

Nonrelativistic phase-shift analysis of impurity scattering in noble-metal hosts

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A general framework is developed for the self-consistent analysis of experimental measurements of quasiparticle scattering by dilute substitutional impurities in metallic hosts. The development is based on phase-shift analysis in the muffin-tin approximation, and departures from free-electron behavior in the host lattice are taken into account. Expressions are given for the Dingle-temperature anisotropy, the impurity resistivity, and the Friedel sum. These quantities depend upon scattering coefficients of the host metal, and on a set of effective ("Friedel") scattering phase shifts. The scattering coefficients for s -, p -, and d -wave scattering in noble-metal hosts are calculated from wave functions determined from nonrelativistic Korringa-Kohn-Rostoker (KKR) phase-shift parametrizations of their Fermi-surface anisotropies. The Friedel phase shifts are determined from analyses of the Dingle-temperature anisotropies and residual resistivities of a series of alloys of nonmagnetic impurities in noble-metal hosts. The Friedel phase shifts are independent of the choice of the Fermi-energy parameter in the phase-shift analysis, and are found to be consistent with the Friedel sum rule whenever lattice distortions and spin-orbit effects can be neglected.

I. INTRODUCTION

The electronic properties of the noble metals, copper, silver and gold, have been studied in great detail. The shapes of the Fermi surfaces have been determined experimentally with a radial accuracy of about 1 part in 10^5 , and the velocity has been mapped over the Fermi surface with an accuracy of about 1%. The band structures have been calculated *ab initio* and also fitted successfully to the experimentally determined Fermi surface (FS) using as parameters the scattering phase shifts. In a recent review,¹ Springford has discussed the scattering of conduction electrons and emphasizes that a satisfactory explanation of the transport properties requires that impurity scattering be anisotropic over the Fermi surface. In the low-temperature limit, where the scattering is impurity dominated, the anisotropy is found to vary with different impurities.

Reference to Springford's review shows that the most extensive experimental results have been obtained using the de Haas-van Alphen effect (dHvA); details of the experimental procedure are discussed therein. The noble metals are particularly convenient for such a study because they are metallurgically fairly simple to handle and dissolve a wide variety of solutes in the appropriate concentration range. Also, because the Fermi surfaces are multiply connected, it is possible to study the effect of impurity scattering on regions of the Fermi surface where wave functions vary significantly in symmetry character.

This paper is concerned with the analysis of such experiments assuming a muffin-tin model of the host metal and incoherent scattering by substitutional impurities. Our theoretical approach is based on a treatment of scattered Bloch states by Morgan² and a preliminary report of our method applied to silver has been published elsewhere.³ By using a partial-wave description of the host metal and of the impurity potential^{2,4} the anisotropic behavior of the Dingle temperatures (i.e., the scattering as measured in the dHvA effect) and the corresponding impurity scattering rates are analyzed in relatively straightforward terms. The scattering rate is expressed as a sum over partial-wave contributions. The discussion will be confined to alloys where only s -, p -, and d -wave scattering is important. In this case, the anisotropy of each partial-wave contribution to the scattering rate depends in a simple way on the anisotropy of the host-metal wave functions at the Fermi energy; the impurity phase shifts determine the weight factor (which we term "scattering parameter") for each partial-wave component. One can therefore make some immediate predictions of the scattering behavior. For example, the host wave function on the neck orbit contains no s -wave component, predominant p -wave, and a small amount of d -wave component, so that a scatterer of predominantly s -like character will cause little scattering of the neck electrons. In order to analyze the experimental Dingle temperature data within this framework, one must first determine, for each extremal orbit, the orbital average of the

anisotropic partial wave coefficient. Quite generally, these coefficients can be calculated from the host wave functions. However, a convenient identity exists⁵ which relates these orbitally averaged coefficients to quantities easily calculated in the course of a phase-shift analysis of the Fermi-surface data on the host metal.

This approach is strictly correct only for *s*- and *p*-like scatterers, but is a satisfactory approximation for *d*-like scatterers provided that differences between the Γ_{12} and Γ_{25} coefficients are small. Once the scattering parameters have been determined it is straightforward to invert the dHvA data to give a map of the scattering anisotropy.⁶⁻⁹ Inversion based on phase-shift analysis has several advantages over other empirical techniques. The expansion takes into account the translational symmetry of the reciprocal lattice, it is rapidly convergent in the expansion parameters, and the parameters themselves have a direct physical significance. In this paper we describe the results of a phase-shift analysis of impurity scattering in the noble metals and apply the results to interpreting anisotropic Dingle temperatures for various impurities. Our description of the electronic structure of the host metals is obtained by fitting very accurate Fermi-surface dimensions, so the calculated phase shifts should be very close to the phase shifts corresponding to the true potential at the Fermi energy. Phase-shift analysis does not give any information on the phase shifts away from the Fermi energy, but this is not important because impurity scattering is elastic and depends only on the wave functions at the Fermi surface.

A unique feature of our approach is that it yields not only the total scattering rate at each point on the Fermi surface as measured by the dHvA effect, but also $P(\vec{k}, \vec{k}')$ the probability of scattering between states \vec{k} and \vec{k}' on the Fermi surface. From $P(\vec{k}, \vec{k}')$ it is possible to calculate the residual resistivity, where the scattering probability is weighted by the momentum change involved. In addition to their intrinsic interest, resistivity calculations provide a check on the reliability of the experimental data and can be used to resolve any ambiguities in the analysis.

The calculations reported here are based on non-relativistic treatments of the host metals. For the heavier metals (gold and maybe silver) this will give inaccurate wave functions, although as a parametrization of the scattering it is probably as good as alternative schemes and should still permit calculation of the resistivity to a good approximation. Extension to the relativistic case will be discussed in a later paper.

To calculate the impurity phase shift for each partial wave from the corresponding scattering parameter, it is necessary to determine a set of co-

efficients that describes the backscattering by the lattice of a spherical wave diverging from the impurity. Earlier attempts to solve this problem were based on unsupported assumptions about the backscattering coefficients,^{3,6} but Holzwarth¹⁰ has recently calculated these coefficients from first principles for noble-metal hosts. We defer a description of these calculations and their application to determination of the impurity phase shifts to a subsequent paper. However, there is a set of *effective* ("Friedel") phase shifts which have the important properties of satisfying the Friedel sum rule and being independent of the choice of muffin-tin zero used in the analysis. We use these phase shifts to parametrize the scattering.

A determination of the impurity phase shifts by analysis of experimental data has the advantage that the self-consistent screening of the impurity by conduction electron is taken into account automatically. Any *ab initio* calculation of impurity phase shifts^{11,12} can easily be compared with our results, although care must then be exercised over the choice of the muffin-tin zero. Several previous treatments of the Dingle temperature have utilized tight-binding orthogonalized-plane-wave (OPW) parametrization schemes. Kirkpatrick¹³ was able to make rough estimates of Dingle temperatures for transition impurities in copper by using information from various band-structure calculations and independent experimental data. Riedinger¹⁴ carried out a more detailed calculation using a basis of four OPW's and Slater-type *d* orbitals where the impurity potential was represented by a model potential, the parameters of which were determined by requiring that the Friedel sum rule be satisfied. The advantage of such schemes is that in principle they can represent the extended nature of the impurity potential. In practice the potential contributions of the self-consistent charge oscillations surrounding impurity sites are very difficult to treat explicitly.

Our assumption, that the impurity potential is confined to a muffin-tin sphere within a single unit cell of the host, is a condition less stringent than it might at first appear. It has been shown that in pure metals the phase-shift parameters are an extremely weak function of the muffin-tin radius¹⁵ even for muffin-tin spheres that overlap by approximately 30%, and the same effect has been observed with the derivative. Furthermore, Andersen and Kasowski¹⁶ have shown that if the wave functions are expressed in terms of "muffin-tin orbitals," a procedure that is formally equivalent to conventional band-structure techniques, the wave functions are valid up to distances as far as the center of nearest-neighbor atoms. This implies that a phase-shift description of the scattering should be approximately independent of the muffin-tin radius

chosen to describe the potential. In principle, a sufficiently large radius can be chosen to include the short-range effects of the impurity potential. The residual effects of the impurity potential are small and are long ranged, and are qualitatively similar to those caused by the lattice distortions associated with impurity atoms of a size different from the host. According to the treatment of Blatt,¹⁷ later extended by Béal-Monod and Kohn,¹⁸ this produces a change in the charge localized round the impurity, which can be expressed as a modified Friedel sum. The important point is that the long-range part of the distortion (that part which is not accounted for by the muffin-tin potential) produces only small-angle scattering. The effect of small-angle scattering on the dHvA effect is more conveniently discussed in terms of dephasing. Although the original treatment¹⁹ incorrectly predicted an appreciable contribution from this cause, a more detailed treatment by Watts²⁰ suggests it is appreciable in only a few cases where the lattice distortion is large and potential scattering is small. The effect on the residual resistivity is very small because of the weighting term $(1 - \cos\theta_{vv})$. We therefore feel justified in performing an essentially "exact" calculation of the impurity scattering within the muffin-tin model. This approximation is ideal for the treatment of isoelectronic impurities, e.g., CuAg, AgAu, etc., and compares favorably with previous calculations for nonisoelectronic impurities.

A more important limitation of the partial-wave analysis is the assumption that the impurity potential has spherical symmetry about a lattice site. This approximation is likely to be satisfactory for close-packed metals, particularly those having cubic symmetry. Considerable modification is necessary, however, to describe scattering by interstitial impurities. Dye *et al.*⁷ have used the partial-wave approach to discuss interstitial hydrogen in copper, by assuming the impurity potential to be distributed in a spherical shell around a lattice site. A more realistic treatment, taking the impurity potential to be distributed around an interstitial site, requires an entirely different set of scattering coefficients, which must be derived from Bloch waves shifted in phase by an amount corresponding to the distance between the impurity site and a lattice point. This would require a complete recalculation of the scattering and, unfortunately, one would not be able to exploit directly the simple relationships connecting the scattering with a band-structure calculation.

