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CALCULATIONS OF RESISTIVITY AND SUPERCONDUCTING  $T_c$  IN TRANSITION METALS\*

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## ABSTRACT

A survey is given of various electron-phonon effects which have been calculated for the metals Nb, Mo, Ta, Pd, and Cu. These effects include the mass enhancement  $\lambda$ , superconducting  $T_c$ , electrical and thermal resistivity, Hall coefficient, magnetoresistance, and the successfully tested predictions of linewidths  $\gamma_0$  of phonons. The calculations use local density approximations (LDA) energy bands, experimental phonons, and the rigid muffin tin (RMT) approximation. Mesh size noise is less than 1% and the Bloch-Boltzmann integral equation has been solved to unprecedented accuracy.

## 1. INTRODUCTION

Over the past 8 years, electron-phonon effects in transition metals have been systematically calculated for the metals Nb, Mo, Ta, Pd, and Cu by a Stony Brook-Oak Ridge consortium. A complete bibliography of this work is given as table IV at the end of this report.

The conductivity  $\sigma$  is the current per unit applied field  $E$ , or in terms of the distribution  $f(k)$  of occupied states  $k \equiv (kn)$

$$\sigma = -(2e/\Omega) \sum_k v_{kx} df(k)/dE_x \quad (1)$$

where the factor of 2 is for spin degeneracy. Lowest-order theory says that  $f(k)$  is the equilibrium Fermi distribution  $f_0(k)$  displaced by an amount  $\delta_x = -eE_x \tau/\hbar$ , yielding

$$\sigma(0) = (2e^2\tau/\Omega) \sum_k v_{kx}^2 (-\partial f/\partial \epsilon_k) = (n/m)_{\text{eff}} e^2\tau \quad (2)$$

$$(n/m)_{\text{eff}} \equiv (2/\Omega) \sum_k v_{kx}^2 \delta(\epsilon_k) \quad (3)$$

where  $(-\partial f/\partial \epsilon_k)$  is approximated by  $\delta(\epsilon_k - \mu)$  and  $\mu$  is set to zero. Thus  $\sigma$  depends on two parameters,  $(n/m)_{\text{eff}}$  which is easily calculated from band theory, and  $1/\tau$  which measures the scattering.

In pure crystals, electron-phonon scattering dominates except at low  $T$ . In the limit  $T \geq \theta_D$  there is a simple expression for the electron-phonon

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scattering rate

$$\hbar/\tau = 2\pi \lambda_{tr} k_B T \quad (4)$$

where  $\lambda_{tr}$  is an electron-phonon coupling constant very similar to the mass enhancement  $\lambda$  which determines the superconducting  $T_C$ :

$$\lambda_w = \frac{N(0) \sum_{kk'} w(k,k') |M(k,k')|^2 \delta(\epsilon_k) \delta(\epsilon_{k'}) / \hbar \omega_{k-k'}}{\sum_{kk'} w(k,k') \delta(\epsilon_k) \delta(\epsilon_{k'})} \quad (5)$$

Here  $N(0)$  is the (single spin) density of states per atom at the Fermi energy,  $M(k,k')$  is the electron-phonon matrix element and  $w(k,k')$  is a weight function equal to 1 for  $\lambda$  and  $(v_{kx} - v_{k'x})^2$  for  $\lambda_{tr}$ . This equation follows rigorously when the Bloch-Boltzmann equation for  $f(k)$  is solved variationally<sup>2</sup> for  $\sigma$  in lowest order. These equations (2-5) reveal an intimate connection between  $T_C$  and  $\sigma$ . Both are described by integral equations (the Eliashberg<sup>3</sup> equations in the case of  $T_C$ ) which have been rigorously justified to lowest order in the small parameter  $N(0)\hbar\omega_D$  by many-body perturbation theory using procedures invented by Migdal<sup>4</sup>. Our aim has been to do numerical studies of  $\sigma$  and  $T_C$  simultaneously. By computing many different physical properties on the same basis we are able to test accuracy much more reliably than if we had focussed only on  $T_C$ .

