

$\times 10^{-5} \Omega^{-1}$ for all materials. We find that our experimental results are in extremely good agreement with this result which predicts that τ_0 will go inversely as l for films of a given thickness. For the data in Fig. 1, R_{square} is $8.7 \times 10^3 \Omega$ and therefore τ_0/R is $1.15 \times 10^{-5} \Omega^{-1}$; for the data in Fig. 2, R_{square} is $= 2.5 \times 10^2 \Omega$ with $\tau_0/R_{\text{square}} \sim 4 \times 10^{-5} \Omega^{-1}$. We consider this to be good agreement with the value of Aslamazov and Larkin of $\tau_0/R_{\text{square}} \sim 1.5 \times 10^{-5} \Omega^{-1}$, especially since our τ_0 values were obtained from a fit to the data near 4°K .

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ACCURATE CALCULATION OF LOW-ENERGY ELECTRON-DIFFRACTION INTENSITIES BY THE PROPAGATION-MATRIX METHOD

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A necessary step in relating low-energy electron-diffraction (LEED) observations to crystal structure is the calculation of accurate values of the intensities of electrons scattered coherently from a given periodic potential (or pseudopotential) terminating at a plane surface. Several methods have been discussed in recent papers,¹⁻³ but they do not seem to give complete and accurate results, which we believe the method described here can provide. Our method uses the "mixed" (Fourier and coordinate) representation of von Laue,⁴ employed recently by Hirabayashi and Takeishi,⁵ but develops a systematic computational procedure whose convergence toward the correct solution can be estimated. The calculation of a "propagation" matrix P defined lat-

er is central to this procedure, since the problem is then reduced to finding the eigenvectors of P , for which new high-speed computer techniques are available.

The calculation has a natural division into two parts, as is emphasized by Heine⁶ and also adopted here. First, solutions are required of the energy-band problem for the infinite crystal, but just for the particular discrete set of Bloch functions with the same energy ϵ and the same (reduced) component of wave number parallel to the surface \vec{k}_ρ as the incident electron has; this set includes solutions which attenuate. Second, the reflection coefficients are found from linear equations which match the wave function and its normal derivative at the surface. In the crystal,

these functions to be matched are sums of members of the above set of Bloch functions, but including only those which propagate or attenuate into the crystal from the surface (outgoing functions); similarly, in the vacuum, sums of plane waves are used (and only the incident electron is an incoming wave). The importance of P is that its eigenvectors are just this discrete set of Bloch functions.

This procedure has been applied in a detailed calculation of reflected intensities over a large range of energies for the potential produced by a simple cubic lattice of point ions of charge Z compensated by a uniform negative charge. This is analytically simple but is not an unrealistic test of the power of the method, since the Coulomb singularity, which provides the chief convergence difficulty for plane-wave expansions, is still present at each nucleus. Both the energy-band structure and the reflection intensities are found in the same calculation; comparison exhibits strikingly the close relation of the reflection peaks to band edges.

Mixed representation and matrix formulation.

Both the wave function $\psi(r)$ and the given potential $V(r)$ are expanded in Fourier series of the form (1) in $\vec{\rho} = (x, y)$ (in planes parallel to the surface), whose coefficients ψ_n and V_n , respectively, are functions of z (normal to the surface):

$$\psi(\vec{\rho}, z) = \sum_n \psi_n(z) \exp[i(\vec{k}_\rho + \vec{K}_n) \cdot \vec{\rho}]. \quad (1)$$

In (1) $n=1$ to N enumerates the reciprocal lattice vectors \vec{K}_n in the plane in some arbitrary, but definite order, e.g., by shells, and gives $\psi(r)$ in an N th order approximation. A convenient vector notation uses the coefficients to define column vectors⁷ $\vec{\psi}(z) \equiv (\psi_1(z), \psi_2(z), \dots, \psi_N(z))^T$, $\vec{\psi}'(z) \equiv (\psi_1'(z), \psi_2'(z), \dots, \psi_N'(z))^T$, $\vec{\Psi}(z) \equiv (\vec{\psi}(z)^T, \vec{\psi}'(z)^T)^T$, where $\psi_n'(z) \equiv d\psi_n(z)/dz$, and $\vec{\Psi}(z)$ has $2N$ components. Insertion of (1) and the expansion of $V(\vec{r})$ in the Schrödinger equation gives differential equations for $\vec{\psi}(z)$ and $\vec{\Psi}(z)$ of the forms