II. ELECTRONIC PROPERTIES OF THE HOST METAL

In Secs. III and IV we shall show how one can analyze experimental Dingle-temperature anisotropy

data, properly taking into account departures from free-electron behavior of the host metal. It is necessary to have an accurate knowledge of the shape of the Fermi surface of the host metal. Moreover, in order to discuss scattering between states on the Fermi surface, we shall need to know the wave-function amplitudes in the initial and final states. In this section, we describe briefly how phase-shift analysis of Fermi-surface data can yield the parameters of the host metal that will be needed in the subsequent discussion of impurity scattering. It has been established that the usual approaches to the calculation of energy bands in a muffin-tin lattice, the Korringa-Kohn-Rostoker (KKR), Korringa-Kohn-Rostoker-Ziman (KKRZ), and augmented-plane-wave (APW) methods all yield rapidly converging energy eigenvalues,²¹ and for calculating surfaces of constant energy any one of these methods is likely to prove satisfactory.²² However, the KKR method alone yields a secular matrix expressed in the angular momentum representation. The eigenvector of the secular matrix at a point on the Fermi surface represents a spherical harmonic expansion of the wave function, and this is the form most naturally adopted when discussing impurity scattering. Moreover, the eigenvectors are easily normalized. We begin therefore by outlining the KKR method applied to the analysis of Fermi-surface data.

The wave function in the N th unit cell of an ideal lattice can be expanded in spherical harmonics. The result is a Bloch function of the form

$$\psi_E(\vec{k}, \vec{r}) = e^{i\vec{k}\cdot\vec{r}} \sum_{l_m} i^{l_m} \alpha_{l_m}(\vec{k}, E) \times \phi_{E l}(\vec{r}_N) Y_{l_m}(\hat{r}_N), \quad (1)$$

where ϕ is the radial wave function and r_N is the radius measured from the center of the N th unit cell. Because the potential is assumed to be spherically symmetric within nonintersecting spheres of radius r_s , and constant elsewhere, the radial wave function in the interstitial region $r_N > r_s$ is of the form

$$\phi_{E l}(r_N) = j_l(\kappa r_N) + i \sin \eta_l^h e^{i\eta_l^h} h_l(\kappa r_N), \quad (2)$$

where the energy $E = \hbar^2 \kappa^2 / 2m$ is measured with respect to the muffin-tin zero, and j_l and h_l are spherical Bessel and Hankel functions. The $\alpha_{l_m}(k, E)$ coefficients are related to the eigenvectors of the KKR secular equations

$$\sum_{l'_m} \mathfrak{K}_{l_m l'_m} V_{l'_m}^0 = \lambda^0 V_{l_m}^0 = 0, \quad (3)$$

where

$$\mathfrak{K}_{l_m l'_m} \equiv \cot \eta_l^h \delta_{l_m l'_m} + (1/\kappa) A_{l_m l'_m}(\vec{k}, E) \quad (4)$$

is the KKR matrix. The lattice potential enters only through the phase shifts η_l^h . Details of the

TABLE I. Fermi energy parameter (E_F) and phase shifts used to parametrize the Fermi surfaces of the noble metals. The lattice constants used in the calculation are also given.

	Fermi energy parameter (Ry)	Phase shifts (rad)				Lattice constant (Å)
		η_0	η_1	η_2	η_3	
Copper	0.55	0.063779	0.126115	-0.116754	0.000753	3.60301
Silver	0.41	0.19356	0.11459	-0.099705	0.000868	4.06920
Gold	0.41	0.449356	0.155318	-0.142485	0.00468	4.06520

calculation of the structure-dependent matrix elements $A_{lm'l'm}(\vec{k}, E)$ are readily available.²³ When applied to the phase-shift analysis of experimental Fermi surface data, surfaces of constant energy $E(\vec{k})=E$ are determined from the locus of k vectors which satisfy $\lambda^0(\vec{k}, E)=0$. The phase shifts η_l^h are treated as parameters, and adjusted to bring a surface of constant energy $E(\vec{k})=E_F$ into agreement with the Fermi-surface data. In this way a set of phase shifts can be deduced which characterizes the interaction between the conduction electrons and the lattice. The phase shifts depend on the choice of the Fermi-energy parameter E_F , but are uniquely defined for a given value of E_F . It has been shown elsewhere²⁴ that different choices of E_F correspond to different ways of representing the crystal potential and that in first approximation all values of E_F lead to equivalent results. There are, however, small differences in the treatment of the interstitial potential for different values of E_F and calculations show that the best approximation to the true crystal potential in the noble metals is obtained with a value of E_F close to the minimum perturbation value. This motivated our choices of E_F in Table I, where we report phase shifts determined by fitting the major cross-sectional areas of the Fermi surfaces of copper, silver, and gold as measured by the dHva effect.²⁵ Comparison of the fit with the experimental frequencies is made in Table II and the phase shifts are in good agreement with other fits.²² Although, as we demonstrate below, calculation of the impurity scattering is also independent of the choice of E_F , the values given in Table I have the additional advantage of allowing direct comparison with previous scattering calculations.^{6,8,9}

If, for a given \vec{k} and E , the eigenvector $V_{lm}(\vec{k}, E)$ is normalized to unity, i. e.,

$$\sum_{lm} |V_{lm}^0(\vec{k}, E)|^2 = 1, \quad (5)$$

then the corresponding Bloch expansion coefficients can be calculated from the expression¹⁰

$$\alpha_{lm}(\vec{k}, E) = \frac{V_{lm}^0(\vec{k}, E)}{[(\hbar^2/2mk)(-\partial\lambda^0/\partial E)]^{1/2} i^l \sin\eta_l^h e^{i\eta_l^h}}. \quad (6)$$

These coefficients yield Bloch wave functions that are normalized to unity²³ within a unit cell of volume Ω :

$$\int_{\Omega} |\psi_E(\vec{k}, \vec{r})|^2 d^3r = 1. \quad (7)$$

Since within our model the impurity site is characterized by the full point symmetry of the lattice, we shall find it convenient to express wave functions in the cubic harmonic representation, which is related to the spherical-harmonic representation by a unitary transformation:

$$Y_{l\Gamma\gamma}(\hat{r}) = \sum_m U_{lm}^{l\Gamma\gamma} Y_{lm}(\hat{r}), \quad (8)$$

where Γ denotes the representation and γ is a particular member of that representation. Expanding the Bloch wave function of Eq. (1) in cubic harmonics yields

$$\psi_E(\vec{k}, \vec{r}) = e^{i\vec{k}\cdot\vec{R}_N} \sum_{l\Gamma\gamma} i^l a_{l\Gamma\gamma}(\vec{k}, E) \phi_{E1}(\vec{r}_N) Y_{l\Gamma\gamma}(\hat{r}_N), \quad (9)$$

where

$$a_{l\Gamma\gamma}(\vec{k}, E) = \sum_m (U_{lm}^{l\Gamma\gamma})^{-1} \alpha_{lm}(\vec{k}, E). \quad (10)$$

Explicit expressions for the wavefunction amplitudes corresponding to $l \leq 2$ in the cubic harmonic representation are²⁶

$$\begin{aligned} a_{0\Gamma_1} &= \alpha_{00}, \\ a_{1\Gamma_{15^x}} &= (1/2)^{1/2} (\alpha_{1-1} - \alpha_{11}), \\ a_{1\Gamma_{15^y}} &= -i(1/2)^{1/2} (\alpha_{1-1} + \alpha_{11}), \\ a_{1\Gamma_{15^z}} &= \alpha_{10}, \\ a_{2\Gamma_{12^u}} &= \alpha_{20}, \\ a_{2\Gamma_{12^v}} &= (1/2)^{1/2} (\alpha_{2-2} + \alpha_{22}), \\ a_{2\Gamma_{25^t}} &= -i(1/2)^{1/2} (\alpha_{2-1} + \alpha_{21}), \\ a_{2\Gamma_{25^t\eta}} &= (1/2)^{1/2} (\alpha_{2-1} - \alpha_{21}), \\ a_{2\Gamma_{25^t\epsilon}} &= -i(1/2)^{1/2} (\alpha_{2-2} - \alpha_{22}). \end{aligned} \quad (11)$$

III. CALCULATION OF SCATTERING PARAMETERS

For a single impurity atom, the scattering probability $P(\vec{k}, \vec{k}')$ between Bloch states \vec{k} and \vec{k}' can

be expressed in the form of the golden rule

$$P(\vec{k}, \vec{k}') = \frac{2\pi}{\hbar N^2} |T_{\vec{k}\vec{k}'}|^2 \delta[E(\vec{k}) - E(\vec{k}')] \quad , \quad (12)$$

where N is the number of primitive unit cells in the crystal,²⁷ and where, following Morgan,² the transition matrix is given by

$$T_{\vec{k}\vec{k}'}(E) = -\frac{\hbar^2}{2m\kappa} \sum_{L,\gamma} a_{L\gamma}^*(\vec{k}', E) a_{L\gamma}(\vec{k}, E) \times A_{L\gamma}(\vec{k}, E) \sin\Delta\eta_l e^{i\Delta\eta_l} \quad . \quad (13)$$