We have also taken care to evaluate quantities like  $\lambda$  in such a way that numerical convergence errors (from finite mesh size) are less than 1%. This enables us to study the possibility<sup>5</sup> that there are systematic errors inherent in present day band theory which alter the value of quantities like  $\lambda$ . The sums in eq. (5) were performed using meshes of  $\sim 5 \times 10^4$  k-points on the Fermi surface of each metal. An outline of the calculations is sketched in fig. 1. Energies  $\epsilon_k$  and wavefunctions  $\psi_k$  were derived from KKR programs. Technically these were non-self-consistent Mattheiss-prescription energy bands<sup>6</sup>, but for d-band elements these agree extremely well with experiment and very well with more sophisticated band theory. The phonon frequencies  $\omega_Q$  came from Born-von Karman interpolations fitted to neutron scattering data.

The matrix element is formally

$$M(k,k') = \int dr dr' \psi_{k'}^*(r) \epsilon^{-1}(r,r') u_Q \cdot \nabla V_0(r') \psi_k(r) \quad (6)$$

but in practice the screening function  $\epsilon^{-1}(r,r')$  is too difficult to compute. Therefore we have used

$$M(k,k')_{RMT} = \int dr \psi_{k'}^*(r) u_Q \cdot \nabla V(r) \psi_k(r) \quad (7)$$

where  $V(r)$  is the total muffin tin potential around the atom at the origin, while  $V_0(r)$  is the bare potential of this atom. This procedure, known as the rigid-muffin-tin (RMT) model<sup>7</sup>, is expected to be very accurate in the core region, less accurate in the interstitial region, and totally fails to give the long range Friedel oscillations contained in (6). For d-band elements, the Fermi-surface wavefunctions  $\psi_k(r)$  are fairly well localized near the core, so the model should be good. Copper, however, is a cross-over case, intermediate between d and (S/P) elements, and the procedure is questionable. To overcome this problem, we exploit the arbitrariness<sup>8</sup>

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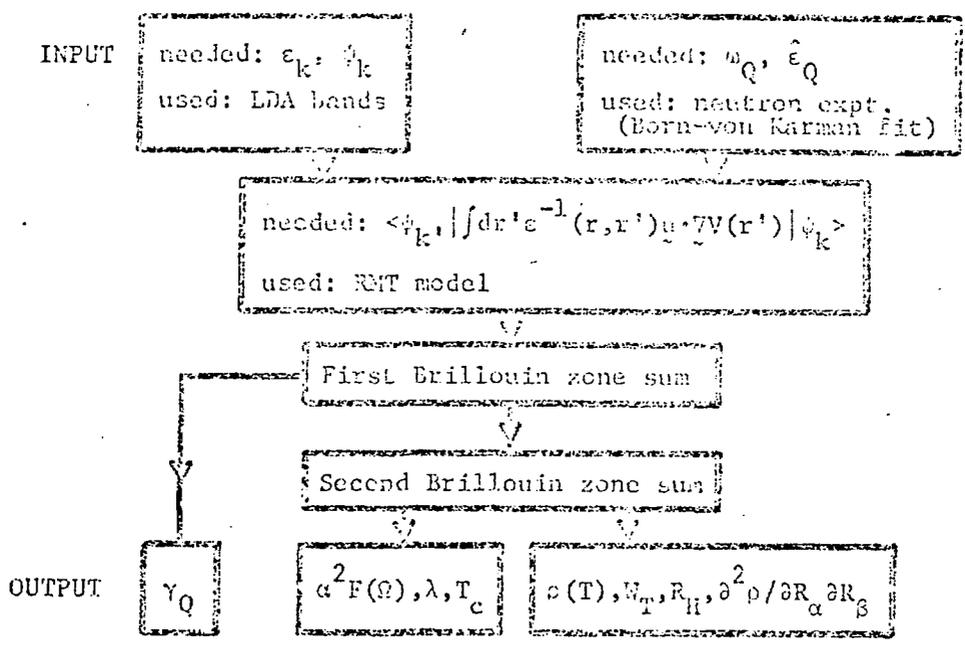


