combined error in evaluating f may be as great as 20%.

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[12]Such a least-squares procedure would have required repeated calculation of $\Delta\alpha(\omega, F)$ for several values of $f=|e|Fa/R$, and would have been unjustifiably expensive.

[13]We have only considered the contribution to the absorption due to the heavy-hole valence band. The contribution of the light-hole band should be smaller by a factor of $[(m_e+m_{h,l})/(m_e+m_{h,h})]^{3/2}\approx 0.3$. The interaction between valence bands has also been neglected.

[14]Note that this is a reversal of our previous pessimism engendered by discouraging results in attempts at fitting the direct absorption in Ge [J. D. Dow, B. Y. Lao, and S. A. Newman, Phys. Rev. B (to be published)]. We believe that, in light of these results, the electroabsorption at the direct edge of Ge should be carefully remeasured.

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Electronic Phase Shifts at the Fermi Surface of Copper—A Reply*

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It is shown that, contrary to a recent claim by Cooke, Davis, and Wood, the results of their phase-shift analysis of the Fermi surface of copper by the Korringa-Kohn-Rostoker method are consistent with those of an earlier augmented-plane-wave calculation by Lee.

In a recent Letter,[1] Cooke, Davis, and Wood presented a phase-shift analysis of the Fermi surface of copper that was based on the Korringa, Kohn, and Rostoker (KKR) method of band-structure calculation, and compared their results with those of an augmented-plane-wave (APW) phase-shift calculation by the present author.[2] Discrepancies between the results of the two analyses led them to question the accuracy of my calculations. The purpose of this reply is to point out that a large apparent discrepancy arose simply because Cooke, Davis, and Wood compared sets of phase shifts corresponding to the different values of the Fermi-energy parameter. I will show that the real discrepancies between the two sets of phase shifts are too small to be of physical significance.

Jan and Templeton[3] and O'Sullivan and Schirber[4] have made precision measurements of the cross-sectional areas of certain extremal orbits on the Fermi surface of copper, while Joseph, Thorsen, Gertner, and Valby[5] and Halse[6] have measured the angular variations of the extremal belly areas in the (100) and the (110) symmetry zones. In a phase-shift analysis, one adjusts the phase shifts η_l and the Fermi-energy parameter E_F that enter into the APW or the KKR secular determinant, in order to bring the shape of the surface of constant energy $E(\vec{k})=E_F$ into agreement with the experimental data.

My calculations showed that E_F is essentially a free parameter in a phase-shift fit to the Fermi surface of copper, but that certain fine details of the shape of the computed surface (the belly an-

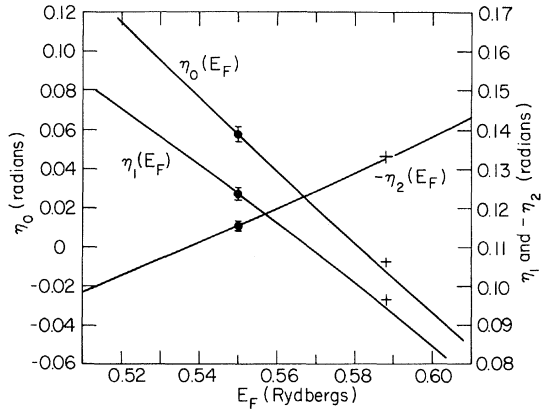

FIG. 1. Phase shifts derived from the experimental Fermi-surface data for copper, plotted as a function of the value of the Fermi-energy parameter. The points and error bars are the best phase shifts deduced by this author from a 30-APW secular determinant, and correspond to $E_F = 0.550$ Ry. The curves, which show the dependence of the phase shifts on the value of the Fermi-energy parameter, are plotted from data given in Table II of Ref. 2. The crosses are the phase shifts deduced by Cooke, Davis, and Wood from their KKR calculation, in which they set $E_F = 0.587\,94$ Ry.

isotropy parameters) depend significantly on the value of E_F. For this reason, I presented in Eq. (6) of Ref. 2 the phase shifts that correspond to my best value of the Fermi-energy parameter ($E_F = 0.550$ Ry); and I suggested that the phase shifts appropriate to any other value of the Fermi-energy parameter be estimated by taking the dependence of the phase shifts on the value of this parameter from Table II of the same paper. Figure 1 shows the relationship between the phase shifts and the Fermi-energy parameter obtained in this way. A direct comparison between these phase shifts (in radians) and those of Cooke, Davis, and Wood, where both sets of phase shifts correspond to $E_F = 0.58794$ Ry, is set out below.

	30 APW	KKR
η_0	−0.0112(42)	−0.007 17
η_1	+0.0953(14)	+0.096 82
η_2	−0.1318(9)	−0.133 24
η_3	+0.0014(3)	+0.000 94

A small discrepancy arises mainly because the convergence of the KKR calculation is more complete than that of my 30-APW calculation by about 0.0008 Ry. Since the two sets of phase shifts agree with one another to within the accuracy with which my phase shifts could be determined from the experimental data (the discrepancy is slightly larger for η_2), I believe that I was justified in truncating the secular determinant beyond 30 APW's.

The aim of the investigation reported in Ref. 2 was to determine the relationship between the phase shifts and the value of the Fermi-energy parameter that is implied by the shape of the Fermi surface of copper. In addition, I attempted to construct a geometrical model of the Fermi surface that is fully consistent with the experimental data. The parameters that specify my model surface include not only my best value of E_F and the corresponding set of phase shifts $\eta_l(E_F)$, but also the number of partial waves and of APW's that I included in the secular determinant. Cooke, Davis, and Wood correctly point out that the value of E_F which gives the best model surface in a 30-APW calculation is no longer appropriate for a KKR (or 60-APW) calculation. I would emphasize that my best value of E_F is a parameter of my model surface, and that my numerical value of this parameter should not be regarded as of fundamental significance.

My results suggest that a 60-APW calculation can lead to no physically significant improvement either in the accuracy of the phase shifts computed as a function of E_F, or in the agreement between the model Fermi surface and the features of the experimental Fermi-surface data on which my analysis is based.[7] I find no evidence to support Cooke, Davis, and Wood's tentative conclusion that "Lee has probably overestimated the accuracy of some of his calculations due to not always carrying the APW method to the necessary convergence." Their results to no extent diminish my confidence that, within the limits set by the accuracy of the experimental data, the aims of my work were fulfilled.

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