Here, for brevity, L denotes l , Γ and, because we are interested in scattering between states on the Fermi surface, the expression is evaluated at $E = E_F$. $\Delta\eta_l \equiv \eta_l^i - \eta_l^h$ is the difference between the impurity phase shift and the host phase shift for a given l . $A_{L\gamma}(\vec{k}, E)$ is the renormalization factor, $(1 + \sum T b/a)$ in Morgan's notation, which describes the effects of backscattering by the host lattice. Its significance is that the wave-function amplitude in the impurity cell takes the form [cf. Eq. (9)]

$$\psi_E^I(\vec{k}, \vec{r}) = e^{i\vec{k}\cdot\vec{r}_I} \sum_{L\gamma} i^l a_{L\gamma}(\vec{k}, E) A_{L\gamma}(\vec{k}, E) \times \phi_{E l}^I(\vec{r}_I) Y_{L\gamma}(\hat{r}_I) \quad , \quad (14)$$

where $\phi^I(\vec{r}_I)$ is the radial wave function in the impurity cell. In the present paper we shall assume that scattering into partial waves $l \geq 3$ can be neglected. The impurity site is characterized by cubic symmetry so that, in general, angular momentum is not a good quantum number. However, for $l \leq 2$, each representation of the cubic point group is associated with only a single angular momentum state, so the renormalized impurity wave amplitude must be directly proportional to the corresponding Bloch wave amplitude. Then the renormalization factor takes the simple form

$$A_{L\gamma}(k, E) \equiv A_L(E) \quad , \quad l \leq 2 \quad . \quad (15)$$

If f -wave scattering is included however, the impurity wave amplitude of symmetry Γ_{15} contains contributions for the $l=1$ and $l=3$ components of the Bloch wave, and the simple proportionality between the renormalized impurity wave amplitude and the Bloch wave amplitude no longer applies. Blaker and Harris⁴ also introduce a factor $A_L(E)$, but with a different normalization. Their term $N_L^i N_L A_L(E)$ is equivalent to our term $A_L(E) e^{i\Delta\eta_l}$ and for $l \geq 3$, their $A_L(E)$ must be interpreted as a matrix multiplying the Bloch wave coefficients of different l belonging to a given representation.

It is convenient to introduce the scattering parameters

$$S_L \equiv A_L \sin\Delta\eta_l e^{i\Delta\eta_l} \quad . \quad (16)$$

Then the forward-scattering matrix element of the T matrix can be written in the form

$$T_{\vec{k}\vec{k}} = -\sum_L t_k^L S_L \quad , \quad (17)$$

where

$$t_k^L = \frac{\hbar^2}{2m\kappa} \sum_{\gamma} |a_{L\gamma}(\vec{k})|^2 \quad . \quad (18)$$

The inverse relaxation time due to impurity scattering at a point k on the Fermi surface due to scattering by an atomic fraction c of impurities is given by

$$1/\tau(\vec{k}) = -(2c/\hbar) \text{Im} T_{\vec{k}\vec{k}} \quad (19)$$

$$= (2c/\hbar) \sum_L t_k^L \text{Im} S_L \quad , \quad (20)$$

where it is assumed that the impurities scatter independently.

Using Eqs. (6) and (18), t_k^L can be expressed in terms of the eigenvalues and eigenvectors of the KKR secular matrix

$$t_k^L = \frac{\sum_{\gamma} |V_{L\gamma}^0(\vec{k}, E)|^2}{\sin^2 \eta_l^h [-\partial \lambda^0(\vec{k}, E)/\partial E]} \quad . \quad (21)$$

This is the most convenient form for direct evaluation of the t_k^L coefficients. Alternatively, if we ignore the distinction between different representations of the cubic group for each angular momentum l , the t_k^L can be obtained from the identity

$$t_k^L \equiv \sum_{\Gamma} t_k^{l\Gamma} = \left(\frac{\partial k}{\partial \eta_l^i} \right)_{E_F} \hbar v_k \quad , \quad (22)$$

where v_k is the Fermi velocity at wave vector \vec{k} , and $(\partial k/\partial \eta_l^i)_{E_F}$ is the derivative of the wave vector \vec{k} with respect to the host phase shift η_l^i .

The experimental quantity, the Dingle temperature X , is a weighted average of $1/\tau(\vec{k})$ around the orbit and can be written

$$m_c X = \frac{\hbar^3}{4\pi^2 k_B} \oint_{\text{orbit}} k \frac{dk}{dE} \frac{1}{\tau} d\theta \quad (23)$$

$$= \frac{\hbar^2 c}{2\pi^2 k_B} \sum_L \text{Im} S_L \oint_{\text{orbit}} k \frac{t_k^L}{v_k} d\theta \quad . \quad (24)$$

In order to determine the scattering parameters $\text{Im} S_L$ from experimental Dingle-temperature data, it is necessary to evaluate the orbital averages of t_k^L , and numerical integration is feasible. However, whenever the identity is applicable a useful simplification is obtained by substituting Eq. (22) in Eq. (24). Then the Dingle temperature is given by

$$m_c X = \frac{\hbar^2 c}{2\pi^2 k_B} \sum_L \text{Im} S_L \left(\frac{\partial \alpha}{\partial \eta_l^i} \right)_{E_F} \quad , \quad (25)$$

where the coefficients $(\partial \alpha/\partial \eta_l^i)_{E_F}$ are the derivatives of the area of the orbit with respect to the phase shifts. Not only are these coefficients readily available from a phase-shift analysis of Fermi-surface data, but also they can be calcu-

TABLE II. Comparison between experimental and fitted de Haas-van Alphen frequencies in units of 10^8 G. Also given are the derivatives of the areas in units of free-electron area per radian. The derivatives are related to the Dingle temperatures X by $m^*X/c = \alpha \sum_l (\partial \alpha / \partial \eta_l) \text{Im} S_l$ where α is 261.4, 204.9 and 205.3 K/at. % for copper, silver, and gold, respectively. The notation for the orbits is B belly, N neck, R rosette, D dogbone, T - P the turning point in the (110) plane, and S - P the saddle-point in the (100) plane.

	B_{100}	B_{111}	N_{111}	R_{100}	D_{110}	T - P	S - P
Copper							
Experiment ^a	5.99551	5.80724	0.217357	2.46035	2.50947		
Fit	5.99543	5.80728	0.217373	2.46020	2.50948		
$\partial \alpha / \partial \eta_0$	0.304	0.264	0	-0.185	-0.188	0.280	0.290
$\partial \alpha / \partial \eta_1$	0.965	0.872	0.585	-1.058	-1.128	0.919	0.938
$\partial \alpha / \partial \eta_2$	2.270	2.726	0.361	-2.219	-1.840	2.378	2.318
Silver							
Experiment ^a	4.74508	4.60573	0.089232	1.96122	2.01324		
Fit	4.74507	4.60573	0.089233	1.96122	2.01330		
$\partial \alpha / \partial \eta_0$	0.322	0.287	0	-0.210	-0.211	0.295	0.305
$\partial \alpha / \partial \eta_1$	0.926	0.845	0.646	-1.260	-1.310	0.901	0.908
$\partial \alpha / \partial \eta_2$	2.373	2.795	0.201	-2.272	-1.944	2.470	2.409
Gold							
Experiment ^a	4.84309	4.49280	0.153119	2.00148	1.93579		
Fit	4.84309	4.49279	0.153120	2.00086	1.93580		
$\partial \alpha / \partial \eta_0$	0.346	0.325	0	-0.246	-0.205	0.289	0.306
$\partial \alpha / \partial \eta_1$	0.784	0.581	0.370	-0.730	-0.845	0.679	0.717
$\partial \alpha / \partial \eta_2$	3.204	3.749	0.412	-3.204	-2.444	3.198	3.091

^aReference 25.

lated without explicit consideration of either the host wave functions or the Fermi velocities. For $l < 2$ there is only a single representation of the cubic group for each partial wave, so Eqs. (22) and (25) are exact. For d waves there are two representations, Γ_{12} and $\Gamma_{25'}$ and correspondingly two values of $\text{Im} S_L$. Only if these values are equal is the use of the identity strictly valid. A quantitative estimate of the error in using the identity with $l=2$ can be made in any particular case if the renormalization factors A_L are known, and this will be discussed more fully in a subsequent paper. Preliminary estimates show that for weak d scattering in noble-metal hosts, the use of the identity is valid and it may well be an adequate approximation even for strong scattering.

As written, Eqs. (20) and (22)–(25) depend upon quantities determined from a band-structure calculation at the Fermi energy. In a real metal the cyclotron mass m^* , the Fermi velocity v_k^* , the apparent scattering rate due to impurities $1/\tau^*(\vec{k})$, and the Dingle temperature X^* are all renormalized by the electron-phonon interaction. (We shall use an asterisk to denote renormalized quantities.) It is important to determine how these equations must be modified to take into account the electron-phonon interaction.