Fig. 1. Schematic outline of electron-phonon calculations

available in fixing the "muffin-tin zero." This arbitrariness is unimportant in Nb, Mo, Ta, and Pd, but serious for Cu. We choose a fixed value for the muffin-tin zero which gives a "forward scattering" matrix element  $M(k,k')$  in accord with nearly free electron theory. This turns out to yield very sensible answers for  $M(k,k')$ . One of the biggest virtues of the RMT model is that the expression for  $M(k,k')$  turns out to be quite simple and depends only on wave-function coefficients and scattering phase shifts  $\delta_k(\epsilon_F)$  which are fixed once the muffin-tin zero is chosen. There is no opportunity or temptation for further adjustment.

## 2. PHONON LINEWIDTHS

An early triumph of this program was the successful prediction of unanticipated structure in the phonon linewidth  $\gamma_Q$  as a function of  $Q$  in Nb and Pd (see table IV part B.) This linewidth describes the decay of a phonon as it excites an electron from a state  $k$  just below  $\epsilon_F$  to a state  $k+Q$  just above  $\epsilon_F$ . A complicated one-dimensional manifold of state  $k$  contributes for fixed  $Q$ . As  $Q$  varies,  $\gamma_Q$  can change quite rapidly through a complicated interplay of Fermi surface geometry, wavefunction variation, and phonon dispersion. Experimental observation of these effects is inhibited by the low resolution and difficult background subtraction of inelastic neutron scattering. Thus although experiment has qualitatively confirmed our calculations, detailed quantitative comparison is not possible in most cases. Nevertheless, this success gave us considerable confidence in the correctness of our algorithms and the validity of the model. Our predictions for Ta have not yet been tested.

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states

~~$\gamma(Q)$~~  not  ~~$\gamma(Q)$~~

3.  $\lambda$  and  $T_c$

From  $\gamma_{0j}$  it is straightforward to compute  $\lambda$  using the identity (table IV, A.1)

$$\lambda = (N/m) N(\epsilon)^{-1} \sum_j \gamma_{0j}^2 / \omega_j^2 \quad (8)$$

Our calculations of  $\lambda$  and  $\lambda_{tr}$  are summarized in table I. We have only small

Table I. Calculations of  $\lambda$ ,  $\lambda_{tr}$ , and  $T_c$

	present work		ref. <del>SS</del>	present	ref. <del>SS</del>	$T_c^{expt}$
	$\lambda_{tr}$	$\lambda$	$\lambda$	$T_c^{calc}$	$T_c^{calc}$	
Cu	0.116	0.111	-	-	-	-
Nb	1.07	1.12	1.3	12.1	17.4	9.2
Ta	0.57	0.88	0.9	7.0	8.0	4.5
Mo	-	0.40	0.4	0.8	0.8	0.91
Pd	0.46	0.41	0.5	0.3	1.4	<0.002

disagreements with the numerical values of Glötzel et al<sup>5</sup> also shown in table I. However, we have a major difference in interpretation. Glötzel et al. state "...theory is incapable of producing reliable  $T_c$ 's... The most probable reasons for this failure are [1] the rigid ion approximation ... or ...[2] conventional local density schemes..." Our view is that  $T_c$ 's are adequately well accounted for, considering the sensitivity of  $T_c$  and the uncertainty in the Coulomb parameter  $\mu^*$ . The computed  $T_c$ 's of table I all assume  $\mu^* = 0.13$ , which is likely to be a significant underestimate in the case of Pd which has fairly long-lived spin fluctuations. Uncertainty in  $\mu^*$  might account for the discrepancy between theory and experiment in Nb and Ta also. We find strong evidence that electron-phonon effects are well explained by [1] the RMT model, and [2] conventional local density schemes. We base this (move) on our transport calculations and  $\gamma_{0j}$  predictions than on the sole criterion of  $T_c$  chosen in ref. ~~SS~~.

