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 12 In Eq. (27) we use the speed ν instead of the actual speed of the Auger electron with no plasmon emission. This approximation is valid : for fast Auger electrons.

¹³This choice of integration limits is perfectly acceptable as far as our derivation of the generalized Poisson distribution is concerned.

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¹⁵For example, the expansion in Eq. (A8) is not valid too close to glancing exit.

¹⁶For data on Ag, see F. Jona, D. W. Jepsen, and P. M. Marcus, in Proceedings of Sixth LEED Seminar, Washington, D. C. (unpublished); for Cu, see S. Andersson, Surf. Sci. **18**, 325 (1969).

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Electron-Electron Scattering in the Transport Coefficients of Simple Metals^{*}

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The parametrization of simple-metal Fermi surfaces by a set of band gaps leads to a model for umklapp electron-electron (Coulomb) scattering and its contribution to electrical resistivity. We discuss transport coefficients in general, but emphasize electrical resistivity, which would vanish without umklapp processes. We treat deviations from Matthiessen's rule resulting from the energy dependence of the deviation function, for the case in which both electron-electron and electron-impurity scattering are present. The resulting T^2 power law is too small to be seen in polyvalent metals. In potassium, the T^2 term is comparable to the phonon contribution at about 2 °K.

I. INTRODUCTION

This quantitative study of simple-metal electronelectron scattering and its contribution to transport was motivated by the experimental search¹ for a T^2 component in the low-temperature electrical resistivity. The results of this calculation, compared with the experimental findings, 1,2 help us to conclude that electron-electron scattering is not responsible for the observed effects. Our results for the *electrical* resistivity are as follows: (i) The contribution from electron-electron scattering is as large in the alkali metals studied (Na and K) as in the simple polyvalent metals; this is the primary result. (ii) Estimated deviation from Matthiessen's rule (DMR) (in the presence of electron-electron and electron-impurity scattering) are small in general, but considerably smaller in the alkali than in the polyvalent metals.

The first result may seem paradoxical since the polyvalent metals offer far more possibility for umklapp scattering (without which there would be no contribution at all). However, the low electron density in the alkali metals compensates for the relative lack of umklapp character in the scattering. As we shall see later, the resistivity can be factored,

 $\rho \sim (m/ne^2\tau_0) \Lambda , \qquad (1.1)$

into a basic electron-electron scattering rate τ_0^{-1} and a quantity Δ , the "fractional umklapp scattering." (As usual m is the electron's mass, e is its charge, and n is the electron density.) The resistivities and the values of Δ are listed in Table I. We shall also see later that (crudely) $\tau_0 \sim n$, so $\rho \sim n^{-2}\Delta$. The relative smallnesses of both n and Δ in the alkali metals tend to compensate, giving a resistivity comparable with that of the polyvalent metals. Because of this we can conclude that electron-electron scattering should be more evident experimentally in the alkali metals. The reason is that, as shown recently by the authors, ³ umklapp electronphonon scattering is much more important in polyvalent metals at very low temperatures. In aluminum, for example, the electron-electron contribution dominates the electron-phonon contribution only for temperatures below a small fraction of a degree. In potassium the electron-electron contribution may dominate below about two degrees, $^{\rm 4}$ so that experimental identification, although tentative at present, may be possible.

Our second result follows from the fact that the estimated DMR are roughly proportional to the "fractional umklapp scattering" Δ , which is quite small in the alkalis. Estimated DMR in the thermal resistivity are also found to depend on Δ , but to a lesser extent. These will be discussed later. Let us now sketch the plan of this paper and list

some previous works upon which we shall draw. First, Jensen, Smith, and Wilkins^{5,6} (JSW) have found the exact transport coefficients of an isotropic Fermi liquid subject to both particle-particle and particle-impurity scattering. That calculation requires solution of the Boltzmann equation for the energy dependence of the deviation (from equilibrium) function. In this work, an exact calculation of transport coefficients would require solving for the angular dependence as well, since the scattering kernel in the Boltzmann equation is itself anisotropic (i.e., depends on the positions of individual wave vectors in addition to wave-vector differences). Such a full calculation is not feasible, but we can nevertheless solve for an "optimal" energy dependence subject to a plausible assumed angular dependence. According to the Kohler variational principle⁷ this would provide an upper bound to the electrical and thermal resistivities. The optimal energy dependence referred to would provide the lowest upper bound, subject to the assumed angular dependence. In Sec. II we describe the use of the JSW formalism in finding the optimal energy dependence. The formalism permits a general discussion of the transport coefficients, including an estimate of the possible DMR, in terms of a set of surface integrals involving the transition probability.

In Sec. III we address the problem of evaluating the surface integrals, with close attention to umklapp processes. The form of the integrals is simple, and most of the work in evaluating them has already been done by Ziman⁸ and by Rösler.⁹ Those authors have treated the case of a spherical Fermi surface with an isotropic umklapp-transition probability. Rösler writes down an explicit expression for the probability, which there arises from the core-orthogonalization components of the wave functions, but does not evaluate the expression. The difference between those and the present work (Sec. III) is that in our model the umklapp scattering arises from the multi-plane-wave nature of the states as it enters the description of simplemetal Fermi surfaces. This results in an explicit form for the umklapp-transition amplitudes which permits easy numerical evaluation of the transport coefficients. The model of course produces an anisotropic scattering probability, but our formalism encompasses that case. Where possible we naturally choose states which conform to the known Fermi-surface distortions. As expected there is a close relationship between surface distortion and the fractional umklapp scattering.

In Sec. III we treat the simplest case, in which only one set of Bragg planes (B.P.) intersects the Fermi surface. In Secs. IV and V we attempt to generalize the result to the case in which many B. P. are involved, to permit the treatment of specific metals.

We should point out that except for its final equations Sec. II is not essential to the rest of the paper, and some readers may wish to pass directly from here to Sec. III.

II. GENERAL PRELIMINARIES

The goal of this section is to obtain formulas for the electrical and thermal resistivities, and estimates of possible DMR's. We begin with a discussion of the Boltzmann equation for electronelectron scattering. As usual we linearize the Boltzmann equation by expanding the Fermi distribution function n_k about its equilibrium $n_k^0 = (e^t + 1)^{-1}$, where $t = (\epsilon_k - u)/k_B T$ is the reduced energy variable with u the chemical potential, at each wave vector \vec{k} :

$$n_k = n_k^0 + \Psi_k \frac{\partial n_k^0}{\partial \epsilon_k} \quad . \tag{2.1}$$

We write the resulting linearized Boltzmann equation as

$$X = P\Psi \quad . \tag{2.2}$$

The driving term X may contain a temperature

$\frac{\rho}{T^2 \Delta} = \frac{2\pi^2 m}{3ne^2 \tau_0 T^2}$ (10 ⁻¹⁴ Ω cm °K ⁻²)	dominant contribu- tion N_u/N_0 from [G]=	number of pairs	$\frac{V_G}{\epsilon_F}$	Total $\frac{N_u}{N_0}$	$\begin{pmatrix} \underline{\Delta_{\min}} \\ \underline{\Delta} \end{pmatrix}$ Eq. (4.10)	Δ ^a Eq. (4.16)	$\rho(\beta = \infty)/T^{2}$ infinite- impurity limit (10 ⁻¹⁴ \Omega cm °K; ⁻²)	$\rho(\beta=0)/\rho(\infty)$ zero- impurity limit
Al 3.1	[200]	3	0.066	0.14	0.80	2/5	1,2	0.96
In 6.1	[111]	4	0.076	0.15	0.79	2/5	2.4	0.96
Mg 12	[101]	6	0.069	0.18	0.76	3/5	7.2	0.95
Zn 5.2	[101]	6	0.048	0.14	0.80	1/2	2.6	0.95
Cd 10						$\gtrsim 1/2$	~ 5	0.95
K 290	[110]	6	0.11	0.011	0.95	0.06	17	
Na 100	[110]	6	0.056	0.0029		0.015	1.5	

TABLE I. Values of resistivity and Δ , and parameters which determine Δ .

^aIn all cases, our quoted value of Δ [from Eq. (4.16)] differs from Δ_{max} by less than 4%. The values of Δ_{min} are included as an estimate of error to be expected from ignorance of interference effects.

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gradient or an electric field \vec{E} :

$$X_{k} \equiv t \vec{\nabla}_{k} \cdot \vec{\nabla}_{x} (k_{B} T) \frac{\partial n_{k}}{\partial \epsilon_{k}} \quad \text{(thermal case)} \quad (2.3a)$$

$$\equiv e \vec{\mathbf{v}}_k \cdot \vec{\mathbf{E}} \frac{\partial n_k}{\partial \epsilon_k} \qquad \text{(electrical case)}, \quad (2.3b)$$

where $\overline{v}_k = \nabla_k \epsilon_k$ is the velocity in state \overline{k} . The collision term is

$$(P\Psi)_{k} \equiv \frac{1}{k_{B}T} \frac{2}{(2\pi)^{6}} \int d^{3}k_{2} d^{3}k_{3} d^{3}k_{4} P(1, 2 - 3, 4)$$
$$\times (\Psi_{k} + \Psi_{2} - \Psi_{3} - \Psi_{4}) . \qquad (2.4)$$

Numerical subscripts and arguments represent the wave-vector indices, $n = k_n$. For the case n = 1, $1 = k_1 = k$ will all be used interchangeably. The collision operator is

$$P(1, 2 \rightarrow 3, 4) = W(1, 2 \rightarrow 3, 4) n_1^0 n_2^0 (1 - n_3^0) (1 - n_4^0)$$
$$\times \delta(\epsilon_1 + \epsilon_2 - \epsilon_3 - \epsilon_4) . \quad (2.5)$$

The transition probability W is given by Fermi's "Golden Rule" and defined in (2.4) and (2.5) to include an average over spins and exchange. For scattering between plane-wave states it is

$$W(1, 2 \rightarrow 3, 4) = (2\pi/\hbar) [V^2(\vec{k}_3 - \vec{k}_1) - \frac{1}{2}V(\vec{k}_3 - \vec{k}_1) V(\vec{k}_4 - \vec{k}_1)] \times \delta(\vec{k}_1 + \vec{k}_2 - \vec{k}_3 - \vec{k}_4) \quad (2.6)$$

[note $W(1, 2 \rightarrow 3, 4) = W(3, 4 \rightarrow 1, 2) = W(2, 1 \rightarrow 4, 3)$]. For V we take the Thomas-Fermi screened-Coulomb interaction

$$V(q) = 4\pi e^2 / (q^2 + k_s^2) , \qquad (2.7)$$

where the Thomas-Fermi screening length k_s^{-1} is given by

$$k_s^2 \equiv 6\pi n e^2/\epsilon_F$$
.