Because of the scattering of electrons by phonons, the probability that a given initial Bloch state $E(\vec{k})$ is occupied must be less than unity. It

is convenient to describe this effect as a renormalization of the Bloch wave amplitude by a real anisotropic factor $\beta(\vec{k})$. The renormalized transition matrix must satisfy the optical theorem, so that [see Eq. (30) below]

$$\beta^2(\vec{k}) \text{Im} T_{\vec{k}\vec{k}} = -\frac{\Omega \beta^2(\vec{k})}{8\pi^2} \int \frac{\beta^2(\vec{k}') |T_{\vec{k}\vec{k}'}|^2 dS_{k'}}{h v_{k'} / [1 + \lambda(\vec{k})]} \quad (26)$$

for all k . But the single-particle transition matrix must also satisfy the optical theorem, so we infer that the renormalization of the Fermi velocity is compensated by renormalization of the wavefunction amplitude, i. e.,

$$\beta^2(\vec{k}) = 1 / [1 + \lambda(\vec{k})] \quad (27)$$

This simple argument can be justified by more detailed analysis. It follows that the ratio t_k^L / v_k which appears in Eq. (24) is unaffected by the electron-phonon interaction, and that Eq. (25) is still correct. Moreover, the experimental quantities $\tau_k v_k$ and $m_c X$ are unaffected by the electron-phonon interaction, in agreement with previous discussions.²⁸ So the renormalized impurity scattering rate $1/\tau^*(\vec{k})$ can be determined from the Dingle-temperature data by use of

$$t_k^L = \frac{\hbar \vec{v}_k^* \sum_{\alpha} |V_{L\alpha}^0(\vec{k}, E)|^2}{\sin^2 \eta_l^* [\partial \lambda^0(\vec{k}, E) / \partial \vec{k}]_{E_F}} \quad (28)$$

or

$$t_k^{i*} = \bar{w}_k^* (\partial \bar{\alpha} / \partial \eta_i)_{E_F} \quad (29)$$

A. Partial scattering coefficients

The coefficients $(\partial \alpha / \partial \eta_i)_{E_F}$ that appear in the expansion of the Dingle temperature are given for several high-symmetry orbits of the noble metals in Table II. Partial scattering rates (t_k^i / v_k) calculated at 19 points with a $\frac{1}{48}$ sector of the Fermi surface using Eq. (22) are listed in the Appendix. These results are derived from nonrelativistic phase-shift analyses of Fermi-surface data using the phase shifts and Fermi energy in Table I. The results quoted here were obtained from a 40×40 APW secular determinant, and direct comparison with KKR calculations showed differences of about 1–2% in the scattering. Tests with larger APW secular determinants confirm that the partial scattering rates are converged to 1–2%.

The results presented here can be compared with other calculations. For copper, Coleridge⁶ used a very similar potential in a KKRZ calculation. Discrepancies of approximately 5% are attributed to slow convergence of the KKRZ method. Harris⁸ also used a very similar potential, and agreement with his results is typically better than 10%. For silver and gold, Harris and Mulimani⁹ have carried out calculations based on empirical potentials, and their results show the same general behavior as ours, although discrepancies in the anisotropy are as great as a factor of 2 in certain directions, especially in gold. The absolute magnitudes of their partial scattering rates are different from ours, and they do not quote the normalization factors required to compare their results with ours and to calculate scattering phase shifts.

B. Optical theorem

The optical theorem²⁹ is an expression of the conservation of particle flux in a scattering process. It states that the rate of scattering from a given state \vec{k} is equal to an integral of the probability that an electron from state \vec{k} will be scattered to any other state \vec{k}' :

$$\text{Im} T_{\vec{k}\vec{k}'} = -\frac{\Omega}{8\pi^2} \int \frac{|T_{\vec{k}\vec{k}'}|^2 dS_{k'}}{\bar{w}_{k'}} \quad (30)$$

The optical theorem imposes a constraint on the scattering parameters S_L . Substituting Eqs. (13) and (16) in Eq. (30), it is easy to show that

$$\text{Im}(S_L) = |S_L|^2 I_L(E_F) \quad (31)$$

or, equivalently,

$$\text{Im}(S_L^{-1}) = -I_L(E_F) \quad (32)$$

where I_L is defined by

$$I_L(E_F) = \frac{\hbar^2}{2mk} \frac{\Omega}{8\pi^2} \int \frac{|a_{L\gamma}(\vec{k}, E_F)|^2 dS_k}{\bar{w}_k} \quad (33)$$

$$= \frac{1}{n(L)} \frac{\Omega}{8\pi^2} \int \frac{t_k^L dS_k}{\bar{w}_k} \quad (34)$$

where $n(L)$ is the degeneracy of the representation Γ . $I_L(E_F)$ depends only on t_k^L / v_k and, according to Eq. (22), $t_k^i / \bar{w}_k = (\partial \bar{\alpha} / \partial \eta_i)_{E_F}$ (we recall that this equation holds even in the presence of the electron-phonon interaction). Thus I_L can be calculated from quantities which depend only on the phase shifts of the host metal at the Fermi energy. The evaluation of I_L is described more fully in the Appendix.

As we have seen, the effect of the dilute substitutional impurities in a given host is characterized by the scattering parameters

$$S_L \equiv A_L \sin \Delta \eta_i e^{i \Delta \eta_i} \quad (16)$$

whose imaginary parts $\text{Im} S_L$ can be determined from the observed Dingle-temperature anisotropies. The optical theorem sets an additional constraint on the scattering parameters, given by Eq. (32). If A_L is written in the form

$$A_L = |A_L| e^{i \theta_L} \quad (35)$$

in Eq. (16), then requiring that the resulting expression for the scattering parameters should satisfy the constraint given by Eq. (32), we find

$$S_L = I_L^{-1} \sin \phi_L e^{i \phi_L} \quad (36)$$

where we have introduced the effective phase shifts ϕ_L , defined by

$$\phi_L \equiv (\Delta \eta_i + \theta_L) \quad (37)$$

Assuming I_L has been calculated for the host metal, experimental Dingle-temperature anisotropies can be interpreted to yield the values of $\sin^2 \phi_L$, but an ambiguity of sign occurs in the values of ϕ_L . Fortunately, this ambiguity can usually be resolved by requiring that the calculated impurity resistivity should be consistent with the experimental value and that the screening charge has the correct sign. Such calculations will be described more fully in Secs. III D and IV.

We conclude this section by showing how quantities which describe impurity scattering in our model depend on the choice of the Fermi-energy parameter E_F , which is an undetermined parameter in a phase-shift analysis of the host metal. The electron-phonon interaction is fully taken into account in this discussion. It has been found that over a wide range of values of E_F , the partial scattering rate t_k^L / v_k has a constant anisotropy with a multiplicative scaling factor which depends weakly on the choice of E_F .⁵ Recalling that $t_k^{L*} / v_k^* = t_k^L / v_k$, Eq. (34) can be rewritten to express I_L as a Fermi surface average of t_k^{L*} / v_k^* . Combining

these results it follows that $t_k^{L^*}/I_L$ must be independent of E_F . Furthermore, the value of S_L must depend on E_F in such a way that the observed partial scattering rate $\text{Im}S_L t_k^{L^*}$ is independent of E_F , so $S_L I_L$ must also be independent of E_F . It follows therefore that the effective phase shifts of ϕ_L , derived from $S_L I_L$ in Eq. (36), have the important property of being independent of the choice of Fermi parameter E_F .

C. Friedel sum rule

The Friedel sum rule describes the displacement of conduction charge in the vicinity of a charged impurity immersed in an electron gas. Friedel³⁰ showed that if the impurity is immersed in a free-electron gas the scattering phase shifts must satisfy the condition

$$\mathcal{F} = (2/\pi) \sum_l (2l+1) \eta_l(E_F) \quad , \quad (38)$$

where \mathcal{F} is the number of electrons displaced in the vicinity of the impurity. Langer and Ambegao-kar³¹ have discussed the form taken by the Friedel sum rule for an impurity placed in a gas of interacting electrons in a metallic lattice. They found that the number of displaced electrons is given by

$$\mathcal{F} = (2\pi i)^{-1} \text{Tr} \ln S(E_F) \quad , \quad (39)$$

where S is the S matrix, which is related to the T matrix by

$$s_{\vec{k}\vec{k}'}(E_F) = \frac{(2\pi)^3}{N\Omega} \delta(\vec{k} - \vec{k}') - \frac{2\pi i}{N} \delta(E_{\vec{k}} - E_{\vec{k}'}) T_{\vec{k}\vec{k}'} \quad . \quad (40)$$

It will be shown in a later paper¹⁰ that the eigenvalues of the S matrix are

$$s_L = (S_L/S_L^*) \quad , \quad (41)$$

where S_L are the scattering parameters introduced in Eq. (16). Substituting in Eq. (41) and evaluating the trace yields

$$\mathcal{F} = (2/\pi) \sum_L n(L) \tan^{-1} (\text{Im}S_L/\text{Re}S_L) \quad (42)$$

$$= (2/\pi) \sum_L n(L) (\Delta\eta_L + \theta_L) \quad (43)$$

$$= (2/\pi) \sum_L n(L) \phi_L \quad , \quad (44)$$

where we have introduced Friedel phase shifts ϕ_L which are equal to the effective phase shifts discussed above [Eq. (37)]. It was shown in Sec. III B that the Friedel phase shifts ϕ_L , and hence the displaced charge \mathcal{F} , are independent of the choice of the Fermi-energy parameter E_F in the phase-shift analysis of the host metal. Equivalent phase shifts have been introduced by Lasseter and So-ven.¹²

This form of the sum rule assumes negligible distortion of the lattice surrounding the impurity. We extend the treatment to real alloys with lattice distortions by identifying \mathcal{F} with the modified sum rule first introduced by Blatt.¹⁷ Such an extension is approximate and certainly goes beyond the muffin-tin model, although the corrections are frequently small.