4. ELECTRICAL RESISTIVITY

Few calculations have been made of  $\rho(T)$  for transition metals which take the true band structure into account. Pioneering work was done by Yamashita and Asano<sup>10</sup> who demonstrated feasibility. Their mesh of  $k$  and  $T$  points was coarse compared to ours, and permitted only semiquantitative comparison with experiment. Apart from this work and our own, we are aware of no quantitative work on the phonon-limited resistivity.

Table I shows an interesting regularity, namely that  $\lambda_{tr}$  and  $\lambda$  are usually quite similar. This was anticipated by Chakraborty et al<sup>11</sup> who proposed using eqs. (2-4) to estimate  $\sigma$  with  $\lambda_{tr}$  replaced by  $\lambda$  and derived from  $T_c$  experiments, and  $(n/m)_{eff}$  derived from band theory. This procedure is now thoroughly vindicated, and it is a pity that band theorists seldom evaluate  $(n/m)_{eff}$  which would be very useful in analyzing transport coefficients.

The calculation of  $\rho(T)$  for  $T < \epsilon_D$  as well as  $T \geq \epsilon_D$  requires a more

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elaborate scheme than given in eqs. (2-5). Rigorous procedures for solving the Bloch-Boltzmann equation are described in the papers listed in table IV parts A and E. Our results are summarized and compared with experiment<sup>12</sup> in fig. 2. Considering that no adjustable parameters have entered (apart from

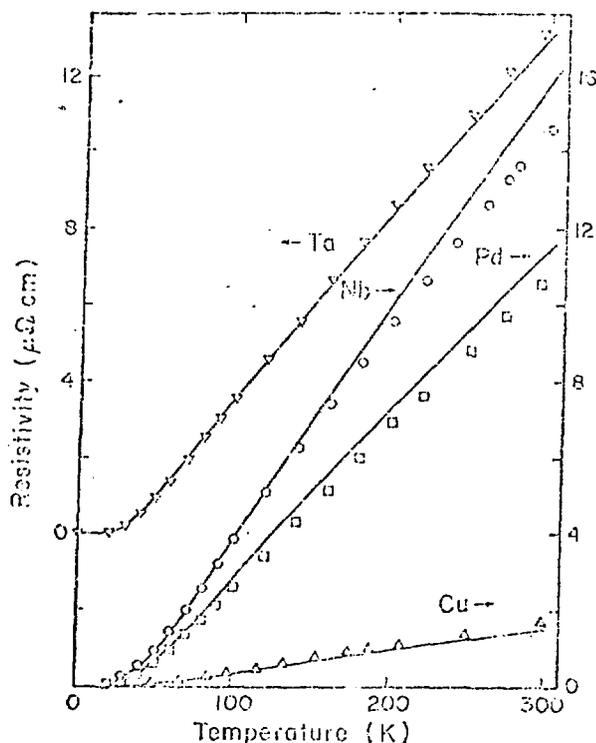


Fig. 2. Resistivity versus temperature. The solid lines for Nb, Pd, and Cu are calculations which include both  $\epsilon$ -dependence and anisotropy; the curve for (Pd) is a lowest order variational calculation and thus somewhat too large for  $T \leq 100K$ . Data are from ref. 12.

the choice of muffin-tin zero in Cu) the spectacular agreement between theory and experiment can be taken as a refutation of the pessimism of ref. 5 and as confirmation of our view that band theory is fully capable of accounting for electron-phonon effects in transition elements.

