ACKNOWLEDGMENT

The authors wish to express their gratitude to John Peech for the generous loan of his crystal-facing instrument and for his valuable assistance in developing sample preparation techniques.

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*Work supported mainly by the U. S. Atomic Energy Commission under Contract No. AT(11-1)-3150, Technical Report No. C00-3150-9. Additional support was received from the Advanced Research Projects Agency and the National Science Foundation through use of the technical facilities of the Materials Science Center, Cornell University, MSC Report No. 1910.

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Phase-Shift Analysis of Impurity Scattering in Copper

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(Received 27 October 1972)

An identity is proved that allows impurity scattering to be calculated in terms of partial waves by using conventional band-structure programs. It is particularly simple when used in conjunction with a phase-shift parametrization of the Fermi surface and it then conveniently gives the average scattering as sampled by the de Haas–van Alphen effect. The technique is illustrated by applying it to impurity scattering in copper.

There has recently been some interest in parametrizing Fermi surfaces with band-structure calculations by adjusting the phase shifts, which characterize the scattering of the muffin-tin potentials, to obtain agreement with experimentally measured areas. It has been demonstrated in some detail[1–4] that not only can an accurate fit to the Fermi surface be obtained with the first few phase shifts ($l = 0$, 1, 2 in copper) but also the accuracy is remarkably independent of the choice of the energy parameter E_F which measures the Fermi energy relative to the muffin-tin zero. The significance of different choices of E_F and the corresponding pseudopotentials has been discussed by Lee and Heine.[5]

One property that is sensitive to the choice of potential and the corresponding wave functions is the scattering of the electrons by impurities. The de Haas–van Alphen (dHvA) effect provides a powerful technique for studying this scattering, and the results—for example, in the noble metals—frequently show considerable anisotropy.[6] Expressed in terms of partial waves, the anisotropy of scattering for each angular momentum component is simply proportional to the intensity of the appropriate component of the wave function. In the case of copper this impurity scattering has been calculated for the $l=0$, 1, 2 partial waves in two independent calculations.[7,8] It is interesting to note the good agreement between the two calculations, one of which used Korringa-Kohn-Rostoker-Ziman (KKR-Z) wave functions[7] and the other augmented-plane-wave (APW) wave functions,[8] because although they both used essentially the same band structure, the formalism was somewhat different. Both calculations involved the relatively complicated procedure of determining the wave function at different points on the Fermi surface, although this was simplified by access to an existing band-structure calculation (or a fit to a set of phase shifts). Also, having calculated the scattering on a point-by-point basis, there is a further complication of having to take a suitably weighted average of the scattering to obtain the quantity measured in dHvA experiments. However, fitting such a calculation to experimental data has the advantage of automatically providing not only a physically significant inversion scheme for the measured results but also an experimental estimate of $P(\vec{k},\vec{k}')$, the probability of scattering between points $\vec{k}$ and $\vec{k}'$ on the Fermi surface.

The purpose of this paper is to draw attention to an identity which significantly simplifies calculation of the scattering. Although the identity is proved within the nonrelativistic KKR-Z formalism, it is also valid for APW matrix elements. We heavily exploit the work of Morgan[9] showing the connection between the two representations. An equivalent identity presumably exists for the relativistic case.

Following Morgan,[9] and assuming both the host and impurity to have potentials confined to muffin-tin wells of radius R_s, the KKR-Z equation can be written as a sum over reciprocal-lattice vectors $\vec{g}'$:

$$\sum_{g'} \alpha_{\vec{k}+\vec{g}'} \left[\Gamma_{gg'} + \rho(g)\delta_{gg'}\right] = 0 \,, \tag{1}$$

where $\rho(g) = |\vec{k}+\vec{g}|^2 - \kappa^2$, $\kappa^2 = E$, where E is the energy, and $\alpha_{\vec{k}+\vec{g}}$ are the coefficients of the Fourier expansion outside the muffin tin. $\Gamma_{gg'}$ is the KKR-Z matrix element given by

$$\Gamma_{gg'} = -\frac{4\pi N}{\kappa} \sum_{l} (2l+1)\tan\eta_l' \times \frac{j_l(|\vec{k}+\vec{g}|R_s)\, j_l(|\vec{k}'+\vec{g}'|R_s)}{j_l^2(\kappa R_s)} P_l^0(\cos\theta_{gg'}) \,, \tag{2}$$

with

$$\tan\eta_l' = \left(\cot\eta_l - \frac{n_l(\kappa R_s)}{j_l(\kappa R_s)}\right)^{-1} \,,$$

where η_l is the lth scattering phase shift, j_l and n_l are spherical Bessel and Neumann functions, and $P_l^0(\cos\theta_{gg'})$ is a Legendre polynomial, with $\theta_{gg'}$ the angle between $\vec{k}+\vec{g}$ and $\vec{k}'+\vec{g}'$.