D. Calculation of residual resistivity

The resistivity ρ of an isotropic metal can be expressed as a Fermi-surface integral of the vector mean free path $\vec{\Lambda}_k$:

$$\frac{1}{\rho} = \frac{e^2}{12\pi^3 \hbar} \int_{\text{FS}} \vec{v}_k \cdot \vec{\Lambda}_k \frac{dS_k}{v_k} \quad . \quad (45)$$

The vector mean free path can be calculated by iterative solution of the equation

$$\vec{\Lambda}_k = \tau_0(\vec{k}) \left(\vec{v}_k + cN \sum_{\vec{k}'} P(\vec{k}, \vec{k}') \vec{\Lambda}_{\vec{k}'} \right) \quad , \quad (46)$$

where

$$\tau_0(k) = \left(cN \sum_{\vec{k}'} P(\vec{k}, \vec{k}') \right)^{-1} \quad . \quad (47)$$

Using as starting values $\vec{\Lambda}_k = \vec{v}_k \tau_0(k)$ it has been shown⁶ that for copper the solution converges within a few iterations, and that the direction of the resulting vector mean free path deviates very little from the direction of the velocity. Furthermore, a good approximation to the resistivity is obtained by assuming that the vector mean free path is in the same direction as the velocity, and given by

$$\frac{1}{\Lambda_k} = \frac{cN}{v_k} \sum_{\vec{k}'} P(\vec{k}, \vec{k}') (1 - \cos\theta_{v\vec{v}'}) \quad (48)$$

where $\theta_{v\vec{v}'}$ is the angle between \vec{v}_k and $\vec{v}_{\vec{k}'}$. Using Eq. (12) for $P(\vec{k}, \vec{k}')$, with an atomic fraction of impurities c , yields

$$\frac{1}{\Lambda_k} = \frac{\Omega c}{4\pi^2 \hbar v_k} \oint_{\text{FS}} |T_{\vec{k}\vec{k}'}|^2 (1 - \cos\theta_{v\vec{v}'}) \frac{dS_{\vec{k}'}}{\hbar v_{\vec{k}'}} \quad (49)$$

in terms of which the resistivity is given by

$$\frac{1}{\rho} = \frac{e^2}{12\pi^3 \hbar} \oint_{\text{FS}} \Lambda_k dS_k \quad . \quad (50)$$

In practice the term $|T_{\vec{k}\vec{k}'}|^2 \cos\theta_{v\vec{v}'}$ is expanded in terms of the form $d_{LL'}(\vec{k}) d_{LL'}(\vec{k}')$ proportional to $\sum_{\gamma, \gamma', i} |a_{L\gamma}(\vec{k})|^2 |a_{L'\gamma'}(\vec{k}')|^2 v_i v'_i$, where v_i is (v_x/v) , (v_y/v) , or (v_z/v) . Use of symmetry properties leads to a significant simplification and only terms with $|l-l'|=1$ remain. The expression for the mean free path can be written in the form

$$\frac{1}{\Lambda_k} = \frac{1}{v_k \tau_0(\vec{k})} - 2c \sum_L \frac{d_{LL'}}{v_k} J_{LL'} \text{Re}(S_L S_{L'}^*) \quad (51)$$

where L' is such that $|l-l'|=1$. Here the wavefunction dependence of $P(\vec{k}, \vec{k}') \cos\theta_{v\vec{v}'}$ is written

as a product of $d_{LL'}(\mathbf{k})$ (defined as a sum over x , y , and z directions of $|a_{L'}(\mathbf{k})|^2 v_i$) and an average value $J_{LL'}$, analogous to I_L :

$$J_{LL'} = \frac{\hbar^2 \Omega}{16\pi^2 m \kappa} \int_{\text{FS}} \frac{d_{LL'}(\mathbf{k}) dS_{\mathbf{F}}}{\hbar v_{\mathbf{k}}} . \quad (52)$$

This integral involves only the quotient $d_{LL'}/v_{\mathbf{k}}$, so that evaluating the mean free path does not require that one know the velocity $v_{\mathbf{k}}$ explicitly. Also, by using the arguments above, it can be shown that electron-phonon enhancement terms cancel out. The impurity contribution $\text{Re}(S_L S_L^*)$ can be written as $\sin\phi_L \sin\phi_{L'} \cos(\phi_L - \phi_{L'})/I_L I_{L'}$, and it is easy to show that the calculated resistivity is independent of the choice of $E_{\mathbf{F}}$.

Values of $d_{LL'}/v_{\mathbf{k}}$ and $J_{LL'}$ are listed in the Appendix. To calculate the impurity resistivity from the scattering parameters $\text{Im}S_L$ requires an evaluation of $\Lambda_{\mathbf{k}}^{-1}$ at each point on the Fermi surface from the Friedel phase shifts ϕ_L , and a summation of $\Lambda_{\mathbf{k}} \Delta S$ over the Fermi surface. A suitable mesh for integration is given in the Appendix.

IV. ANALYSIS OF EXPERIMENTAL RESULTS

The experimental Dingle-temperature anisotropies of dilute noble-metal alloys have been interpreted to yield the scattering parameters $\text{Im}S_i$. The data were fitted in a least-squares sense to Eq. (25), using the coefficients ($\partial\alpha/\partial\eta_i$) listed in Table II together with experimental values of the cyclotron masses.³² The differences between the Γ_{12} and Γ_{25} representations were neglected because the available experimental data are not sufficiently precise to distinguish between them.

A difficulty in this type of analysis is the lack of independence of the s , p , and d partial scattering rates that is encountered in practice. Poulsen *et al.*³³ note, for example, that in copper, 6.5 times the s rate plus 0.63 times the p rate reproduces the d rate to within 11%. To resolve such ambiguities the impurity resistance was calculated. Because this involves mixing between the various partial scattering rates, it was then possible to choose one set of scattering parameters that, within experimental accuracy, gave not only the correct Dingle temperatures but also the correct resistivity.

Resistivity calculations also help to determine the signs of the Friedel phase shifts ϕ_L . The dHvA scattering, which is proportional to $\sin^2\phi_L$ gives no information about the signs of the phase shifts, but the resistivity often depends sensitively on the relative signs and can be used to eliminate most combinations of signs. To obtain the absolute signs it is necessary to appeal to the Friedel sum rule, because reversing the signs of *all* the phase shifts leaves the calculated resistivity unchanged.

Two complementary homovalent alloy pairs, Ag(Au)/Au(Ag) and Cu(Au)/Au(Cu) are included in our analysis. If lattice distortions are neglected, the impurity potentials can be approximated by potential wells of strength equal to the difference in the binding energies of the two metals, and screened by the conduction electrons. In homovalent alloys the impurity potentials are weak, the scattering phase shifts are linear in the impurity potentials, and the corresponding phase-shift differences $\Delta\eta_i$ for complementary alloy pairs are expected to be of opposite sign. Therefore, whenever backscattering corrections are small, the analysis of data for complementary alloy pairs provides a useful check on the signs and approximate magnitude of the Friedel phase shifts.

Results of the analysis of Dingle-temperature data are summarized in Table III, where values of the scattering parameters $\text{Im}S_i$ are given, together with the corresponding Friedel phase shifts and the calculated resistivity. The results for the various alloys are discussed in detail below.

A. Copper-based alloys

The most recent and most accurate results in copper-based alloys are those of Poulsen, Randles, and Springford,³³ hereafter denoted as PRS. They have measured the Dingle-temperature anisotropies in the Cu(Ni), Cu(Ge), and Cu(Au) systems, and analyze their results both in terms of an empirical Fourier expansion and also by the phase-shift technique. We use the results of their phase-shift analysis, but prefer to express the quality of fit as an rms error in the deviation between experimental results and fit rather than as an error in the fractional deviation. To express the rms error as a percentage we divide by the mean Dingle temperature. We believe that this is a slightly more appropriate procedure because it is the absolute experimental errors, rather than the fractional errors, that are approximately constant. In fact, the resulting percentage errors are generally close to those quoted by PRS.

The maps of scattering anisotropy given by PRS are in good agreement with those obtained by the phase-shift inversion scheme, so we do not present maps of our results. The agreement is typically better than 10% except near $\langle 100 \rangle$ where our maps are somewhat more peaked than those of PRS.

1. Cu(Ni)

The rms error in the experimental data quoted by PRS is 10.8%. Fitting our data with only a d -wave phase shift, we find that the rms deviation between fit and experiment is 7.4%, whereas the best fit with s -, p -, and d -phase shifts gives an rms error of 5.3%. Assuming d -wave scattering

TABLE III. Analysis of Dingle-temperature results. Z_{Blatt} denotes the expected valence difference using Blatt's procedure (Ref. 17). The scattering parameters $\text{Im}S_j$ are fitted to the experimental Dingle temperatures as discussed in the text and ϕ_j are the corresponding "Friedel phase shifts." The calculated Friedel sum \mathcal{F} and resistivity ρ_{calc} should be compared with Z_{Blatt} and the ρ_{expt} , the experimental resistivity. For the results denoted "phase smearing," the experimental neck scattering has been decreased to allow for possible phase smearing effects. For each alloy the "best" set of phase shifts is underlined.

Alloy	Z_{Blatt}	ρ_{expt} ($\mu\Omega$ cm/at. %)	$\text{Im}S_0$	$\text{Im}S_1$	$\text{Im}S_2$	ϕ_0	ϕ_1 (rad)	ϕ_2	\mathcal{F}	ρ_{calc} ($\mu\Omega$ cm/at. %)
Cu(Ni)	-0.94	1.11 ^a	0	0	0.0605	0	0	-0.259	-0.83	1.19
			0.008 ₅	0.001 ₇	0.059 ₇	<u>-0.069</u>	<u>-0.038</u>	<u>-0.258</u>	-0.94	1.11
Cu(Ge)	2.81	3.79 ^a	0	0.599	0	0	0.785	0	1.49	5.14
			0.04	0.553	0.029	<u>0.15</u>	<u>0.748</u>	<u>0.18</u>	2.09	3.79
Cu(Au)	-0.32	0.55 ^a	0.0585	0.009	0.0194	<u>0.182</u>	<u>-0.087</u>	<u>-0.147</u>	-0.52	0.55
						0.182	0.087	-0.147	-0.19	0.69
			(phase smearing)	0.073	0.008 ₄	0.017 ₄	0.203	-0.084	-0.139	-0.47
Cu(Fe)	0	0	0.59	<u>0</u>	<u>0</u>	<u>-0.93</u>	-1.47 ^b	12.0
Ag(Au)	0	0.38 ^c	0.050 ₃	0.008 ₈	0.006 ₅	<u>0.176</u>	<u>0.087</u>	<u>-0.085</u>	0.01	0.39
						0.176	-0.087	-0.085	-0.32	0.39
Ag(Sn)	2.76	4.3 ^d	0.342	0.622	0	0.474	0.813	0	1.86	4.65
			0.065	0.588	0.044	<u>0.201</u>	<u>0.786</u>	<u>0.223</u>	2.34	4.30
Au(Ag)	0	0.36 ^e	0.118 ₅	0.008 ₈	0.001 ₈	<u>-0.277</u>	<u>-0.072</u>	<u>0.051</u>	-0.15	0.36
						-0.277	0.072	0.051	0.12	0.48
						-0.277	-0.072	-0.051	-0.48	0.25
Au(Cu)	0.21	0.45 ^e	0.069	0.010	0.007 ₂	<u>-0.210</u>	<u>0.077</u>	<u>0.103</u>	0.34	0.46
						-0.210	-0.077	0.103	0.05	0.48
			(phase smearing)	0.094	0.004 ₁	0.006 ₂	-0.245	0.049	0.095	0.24
Au(Zn)	1.10	0.95 ^e	0.102	0.056	0.039	<u>0.255</u>	<u>0.180</u>	<u>0.237</u>	1.26	1.00

^aReference 33.