In standard transport calculations the Boltzmann equation is solved only approximately, and the resulting transport coefficients must be interpreted variationally.⁷ So at this point we state the variational principle and explain our use of it in this calculation. We write a conductivity functional

$$T\{\Psi'\} \equiv (\Psi', X)^2 / (\Psi' \cdot, P\Psi'), \qquad (2.8)$$

where X is defined with unit electric field or temperature gradient. The inner products are defined by

$$(\Psi', X) \equiv (1/4\pi^3) \int d^3k \, \Psi'_k X_k$$
, (2.9)

$$(\Psi', P\Psi') \equiv (1/4\pi^3) \int d^3k \, \Psi'_k (P\Psi')_k \,.$$
 (2.10)

As discussed by Kohler, ${}^7 T{\{\Psi'\}}$ attains its maximum value, the physical conductivity, if and only if $\Psi' = \Psi$, the solution of the Boltzmann equation

(2.2).

It is standard procedure, and quite adequate for many purposes (e.g., where electron-impurity scattering dominates), to select the trial solutions

$$\Psi'_{k} = t \, \overline{\nabla}_{k} \cdot \overline{\nabla}_{x}(k_{B} T)$$

for thermal conductivity, (2.11a)

$$= \vec{v}_k \cdot \vec{E}$$
 for electrical conductivity . (2.11b)

It is feasible for our purposes to generalize the trial functions to include additional energy dependence:

$$\Psi'_{k} = \vec{v}_{k} \cdot \vec{\nabla}_{x} (k_{B}T) \psi(t) \quad \text{(thermal)} \quad (2.12a)$$
$$= \vec{v}_{h} \cdot \vec{E} \psi(t) \quad \text{(electrical)} \cdot (2.12b)$$

 ψ is a general function of t, but should be odd in the thermal case and even in the electrical case, as are the particular choices in (2.11). By maximizing $T\{\Psi'\}$ over the subspace of functions (2.12) we derive a reduced Boltzmann equation for the energy dependence $\psi(t)$. The equation is identical to that of JSW.⁵ So we can simply carry over their exact expressions for the conductivities, except that in this treatment the conductivities are no longer exact but only lower bounds, because the angular dependence of Ψ'_k is restricted. But the advantage of this formulation is that we can calculate the JSW parameters in the presence of anisotropic scattering, which we will have to do in order to treat umklapp scattering in Sec. III.

The integrals in (2.9) and (2.10) can be decomposed into surface and energy integrals

$$d^{3}k = \frac{k_{B}T}{\hbar} \frac{dS_{k}}{|v_{k}|} dt, \quad \hbar \vec{\nabla}_{k} = \vec{\nabla}_{k} \epsilon_{k} .$$
 (2.13)

The actual physical input of our model affects only the surface integrals (through the velocity field \vec{v}_k and the transition probability W). All the necessary energy integrals have been done by JSW and will not be repeated here. If we set $\delta T/\delta \psi = 0$ and "do" all the energy integrals, we are left with the JSW reduced Boltzmann equation for $\psi(t)$. (This complicated procedure is carried out in Appendix A.) The parameters of the equation, and hence the conductivity, can be written in terms of four surface integrals which we now write out in detail.

Surface Integrals

The natural occurrence of the following four surface integrals in the derivation of the JSW equation is described in Appendix A.

The simplest surface integral enters through (2.9). If we take the simplest trial solution [(2.11b) for the electrical conductivity], with unit electrical field \hat{E} , then

$$(\Psi'_k, X) = (\overline{\mathbf{v}}_k \cdot \widehat{E}, X) = \frac{1}{4\pi^3 \overline{h}} \int \frac{dS}{|v|} (\widehat{E} \cdot \overline{\mathbf{v}})^2 = \frac{n}{m_{opt}},$$
(2.14)

 m_{opt} is the optical mass,

$$m/m_{opt} \equiv (S_F v_F)^{-1} \int dS \left| \vec{v} \right|$$

 V_F is the free-electron Fermi velocity and S_F the area of the free-electron Fermi sphere $4\pi k_F^2$. We take (2.14) to be independent of field direction, which is valid for a cubic material or for a polycrystalline sample, in which we can average over directions of the field.

The three remaining surface integrals occur in (2.10). We symbolize these fourfold integrations with the average over field directions by angular brackets,

$$\langle f(\hat{E}, \{S_i\}) \rangle = \left(\prod_{i=1}^4 \int \frac{dS_i}{|v_i|}\right) \int \frac{d\Omega_E}{4\pi} f(\hat{E}, \{S_i\}) .$$
(2.15)

The simplest fourfold integration defines a basic relaxation time for electron-electron scattering:

$$\frac{n}{\tau_0 m_{\text{opt}}} = \frac{4}{3(2\pi)^9} \frac{(k_B T)^2}{\hbar^4} \langle |\vec{v}_1|^2 W(1, 2-3, 4) \rangle .$$
(2.16)

Since all indices inside the angular brackets are dummy variables we can write unambiguously

$$\frac{n}{\tau_0 m_{\text{opt}}} \equiv \frac{4}{3(2\pi)^9} \frac{(k_B T)^2}{\hbar^4} \left\langle \left| \overrightarrow{\mathbf{v}} \right|^2 W \right\rangle$$

Precisely defined, $\pi^2/2\tau_0$ is the surface-averaged relaxation rate for an electron at the Fermi surface (t=0), due to electron-electron scattering. In Appendix B it is shown that to a good approximation,

$$\langle \left| \vec{\mathbf{v}} \right|^2 W \rangle = (2\pi)^5 \frac{m_{\rm sh}^3}{\hbar^2} \frac{n}{m_{\rm opt}} W \left(\frac{2k_F}{k_s} \right) , \qquad (2.17)$$

where neglecting exchange and using (2.7),

$$W(x) = (2\pi/\hbar) V^2(0) \gamma(x), \qquad (2.18)$$

with

$$\gamma(x) = \frac{1}{x} \int_0^x \frac{dy}{(y^2+1)^2} = \frac{1}{2x} \arctan x + \frac{1}{2}(x^2+1)^{-1} .$$

Exchange corrections (2.6) are discussed in Ap-

TABLE II. Including exchange reduces $1/\tau_0$ by about $\frac{2}{3}$ for all metals studied. The product of effective masses which occurs in the prefactor of Δ in the resistivity formula (1.1) and (2.26) is close to unity (column 4).

	Exchange correction to $1/\tau_0$	$rac{{m_{\mathrm{sh}}}^{\mathrm{a}}}{m}$	$\frac{m^{b}}{m_{opt}}$	$\frac{m_{\rm opt}m_{\rm sh}^3}{m^4}$
к	0.66	1	1	1
Na	0.67	1	1	1
In	0.70	9	7	1
Al	0.71	ĩ	$\frac{4}{5}$	5-

^aReferences 12-14.

^bSum of contribution from each B. P.



FIG. 1. (a) Scattering rate τ_0^{-1} as a function of $2k_F/k_S$, normalized to its value in potassium τ_0^{-1} (K). (b) γ and $\langle \cos\theta \rangle$ depend only weakly on $2k_F/k_S$. Owing to the weak dependence of γ on $n \sim (k_F/k_S)^6$ the scattering rate τ_0^{-1} [(2.18) and (2.20)] is roughly proportional to $V^2(0) \sim n^{-2/3}$.

pendix C, and tabulated in Table II. $m_{\rm sh}$ is the (unenhanced) specific-heat effective mass, defined by

$$\frac{m_{\rm sh}}{m} = \frac{v_F}{S_F} \int \frac{dS}{|v|} \quad . \tag{2.19}$$

Combining (2.16) and (2.17) we write

$$\frac{1}{\tau_0} = \frac{1}{4\pi^4} (k_B T)^2 \frac{m_{\rm sh}^3}{\hbar^6} W\left(\frac{2k_F}{k_s}\right).$$
(2.20)

From (2.20) it is easy to show that τ_0 is identical to the τ_0 defined by JSW⁵ in the case of a spherical Fermi surface with an isotropic scattering probability. This equivalence is demonstrated in Appendix C.

The crude proportionality $\tau_0 \sim n$ can be seen from (2.18) and (2.20) by noting that $V(0) = \frac{2}{3} (\epsilon_F/n) \sim n^{-1/3}$. $\gamma (2k_F/k_s)$ contributes a weaker density dependence. The dependence of both τ_0 and γ upon *n* is shown in Fig. 1.

The remaining two surface integrals are defined as ratios:

$$\Delta \equiv \frac{1}{4} \left\langle \left| \vec{v}_1 + \vec{v}_2 - \vec{v}_3 - \vec{v}_4 \right|^2 W \right\rangle \left\langle \left| \vec{v} \right|^2 W \right\rangle^{-1}, \qquad (2.21)$$

$$\langle \cos\theta \rangle \equiv \langle \vec{\mathbf{v}}_1 \cdot \vec{\mathbf{v}}_2 W \rangle \langle |\vec{\mathbf{v}}|^2 W \rangle^{-1}$$
 (2.22)

 Δ is a measure of the relative amount of umklapp

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scattering, and will be the focus of Secs. III and IV. Note that it vanishes on a spherical Fermi surface with normal scattering only. $\langle \cos\theta \rangle$ is analogous to the angular average of " $\cos\theta$ " which ordinarily appears in the theory with a spherical Fermi surface, where θ is the angle between the two initial wave vectors. It is treated in Appendix C for the case of normal scattering only. The weak dependence on *n* is shown in Fig. 1.

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The appearance of the velocity field instead of momentum or crystal momentum is not only plausible [as suggested by the form of X (2.3)], but it is necessary for an unambiguous and physically reasonable distribution function (2.11). It also means that one cannot always distinguish a given scattering process as normal or umklapp, since the "velocity transfer" (2.21) is not restricted to a discrete set of values, i.e., to reciprocal lattice vectors.

In terms of the surface integrals just presented we now write down the electrical and thermal resistivities $T^{-1}{\{\Psi\}}$. We shall write the resistivities for the case in which both electron-electron and electron-impurity scattering are present. Smith and Wilkins⁸ have treated this case and found, as with pure electron-electron scattering, that the conductivities can be written as rapidly converging series. The effect of impurities enters through the parameter

$$\beta \equiv (2/\pi^2) \left(\tau_0 / \tau_{\rm imp} \right) \,, \tag{2.23}$$

where τ_{imp} is the relaxation time due to impurities. The series is well approximated over the whole range of accessible values of the parameters by

$$\rho = \sigma^{-1} = \frac{2\pi^2}{3} \frac{m_{\text{opt}}}{ne^2 \tau_0} \Delta \left(1 - \frac{\Delta}{10.4 + \Delta + 5.0\beta} \right) \quad (2.24)$$

for electrical resistivity, and

$$K^{-1} = \frac{6}{5} \frac{m_{\text{opt}}}{nk_B^2 T \tau_0} \Gamma \left(1 - \frac{\Gamma}{8.4 + 1.8\Gamma + 4.35\beta} \right),$$
(2.25)

where $\Gamma \equiv 2 - 2\langle \cos\theta \rangle + \Delta$, for the thermal resistivity. We have dropped the temperature-independent resistivities due to electron-impurity scattering only, which would add to (2.24) and (2.25). As expressed by those equations, however, the presence of impurities does increase the (temperature-dependent) resistivity due to electron-electron scattering. Pure and impure limits correspond to

pure:
$$\beta \rightarrow 0$$
, impure: $\beta \rightarrow \infty$.