The scattering by an impurity, characterized by phase shifts $\eta_l + \Delta\eta_l$, is given by the T matrix, and Morgan[9] shows that

$$T_{kk'} = \sum_{gg'} \alpha^*_{\vec{k}'+\vec{g}'} \alpha_{\vec{k}+\vec{g}} V_{\text{eff}}(\vec{k}+\vec{g}, \vec{k}'+\vec{g}') \,,$$

where

$$V_{\text{eff}}(\vec{k}+\vec{g}, \vec{k}'+\vec{g}') = -\frac{4\pi}{\kappa} \sum_{L} (2l+1) \frac{\tan^2\eta_l'}{\sin^2\eta_l} A_L \sin(\Delta\eta_l) e^{i\Delta\eta_l} \times j_l(|\vec{k}+\vec{g}|R_s)\, j_l(|\vec{k}'+\vec{g}'|R_s) \frac{P_l^0(\cos\theta_{k+g,k'+g'})}{j_l^2(\kappa R_s)} \,, \tag{3}$$

and $\theta_{k+g,k'+g'}$ is the angle between $\vec{k}'+\vec{g}'$ and $\vec{k}+\vec{g}$. The term $A_L, (1+\sum_{L'} T_{LL'} b_{L'}/a_L)$ in Morgan's notation, represents the incoming spherical wave produced by the outgoing scattered wave being back-scattered by the surrounding lattice. Using somewhat different formalism, Blaker and Harris[10] have demonstrated that in a cubic environment, A_L (L being a representation of the cubic group) is independent of $\vec{k}$ and is a function of energy only, and is a renormalizing constant for the impurity-atom wave functions inside the muffin tin. For the purpose of illustration (in copper) the differences between the A_L's for the $\Gamma_{25'}$ and Γ_{12} representations can be neglected[7,8] and L replaced by l, with $l_{\max} = 2$. The generalization is trivial.

At a point $\vec{k}$ on the Fermi surface, the total scattering rate is given by $1/\tau_0(\vec{k}) = (-2/\hbar)\operatorname{Im} T_{kk}$, and it is convenient to write the forward scattering part of the T matrix as

$$T_{kk} = -\sum_{l} t_k^l A_l \sin(\Delta\eta_l) e^{i\Delta\eta_l} \,.$$

Consider the function $f(\vec{k}, E, \eta_l)$ defined by

$$f \equiv \sum_{gg'} \alpha^*_{\vec{k}'+\vec{g}'} \alpha_{\vec{k}+\vec{g}} \left[\Gamma_{gg'} + \rho(g)\delta_{gg'}\right] \,.$$

Equation (1) shows that (a) $f = 0$ and (b) partial differentiation with respect to any of the independent variables x ($x=\vec{k}$, E, or η_l) means that

$$\frac{\partial f}{\partial x}=\sum_{gg'} \alpha^*_{\vec{k}+\vec{g}'}\alpha_{\vec{k}+\vec{g}}\,\frac{\partial(\Gamma_{gg'}+\rho(g)\delta_{gg'})}{\partial x} \;.$$

Differentiation with respect to a phase shift and comparison with Eq. (3) shows that

$$\frac{\partial f}{\partial \eta_l}=-Nt^l_k \;.$$

For a band-structure calculation there is a constraint on the phase shifts, namely, that they are a function of energy specified by the particular potential used. Therefore, the reciprocal of the component of velocity in the direction $\vec{k}$, i.e., $\hbar(dk/dE)_{\mathrm{BS}}$, is given by[11]

$$\left(\frac{dk}{dE}\right)_{\mathrm{BS}}=-\left[\left(\frac{\partial f}{\partial E}\right)_{k,\eta}+\sum_l\left(\frac{\partial f}{\partial \eta_l}\right)_{k,E,\eta}\frac{d\eta_l}{dE}\right]\bigg/\left(\frac{\partial f}{\partial k}\right)_{E,\eta} \;.$$