$$\vec{\psi}''(z) = [V(z) + D(\epsilon, \vec{k}_\rho)] \vec{\psi}(z), \quad (2)$$

$$\vec{\Psi}'(z) = \begin{pmatrix} \mathbf{O}_N & \mathbf{I}_N \\ V + D & \mathbf{O}_N \end{pmatrix} \vec{\Psi}(z), \quad (3)$$

where $V(z)$ is an $N \times N$ matrix whose components V_{mn} are matrix elements of $V(r)$ between two-dimensional plane waves \vec{k}_m and \vec{k}_n , D is a diagonal matrix with components $D_{mn} = [-\epsilon + (\vec{k}_\rho + \vec{K}_n)^2] \delta_{mn}$, and \mathbf{O}_N is the $N \times N$ null matrix and \mathbf{I}_N the $N \times N$ identity matrix. The band problem

for given ϵ and \vec{k}_ρ is now reduced formally and conceptually to solution of the one-dimensional linear vector differential equations (2) or (3). Because of the linearity of (3), a $2N \times 2N$ matrix $P(z, z_s; \epsilon, \vec{k}_\rho)$ can be introduced which relates the values of any solution of (3) at initial position z_s to values at position z by

$$\vec{\Psi}(z) = P(z, z_s) \vec{\Psi}(z_s). \quad (4)$$

Then P also satisfies (3), with initial value $P(z_s, z_s) = \mathbf{I}_{2N}$, and can be found accurately by stepwise integration. If that integration is carried through a full period a along z , the column eigenvectors of $P(z_s + a, z_s)$ are seen from (4) to be the Bloch functions (evaluated at z_s), with eigenvalues $\exp(ik_z a)$, the multiplying factor on translation through a .

Matching equations and reflection coefficients.

From the $2N$ column eigenvectors $\vec{\Psi}_j(z_s)$ of the full-period P , the N outgoing Bloch functions $\vec{\Psi}_j^+$ are selected by using the velocity formula

$$V_{jz} \equiv V_{jz}^u / \pi \\ = \text{Im}[\vec{\psi}_j^*(z_s) \cdot \vec{\psi}_j'(z_s)] \\ \times \left(\int_{z_s}^{z_s+a} \frac{dz \vec{\psi}_j^*(z) \cdot \vec{\psi}_j'(z)}{a} \right)^{-1}, \quad (5)$$

where V_{jz}^u is the un-normalized velocity obtained directly from the values of the un-normalized Bloch function and its derivative at z_s , and π is the (positive) normalization integral. Then the M_C outgoing propagating waves can be obtained from the sign⁸ of V_{jz}^u , without evaluation of π ; the $N - M_C$ outgoing attenuating waves are determined by the sign of the imaginary part of k_z .

Now the total wave function in the crystal $\vec{\Psi}^C(z)$ is a linear combination of the $\vec{\Psi}_j(z)$ with coefficients given by the complex transmission coefficients T_j . Similarly the wave function in the vacuum $\vec{\Psi}^V(z)$ is a linear combination of outgoing plane waves whose coefficients are the complex reflection coefficients R_n , plus a single incoming wave, the incident plane wave with unit amplitude. Since $\vec{\Psi}_j^+(z_s)$ has known components, which are the expansion coefficients in plane waves in the $\vec{\rho}$ plane, $\vec{\Psi}^C(z_s)$ and $\vec{\Psi}^V(z_s)$ can be matched component by component at the surface $z = z_s$. This provides just $2N$ linear equations for the $2N$ R 's and T 's; the values of the R 's (but not the T 's) are independent of the normalization of the $\vec{\Psi}_j^+$.