The impure limits of (2.24) and (2.25) correspond to the simplest trial functions $\psi(t) = 1$ for electrical resistivity, and $\psi(t) = t$ for thermal resistivity:

$$\rho\{\psi=1\} = \frac{2\pi^2}{3} \frac{m_{\text{opt}}}{ne^2 \tau_0} \Delta , \qquad (2.26)$$

$$K^{-1}\left\{\psi = t\right\} = \frac{6}{5} \frac{m_{\text{opt}}}{nk_B^2 T \tau_0} \left(2 - 2\left\langle \cos\theta \right\rangle + \Delta\right) . \quad (2.27)$$

The familiar temperature dependences are now apparent. Since $\tau_0 \sim T^{-2}$ it follows that $\rho \sim T^2$ and $K^{-1} \sim T$. In the pure case the temperature dependence will not be drastically altered, as shown in Fig. 2. Note that in the electrical case both ρ and the DMR vanish with Δ .

III. A SIMPLE MODEL FOR UMKLAPP SCATTERING

We direct our attention for the rest of the paper to the "fractional umklapp scattering"

$$\Delta = \frac{\langle |\vec{v_1} + \vec{v_2} - \vec{v_3} - \vec{v_4} |^2 W \rangle}{4 \langle |\vec{v}|^2 W \rangle}, \qquad (2.21)$$

whose physical meaning is most apparent from the simple-trial-function result for electrical resistivity

$$\rho = \frac{2\pi^2}{3} \frac{m_{\rm opt}}{ne^2 \tau_0} \Delta$$
 (2.26)

due to electron-electron scattering. We calculate Δ using two plane-wave states, ignoring the coreorthogonalization components of the wave functions.



FIG. 2. Ratio of temperature-dependent resistivity as a function of β [(2.24) and (2.25)] to its value at $\beta = \infty$, the latter corresponding to infinite impurity concentration and the simplest trial deviation function $\psi(t) = 1$. Resistivities are plotted versus $(50/\beta)^{1/2}$, which at fixed τ_{imp} is linear in the temperature, since β (2.23) is proportional to T^{-2} . DMR are small in electrical resistivity, but depend strongly on Δ . In the thermal resistivity the DMR are larger and depend only weakly on the material parameters, potassium and indium representing small and large values of Δ , respectively (Table I).

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FIG. 3. Fermi surfaces in extended zone scheme (a). given by (3.2) and (3.4), and in extended-reduced zone scheme (b), given by (3.4) with $(\alpha_k/\beta_k)_{\pm} = \eta \pm \operatorname{sgn}(V_G)$ $\times (\eta^2 + 1)^{1/2}$.

The result depends solely on Fermi-surface geometry—in part through the band gaps V_G which parametrize its distortions near the B.P. The point of such an approach is to demonstrate that Fermi-surface distortions alone guarantee a certain minimum value of Δ .

In this section we proceed to treat the case of a Fermi surface which intersects, or passes close to a single pair of Bragg planes $(\pm \vec{G})$. If k lies close to the B. P. (\vec{G}) its simple-metal pseudowave-function is

$$\psi_k(\mathbf{r}) = \alpha_k e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}} + \beta_k e^{i(\vec{\mathbf{k}}-\vec{\mathbf{G}})\cdot\vec{\mathbf{r}}}, \quad \alpha_k^2 + \beta_k^2 = 1. \quad (3.1)$$

To work in the extended-zone scheme we choose

$$\frac{\alpha_k}{\beta_k} = \eta \left[1 + (1 + \eta^{-2})^{1/2} \right], \quad \eta \equiv \frac{\hbar^2}{2m V_G} \quad (\vec{k} \cdot \vec{G} - \frac{1}{2}G^2), \quad (3.2)$$

which puts ψ_k in the upper of two bands when $\vec{k} \cdot \vec{G} > \frac{1}{2}G^2$, and in the lower band when $\vec{k} \cdot \vec{G} < \frac{1}{2}G^2$. V_G is the Gth Fourier component $\langle \vec{k} - \vec{G} | V_{ps} | \vec{k} \rangle$ of the electron-ion pseudopotential V_{ps} . The velocity and energy of (3.1) are given by

$$\frac{m}{\hbar} \vec{\mathbf{v}}_k = \vec{\mathbf{k}} - \beta_k^2 \vec{\mathbf{G}}$$
(3.3)

and

$$\epsilon_k = \frac{\hbar^2 k^2}{2m} + V_G \frac{\beta_k}{\alpha_k} \quad . \tag{3.4}$$

With the convention (3.2) the Fermi surface $\epsilon_{\rm b} = \epsilon_{\rm F}$ (Fig. 3) becomes a sphere as $V_G \rightarrow 0$.

In order to construct the transition probability W we write the Coulomb matrix elements for scattering from $(\vec{k_1}, \vec{k_2})$ into $(\vec{k_3}, \vec{k_4})$ in terms of the single-plane-wave matrix elements (2.6)-(2.7). Since the expression in general contains 16 terms we simplify the problem by supposing that only one of the coefficients β , say β_1 , is nonzero. Then (neglecting exchange)

$$\langle \vec{k}_{3}, \vec{k}_{4} | V_{Coul} | \vec{k}_{1}, \vec{k}_{2} \rangle = \alpha_{1} V (| \vec{k}_{3} - \vec{k}_{1} |) \delta (\Delta \vec{k})$$

$$+ \beta_{1} V (| \vec{k}_{3} - \vec{k}_{1} + \vec{G} |) \delta (\Delta \vec{k} - \vec{G}) , \quad (3.5)$$

$$\Delta \vec{k} = \vec{k}_{1} + \vec{k}_{2} - \vec{k}_{3} - \vec{k}_{4} ,$$

where V(q) is given by (2, 7). In performing the

surface integrals of Δ (2.21) we shall in fact permit only one of the β 's to be nonzero at a time.

To estimate the consequent error, note (Fig. 4) that $|\beta|$ is much smaller than $|\alpha|$ except within a small distance $\Delta k \sim 2m V_G / \hbar^2 G$ of the B.P. where they are comparable. (In general $\alpha^{2} > \frac{1}{2}$ and $\beta^2 \leq \frac{1}{2}$.) As we shall see, our approximation scheme will provide a contribution to Δ which is first order in $|V_G|/\epsilon_F$. A "second-order" calculation, which would allow *two* of the coefficients β to be nonzero at a time would add a contribution of order $O(V_G^2/\epsilon_F^2)$ to Δ , and so on for third- and fourthorder calculations. For the moment we retain only the first-order contribution, as $|V_G|/\epsilon_F$ is less than 10% in most of the cases we shall consider (see Table I).

From (3.3) we find the velocity factor in (2.21),

$$\Delta \vec{v} \equiv \vec{v}_1 + \vec{v}_2 - \vec{v}_3 - \vec{v}_4$$

= $(\hbar/m) (\Delta \vec{k} - \beta_1^2 \vec{G}_1 - \beta_2^2 \vec{G}_2 + \beta_3^2 \vec{G}_3 + \beta_4^2 \vec{G}_4) , \quad (3.6)$

where \vec{G}_n is the reciprocal lattice vector associated with the two-plane-wave description of ψ_n . Letting only β_1 be nonzero and observing the arguments in the δ functions of (3.5), i.e., if $\Delta k = 0$, then

$$(m/\hbar) \Delta \vec{\mathbf{v}} = -\beta_1^2 \vec{\mathbf{G}},$$

and if $\Delta \vec{\mathbf{k}} - \vec{\mathbf{G}} = 0$, then
 $(m/\hbar) \Delta \vec{\mathbf{v}} = \alpha_1^2 \vec{\mathbf{G}};$
the product in (2. 21) is
 $(\hbar/2\pi) (m^2/\hbar^2) |\Delta \vec{\mathbf{v}}|^2 W$
 $= \alpha_1^2 \beta_1^4 G^2 V^2 (|\vec{\mathbf{k}}_3 - \vec{\mathbf{k}}_1|) \delta (\Delta \vec{\mathbf{k}})$
 $+ \alpha^4 \beta_1^2 G^2 V^2 (|\vec{\mathbf{k}}_3 - \vec{\mathbf{k}}_1 + \vec{\mathbf{G}}|) \delta (\Delta \vec{\mathbf{k}} - \vec{\mathbf{G}}).$ (3.7)

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Since the common factor $\alpha_1^2 \beta_1^2$ is sharply peaked



FIG. 4. β^2 falls rapidly from $\frac{1}{2}$ to 0 as $|\eta|$ increases from zero, and $\alpha^2 = 1 - \beta^2$ rises from $\frac{1}{2}$ to 1. β^2 is relatively large only within a distance of about GV_G/ϵ_F from the B. P. $\eta = 0$.

for \bar{k}_1 near the B. P. (as shown on Fig. 4), it is clear that the contributions to Δ come from regions where at least one of the four wave vectors is close to a B. P.

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One might think of the $\delta(\Delta \vec{k} - \vec{G})$ term in (3.7) as representing umklapp processes, and the $\delta(\Delta \vec{k})$ term normal processes, although the distinction fades near the B. P. If one makes the distinction then umklapp contributions to Δ dominate normal ones since $\alpha^2 \ge \beta^2$. In fact if $2k_F > G$ the dominance is by about a factor of 4.