Inspection of the condition for normalizing KKR-Z or APW wave functions (see, e.g., Loucks[12]) shows that the numerator is just N (if we take the usual normalization); so

$$\left(\frac{dk}{dE}\right)_{\mathrm{BS}}=N\bigg/\left(\frac{\partial f}{\partial k}\right)_{E,\eta} \;.$$

From the properties of partial derivatives

$$\left(\frac{\partial k}{\partial \eta_l}\right)_E=-\left(\frac{\partial f}{\partial \eta_l}\right)_{E,k}\bigg/\left(\frac{\partial f}{\partial k}\right)_{E,\eta}$$

so one obtains the desired identity

$$\left(\frac{\partial k}{\partial \eta_l}\right)_E=\left(\frac{dk}{dE}\right)_{\mathrm{BS}} t^l_k \;; \tag{4}$$

i.e., the partial scattering rate, which has an anisotropy given by t^l_k, is obtained from the rate of change of $\vec{k}$ vector with appropriate phase shift weighted by the velocity component in the k direction.

This relationship is somewhat more useful in interpreting experiments than might at first appear. The quantity involved in fitting "Dingle temperatures"—the average scattering measured by the dHvA effect—is the point scattering weighted by the time an electron spends at each point on the orbit.[6] When fitting extremal areas to a set of phase shifts at a given value of E_F, a convenient procedure is to use an approximate set of phase shifts and calculate the area A_0 of the various orbits and the derivatives of this area with respect to phase shift $(\partial A_0/\partial\eta_l)_{E_F}$. Provided the initial set of phase shifts is a sufficiently good trial, the corrections to the phase shifts can be obtained by a least-squares fit to the set of linear equations. If the orbit is specified by a radius vector k_r measured from the center and an angle around the orbit θ, then the integral involved in calculating the area changes is

$$\left(\frac{\partial A_0}{\partial \eta_l}\right)_{E_F}=\int_{\mathrm{orb}} k_r\left(\frac{\partial k_r}{\partial \eta_l}\right)_E d\theta$$

$$=\int_{\mathrm{orb}} k_r t^l_k\left(\frac{dk}{dE}\right)_{\mathrm{BS}} d\theta \;.$$

But $k_r(dk/dE)_{\mathrm{BS}}$ is just the weight factor required to calculate the dHvA Dingle temperature x, in the form[6]

$$m_c x=\frac{-\hbar^2}{2\pi^2 k_B}\int_{\mathrm{orb}} k_r\frac{dk}{dE}\,\mathrm{Im}\,T_{kk}\,d\theta \tag{5}$$

(m_c is the cyclotron mass of the orbit).

Thus the coefficients $\partial A_0/\partial\eta_l$ for each orbit, which are frequently available from the process of fitting Fermi-surface areas to a set of host phase shifts, give directly the coefficients which must be combined with the scattering phase shifts and the normalizing factor A_l to obtain the measured dHvA scattering $m_c x$ in the form

$$m_c x=\frac{\hbar^2}{2\pi^2 k_B}\sum_l \frac{\partial A_0}{\partial \eta_l}\,\mathrm{Im}[A_l\sin(\Delta\eta_l)\,e^{i\Delta\eta_l}] \;. \tag{6}$$

This formula may not be strictly correct, because the weight factor used for averaging the scattering around the orbit should presumably be a quasiparticle velocity, while Eq. (5) uses a band-structure value. Although we are unaware of any explicit treatment of the effect of the electron-phonon interaction on impurity scattering, it seems reasonable to assume that, by analogy with the free-electron case, the products $t^l_k(dk/dE)_{\mathrm{BS}}$ and $t^{l*}_k(dk/dE)^*$ are the same (an asterisk indicating the value with the electron-phonon effects in-

TABLE I. Values of $\partial A_0/\partial\eta_l$ compared with previously calculated scattering. Fermi-surface extremal areas are given in free-electron units (5.8363 Å^{-2}) and phase shifts in radians. For purposes of comparison, the ratio of $\partial A_0/\partial\eta_l$ to the equivalent quantity deduced from the scattering is obtained by using Eq. (6) and correcting the results in Ref. 7 to remove electron-phonon enhancements and normalizing coefficients A_l. A value of E_F $=0.55$ Ry was used with phase shifts; $\eta_0=0.0638$, η_1 $=0.1261$, $\eta_2=-0.1168$, $\eta_3=0.0007_5$. The errors in $\partial A/\partial\eta_l$ are estimated to be $\lesssim 1\%$. The orbit notation is B for belly, D for dog's bone, R for rosette, and N for neck, with the appropriate orientation of magnetic field; the ⟨511⟩ direction refers to turning point ~16° from ⟨100⟩ in the (110) plane.