^bFor one spin state.

^cReference 11.

^dMyers (private communication).

^eReference 42.

alone, our calculated resistivity is 1.19 $\mu\Omega$ cm/at. %, in good agreement with the value of 1.2 $\mu\Omega$ cm/at. % obtained by PRS. A linear combination of the two fits was constructed to give correctly the observed resistivity (1.11 $\mu\Omega$ cm/at. %³⁴) and to fit the data with an rms error of 6.6%, which is not significantly worse than the best three-phase-shift fit. The calculated Friedel sum $\mathcal{F} = -0.94$ is close to the valence difference $\Delta Z = -1$, and is in excellent agreement with the value predicted by Blatt's argument which takes into account the lattice strain surrounding the impurity site. The results show dominant d wave scattering which is in agreement with the predictions of an *ab initio* calculation by Harris.⁸

2. Cu(Ge)

The RMS error in the experimental data quoted by PRS is 10%. Our best fit to the data assuming only a p -wave scattering has an rms error of 10.7%, and the calculated resistivity is 5.14 $\mu\Omega$ \times cm/at. %, which is in satisfactory agreement with the value of 5.0 $\mu\Omega$ cm/at. % calculated by PRS. Addition of small s - and d -wave phase shifts re-

duced the resistivity to the experimental value, 3.79 $\mu\Omega$ cm/at. %, and the rms error of the fit fell to 9.2%.

The exact proportion of s - and d -phase shifts cannot be determined precisely, so we have chosen values that maximize the calculated Friedel sum (2.09). This is significantly lower than the value predicted by Blatt of 2.81. In this context we note that the experimental value for the specific resistivity of Cu(Ge) is an old value³⁵ and errors of ~20% in these values are not unusual [e.g., the case of Cu(Ni) cited above]. An increase in the specific resistivity would certainly increase the Friedel sum without affecting the fit to the Dingle-temperature data. However, a more reasonable explanation of the discrepancy lies in breakdown of the muffin-tin approximation in the presence of lattice distortions associated with an impurity of a different size. This means the lattice sites near the impurity will be moved from the positions they had in the host. In particular the backscattering coefficients A_L will be directly affected by the distortion so the derivation of a Friedel sum rule will be invalid. We note that the work of Béal-Monod

and Kohn,¹⁸ which improves on Blatt's argument by treating the host ions as discrete, leads to the same value for the displaced charge.

Notwithstanding the uncertainties in the *s*- and *d*-phase shifts and the incorrect Friedel sum, the analysis shows clearly the strong dominance of the *p*-wave scattering.

3. Cu(Au)

In this system precise determination of the phase shifts is a little more involved. The Friedel sum is expected to be close to zero, and therefore the signs of the phase shifts are expected to vary. There is also a large lattice distortion surrounding the impurity site, which suggests the possibility of impurity-induced phase smearing,^{19,20} but in the first instance this possibility is neglected.

The rms error in the experimental data quoted by PRS is 9%. Consideration of the electronic structures of the pure metals suggests that either *s* or *d* scattering might be dominant. Although a single *s*-phase shift does not produce an acceptable fit to the Dingle-temperature anisotropy, a single *d*-phase shift produces a reasonable fit with an rms error of 10.5%. The corresponding resistivity, $0.60 \mu\Omega \text{ cm/at.}\%$ is also close to the experimental value of 0.55. The three-phase-shift fit of PRS implies predominantly *s*-wave scattering, but this fit to the data has an rms error of 11% and is marked by an uncharacteristically bad fit to the $\langle 111 \rangle$ belly orbit. (This is one of the few instances where the different convention used by PRS yields significantly different estimates of the error.) Our preferred three-phase shift fit has, by contrast, predominant *d*-wave scattering, and yields an rms error of 9%. In particular, we find a rather good fit to the scattering on the $\langle 111 \rangle$ belly orbit. Our fit certainly provides a better least-squares fit to the data than that of PRS if our assessment of errors is adopted. The difference between the two fits might be considered a measure of the basic accuracy of the analysis.

The relative signs of the phase shifts can be determined by calculating the resistivity. The two best choices of sign are shown in Table III (the others gave resistivities of 0.27 and $0.93 \mu\Omega \text{ cm/at.}\%$) and the absolute signs of the phase shifts has been determined from the Friedel sum. The discrepancy between the calculated sum $\mathcal{F} = -0.52$, and the expected value based on Blatt's arguments, $\mathcal{F} = -0.32$ can be attributed to our nonrelativistic treatment, which ignores the relativistic effects in the heavy gold atom and to the effect of lattice distortion.

Some doubt may remain over the choice of signs, but we believe that the magnitudes of the phase shifts are fairly accurately determined. This is indicated by repeating the fit after making a phase-

smearing correction to the neck Dingle temperatures. Qualitatively the result is unchanged, although the phase shifts change by 10% or so. The scattering is seen to involve *s*-, *p*-, and *d*-phase shifts of similar magnitude, but with the anisotropy predominantly *d*-like because of the weighting factors $\sim (2l+1)$.

4. Cu(Fe)

This alloy system has a localized magnetic moment and therefore the scattering rate depends on the alignment of the impurity spins. The dHvA results^{6,36} show scattering from only one orientation of conduction electron spin, so a complete discussion would require more experimental information than that available from the Dingle temperature anisotropy. We mention the problem briefly because new results have become available,³⁶ which confirm the validity of a rather simple explanation of the observed dHvA amplitude. In an earlier treatment⁶ a single *d*-phase shift was found to account rather well for the measured scattering rate except for the scattering on the neck which was too low. More recent work³⁶ shows that on the neck (and only on the neck) the measured scattering rate is affected by a beat between oscillations arising from electrons in the two spin orientations. Furthermore, the scattering rate for the dominant spin state in the neck (121 K/at.%) is in very good agreement with results for the other orbits. Thus a single *d*-wave phase shift fits *all* the orbits with an rms error of 4% compared with the experimental error of 7%. By extrapolating from the experience in Cu(Cr),³⁷ the anisotropy of the differential scattering might also be explained by a single *d*-like term, so the two spin states should each be described by a separate *d*-phase shift which depends now on the magnetization of the impurity.³⁸ To explain the resistivity of this model (following the discussion in Ref. 6) would require introducing *s*- and *p*-phase shifts ≈ 0.15 rad, but these will have a negligible effect on the quality of the fit to the Dingle-temperature data.

B. Silver-based alloys

For silver-based alloys, we have analyzed the experimental data of Brown and Myers.³⁹ Phase-shift fits and maps of the scattering anisotropy in Ag(Au) and Ag(Sn) have been published elsewhere⁴⁰ (denoted as CL), and for these aspects of the analysis we refer the reader to Ref. 3. The experimental results for Ag(Cd) and Ag(Ge) are insufficiently extensive to justify a complete analysis, but are qualitatively the same as for Ag(Sn). In discussing the errors we adopt the same conventions as for the copper alloys.

1. Ag(Au)

The rms error experimental data of Brown and Myers is 8.5%. Our best fit with s -, p -, and d -wave scattering has an rms error of $\approx 1\%$ which is significantly better than the best fit with s and p waves alone. For two choices of sign, the resistivity calculated from the parameters of our best fit was $0.39 \mu\Omega\text{cm/at.}\%$, in good agreement with the experimental value $0.38 \mu\Omega\text{cm/at.}\%$, and was markedly different for the other possibilities. Our final choice of signs of the phase shifts gave a Friedel sum of 0.01, very close to the expected value of zero, compared with the other possibility $\mathcal{F} = -0.32$. Comparison with the host phase shifts (see CL) determines the absolute signs. Although the various phase shifts are not strictly independent, we believe that our fit is a fair representation of the true scattering and that the phase shifts are accurate to within 20%.

2. Ag(Sn)

The rms error of the revised experimental data of Brown and Myers,³⁹ as revised by Myers and quoted in CL is 6.8%. Our best least-squares fit, rejecting negative d -wave scattering as being nonphysical, had an rms error of 4%. Compared with the experimental resistivity of $4.3 \mu\Omega\text{cm/at.}\%$ this fit gave $4.65 \mu\Omega\text{cm/at.}\%$. Progressively introducing d scattering reduced the resistivity and then caused it to increase again. For the smallest d -phase shift compatible with the correct resistivity the Friedel sum was approximately 2.0, markedly lower than the expected value of 2.76. We therefore choose a stronger d -wave phase shift, which gave a Friedel sum of 2.34 and an rms error of fit of 4.2%, marginally worse than the best fit. Contrary to the discussion in CL, we do not believe it valid to use the procedure of Alfred and van Ostenburg⁴¹ to correct for higher-order phase shifts, because the d -phase shift is associated predominantly with the d -band resonance in silver. As in Cu(Ge), we attribute the discrepancy in the Friedel sum to the effects of lattice distortions.