To calculate Δ we separately let each of the β_n 's become nonzero. Since the contribution of each is identical and the contributions are (by assumption) additive, the total is four times the individual contributions and

$$\Delta = \frac{G^2}{k_F^2} \left(v_F^2 \prod_{i=1}^4 \int \frac{dS_i}{|v_i|} \right) \alpha_1^2 \beta_1^2 \left[\beta_1^2 V^2(|\vec{k}_3 - \vec{k}_1|) \delta(\Delta \vec{k}) + \alpha_1^2 V^2(|\vec{k}_3 - \vec{k}_1 + \vec{G}|) \delta(\Delta \vec{k} - \vec{G}) \right] \langle |\vec{v}|^2 W \rangle^{-1}.$$
(3.8)

The denominator is treated in Appendix A, where it is shown that umklapp processes after its value by $O(V_G^2/\epsilon_F^2)$. The routine integrations over S_2 and S_4 give

$$\Delta = \left(\frac{G^2}{k_F^2}\right) \left[v_F^2 \int \frac{dS_1}{|v_1|} \frac{dS_3}{|v_3|} \alpha_1^2 \beta_1^2 \left(\beta_1^2 \frac{V^2(|\vec{k}_3 - \vec{k}_1|)}{|\vec{k}_3 - \vec{k}_1|} \Delta(\Delta \vec{k}) + \alpha_1^2 \frac{V^2(|\vec{k}_3 - \vec{k}_1 + \vec{G}|)}{|\vec{k}_3 - \vec{k}_1 + \vec{G}|} \Delta(\Delta \vec{k}) + O \frac{V_G^2}{\epsilon_F^2} \right) / \int |\vec{v}_1| dS_1 \frac{dS_3}{|v_3|} \frac{V(|\vec{k}_3 - \vec{k}_1|)}{|\vec{k}_3 - \vec{k}_1|} \Delta(\Delta \vec{k}) + O \frac{V_G^2}{\epsilon_F^2} \right] \cdot (3.9)$$

The Δ functions merely serve to restrict the S_1 and S_3 integrations to regions where the wave-vectorconservation conditions can be fulfilled. In the "normal" term $\Delta(\Delta \vec{k})$ the S_3 integral contributes the same as in the denominator—the result is proportional to $V^2(0)\gamma(2k_F/k_s)$. In the "umklapp" term, however, $(\vec{k}_1 - \vec{G})$ does not in general lie on the Fermi surface, so the "wave-vector transfer" $(\vec{k}_3 - \vec{k}_1 + \vec{G})$ is restricted from zero and the S_3 integral is thereby reduced, the amount of reduction depending on \vec{k}_1 . We introduce a new func tion $\gamma_u(\vec{k}_1)$ to denote this contribution (see Appendix B), so (3.9) becomes

$$\Delta = \frac{G^2}{k_F^2} \frac{\hbar m_{\text{opt}}}{4\pi k_F m} \int \frac{dS_1}{|v_1|} \alpha_1^2 \beta_1^2 \left(\beta_1^2 + \frac{\alpha_1^2 \gamma_u(\vec{k}_1)}{\gamma}\right).$$
(3.10)

The factor containing m_{opt} results from the S_1 integration in the denominator. The S_3 integrations cancel in the normal term—in the umklapp term the factor $\gamma_u(\vec{k}_1)/\gamma \leq 1$ represents the failure of complete cancellation. To estimate $\gamma(\vec{k}_1)$ we derive simple formulas by assuming the Fermi surface is spherical and ψ_3 is a single plane wave¹⁰:

$$\begin{aligned} \gamma_{u}(\vec{k}_{1}) \\ &= \frac{1}{2}(x_{F} + x_{\min})^{-1} \int_{x_{\min}}^{2x_{F}} \frac{ds}{(s^{2} + 1)^{2}} \quad \text{for } \vec{k}_{1} \cdot \vec{G} < \frac{1}{2}G^{2} \\ &= \frac{1}{2}(x_{F} - x_{\min})^{-1} \int_{x_{\min}}^{2x_{F} - x_{\min}} \frac{ds}{(s^{2} + 1)^{2}} \quad \text{for } \vec{k}_{1} \cdot \vec{G} > \frac{1}{2}G^{2}; \end{aligned}$$

$$(3.11)$$

where

$$x_F = k_F/k_s$$
,

$$\begin{aligned} x_{\min} &= (1/k_s) \mid (k_F^2 + G^2 - 2\vec{k}_1 \cdot \vec{G})^{1/2} - k_F \mid \\ &= (1/k_s) [\text{distance from } (\vec{k}_1 - \vec{G}) \\ & \text{to the Fermi surface}]. \end{aligned}$$

Consider (3.11) separately for the following cases. (i) The Fermi surface intersects the B. P.

 $[k_F > \frac{1}{2}G$ or more precisely, $\epsilon_F > (\hbar^2 G^2/8m) + |V_G|$.] In this case, the prefactor $(\beta_1 \alpha_1)^2$ in the integrand of (3.10) peaks when \vec{k}_1 is on the B. P. $(\vec{k}_1 \cdot \vec{G} = \frac{1}{2}G^2)$, and falls rapidly as \vec{k}_1 moves away (Fig. 4). It is precisely when \vec{k}_1 is on the B. P. that $\vec{k}_1 - \vec{G}$ lies on the Fermi surface, which means in turn that $x_{\min} = 0$, and $\gamma_u(\vec{k}_1$ on the B. P.) = γ . If we rewrite the term in large parentheses in (3.10) as

$$\{1 + \alpha_1^2[\gamma_u(\vec{k}_1)/\gamma - 1]\},\$$

then the second term is zero for \vec{k}_1 on the B. P. As it can be shown to give only a small contribution (see Appendix B), we neglect it for all \vec{k}_1 .

(ii) The Fermi surface does not intersect the B. P. $[k_F < \frac{1}{2}G$, or $\epsilon_F < (\bar{n}^2 G^2/8m) - |V_G|$.] For the simple alkali metals we find that $(\beta_1/\alpha_1)^2$ is at most of order V_G^2/ϵ_F^2 everywhere on the Fermi surface. It is therefore useful to rewrite the term in large parentheses of (3.10) as

$$\left\{\gamma_{u}(\vec{k}_{1})/\gamma + \beta_{1}^{2}\left[1 - \gamma_{u}(\vec{k}_{1})/\gamma\right]\right\},\$$

and to neglect this second term, which results in a relative error ~ $O(V_G^2/\epsilon_F^2)$. In case (i) (3.10) becomes

$$\Delta = \left(\frac{G}{k_F}\right)^2 \frac{\hbar m_{\text{opt}}}{4\pi k_F m^2} \int \frac{dS_1}{|v_1|} (\beta_1 \alpha_1)^2, \quad k_F > \frac{1}{2}G \ . \tag{3.12}$$

In case (ii) the only alteration in the expression is that $\gamma_u(\vec{k}_1)/\gamma$ appears in the integrand. This reduces Δ by some fraction, denoted by $\overline{\gamma}_u/\gamma$:

$$\Delta = \Delta^{(3,12)} \overline{\gamma}_{u} / \gamma, \quad k_{F} < \frac{1}{2}G, \qquad (3.13)$$

$$\frac{\overline{\gamma}_{u}}{\gamma} = \int \frac{dS}{|v|} (\alpha\beta)^{2} \gamma_{u}(\vec{k}) \left[\gamma \left(\frac{2k_{F}}{k_{s}}\right) \int \frac{dS}{|v|} (\alpha\beta)^{2} \right]^{-1}.$$

For a nearly spherical Fermi surface $\overline{\gamma}_u/\gamma$ depends almost solely upon geometrical factors. We have evaluated the fraction numerically for the geometry of the simple alkali metals and find $\overline{\gamma}_u/\gamma$ (alkali) $\approx \frac{5}{9}$.

A more important distinction between the polyvalent and alkali geometries arises from the integral in (3.12) itself. To evaluate that expression, for a single set of Bragg planes, we write

$$\frac{dS}{|v|} = \frac{|k_{\perp}|}{|v_{\perp}|} d\varphi dk_{\parallel} = \frac{m}{\hbar} d\varphi dk_{\parallel},$$

where k_{\parallel} and \vec{k}_{\perp} are components of \vec{k} parallel and perpendicular to \vec{G} . *m* is the free-electron mass since \vec{v}_{\perp} is unperturbed by the lattice potential. Integration over the azimuthal angle φ contributes 2π , so (3.12) becomes

$$\Delta = \frac{G^2}{k_F^2} \frac{m_{\text{opt}}}{2k_F m} \int dk_{\parallel} (\alpha \beta)^2. \qquad (3.14)$$

The width of the peak of the integrand $(\alpha\beta)^2$ is (from Fig. 4) $\Delta k \sim 4m V_G/\hbar^2 G$, so the fraction of the Fermi surface which contributes to Δ is proportional to V_G/ϵ_F . Since the maximum value of $(\alpha\beta)^2$ is independent of V_G , Δ is a direct measure of that fraction.

The integral in (3.14) is evaluated most simply by using the identity (from 3.2)

$$dk_{\parallel} = (m V_G / \hbar^2 G) (\alpha \beta)^{-2} d(\tan^{-1} (\alpha / \beta)), \qquad (3.15)$$

which holds everywhere except at $k_{\parallel} = \frac{1}{2}G$, where α/β suffers a discontinuity in the extended zone scheme [(3.2) and Figs. 3 and 5(a)]. Because of the discontinuity the integral must be taken separately over the first and second Brillouin zones, a procedure implied by the notation \int_{FS} :

$$\Delta = \frac{1}{4} \left(G V_G m_{\text{opt}} / k_F \epsilon_F m \right) \int_{FS} d(\tan^{-1}(\alpha/\beta)) \quad (3.16)$$

Figure 5 shows the integral as a function of $2k_F/G$. It is apparent that

$$\lim_{V_G \to 0} \int_{FS} d(\tan^{-1}(\alpha/\beta)) = \pi \theta (2k_F/G - 1), \qquad (3.17)$$

where θ is the unit step function. The identity

$$\tan^{-1}\eta[1+(1+\eta^{-2})^{1/2}] = -\frac{1}{2}\cot^{-1}\eta = -\frac{1}{2}\tan^{-1}\eta^{-1}$$

is useful in evaluating the integral explicitly: (i) For $k_F > \frac{1}{2}G$,¹¹

$$\int_{\mathbf{FS}} d\left(\tan^{-1}\left(\frac{\alpha}{\beta}\right) \right) = \left(\frac{\pi}{2} - \tan^{-1} \nu_{G} \right)$$

+
$$\left[\frac{\pi}{2} - \tan^{-1}\left(\frac{G\nu_G}{2k_F - G}\right)\right]$$
 + (3. 18a)
 $\simeq \pi - \frac{2k_F}{2k_F - G}\nu_G + O(\nu_G^2)$ (3. 18b)

where $\nu_G \equiv 4 m V_G / \hbar^2 G^2$, and where the first term within the parentheses on the right-hand side is associated with the first zone, and the second term with the second zone. (ii) For $k_F < \frac{1}{2}G$, the integration is over the first zone only and

$$\int_{FS} d\left(\tan^{-1}\left(\frac{\alpha}{\beta}\right)\right) = \tan^{-1}\left(\frac{G\nu_G}{G-2k_F}\right) - \tan^{-1}\nu_G$$
(3.19a)
$$\approx \frac{2k_F}{G-2k_F}\nu_G + O(\nu_G^2).$$
(3.19b)

The approximate forms (3.18b) and (3.19b) are valid if k_F is not too close to $\frac{1}{2}G$, and together with (3.16) show that to lowest order in ν_G

$$\Delta \approx \frac{\pi}{4} \frac{G V_G m_{\text{opt}}}{k_F \epsilon_F m} \quad \text{for } 2k_F > G \quad (3.20)$$

and



FIG. 5. (a) Plot of the function which appears as a differential in (3.15) and in the expression for Δ (3.16). (b) Fractional umklapp scattering Δ as a function of Fermi wave vector, normalized to its limiting value at large $2k_F/G$ (large η). The two plots correspond to the band gaps of the (200) and (111) planes of aluminum, and the corresponding values of $2k_F/G$ are indicated on the abscissa. The plots of (b) are equivalent to that of (a) with its discontinuity removed.