Orbit	$\partial A_0/\partial\eta_0$	Ratio	$\partial A_0/\partial\eta_1$	Ratio	$\partial A_0/\partial\eta_2$	Ratio
B_{111}	0.265	1.00_5	0.869	1.02	2.74_9	1.00
B_{100}	0.305	1.03	0.963	1.00_5	2.29_5	1.02
B_{511}	0.279	1.01_5	0.919	0.99	2.39_6	1.01
D_{110}	−0.188	1.05	−1.129	1.02	-1.85_7	1.04
R_{100}	−0.185	1.00_5	−1.061	1.04	−2.243	0.98_5
N_{111}	0	...	0.582	1.04	0.362	0.91

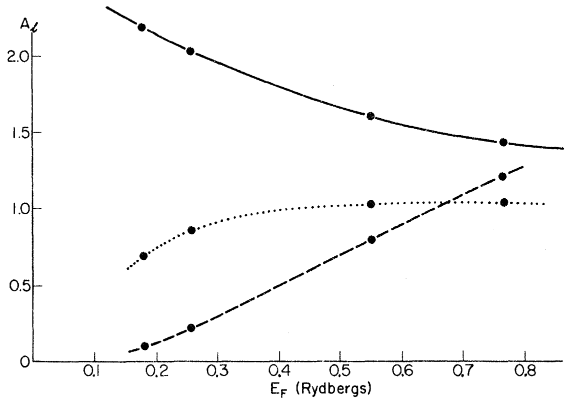

FIG. 1. Estimates of the renormalization factor A_l obtained by the method discussed in the text. The solid line refers to $l=0$, the dotted line to $l=1$, and the dashed line to $l=2$.

cluded). We would point out that the experimental quantity in the dHvA effect is the product m^*x^* (or $m_c x$), and to estimate the x or x^* independently it is necessary to use the appropriate value of the cyclotron mass.

Fitting the dHvA scattering to the adjustable parameters, $\mathrm{Im}[A_l \sin(\Delta\eta_l)e^{i\Delta\eta_l}]$ automatically provides an inversion scheme because the point scattering can also be calculated with the same parameters by using calculated values of $\partial k_r/\partial\eta_l$ (see below) and the velocity component $(1/\hbar)(dE/dk_r)$. Furthermore, as inspection of Eqs. (27) and (38) of Morgan's paper shows,[9] it is relatively easy to obtain from such an inversion the scattering probability $P(\vec{k}, \vec{k}')$ between points $\vec{k}$ and $\vec{k}'$.

Values of $(\partial A_0/\partial\eta_l)_E$ calculated using the APW method (using 30 reciprocal-lattice vectors and $l_{\max}=12$) are compared in Table I with equivalent numbers obtained using explicit KKR-Z wave functions[7] (at the same E and phase shifts). As expected, Eq. (6) is confirmed for each of six orbits on the Fermi surface of copper and three values of l (0, 1, 2).

All the deviations, even the rather large difference observed at the neck with $l=2$, are consistent with the estimated errors in the full-length KKR-Z calculation. It should be emphasized that the less complicated and more fully converged calculation of $\partial A_0/\partial\eta_l$ are inherently more accurate than the KKR-Z wave-function calculation. The agreement between the two calculations confirms that the scattering is indeed independent of choice of APW or KKR-Z wave functions provided the calculation is carried to convergence.

For completeness, Table II gives values of $\partial k/\partial\eta_l$, which can be used, in conjunction with the appropriate velocity component, for inverting dHvA scattering to a point quantity [Eq. (4)].

With this ability to calculate scattering with relatively little expenditure of computation time it is of interest to investigate the effects of changing the energy parameter E_F. Over a range 0.18–0.76 Ry (using the phase shifts given by Lee and Heine[5] and Shaw *et al.*[4]) the calculated values of $\partial A_0/\partial\eta_l$ showed exactly the same anisotropy for all values of E_F but the magnitudes varied with E_F. A convenient measure of this magnitude is to estimate A_l by assuming it to be real and applying the optical theorem,[7] i.e.,

$$-\mathrm{Im}\,T_{kk}=\sum_{k'}|T_{kk'}|^2\,\delta(E_k-E_{k'})\,,$$

for each value of l. Figure 1 shows a plot of the estimates of A_l obtained in this fashion (using quasiparticle values for the density of states), and although there is no simple systematic behavior,

TABLE II. Derivatives with respect to phase shift of Fermi-surface radius vector measured from the center of the Brillouin zone and given in spherical polar coordinates. The calculation parameters and estimated accuracy are the same as in Table I, with radii measured in free-electron units (1.3630 Å^{-1}) and phase shifts in radians. The partial scattering coefficients t_k^l can be obtained by multiplying by the component of band-structure velocity parallel to k (see, e.g., Ref. 13).