Although the precise magnitude of the s - and d -phase shifts cannot be determined very accurately, the scattering is certainly predominantly p wave, just as Brown and Myers suggest.

C. Gold-based alloys

For gold-based alloys, we have analyzed the experimental data of Lowndes, Miller, Poulsen, and Springford⁴² (LMPS). By allowing empirically for mosaic spread in their crystals, they were able to fit with a Fourier expansion both their data taken with the magnetic field along symmetry directions and also data taken with other field orientations. The coefficients for phase-shift analysis have been

calculated only in symmetry directions. We have therefore attempted to fit (i) the experimental data in symmetry directions, and (ii) the values at symmetry directions derived from the LMPS Fourier expansion. Sometimes there were discrepancies between these two procedures which are due either to the different inversion procedure of the phase-shift analysis or to the presence of errors in the corrections for mosaic spread but these discrepancies are comparable with the errors of the data. Maps of the scattering are the same, within about 10% as those presented by LMPS. All errors for gold alloys are expressed as fractional errors, in contrast to our procedure for copper and silver alloys.

In the gold-based alloys, relativistic terms are expected to be important. Our fitting procedure is based on a nonrelativistic treatment of the host metal, and although this is probably as good as a Fourier expansion for inverting the data, the derived phase shifts will certainly be in error. A relativistic treatment of scattering in gold alloys will be presented in a later paper.

1. Au(Ag)

Our preferred fit for this alloy is the mean of (i) and (ii). Compared with an rms error of 5.6% between the data and the LMPS fit, our phase-shift fit deviates from the LMPS fit at the symmetry directions by 2.6%. Also, our fit is in rather better agreement with the experimental data in symmetry directions than the LMPS fit. Varying the signs of the phase shifts gave calculated resistivities of 0.25, 0.36, and $0.48 \mu\Omega\text{cm/at.}\%$, whereas the experimental value is $0.36 \mu\Omega\text{cm/at.}\%$. For the choice of signs giving the correct resistivity, the Friedel sum is -0.15 if the signs of the phase shifts are chosen to be the opposite of those for the complementary alloy Ag(Au). The small difference from the expected value of zero is attributed to relativistic effects.

In Au(Ag), s -wave scattering is dominant, and the phase shifts are rather similar in magnitude to those in the Ag(Au) system. Comparing the results with the work of Harris and Mulimani,⁹ a rough estimate of their normalization integrals I_i suggests that their fit to the same data yields scattering parameters that may differ by as much as a factor of 2. The differences must be associated with their rather different values for the wave functions in the neck region.

2. Au(Cu)

As in the case of Cu(Au), it is reasonable *a priori* either to take into account or to neglect the effect of impurity-induced phase-smearing on the neck scattering. The Fourier expansion of the LMPS fits their data with an rms error of 4.8%,

and our phase shift fits to the Fourier expansions with and without a phase-smearing correction have rms errors of 1.8% and 1.9%, respectively; the corresponding calculated resistivities are 0.45 and 0.46 $\mu\Omega\text{cm/at.}\%$. Therefore it is not possible to decide on this basis whether phase smearing is important. It is interesting to note that the analysis of the same data by Harris and Mulimani,⁹ whose wave functions near the neck are different from ours, yields parameters in very good agreement with those we deduced taking into account phase smearing (the agreement is within 10% as accurately as their normalization terms can be estimated).

Our choice of the signs of the phase shift as determined from the resistivity data is confirmed by calculating the Friedel sum, which is in good agreement with the expected value considering the uncertainties due to possible relativistic effects. As expected, the phase shifts, are opposite in sign to those for Cu(Au) but of comparable magnitude, making the two choices self-consistent. The scattering in Au(Cu) is predominantly *s*-like, but with appreciable *p* and *d* admixture.

3. Au(Zn)

Because of metallurgical difficulties, the experimental data of LMPS for Au(Zn) were based on samples of only one alloy concentration. The data must therefore be considered somewhat less reliable than for the other alloys. Harris and Mulimani⁹ found difficulty in fitting the data, but our fit to the data in symmetry directions has an rms error of 5.3%, which is only marginally worse than the LMPS four-term Fourier expansion with an rms error of 5.1%. Although the calculated resistivity is about 5% high, we did not consider the accuracy of the results justified our modifying the scattering parameters to achieve a better value. Considering the accuracy of the data the Friedel sum (1.26) is in good agreement with the expected value of 1.10.

4. Au(Fe)

We found it impossible to achieve a significant fit to the experimental data for this alloy. For the reasons discussed by LMPS we believe that the data do not represent scattering by isolated substitutional impurities and the present formulation of the phase-shift analysis is therefore not appropriate.

V. DISCUSSION

A phase-shift analysis of anisotropic Dingle temperature data for several dilute alloys in noble-metal hosts has yielded a satisfactory fit to the data. In most alloys a three-phase-shift fit agrees with the data as well as, or better than, other three- or four-parameter empirical inversion

schemes. The experimental impurity resistivity of each alloy is consistent with the value calculated from the phase-shift fit. Furthermore, in the complementary systems Ag-Au and Cu-Au corresponding phase shifts deduced only from the scattering data have opposite signs and comparable magnitudes, as expected on the basis of a simple model of the electronic structures of complementary alloys.

Friedel phase shifts which describe the redistribution of conduction charge on the impurity site have been determined with reasonable precision, although the uncertainty in the *s*-phase shift is large wherever *s*-wave scattering is dominated by the other *l* values. For isoelectric alloys and Cu(Ni) the values of the Friedel sum are in good agreement with the expected values, provided allowance is made for possible relativistic effects in gold. There is a substantial discrepancy in Cu(Ge) and Ag(Sn), although in these alloys the analysis demonstrates clearly the dominant *p* character of impurity scattering, and only a minor modification is needed to reproduce the experimental resistivities.

It may be that disagreement with the value of the Friedel sum predicted by Blatt's theory is a real effect which indicates a failure of the theory for large distortions. This is not just the assumption of an elastic continuum model for the host, because the improved theory which uses a point-ion model¹⁸ predicts the same displaced charge. Unfortunately, any treatment of the lattice distortion is inconsistent with the basic assumption of the muffin-tin model, which is that the lattice is unchanged except within the impurity cell. The calculation of the Friedel sum involves this approximation and any lattice distortion will surely affect the backscattering coefficients A_L in a direct fashion. We note, however, that all the discrepancies are in the sense of an *increased* displacement of charge, and the same might also be true for the Cu(Au) system when relativistic effects are taken into account.

The analysis has been restricted to the scattering of electrons, i. e., the imaginary part of the *T* matrix. An exactly parallel discussion may be applied to the real part of the *T* matrix and this can be used to analyze the changes in the size and shape of the Fermi surface observed when alloying.⁴³

In conclusion, we emphasize that the Friedel phase shifts ϕ_L are *not* the phase shifts which characterize the scattering of electrons of energy E_F by an impurity potential of muffin-tin form. These latter phase shifts are denoted $\Delta\eta_l \equiv \eta_l^i - \eta_l^r$, and the scattering parameters $S_L \equiv A_L \sin\Delta\eta_l e^{i\Delta\eta_l}$ include the very important effect of backscattering by the host lattice through the factors A_L . For

TABLE IV. Coordinates for grid over $\frac{1}{48}$ th of Brillouin zone. For points 1–15 the coordinates are the same, but points 16–19 are different for the three metals.

Point	θ (degrees)	ϕ	Point	θ (degrees)	ϕ	Point	θ (degrees)	ϕ
1	87.74	7.13	6	76.07	24.55	11	86.91	40.09
2	83.24	11.81	7	81.88	27.45	12	74.71	36.49
3	82.84	16.70	8	80.85	33.47	13	69.49	33.21
4	87.12	22.28	9	88.07	32.39	14	69.49	27.42
5	76.15	19.25	10	80.99	41.67	15	73.19	42.09
	Copper			Silver			Gold	
16	67.41	49.92	16	66.18	49.49	16	66.77	49.70
17	65.47	54.54	17	64.38	53.68	17	64.92	54.10
18	64.67	48.95	18	62.46	48.14	18	64.14	48.76
19	63.04	52.60	19	61.14	51.01	19	62.59	52.53

different choices of E_F the coefficients $\partial\alpha/\partial\eta_i$, the values of A_L and the scattering phase shifts $\Delta\eta_i$ will be different, although the Friedel phase shifts ϕ_i will be unaltered. Although the values of E_F used in the analysis were chosen to be close to the minimum perturbation values they have no particular significance either in determining the values of ϕ_i or in deriving the terms listed in the Appendix. Details of the calculation of A_L , and the relationship between the Friedel phase shifts ϕ_i and the scattering phase shifts $\Delta\eta_i$ determined with different choices of E_F , will be discussed in a subsequent paper.

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APPENDIX

To aid in analysis of experimental data, we list in Table V the terms needed to calculate, from the scattering parameters $\text{Im}S_L$, the resistivity and the scattering anisotropy. These are presented for the three noble metals and are calculated for the phase-shift parametrization summarized in Tables I and II.

Values are given along the $\langle 100 \rangle$ and $\langle 110 \rangle$ symmetry directions and on the neck. For evaluation of integrals a net of 19 points was used, distributed over the basic $\frac{1}{48}$ of the Brillouin zone, with the coordinates listed in Table IV. The wave-function coefficients $|a_L(k)|^2$ were obtained from a 40×40 APW calculation with the k vector adjusted carefully at each point to agree accurately with the

model Fermi surface. (The agreement with Halse³² radii was typically better than 0.1% but occasionally the deviation was up to 1%.) The wave functions were normalized by comparison with values of $(\partial k/\partial\eta_i)$. The estimated errors in the calculation are $\lesssim 1\%$ and errors from incomplete convergence are of the same orders.