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$$\Delta \approx \frac{k_F^2}{G(G-2k_F)} \frac{V_G^2 m_{\text{opt}}}{\epsilon_F^2 m} \frac{\overline{\gamma}_u}{\gamma} \quad \text{for } 2k_F < G , \quad (3.21)$$

with $\overline{\gamma}_u/\gamma \approx \frac{5}{9}$ for the alkali-metal geometry. The principal results are summarized by (3. 20) and (3. 21). The polyvalent-metal geometry results in Δ proportional to V_G/ϵ_F , which represents the fraction of Fermi-surface area on which umklapp scattering can occur. By contrast Δ is proportional to only V_G^2/ϵ_F^2 in the alkali-metal geometry, dictated by the form of the mixing coefficient β far from the B. P.

We mention in passing that if the Fermi surface contacts the zone boundary but has no second zone, as in the noble metals, then the integral is given correctly by both (3.18a) and (3.19a):

$$\int_{FS} d(\tan^{-1}(\alpha/\beta)) = \frac{1}{2}\pi - \tan^{-1}\nu_G, \quad k_F = \frac{1}{2}G.$$
(3.22)

In the present section we have treated a Fermi surface in the presence of only a single pair of B. P. It has been possible to evaluate the S_1 integral (3.12) exactly, over the distorted Fermi surface. Surface distortions were ignored in the S_3 integration, which averages the transition probability W, but this results in small relative error $O(V_G/\epsilon_F)$. The approximation which we treat in Sec. IV is the assumed independence of the contributions from different coefficients β_n .

IV. APPLICATION TO REAL METALS

Before attempting to discuss real metals, we must first consider the problem of a Fermi surface in the presence of many B. P. In a typical scattering event, more than one of the four scattering states may deviate significantly from a single plane wave. This destroys the approximate additivity of contributions of the separate states to the total scattering probability, and requires that we consider the effects of interference in the surface integrals. Therefore it is probably incorrect to calculate Δ from the equation

where $\Delta_{\underline{G}}$ is the contribution to Δ from the pair of B. P. $(\pm \overline{G})$, as defined by (3.16):

$$\Delta_{G} = \frac{\pi G V_{G}}{4 k_{F} \epsilon_{F}} \frac{m_{opt}}{m} \left[\frac{1}{\pi} \int_{FS} d\left(\tan^{-1} \left(\frac{\alpha_{G}}{\beta_{G}} \right) \right) \right].$$
(4.2)

We define α_G/β_G as if only B. P. $(\pm \vec{G})$ were present. Later we shall assess our neglect of the effect of neighboring B. P.

Since it is unduly complicated to perform the surface integrals when each state contains two (or more) plane waves, we shall suggest (without proof) upper and lower bounds to the **result** which would be obtained by such an exact treatment. To do so we introduce the concept of "umklapp density of states."

A. Umklapp Density of States

Following (3. 12) or alternatively setting $\gamma_u(\vec{k}) = \gamma$ in (3. 10) we can think loosely of $(\alpha_k \beta_k)^2$ as the probability that an electron in state \vec{k} will participate in an umklapp process provided (as assumed in the previous section) that the other three scattering states are single plane waves. We define the surface-averaged probability as the "umklapp densityof-states,"

$$\frac{N_u}{N_0} = \frac{\int (dS/|v|) (\alpha\beta)^2}{4\pi k_F m/\hbar} = \left(\frac{k_F}{G}\right)^2 \frac{m}{m_{opt}} \Delta_G , \qquad (4.3)$$

where the subscript on N_0 refers to the free-electron value. Setting the factor $(1/\pi) \int_{FS} d (\tan^{-1}(\alpha/\beta))$ to unity, we have from (3. 20),

$$\frac{N_u}{N_0} = \frac{\pi}{4} \frac{k_F}{G} \frac{V_G}{\epsilon_F} \,. \tag{4.4}$$

Generalizing to the case in which many B. P. distort the Fermi surface, we assume that the contributions from all pairs of B. P. to $N_{\rm u}/N_0$ are additive:

$$\frac{N_u}{N_0} = \frac{m}{m_{\text{opt}}} \sum_{\text{pairs} \pm G} \left(\frac{k_F}{G}\right)^2 \Delta_G \approx \frac{\pi}{4} \sum_{\text{pairs} \pm G} \frac{k_F}{G} \frac{V_G}{\epsilon_F} .$$
(4.5)

In Table I, we list several values of N_u/N_0 , calculated taking into account the factors $\gamma_u(\vec{k})$ and $(1/\pi)$. $\int_{FS} d(\tan^{-1}(\alpha/\beta))$. Additivity in N_u/N_0 , (4.5), would follow if the different B. P. did not overlap near the Fermi surface. The overlapping produces admixture of three of four plane waves in the states and contributes to the reduction (m_{sh}/m) in the density of states. Presumably it reduces the umklapp density of states N_u/N_0 by $O(N_u^2/N_0^2)$. In any case overlapping is ignored.

Additivity in Δ , (4.1), on the other hand would follow from the assumption that three of the four scattering states are single plane waves. This assumption ignores interference effects (in processes like Fig. 6) which are present whether or not the different B. P. overlap. In the following we estimate the effects of interference by calculating Δ from N_u/N_0 with certain assumptions, rather than from (4.1) directly.

Since the contributions to N_u/N_0 come principally from regions near the B.P., we imagine that a certain fraction (N_u/N_0) of Fermi-surface states is responsible for umklapp scattering. We refer to this imaginary set of states as the "umklapp region." The probability that $n \leq 4$ of four randomly chosen wave vectors lie in the umklapp region is

TABLE III. Probability P(n) that *n* of 4 randomly chosen wave vectors on the Fermi surface lie in the umklapp region. For $N_u/N_0 < \frac{1}{5}$ there is only a small probability that more than two of the wave vectors lie in the umklapp region.

$N_{\rm N} = 0.20$							
n	0	1	2	3	4		
P(n)	0.41	0.41	0.15	0.026	0.0016		

$$P(n) = \frac{4!}{n!(4-n)!} \left(\frac{N_u}{N_0}\right)^n \left(1 - \frac{N_u}{N_0}\right)^{4-n}.$$
 (4.6)

We assume the formula holds for four *scattering* states, which must satisfy some wave-vector conservation rule.

For a typical polyvalent metal, with $N_u/N_0 = 0.20$, we list the probabilities on Table III.

Using N_u/N_0 and some assumption about interference, we may deduce the "relative probability" P_u that an umklapp process will occur. (One might prefer to call P_u the "fraction of umklapp scatterings.") For example, the "additivity assumption" of Sec. III is equivalent to saying $P_u = 4N_u/N_0$. We find the formula for Δ in terms of P_u by generalizing (3.10). Instead of multiplying the contribution from \vec{k}_1 by four [which we did to obtain (3.10)], we replace the surface average of $(\alpha_1\beta_1)^2$ by P_u in, for example, (3.12) and the result is

$$\Delta = \frac{m_{\text{opt}}}{m} \left(\frac{G}{2k_F}\right)^2 P_u . \tag{4.7}$$

Since the different \vec{G} 's have different magnitudes, we weight each according to its contribution to $N_u N_0$, and use the definition of N_u / N_0 (4.5) to write, more generally,

$$\Delta = \frac{P_u}{4(N_u/N_0)} \sum_{\text{pairs} \pm G} \Delta_G . \qquad (4.8)$$

Now the "additivity assumption" of Sec. III, which ignores interference effects, can be stated as follows: "If a scattering state lies in the umklapp region, it contributes to Δ whether or not any of the other three scattering states is in the umklapp region." The contribution to Δ from a given configuration is therefore proportional to the number of states in the umklapp region, so

$$P_u^{\max} = \sum_{n=1}^{4} nP(n) = 4(N_u/N_0).$$

This statement applied to (4, 8) leads to (4, 1) as it should, and provides an upper bound to Δ :

$$\Delta_{\max} = \sum_{\text{pairs} \pm G} \Delta_G , \qquad (4.9)$$

since it probably overestimates the effects of interference. Going to the opposite extreme, we might assume that if one or more of the four scattering states are in the umklapp region, they contribute to Δ as if only one state were in the umklapp region. This leads to the following, which we suggest as a lower bound:

$$P_u^{\min} = \sum_{n=1}^{4} P(n) = 1 - P(0) = 1 - (1 - N_u/N_0)^4$$

and

$$\Delta_{\min} = \frac{1 - (1 - N_u / N_0)^4}{4N_u / N} \sum_{\text{pairs} \pm G} \Delta_G . \qquad (4.10)$$

For the example $N_u/N_0 = 0.20$ (Table III), the upper and lower bounds are quite close: $\Delta_{\min} = 0.74 \Delta_{\max}$.

FIG. 6. Geometry of a doubleumklapp scattering event. The dashed line is the great circle on which \vec{k}_3 and \vec{k}_4 , diametrically opposed, satisfy the condition $\vec{k}_1 + \vec{k}_2 - \vec{k}_3 - \vec{k}_4 - \vec{G}_1 - \vec{G}_2 = 0$.



B. Interference Effects

We now mention a specific case of interference which suggests that the upper bound Δ_{max} (4.9) is closer to the true value of Δ than the lower bound Δ_{\min} (4.10). Noting in Table III that most of the contributions to Δ come from scattering processes in which only one or two of the states are in the umklapp region, one of the authors has repeated the calculation of Sec. III for the case in which two states deviate from single plane waves (Fig. 6. and second paper of Ref. 3). The result of that calculation is as follows: If the two states lie close to different B.P., and if the usual umklapp scattering phase-space factors $\gamma_u(\vec{k})$ are ignored, then the contributions from the two states to Δ are additive. That is, each state contributes to Δ independently of the other.

To estimate P_u we need now only make assumptions about scattering events with three or four states in the umklapp region. Assuming conservtively that three or four states could contribute only as much as two, we deduce that

$$P_u = P(1) + 2 \sum_{n=2}^{4} P(n) = 4(N_u/N_0) - P(3) - 2P(4)$$

 \mathbf{or}

$$\Delta = \Delta_{\max} \left(1 - \frac{P(3) + 2P(4)}{\sum n P(n)} \right) \approx \Delta_{\max}$$
 (4.11)

(for $N_w/N_0 = 0.20$, $\Delta = 0.964 \Delta_{max}$). Because P(3)and P(4) are small the quantitative result (4.11) is practically independent of assumptions about scattering events in which more than two states are in the umklapp region. Calculated values of Δ [from (4.11)] are given in Table I, along with the resulting values of electrical resistivity.