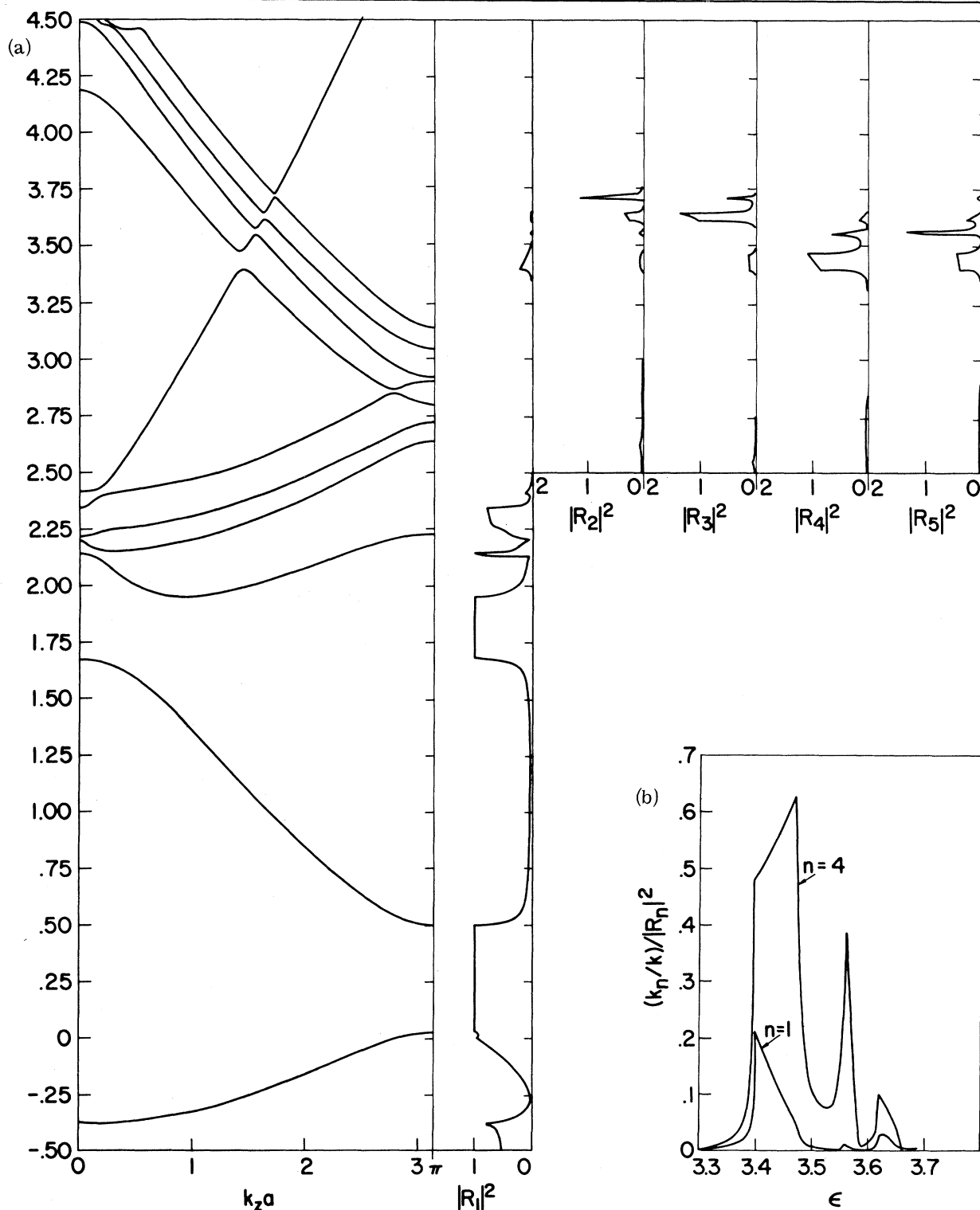


FIG. 1. (a) Band structure $\epsilon(k_z a)$ for the model potential with $Z=1, a=4$, along the line $k_\rho a = (0.2, 0.1)$ between -0.5 and 4.5 Ry, calculated with a nine-Fourier-component approximation ($N=9$). At the right-hand side on the same energy scale are shown all the significant reflected intensities $|R_n|^2$ of all the propagating waves; $n=1, 2, 3, 4, 5$ correspond to $\frac{1}{2}\vec{K}_n a = (00), (10), (01), (\bar{1}0), (0\bar{1})$, respectively; the vacuum potential is zero, and values of $|R_n|^2$ below $\epsilon=0$ correspond formally to an incident damped wave. (b) Enlarged plot of lines in (a) at 3.4 Ry showing the projected intensities on the $\vec{\rho}$ plane of the specularly reflected wave and the fourth propagating wave in vacuum, $(k_1/k)|R_{00}|^2$ and $(k_n/k)|R_{\bar{1}0}|^2$, where $k = \epsilon^{1/2}$.

A check on these R 's and T 's is provided by the conservation theorem for the propagating modes

$$\sum_{n=1}^{M_V} (k_n/k_1) |R_n|^2 + \sum_{j=1}^{M_C} (V_{jz}^u/R_1) |T_j|^2 = 1, \quad (6)$$

where M_V is the number of propagating modes in the vacuum, and $k_n = [\epsilon - (\vec{k}_\rho + \vec{K}_n)^2]^{1/2}$. The proof shows that the current carried by a superposition of propagating Bloch functions with the same ϵ and \vec{k}_ρ is the sum of the individual currents,⁹ so that expressing $\vec{\Psi}^C$ as a sum of $\vec{\Psi}_j^+$ guarantees that the current at infinity is outgoing, and thus never violates the boundary condition at infinity. The relation (6) is exact, even when the R 's and T 's are found in an N -component approximation.