ϕ (deg)	$l=0$				$l=1$				$l=2$			
θ (deg)	0	15	30	45	0	15	30	45	0	15	30	45
0	0.108	0.108	0.108	0.108	0.650	0.650	0.650	0.650	0.28	0.28	0.28	0.28
5	0.109	0.109	0.109	0.109	0.590	0.590	0.590	0.590	0.39	0.39	0.39	0.39
10	0.112	0.112	0.111	0.110	0.486	0.486	0.486	0.486	0.61	0.60	0.60	0.60
15	0.115	0.114	0.112	0.110	0.398	0.400	0.402	0.403	0.80	0.79	0.78	0.77
20	0.118	0.116	0.110	0.107	0.340	0.344	0.353	0.357	0.95	0.93	0.89	0.87
25	0.121	0.117	0.107	0.101	0.304	0.313	0.334	0.346	1.07	1.03	0.96	0.92
30	0.125	0.118	0.101	0.092	0.281	0.299	0.344	0.370	1.16	1.11	0.99	0.93
35	0.127	0.118	0.093	0.078	0.269	0.300	0.385	0.450	1.23	1.16	0.99	0.90
40	0.131	0.117	0.081	0.055	0.261	0.309	0.473	0.665	1.28	1.19	0.98	0.87
45	0.132	0.115	0.066	0	0.260	0.323	0.623	7.25	1.29	1.19	0.96	4.50
50	0.131	0.112	0.49	⋯	0.261	0.333	0.866	⋯	1.28	1.16	0.97	⋯

it is nevertheless interesting to note that in the region of 0.55 Ry (i.e., near the free-electron Fermi energy) the values of A_l are rather close to unity. In the spirit of Lee and Heine's minimum-perturbation potential,[5] this energy corresponds to a host potential chosen so that the atomic cell is electrically neutral, meaning that the perturbation will be confined to and screened within the impurity cell. Considering A_l to be a renormalization factor for the wave function inside the impurity muffin-tin cell, a value of unity therefore could be interpreted to imply that the host has little influence on the wave function inside the impurity cell.

In conclusion, we have proved an identity that allows band-structure calculations—in particular, phase-shift parametrizations—to be used directly to describe impurity scattering in terms of the scattering phase shifts of the impurity. To fit experimentally observed Dingle temperatures requires little or no more calculation than is often already available from the procedure of phase-shift parametrization. When fitted to a set of impurity phase shifts, the calculation automatically provides an inversion scheme for Dingle temperatures that gives not only the point scattering but also, with a little additional calculation, $P(k, k')$, the probability of scattering from a point k to k', required for calculating transport properties.

I wish to thank Dr. R. Harris, Dr. M. J. G. Lee, and Dr. M. Rasolt for helpful discussions, and Dr. I. M. Templeton for help and advice on many aspects of the computation.

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Role of Bulk and Surface Plasmons in the Emission of Slow Secondary Electrons: Polycrystalline Aluminum*

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(Received 26 July 1972)

Measurement of both the low-energy (true-secondary) and high-energy (characteristic-loss regions of the secondary-electron-emission spectrum of several types of polycrystalline aluminum have been made in order to explain structure seen at very low energies (0–20 eV). The data indicate that the structure is due to hot electrons losing energy by the creation of plasmons rather than by excitation of single electrons by decaying plasmons, as had been previously suggested.

I. INTRODUCTION

The strong coupling between electrons and plasmons has made electron-beam transmission and reflection experiments the major source of information on collective electron oscillations in solids. The most extensive work has been done by analyzing the energy of a beam of monochromatic high-energy electrons (primary energy E_p about 10–50 keV) after transmission through a thin solid sample.[1] In addition to the unscattered beam at energy E_p, peaks are found in the energy distribution curve (EDC) which are shifted to lower energy by the energy of one or more bulk plasmon $\hbar\omega_B$ or a surface plasmon $\hbar\omega_s$.[2] These are, of course, electrons that have created one or more plasmons in the material while passing through. Plasmon loss peaks have also been observed in the EDC's