We repeat that we have not taken into account the overlapping effects of the different B.P. in estimating N_u/N_0 . For this reason we do not claim high accuracy in the final result Δ . In calculating Δ from (4.11) we drop the factor m_{opt}/m in (4.2), since the enhancement to Δ which it provides is almost certainly compensated by the overlapping effect we have ignored.

C. Estimates of \triangle and Electrical Resistivity

We have calculated N_u/N_0 as described following (4.5), and Δ from (4.11) as described above, for the metals listed in Table I. Since in every case $N_u/N_0 < \frac{1}{5}$, the value of Δ is within 4% of its upper bound Δ_{max} . The entries in the Table are computed as follows.

(a) In the spirit of our two-plane-wave calculation, we take values of V_G determined by local pseudopotential fits to the Fermi surfaces. We use the values of Ashcroft^{12,13} for Al, K, and Na; Ashcroft and Lawrence¹⁴ for In; Harrison¹⁵ for Zn; and Kimball, Stark, and Mueller¹⁶ for Mg. Falicov and Stark¹⁷ fit the Fermi surfaces of Zn and Cd, using a pseudopotential which is nonlocal through a strong admixture of d states. Using the parameters of their local component in the formula for Δ does not alter our result substantially. Using a similar nonlocal pseudopotential, Lee and Falicov¹⁸ show that an improved fit to the Fermi surface of K is possible. The resulting parameter V_{110} is roughly one-third Ashcroft's value, which would reduce our value of Δ by about nine. The umklapp scattering induced by the admixed d states might compensate the reduction, but we shall not consider that problem here.

(b) Special Fermi-surface characteristics are taken into account in calculating N_u/N_0 for In and Mg. The absence of third-zone arms in the (200) planes of In reduces the contribution from (111) planes by one-third, and the contribution from (200) planes by one-half. In Mg, the important set of B. P. barely intersects the Fermi surface: $(k_F - \frac{1}{2}G)/k_F \approx \frac{1}{17}$. Nevertheless,

$$(1/\pi)\int_{FS} d(\tan^{-1}(\alpha/\beta)) = 0.85$$

for a single set of these planes, which is close to its maxim value of unity. The Fermi surface of Cd is highly distorted, and cannot be well fit by a local pseudopotential. Noting the similarity to Zn (which also requires a nonlocal pseudopotential for a precise fit)¹⁷ we take Δ to be about the same, without special considerations of its Fermi surface.

(c) We use the free-electron mass for both m_{opt} and m_{sh} . To use estimated effective masses would probably change the final result by an amount less than the uncertainty in Δ . Note that the factor $m_{opt}/ne^2\tau_0$ is proportional to $m_{opt}m_{sh}^3$: If we estimate m_{opt} by adding results from each B. P., and take m_{sh} from the references quoted, the resulting product is close to unity (Table II).

V. CONCLUSIONS

Since we have used only the simplest type of wave functions in calculating umklapp scattering probabilities, our estimates of Δ_{\min} can probably be interpreted as the smallest possible values of Δ consistent with observed Fermi-surface distortions. Further complications in the wave functions which we have ignored (admixed d states and coreorthogonalization components) can be expected only to enhance the umklapp scattering. In potassium and sodium, our estimate of umklapp scattering is of the same order of magnitude as that suggested by Ziman and Rösler, which would arise from the core-orthogonalization components of the wave functions. In the polyvalent metals, Δ is so large (about half of the scattering events may be regarded as "umklapp") that further refinements in the wave functions would probably not alter its

value significantly.

The surprising conclusion of this work is that the T^2 component in electrical resistivity resulting from Coulomb electron-electron scattering is as strong in potassium as in the polyvalent metals we have studied. This is possible because the low electron densities in both potassium and sodium compensate their small umklapp scattering probabilities. Our conclusion would not be altered by improvements to the Born approximation, which is known to underestimate the scattering probabilities more severely in metals with low electron density than in metals with high electron density. Smith and Kukkonen¹⁹ use a phase-shift analysis to calculate the scattering cross section due to the Thomas-Fermi screened-Coulomb interaction for relative energy equal to the Fermi energy of sodium. The resulting cross section is reduced only by a factor of 2 over that given by the Born approximation.

Nor would our conclusion be altered by including the exchange term (2.6) in the transition probability. In Appendix C we calculate the exchange contribution to $1/\tau_0$ and find that the relaxation rate is reduced by about $\frac{2}{3}$, the reduction varying by only 5% over the entire range of electron densities represented on Table I. The parameter Δ is affected only minutely by exchange, since almost the same average of W occurs in both its numerator and denominator.

In closing we recall that our improved treatment of the Boltzmann equation, which includes energy dependence in the deviation function, leads to deviations from a pure T^2 power law in electrical $(T^1$ in thermal) resistivity. For the largest values of Δ , the deviations are less than 10% in electrical (25% in thermal) resistivity, and the deviations decrease as Δ decreases.

APPENDIX A

We derive here an equation for the energy dependence $\psi(t)$ [(2.12a) and (2.12b)] which maximizes the conductivity functional (2.8) subject to the assumed angular dependence (2.12a) and (2.12b). We shall treat the case in which there is no impurity scattering and simply quote the more general result at the end.

Setting $\delta T/\delta \psi = 0$ in (2.8) is equivalent to forming the inner product of both sides of the Boltzmann equation (2.2) with the function $\vec{v} \cdot \hat{E}$ without doing the energy integrals, and performing an average over directions of the electric field (or temperature gradient):

$$\begin{pmatrix} e \\ t_1 \end{pmatrix} \frac{\partial n_1^0}{\partial \epsilon_1} \frac{k_B T}{12\pi^3 \hbar} \int dS_1 \left| \vec{\mathbf{v}}_1 \right| = \frac{-4}{3(2\pi)^9 \hbar} \int \frac{dS_1}{|v_1|} d^3 k_2 d^3 k_3 d^3 k_4 P(1, 2-3, 4) \vec{\mathbf{v}}_1 \cdot (\vec{\mathbf{v}}_1 \psi_1 + \vec{\mathbf{v}}_2 \psi_2 - \vec{\mathbf{v}}_3 \psi_3 - \vec{\mathbf{v}}_4 \psi_4),$$
 (A1)

where the factor $e(t_1)$ applies to the electrical (thermal) case. Of course $\psi_i = \psi(t_i)$ is a function only of reduced energy t_i . The directional average of the electric field (temperature gradient) is justified in the cases of polycrystalline samples or single crystals of cubic materials, where the conductivity tensor is diagonal. Noting that $-\partial n_1^0/\partial \epsilon_1 = (4k_BT \cosh^2 \frac{1}{2}t_1)^{-1}$ and that the surface integral on the left-hand side is proportional to n/m_{opt} [definition (2.14)] and using $d^3k = (k_BT/\hbar) (dS_k/|v_k|) dt$ [(2.13)], we write

$$\begin{pmatrix} t_1 \\ e \end{pmatrix} (4 \cosh^{\frac{2i}{2}}t_1)^{-1} \frac{n}{m_{\text{opt}}} = \frac{4}{3(2\pi)^9} \frac{(k_B T)^2}{\hbar^4} \int \frac{dS_1}{|v_1|} \left(\prod_{i=2}^4 \frac{dS_i}{|v_i|} dt_i \right) \\ \times W(1, 2-3, 4) n_1^0 n_2^0 (1-n_3^0) (1-n_4^0) \delta(t_1+t_2-t_3-t_4) \vec{v}_1 \cdot (\vec{v}_1 \psi_1 + \vec{v}_2 \psi_2 - \vec{v}_3 \psi_3 - \vec{v}_4 \psi_4) .$$
 (A2)

Now we rewrite the product $\Pi \equiv \vec{v_1} \cdot (\vec{v_1}\psi_1 + \vec{v_2}\psi_2 - \vec{v_3}\psi_3 - \vec{v_4}\psi_4)$ by making the variable transformations $(t_3 - t_2, t_2 - t_3)$ in the ψ_2 term, and $(t_3 - t_4, t_4 - t_3)$ in the ψ_4 term. Using the identity $n^0(-t) = 1 - n^0(t)$ and noting that $\psi(t)$ is an even (odd) function of t in the electrical (thermal) case²⁰ we rewrite the product Π inside the integrals:

 $\prod (\text{electrical}) = \psi_1 | \vec{v_1} |^2 + \psi_3 \vec{v_1} \cdot (\vec{v_2} - \vec{v_3} - \vec{v_4}),$

$$\Pi \text{ (thermal)} = \psi_1 | \vec{v}_1 |^2 - \psi_3 \vec{v}_1 \cdot (\vec{v}_2 + \vec{v}_3 + \vec{v}_4) \text{ .}$$

Permutation symmetry in the surface variables (2.6) further permits the replacement

$$\vec{v}_1 \cdot \Delta \vec{v} + \frac{1}{4} \left| \Delta \vec{v} \right|^2,$$

where

$$\Delta \vec{v} \equiv \vec{v}_1 + \vec{v}_2 - \vec{v}_3 - \vec{v}_4 ,$$

and so finally

 $\prod \text{ (electrical)} = \psi_1 \left| \vec{\mathbf{v}}_1 \right|^2 - \psi_3 \left(\left| \vec{\mathbf{v}}_1 \right|^2 - \frac{1}{4} \left| \Delta \vec{\mathbf{v}} \right|^2 \right)$

$$\prod (\text{thermal}) = \psi_1 |\vec{v}_1|^2 - \psi_3 [\vec{v}_1 \cdot (\vec{v}_1 + 2\vec{v}_2) - \frac{1}{4} |\Delta \vec{v}|^2].$$

So three distinct surface integrals enter the righthand sides of (A2). Denoting the fourfold surface integration by angular brackets (2.15) the integrals are (i)

$$\langle |\vec{\mathbf{v}}_1|^2 W(1, 2 \rightarrow 3, 4) \rangle \equiv \langle |\vec{\mathbf{v}}|^2 W \rangle$$

proportional to the quasiparticle relaxation rate

due to electron-electron scattering for an electron on the Fermi surface; (ii) $\langle \vec{v_1} \cdot \vec{v_2} W \rangle$, analogous to an angular average in JSW, occurs only in the thermal conductivity; and (iii) $\langle |\Delta \vec{v}|^2 W \rangle$, which vanishes without umklapp scattering.