Results for a simple potential.—We define a precise problem for our simple-cubic-crystal model by choosing a semi-infinite crystal with a (001) surface for scattering, placed halfway between lattice planes; thus if the plane $z=0$ is a lattice plane, the surface is at $z=-\frac{1}{2}a$. The Fourier coefficients of the model potential in the mixed representation for this choice of surface orientation then have the analytical forms, valid over $-\frac{1}{2}a \leq z \leq \frac{1}{2}a$ (and then repeating with period a),

$$V_{\vec{n}}(z) = (-2Z/na) \exp(-2\pi |z|/a) \\ \times \{[\exp(4\pi n |z|/a + 1)/\exp(2\pi n) - 1] + 1\},$$

$\vec{n} \neq (0, 0)$, where $\vec{K}_{\vec{n}} = (2\pi/a)\vec{n}$, $\vec{n} \equiv (n_1, n_2)$, $n = |\vec{n}|$, $n_1, n_2 = 0, \pm 1, \pm 2, \dots$, and $V_{00}(z) = (-4\pi Z/a)[\frac{1}{4} - (|z|/a)(1 - |z|/a)]$. The functions $V_{\vec{n}}(z)$ curve downward to a cusp at $z=0$, and decrease exponentially for increasing n at all z except $z=0$. The periodic crystal potential is assumed cut off abruptly at the crystal surface where it rises discontinuously to the uniform value in the vacuum; the maximum value of the potential between the ion cores, which occurs also on the surface on [001] lattice lines, is -0.2138 Ry for $Z=1$, $a=4a_0$; however, $V_{00}(z)$ is continuous at the surface.

The spectrum of reflected intensities along with the band structure is shown in Fig. 1(a) for $Z=1$, $a=4$ ($=2.12$ Å), $\vec{k}_\rho a = (0.2, 0.1)$ (near normal incidence), $N=9$ [$n = (00), (10), (\bar{1}0), (0\bar{1}), (11), (\bar{1}\bar{1}), (\bar{1}\bar{1}), (1\bar{1})$] up to $\epsilon = 4.5$ Ry ($=61.2$ V). Typically the intensity rises on approaching a band edge from within the band, then breaks sharply as the energy gap is entered. An interesting re-

sult is that $|R_n|^2$ for beams other than the specularly reflected beam $|R_1|^2$ can be greater than 1; however, no violation of matter conservation results, and (6) is satisfied because of the factors $(k_n/k_1) < 1$. In Fig. 1(b) an enlarged view of the first and fourth lines at 3.4 Ry illustrates this.

The absolute accuracy of the calculation has been estimated by finding independently the lowest two energies at $\vec{k}=0$; the energies found from eigenvalues of P for $N=9$ (and normal incidence) are 6 to 7% high. The relative accuracy and shape of the reflection spectrum are probably better, since calculations at $N=13$ show much smaller differences from $N=9$.

In summary, this method appears to provide reasonably accurate values of LEED intensities for a given periodic potential, which could be further refined.¹⁰ It can be straightforwardly extended to films and surface layers; it provides energy bands and wave functions for a particular direction in k space, including attenuating solutions, that may be useful in other connections. The numerical procedures, which consumed most of the effort, will be described elsewhere, but we note that the calculation has been made practicable by a new program for eigenvectors of unsymmetrical real matrices due to Parlett.¹¹

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⁹This is not true for a superposition of arbitrary Bloch functions belonging to the given potential.

¹⁰A limit to the accuracy may be set by the large ei-

genvalues of \mathbf{P} belonging to exponentially increasing Bloch functions, which rapidly increase as N increases.

¹¹A Fortran-IV program for the IBM 7094 called CEEP (Complete Eigenvalue-Eigenvector Program). F. Branin, private communication.