The results in Table V are in the form $C_k t_k^L/v_k$, where $C_k (=k_f^2/2\pi\hbar; k_f$ is the free-electron Fermi radius) is chosen so that the result reduces to $(2L+1)$ in the free-electron case ($\kappa=k_f$, and $n(L)=3$ or 2 for each of the two separate d representations). In these terms the anisotropic scattering time τ_k for an atomic fraction c of impurities is given by (cf. the free-electron case)

$$(v_k\tau_k)^{-1} = (4\pi c/k_f^2) \sum_L C_k(t_k^L/v_k) \text{Im}S_L \quad (A1)$$

As explained in the text $(v_k\tau_k)^{-1}$ is unaffected by electron-phonon renormalization.

Also listed are area elements of the Fermi surface associated with each point and expressed as a fraction of the area of the free-electron sphere, i. e., as $\Delta S_k/S_f$. The integral I_L is then given by

$$I_L = n(L)^{-1} \sum_{k=1}^{19} C_k(t_k^L/v_k) (\Delta S_k/S_f) \quad (A2)$$

Provided the same band-structure parameters (E_F, η_i^A) are used these values of I_L , when calculated for silver and copper, agree within 0.1% with those obtained using a KKR calculation and with a much finer net. We note that previously published values for I_L in silver,³ and copper^{5,6} (expressed there as $1/|A_L|$) are in error by about 15%.⁴⁴

Corresponding cross terms for calculating the resistivity are given as $C_k d_{LL}^2/v_k$, normalized in the same way with the average J_{LL} , corresponding to I_L . As discussed in the text the approximate mean free path Λ_k is given by

TABLE V. Scattering coefficients and cross terms required for the resistivity together with area weights and the mean values I_L, J_{LL} . Along the symmetry directions and on the neck, only the scattering rates C_k^{LL}/v_k are given with the total rate for d scattering, i. e., the sum of the rates for the $\Gamma_{25'}$ and Γ_{12} representations.

	$\Delta S_k/S_F$	s	C_k^{LL}/v_k p	$d_{\Gamma_{25'}}$	$d_{\Gamma_{12}}$	sp	C_k^{LL}/v_k $pd_{\Gamma_{25'}}$	$pd_{\Gamma_{12}}$
Copper								
$\langle 100 \rangle$		0.651	3.925		1.679			
$\langle 110 \rangle$		0.796	1.576		7.688			
neck		0.000	7.280		4.504			
1	0.0643	0.651	3.177	1.164	1.731	0.800	0.363	1.226
2	0.0617	0.656	2.468	2.409	1.851	0.708	0.639	1.004
3	0.0569	0.669	2.157	3.102	1.996	0.678	0.763	0.908
4	0.0723	0.710	1.914	3.732	2.203	0.660	0.872	0.832
5	0.0560	0.632	2.055	3.443	2.060	0.657	0.847	0.827
6	0.0568	0.620	2.034	3.671	2.160	0.645	0.917	0.773
7	0.0543	0.693	1.839	4.066	2.314	0.647	0.957	0.747
8	0.0558	0.696	1.829	4.346	2.438	0.643	1.050	0.670
9	0.0369	0.760	1.658	4.597	2.512	0.646	1.040	0.688
10	0.0553	0.710	1.813	4.588	2.533	0.639	1.137	0.593
11	0.0565	0.780	1.610	4.908	2.627	0.645	1.128	0.608
12	0.0593	0.562	2.271	3.819	2.288	0.620	1.072	0.641
13	0.0621	0.432	2.801	3.197	2.096	0.576	1.009	0.739
14	0.0599	0.497	2.434	3.333	2.083	0.606	0.962	0.754
15	0.0466	0.497	2.540	3.590	2.228	0.591	1.105	0.612
16	0.0315	0.268	4.004	2.703	2.068	0.449	1.068	0.881
17	0.0315	0.257	4.021	2.611	2.028	0.457	1.021	0.914
18	0.0315	0.072	6.167	2.223	2.198	0.176	0.982	1.362
19	0.0315	0.068	6.183	2.196	2.188	0.184	0.960	1.377
I_L, J_{LL}		0.564	0.839	1.111	1.071	0.598	0.907	0.814
Silver								
$\langle 100 \rangle$		0.684	3.467		1.966			
$\langle 110 \rangle$		0.844	1.585		7.893			
neck		0.000	11.066		3.491			
1	0.0632	0.688	2.957	1.048	2.003	0.806	0.287	1.310
2	0.0613	0.696	2.392	2.350	2.087	0.727	0.575	1.091
3	0.0571	0.710	2.114	3.138	2.180	0.695	0.731	0.971
4	0.0729	0.752	1.902	3.857	2.321	0.680	0.855	0.883
5	0.0565	0.678	2.002	3.601	2.186	0.672	0.857	0.851
6	0.0574	0.668	1.977	3.886	2.211	0.662	0.946	0.772
7	0.0550	0.738	1.819	4.294	2.343	0.666	0.978	0.758
8	0.0567	0.741	1.810	4.616	2.360	0.650	1.082	0.682
9	0.0377	0.805	1.659	4.877	2.467	0.665	1.066	0.693
10	0.0560	0.758	1.800	4.906	2.372	0.664	1.187	0.562
11	0.0579	0.827	1.616	5.254	2.491	0.666	1.172	0.593
12	0.0586	0.621	2.203	4.091	2.147	0.654	1.138	0.588
13	0.0595	0.507	2.647	3.438	1.948	0.633	1.100	0.634
14	0.0593	0.561	2.326	3.585	2.038	0.641	1.027	0.700
15	0.0446	0.571	2.474	3.897	2.047	0.651	1.197	0.530
16	0.0370	0.325	4.073	2.625	1.661	0.542	1.163	0.719
17	0.0370	0.356	4.574	2.863	1.854	0.633	1.275	0.796
18	0.0280	0.107	7.580	1.779	1.594	0.338	1.103	1.110
19	0.0280	0.104	7.662	1.767	1.603	0.338	1.091	1.143
I_L, J_{LL}		0.618	0.854	1.164	1.053	0.641	0.948	0.791

TABLE V. (Continued)

	$\Delta S_k/S_F$	s	$C_k t_k^L/v_k$ p	$d_{\Gamma_{25'}}$	$d_{\Gamma_{12}}$	sp	$C_k d_{LL'}^k/v_k$ $p d_{\Gamma_{25'}}$	$p d_{\Gamma_{12}}$
Gold								
(100)		0.545	4.250		1.057			
(110)		1.101	1.051		11.703			
neck		0.000	4.874		5.436			
1	0.0745	0.559	2.533	2.421	1.183	0.619	0.622	0.814
2	0.0699	0.609	1.760	3.936	1.470	0.554	0.798	0.675
3	0.0594	0.660	1.505	4.686	1.796	0.550	0.853	0.652
4	0.0737	0.776	1.312	5.673	2.318	0.580	0.801	0.732
5	0.0565	0.619	1.435	4.716	1.914	0.542	0.868	0.618
6	0.0565	0.640	1.406	5.006	2.212	0.544	0.905	0.614
7	0.0539	0.789	1.254	5.978	2.619	0.567	0.969	0.620
8	0.0551	0.850	1.227	6.483	2.994	0.580	1.048	0.588
9	0.0365	0.957	1.113	7.119	3.140	0.590	1.067	0.610
10	0.0544	0.942	1.209	7.118	3.351	0.600	1.150	0.551
11	0.0556	1.056	1.075	7.807	3.520	0.612	1.163	0.571
12	0.0581	0.681	1.518	5.515	2.816	0.557	1.041	0.569
13	0.0604	0.476	1.873	4.279	2.388	0.502	0.951	0.624
14	0.0590	0.507	1.671	4.314	2.188	0.510	0.905	0.629
15	0.0451	0.639	1.698	5.336	2.869	0.550	1.092	0.548
16	0.0315	0.296	2.769	3.580	2.465	0.390	1.004	0.791
17	0.0315	0.259	2.798	3.322	2.323	0.375	0.938	0.830
18	0.0296	0.077	4.068	2.816	2.497	0.151	0.887	1.173
19	0.0296	0.065	4.211	2.800	2.517	0.146	0.877	1.230
$I_L, J_{LL'}$		0.635	0.586	1.640	1.183	0.523	0.922	0.675

$$\Lambda_k^{-1} = (v_k \tau_k)^{-1} - (4\pi c/k_f^2) \times \sum_L C_k (d_{LL'}^k/v_k) (2J_{LL'}/I_L I_{L'}) \times \sin\phi_L \sin\phi_{L'} \cos(\phi_L - \phi_{L'}) \quad (\text{A3})$$

and the resistivity is obtained from

$$\rho^{-1} = (e^2/12\pi^3 \hbar) \sum_k \Lambda_k \Delta S_k \quad (\text{A4})$$

We note that the values of $C_k t_k^L/v_k$ and $C_k d_{LL'}^k/v_k$ listed in Table V are those appropriate to the values of E_F given in Table I. Alternative choices

of E_F will lead to exactly the same anisotropy, but each L value will have a different magnitude and hence the values of I_L and $J_{LL'}$ will be altered. Such changes will have no effect on using these tables to invert Dingle temperatures or to calculate the resistivity provided the scattering parameters $\text{Im}S_L$ are fitted self-consistently.

Note added in proof. Note that for Dingle-temperature analysis of hole orbits, such as the rosette and dogsbone, the absolute magnitude of $(\partial a/\partial \eta_1)_{E_F}$ should be used in Eq. (25). The same expression which appears in the head of Table II should be similarly modified.

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