The first integral (i) defines the relaxation rate from the text:

$$\frac{n}{\tau_0 m_{\text{opt}}} \equiv \frac{4}{3(2\pi)^9} \frac{(k_B T)^2}{\hbar^4} \langle |\vec{\mathbf{v}}|^2 W \rangle \qquad (2.16)$$

and the remaining two integrals enter as dimensionless ratios:

$$\Delta \equiv \frac{1}{4} \langle | \Delta \vec{\mathbf{v}} |^2 W \rangle \langle | \vec{\mathbf{v}} |^2 W \rangle^{-1}$$
 (2.21)

and

$$\langle \cos\theta \rangle \equiv \langle \vec{\mathbf{v}}_1 \cdot \vec{\mathbf{v}}_2 W \rangle \langle |\vec{\mathbf{v}}|^2 W \rangle^{-1}.$$
 (2.22)

With these parameters we write (A2) as

$$\binom{e}{t} (2\cosh\frac{1}{2}t)^{-2} = \tau_0^{-1} \int \int dt_2 dt_3 dt_4 \,\delta\left(t + t_2 - t_3 - t_4\right)$$
$$\times n^0(t) \, n^0(t_1) \left[1 - n^0(t_3)\right] \left[1 - n^0(t_4)\right]$$
$$\times \left[\psi(t) - \left(\frac{1 - \Delta}{1 + 2\langle\cos\theta\rangle - \Delta}\right) \,\psi(t_3)\right] \,. \quad (A3)$$

The relevant energy integrals are recorded as (B11) and (B12) of JSW. Using those formulas and substituting $\psi(t) \equiv 2\tau_0 \cosh \frac{1}{2}t Q(t)$ we recover the reduced Boltzmann equation (B13) of JSW,

$$\binom{e}{t} \cosh^{-1}\frac{1}{2}t = (\pi^2 + t^2) Q(t) - \alpha \int_{-\infty}^{\infty} ds \ F(t-s) Q(s),$$
(A4)

where

$$F(x) \equiv \frac{x}{2\sinh\frac{1}{2}x}$$

and

$$\alpha = 2 \begin{pmatrix} 1 - \Delta \\ 1 + 2 \langle \cos \theta \rangle - \Delta \end{pmatrix}$$
 (A5)

for the electrical (thermal) conductivity. JSW show that (A4) leads to the *electrical* conductivity

$$\sigma = \frac{ne^2 \tau_0}{2m_{\text{opt}}} \tilde{\sigma} \quad , \tag{A6}$$

where

$$\widetilde{\sigma} = \int_{-\infty}^{\infty} dt \frac{Q(t)}{\cosh \frac{1}{2}t}$$
$$= \frac{1}{3} + \frac{4\alpha}{\pi^2} \sum_{\text{odd n}} \frac{2n+1}{n^2(n+1)^2} \left(\frac{1}{n(n+1)-\alpha}\right) ,$$

and to the thermal conductivity

$$K = \frac{nk_B^2 T \tau_0}{2m_{\text{opt}}} ,$$

where

$$\begin{split} \tilde{K} &= \int_{-\infty}^{\infty} dt \, \frac{t \, Q(t)}{\cosh \frac{1}{2} t} \\ &= \frac{12 - \pi^2}{3} + 4 \, \alpha \, \sum_{\text{even } n} \, \frac{2n + 1}{n^2 (n+1)^2} \left(\frac{1}{n(n+1) - \alpha} \right). \end{split}$$
(A7)

The problem of combined electron-electron and electron-impurity scattering was solved by Smith and Wilkins.⁶ The equation for $\psi(t)$ is of the form (A4), modified only by the introduction of the parameter

$$\beta = (2/\pi^2) \tau_0 / \tau_{\rm imp}, \qquad (2.23)$$

the ratio of electron-electron to electron-impurity scattering times. So the conductivities are again given by series. The resulting temperature-dependent resistivities are given to within 2% by the simple expressions (2. 24) and (2. 25), over the whole range of parameters $0 \le \alpha \le 2$ and $0 \le \beta < \infty$. For $\beta = 0$ the expressions (2. 24) and (2. 25) represent the first two terms of the series and approximate the exact results to within $\frac{4}{3}$ % for $0 \le \alpha \le 2$.

APPENDIX B

We calculate the surface integral $\langle |\vec{\nabla}|^2 W \rangle$, (2.17), related to τ_0 by (2.16), and show that (2.17) is valid to second order in the ratio of the band gap to the Fermi energy V_G/ϵ_F . Equation (2.17) would be exact on a spherical Fermi surface with normal scattering only, but a small $O(V_G^2/\epsilon_F^2)$ reduction occurs because of the reduced density of final states which accompanies umklapp processes. Typically $V_G / \epsilon_F < 0.1$ (Table I) so the correction to $\langle |\vec{v}|^2 W \rangle$ is $\leq 1\%$. This and the analogous correction to Δ will be discussed at the end of the appendix. In order to isolate the correction term in our derivation of (2.17) we shall include umklapp processes, using the notation of Sec. III. For the purposes of Sec. II we point out that a coefficient α^2 accompanies normal processes and β^2 accompanies umklapp processes. To derive (2.17) without the correction one may set $\alpha^2 = 1$ and $\beta = 0$.

To begin we suppose that k_1 lies close to the B. P. (\vec{G}) and write the transition probability (2.6) as (neglecting exchange)

$$(\hbar/2\pi) W(1, 2-3, 4) = \alpha_1^2 V^2(|\vec{k}_3 - \vec{k}_1|) \delta(\Delta \vec{k}) + \beta_1^2 V^2(|\vec{k}_3 - \vec{k}_1 + \vec{G}|) \delta(\Delta \vec{k} - \vec{G}).$$
(B1)

In the fourfold surface integration $\langle |\vec{\nabla}|^2 W \rangle$ we first do the S_2 and S_4 integrals by Ziman's method⁸: On a spherical Fermi surface the surface elements are defined by $dS_k = k^2 d\Omega_k$, where $d\Omega_k$ is the solid angle subtended by dS_k at the distance k. Introducing $q = k_4 - k_2$ we make the replacements dS_2 $+ (k_F^2/q^2) dS_q$ and $dS_4 + 2\pi q dq$ so that

$$dS_2 dS_4 = 2\pi (k_F^2 / q) d^3 q$$

and

$$\int \frac{dS_2}{|v_2|} \frac{dS_4}{|v_4|} \,\delta(\Delta k - Q) = \frac{2\pi m_{gh}^2}{\hbar^2 |\vec{k}_3 - \vec{k}_1 - \vec{Q}|} \,\Delta(\Delta \vec{k} - \vec{Q}), \tag{B2}$$

where $\vec{Q} = 0$ in the first term of (B1) and $\vec{Q} = \vec{G}$ in the second term. $\Delta(\Delta \vec{k} - \vec{Q})$ restricts the S_1 and S_3 integrations to regions in which the condition $\Delta \vec{k} - \vec{Q}$

= 0 can be satisfied with all four wave vectors \vec{k}_i on the Fermi surface. For normal processes $\Delta(\Delta \vec{k})$ is trivially unity for all \vec{k}_1 and \vec{k}_3 on the Fermi surface. The factors of m_{sh} are intended to correct for the distortion of the Fermi surface. We assume the correction is close to the usual definition of the "specific-heat effective mass" (2.19) (In most simple metals $0.9 \le m_{sh}/m \le 1.0$):

$$\langle \left|\vec{\nabla}\right|^{2}W\rangle = \frac{(2\pi m_{\rm sh})^{2}}{\hbar^{3}} \int \frac{dS_{1}}{|v_{1}|} \frac{dS_{3}}{|v_{3}|} \left|\vec{\nabla}_{1}\right|^{2} \left(\alpha_{1}^{2} \frac{V^{2}(\left|\vec{k}_{3}-\vec{k}_{1}\right|)}{\left|\vec{k}_{3}-\vec{k}_{1}\right|} \Delta(\Delta\vec{k}) + \beta_{1}^{2} \frac{V^{2}(\left|\vec{k}_{3}-\vec{k}_{1}+\vec{G}\right|)}{\left|\vec{k}_{3}-\vec{k}_{1}+\vec{G}\right|} \Delta(\Delta\vec{k}-\vec{G})\right). \tag{B3}$$

To evaluate the first term in square brackets we write $dS_3 = 2\pi |k_3 - k_1| d |k_3 - k_1|$ as if the Fermi surface were spherical, and introduce another factor of $m_{\rm sh}$ to denote the correction. Accordingly,

$$\int \frac{dS_3}{|v_3|} \frac{V^2(|\vec{k}_3 - \vec{k}_1|)}{|\vec{k}_3 - \vec{k}_1|} \Delta(\Delta \vec{k}) + 4\pi \frac{m_{\rm sh}}{\hbar} \left(\frac{1}{2k_F} \int_0^{2k_F} dq \ V^2(q)\right) = 4\pi \frac{m_{\rm sh}}{\hbar} V^2(0)\gamma \ (2k_F/k_s) \equiv 2m_{\rm sh} W(2k_F/k_s), \quad (B4)$$

where γ and W are given by (2.18), with $y = q/k_s$. Turning to the second term in large parentheses we can again express the S_3 integration as an integral over momentum transfer, but since $\vec{k}_1 - \vec{G}$ does not in general lie on the Fermi surface the momentum transfer $\vec{k}_3 - \vec{k}_1 + \vec{G}$ is restricted away from zero and the S_3 integral is correspondingly reduced. The $\mathbf{\bar{k}}_1$ -dependent reduction is expressed through the function $\gamma_u(\vec{k}_1)$, (3.11), which replaces $\gamma(2k_F/k_s)$ in (B4). [The estimate (3.11) is done in the approximation of a spherical Fermi surface.] The important point is that β_1^2 is sharply peaked for \overline{k}_1 close to the B. P. (\vec{G}), i.e., for $\vec{k}_1 - \vec{G}$ close to the Fermi surface. So the S_1 integration emphasizes those values of k_1 for which $\gamma_u(k_1)$ is approximately equal to $\gamma (2k_F/k_s)$, and we can isolate the correction term by using $\alpha_1^2 + \beta_1^2 = 1$ (Sec. III) to write (B3) as

$$\langle |\vec{\mathbf{v}}|^2 W \rangle = 8\pi^2 \left(\frac{m_{sh}}{\hbar}\right)^3 W\left(\frac{2k_F}{k_s}\right)$$
$$\times \int dS_1 |\vec{\mathbf{v}}_1| \left[1 + \beta_1^2 \left(\frac{\gamma_u(\vec{\mathbf{k}}_1) - \gamma}{\gamma}\right)\right], \quad (B5)$$

where $\gamma \equiv \gamma (2k_F/k_s)$. Since the difference function $\gamma_u(\vec{k}_1) - \gamma$ vanishes for \vec{k}_1 on the B. P. and grows linearly in the distance of \vec{k}_1 away from the Bragg plane, and since β_1^2 restricts the contribution from the S_1 integration to the region within about $k_F V_G / \epsilon_F$ of the B. P., we can conclude that the correction term in (B5) is second order in V_G / ϵ_F . Ig-

noring the correction term the combined normal and umklapp contributions give exactly what normal processes alone ($\alpha^2 = 1$ and $\beta = 0$) would give.