TEMPERATURE DEPENDENCE OF THE SPIN SUSCEPTIBILITY OF A NEARLY FERROMAGNETIC FERMI LIQUID*

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We have calculated the contribution of spin fluctuations¹⁻³ ("paramagnons") to the temperature dependence of the susceptibility of a nearly ferromagnetic Fermi liquid. We find a term in $\chi(T)/\chi(0)$ proportional to $(T/K_0^2 T_F)^2$, where K_0^{-2} is the Stoner enhancement factor, in contrast to $(T/T_F)^2$ for free fermions. For $K_0^{-2} \gg 1$, the coefficient of this term contains no adjustable parameters, and since $\chi(0) = 3\mu_m^2/(2K_0^2 k_B T_F)^{1/2}$, the theory makes a definite, quantitative assertion, independent of any assumption about T_F , about the relation between $\chi(0)$ and the temperature dependence of $\chi(T)$ for $T < K_0^3 T_F$. Comparison with experiments, discussed in more detail below, is made in Fig. 3.

We calculate the susceptibility per unit volume as⁴

$$\chi = \frac{N}{V} \mu_m^2 \left(\frac{\partial^2 F}{\partial \xi^2} \right)^{-1}, \quad (1)$$

where μ_m is the magnetic moment, N/V the number of particles per unit volume $= \rho_F^3/3\pi$, and F is the free energy per particle. ξ is related to the difference of spin up and spin down:

$$\xi = \frac{N_+ - N_-}{N}. \quad (2)$$

F can be written in the form

$$F(T, \xi) = G_0(T, B) + (IN/4\Omega)(1 - \xi^2) + \Delta F(T, B) - \xi B, \quad (3)$$

where B is determined by $(\partial F/\partial B)_T, \xi = 0$. B is a mathematical object, $G_0(T, B)$ is the free energy of a noninteracting Fermi gas with single-particle energies $\epsilon_{p, \pm} = p^2/2m \pm B$, $IN(1 - \xi^2)/4\Omega$ is the first order of perturbation theory in the interaction I , and ΔF is the contribution of higher orders in I . When only leading terms in the Stoner enhancement factor $K_0^{-2} = [1 - IN(0)]^{-1}$ [$N(0)$ = density of states at the Fermi surface] are retained, ΔF is found to vanish for $T = 0$, the T dependence

of G_0 is negligible, and (1) leads to

$$\chi = \chi(0) \left(1 - \frac{2}{3} \frac{T}{K_0^2} \frac{\partial^2 \Delta F}{\partial B^2} \right), \quad (4)$$

where $\chi(0) = K_0^{-2} \chi_{\text{Pauli}}$ is the Stoner-enhanced zero-temperature susceptibility.

We are interested in those parts of ΔF which represent the correction to F due to paramagnons. We consider for ΔF both the ladder and the ring diagrams (Fig. 1):

$$\Delta F = \Delta F_{\text{ring}} + \Delta F_{\text{ladder}}, \quad (5)$$

$$\left(\frac{N}{V} \right) \Delta F_{\text{ring}} = T \sum_{\vec{k}, \omega} \frac{1}{2} \{ \ln[1 - I^2 \chi^{0+} \chi^{0-}] + I^2 \chi^{0+} \chi^{0-} \}, \quad (6)$$

$$\left(\frac{N}{V} \right) \Delta F_{\text{ladder}} = T \sum_{\vec{k}, \omega} \{ \ln[1 - I \chi^{0+ -}] + I \chi^{0+ -} \}, \quad (7)$$

where

$$\chi^{0\pm}(\vec{k}, \omega) = - \sum_{\vec{p}} \frac{f_{\vec{p}}^{\pm} - f_{\vec{p}+\vec{k}}^{\pm}}{\omega - \xi_{\vec{p}+\vec{k}}^{\pm} + \xi_{\vec{p}}^{\pm}}, \quad (8)$$

$$\chi^{0+-}(\vec{k}, \omega) = - \sum_{\vec{p}} \frac{f_{\vec{p}}^{-} - f_{\vec{p}+\vec{k}}^{\pm}}{\omega - 2B - \xi_{\vec{p}+\vec{k}}^{\pm} + \xi_{\vec{p}}^{-}}, \quad (9)$$

$$f_{\vec{p}}^{\pm} \equiv [\exp(\xi_{\vec{p}}^{\pm} B)/T + 1]^{-1}, \quad (10)$$

$$\xi_{\vec{p}}^{\pm} \equiv p^2/2m - \mu$$

(μ is the chemical potential at $T = 0$).

Notice that, to the lowest order in temperature, the free energy F is equal to μN (N = total number of particles) plus the thermodynamic potential $\Omega(\mu, T)$ evaluated at the chemical potential at $T = 0$. The proof is easy: Let $\mu + \delta\mu$ be