To complete the derivation we note that the S_1 integration is proportional to the inverse optical mass (2.14), so

$$\langle \left| \overrightarrow{\mathbf{v}} \right|^2 W \rangle = 3(2\pi)^5 \frac{m_{\rm sh}^3 n}{\hbar^2 m_{\rm opt}} W \left(\frac{2k_F}{k_{\rm s}} \right) \left[1 + O \left(\frac{V_G^2}{\epsilon_F^2} \right) \right].$$
(B6)

Umklapp Phase-Space Corrections to τ_0 and Δ

We have computed by machine the correction terms to $\langle |\vec{\nabla}|^2 W \rangle$, (B5), and to Δ , (3.10). In $\langle |\vec{\nabla}|^2 W \rangle$ we resolve the direct and correction terms

$$D+C=\int dS \left|\vec{v}\right| \left\{1+\beta^2 \left[\Delta\gamma(\vec{k})/\gamma\right]\right\}, \quad (\tau_0)$$

where $\Delta \gamma(\vec{k}) \equiv \gamma_u(\vec{k}) - \gamma$ and consequently $C \leq 0$. *D* is the same whether or not umklapp processes occur and *C* vanishes in the absence of umklapp. We evaluate *C* using (3.11) for $\gamma_u(\vec{k})$. *C* is quadratic in V_G/ϵ_F to lowest order, and depends only weakly on geometry k_F/G . We show the result on Fig. 7 for $k_F/G = 0.65$ [(111) planes of aluminum]. |C|/D is less than a percent for $V_G/\epsilon_F = 0.2$.

The direct and correction terms of Δ are resolved as in (3.10).

$$D+C=\int \frac{dS}{|\vec{v}|} (\alpha\beta)^2 \left(1+\alpha^2 \frac{\Delta\gamma(\mathbf{k})}{\gamma}\right), \quad (\Delta).$$

Again $C \le 0$ is quadratic in V_G / ϵ_F , but now D is linear in V_G / ϵ_F to lowest order, and (with C) vanishes without umklapp. Again the computation shown on Fig. 7 was done for $k_F / G = 0.65$. |C| / D is as large as 10% for $V_G / \epsilon_F = 0.08$.

APPENDIX C

Angular Averages

Jensen, Smith, and Wilkins, ⁵ following Abrikosov and Khalatnikov, ²¹ express the transition probability W in terms of the angular coordinates depicted in Fig. 8. θ is the angle between the two incident momenta, and φ is the angle between the planes



FIG. 7. Corrections to Δ and τ_0 due to restricted umklapp scattering phase space, for the geometry of (111) planes in aluminum.

defined by the two incident, and the two final momenta.

Our object here is to relate their angular averages to our averages over momentum transfer. We shall show that our definition of τ_0 is equivalent to that of JSW on a spherical Fermi surface, and we shall derive the expression for $\langle \cos \theta \rangle$ as an average over momentum transfer. Finally we calculate the exchange correction to τ_0 .

To convert the angular averages into momentumtransfer averages we introduce the variables

$$z = \sin^2 \frac{1}{2} \theta$$
, $u = \sin \frac{1}{2} \theta \sin \frac{1}{2} \varphi = \left| \mathbf{k}_3 - \mathbf{k}_1 \right| / 2k_F$

the latter proportional to momentum transfer. The following formulae will be useful:

$$d\varphi = \frac{2}{(z-u^2)^{1/2}} du, \quad \cos\theta = 1 - 2z,$$

$$\cos\frac{1}{2}\theta = (1-z)^{1/2}, \qquad d(\cos\theta) = -2 dz.$$
(C1)

The angular average which determined the relaxation time τ_0 is

$$\left\langle \frac{\omega(\theta, \varphi)}{\cos\frac{1}{2}\theta} \right\rangle \equiv \int_{0}^{\pi} \frac{d\varphi}{\pi} \int_{-1}^{1} \frac{d(\cos\theta)}{2} \frac{\omega(\theta, \varphi)}{\cos\frac{1}{2}\theta}$$
$$= \frac{2}{\pi} \int_{0}^{1} dz \int_{0}^{\sqrt{z}} \frac{du\,\omega(u, z)}{(1-z)^{1/2}(z-u^{2})^{1/2}}$$
$$= \frac{2}{\pi} \int_{0}^{1} du \int_{u^{2}}^{1} \frac{dz\omega(u, z)}{(1-z)^{1/2}(z-u^{2})^{1/2}} .$$
(C2)

Ignoring exchange, $\omega(u) = (2\pi/\hbar) V^2(|\vec{k}_3 - \vec{k}_1|)$ is independent of z and we can use the identity

$$\int_{u^2}^{1} dz \, \frac{1}{(1-z)^{1/2}} \, \frac{1}{(z-u^2)^{1/2}} = \pi$$

to get

$$\left\langle \frac{\omega(\theta, \varphi)}{\cos\frac{1}{2}\theta} \right\rangle = 2 \int_0^1 du \,\,\omega(u) = 2W\left(\frac{2k_F}{k_s}\right),\tag{C3}$$

where $W(2k_F/k_s)$ is defined in the text, (2.18), and is associated with the surface average $\langle |\vec{\nabla}|^2 W \rangle$ which determines τ_0 . From (C3) and (2.20) one can see that our τ_0 is identical with that of JSW, on a spherical Fermi surface.

The angular average analogous to our $\langle \cos \theta \rangle$ is

$$\left\langle \frac{\cos \theta \,\omega(\theta, \,\varphi)}{\cos \frac{1}{2}\theta} \right\rangle = \frac{2}{\pi} \int_0^1 du \int_{u^2}^1 dz \,\frac{(1-2z)\,\omega(u)}{(1-z)^{1/2}(z-u^2)^{1/2}} \,.$$

Again ignoring exchange we break up the integrand,

$$\left(2\left(1-z\right)^{1/2}-\frac{1}{\left(1-z\right)^{1/2}}\right)\frac{1}{\left(z-u^2\right)^{1/2}}\,\omega(u)$$

and use

$$\int_{u^2}^{1} \frac{(1-z)^{1/2}}{(z-u^2)^{1/2}} \, dz = \frac{\pi}{2} \left(1-u^2\right)$$

to deduce

$$\left\langle \frac{\cos\theta\omega(\theta, \varphi)}{\cos\frac{1}{2}\theta} \right\rangle = -2\int_{0}^{1} u^{2}\omega(u) \, du$$
$$= 2W\left(\frac{2k_{F}}{k_{s}}\right) \left\langle \cos\theta \right\rangle. \tag{C4}$$

The second equality follows from the definition of $\langle \cos \theta \rangle$, (2.22), which is equivalent to

$$\langle \cos \theta \rangle \equiv \left\langle \frac{\cos \theta \,\omega(\theta, \,\varphi)}{\cos \frac{1}{2} \theta} \right\rangle \left\langle \frac{\omega(\theta, \,\varphi)}{\cos \frac{1}{2} \theta} \right\rangle^{-1}$$

We now calculate the exchange correction to τ_0 .

Exchange

From (2.6) and Fig. 8 we write the transition probability as the sum of direct and exchange terms:

$$\omega(\theta, \ \varphi) = (2\pi/\hbar) \left[V^2(\theta, \ \varphi) - \frac{1}{2} V(\theta, \ \varphi) V(\theta, \ \varphi + \pi) \right]$$
$$\equiv \omega_D(\theta, \ \varphi) - \frac{1}{2} \omega_{ex}(\theta, \ \varphi).$$
(C5)

Using the Thomas-Fermi potential,

$$V(\theta, \phi) = \frac{4\pi e^2}{(2k_F)^2 \sin^2 \frac{1}{2}\theta \sin^2 \frac{1}{2}\varphi + k_s^2},$$

the exchange term is

$$\omega_{\mathrm{ex}}(\boldsymbol{\theta}, \boldsymbol{\varphi}) = (2\pi^3 e^4 / \hbar k_F^4) \left(\sin^2 \frac{1}{2} \boldsymbol{\theta} \sin^2 \frac{1}{2} \boldsymbol{\varphi} + \chi^{-2} \right)^{-1}$$



FIG. 8. Angular variables introduced in Ref. 21. θ is the angle between initial wave vectors and ϕ is the angle between the planes defined by the two initial and the two final wave vectors.

and

$$\times (\sin^2 \frac{1}{2}\theta \cos^2 \frac{1}{2}\varphi + x^{-2})^{-1},$$

ables, we have

$$\omega_{\rm ex}(u, z) = (2\pi^3 e^4 / \hbar k_F^4) (u^2 + x^{-2})^{-1} (z - u^2 + x^{-2})^{-1}$$

where $x \equiv 2k_F / k_s$. Transforming to *u* and *z* vari-

$$\frac{\hbar k_F^4}{2\pi^3 e^4} \left\langle \frac{\omega_{\text{ex}}(\theta, \varphi)}{\cos\frac{1}{2}\theta} \right\rangle = \frac{2}{\pi} \int_0^1 \frac{du}{(u^2 + x^{-2})} \int_{u^2}^1 \frac{dz}{(z - u^2 + x^{-2})} \frac{1}{(1 - z)^{1/2}} \frac{1}{(z - u^2)^{1/2}} \cdot \frac{1}{(z - u^2)^{1/2}} \cdot \frac{1}{(z - u^2)^{1/2}} \frac{1}{(z - u^2)^{1/2}} \cdot \frac{1}{(z - u^2)^{1/2}} \cdot$$

The z integration gives $\pi x (1 + x^{-2} - u^2)^{-1/2}$, so

$$\frac{\hbar k_F^4}{2\pi^3 e^4} \left\langle \frac{\omega_{\text{ex}}(\theta, \varphi)}{\cos\frac{1}{2}\theta} \right\rangle = 2x \int_0^1 \frac{du}{(u^2 + x^{-2})(1 + x^{-2} - u^2)^{1/2}} = \frac{2x^3}{(2 + x^2)^{1/2}} \tan^{-1} x \left(\frac{2 + x^2}{1 + 2x^2}\right)^{1/2} \equiv \frac{\hbar k_F^4}{\pi^3 e^4} W_{\text{ex}}(x), \tag{C6}$$

in comparison with the direct term (C3):

$$\frac{\hbar k_F^4}{2\pi^3 e^4} \left\langle \frac{\omega_D(\theta, \phi)}{\cos\frac{1}{2}\theta} \right\rangle = 2 \int_0^1 \frac{du}{(u^2 + x^{-2})^2} = x^3 \left(\tan^{-1} x + \frac{x}{x^2 + 1} \right) = \frac{\hbar k_F^4}{\pi^3 e^4} W(x), \tag{C7}$$

where W_{ex} is defined by the last equality in (C6), W is the same function defined by (2.18), and (C3), and $x \equiv 2k_F/k_s$. According to (C5)-(C7) the values of $1/\tau_0$ are reduced by about $\frac{2}{3}$ (see Table

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II). The entries in Table I reflect this reduction. The exchange corrections to Δ are negligible because the same average of ω occurs in both its numerator and denominator.

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