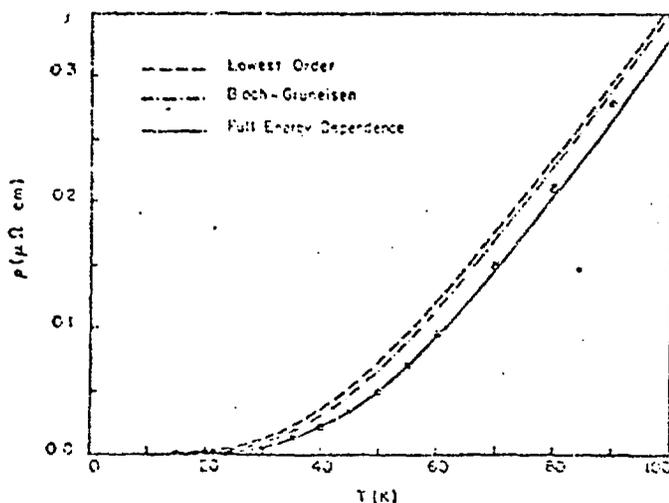


Fig. 3. Low T resistivity of Cu, showing the effect of  $\epsilon$ -dependent corrections to the lowest-order solution. Also a Bloch-Gruneisen formula has been fitted to the theory in the regime  $T \sim \theta_D$  and disagrees for  $T < 100K$ . Data are from refs. 13(O) and 14(x).

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Figure 3 shows the low temperature part of  $\rho(T)$  for Cu in more detail. This illustrates the role of corrections to the lowest order variational solution. In lowest order there is a relatively simple formula for  $\rho(T)$  which consists of eqs. (2-4) with  $\lambda'_{tr}$  replaced by  $\lambda_{tr}(T)$  defined as

$$\lambda_{tr}(T) = 2 \int_0^{\infty} \frac{d\alpha}{\alpha} \alpha_{tr}^2 F(\alpha) \left( \frac{4\alpha/2k_B T}{\sinh(\alpha/2k_B T)} \right)^2 \quad (9)$$

where  $\alpha_{tr}^2 F(\alpha)$  is a close analog of  $\alpha^2 F(\alpha)$  used in  $T_c$  theory. The role of band theory is then to provide  $(n/m)_{off}$  and  $\alpha_{tr}^2 F(\alpha)$ . This approximation is remarkably accurate for  $T \geq \epsilon_D/2$ , but at lower  $T$  interesting corrections enter which can be divided into two classes. The distribution function can be written as  $f_0(k + \delta(k, \epsilon))$  where  $\delta$  is the displacement caused by the applied field. In lowest order,  $\delta$  is a constant, but the exact solution exhibits both a dependence on the position on the Fermi surface,  $k'$  (called the "anisotropy" effect) and a dependence on the elevation  $\epsilon - \mu$  above or below the Fermi energy (called the "energy dependence" effect.) It turns out to require no additional input from band theory to handle the second effect as accurately as desired (neglecting corrections of order  $N(0)k_B T$ .) However, the anisotropy effect requires additional tedious band theory input (e.g. a series of functions  $\alpha_{ij}^2 F(\alpha)$ .) Both are important as illustrated

Table II. Resistivity of Cu calculated at three temperatures at various levels of approximation.

	20K	40K	220K
Lowest order	0.00163	0.0360	1.067
energy dependence	0.00097	0.0210	1.061
anisotropy	0.00143	0.0352	1.063
complete solution	0.00083	0.0200	1.057

in fig.3 and table II. The total correction is a factor of 2 at 20K, but only 1% at 220K, for Cu. Our "complete" solution is actually a truncated series representation of the anisotropy effect which captures > 80% of the anisotropy correction, at a computational expense of a factor of  $\sim 6$  over the lowest order solution. It would not be easy to improve this calculation further.

## 5. DEVIATIONS FROM MATTHIESSEN'S RULE (DMR)

Matthiessen's rule states that  $\rho_{tot}(T) = \rho_0 + \rho_{pure}(T)$  where  $\rho_0$  is the residual resistivity which is sample dependent (usually dominated by impurities) and  $\rho_{pure}(T)$ , the experimental resistivity of the pure material, gives the temperature dependence. The lowest-order variational theory obeys Matthiessen's rule, but the higher order corrections do not, because the displacement  $\delta(k, \epsilon)$  is determined by impurity scattering if  $\rho_{pure} < \rho_0$  and by phonon scattering if  $\rho_{pure} > \rho_0$ . These two scattering mechanisms have very different effects on  $\delta$  (for example, when impurities dominate there is no  $\epsilon$ -dependence) resulting in a well known source of DMR. Our calculations for Cu are shown in fig. 4. The simplest possible model for impurity scattering was used, namely a  $(k, k')$ -independent matrix element, which is a good starting point but cannot explain any differences between

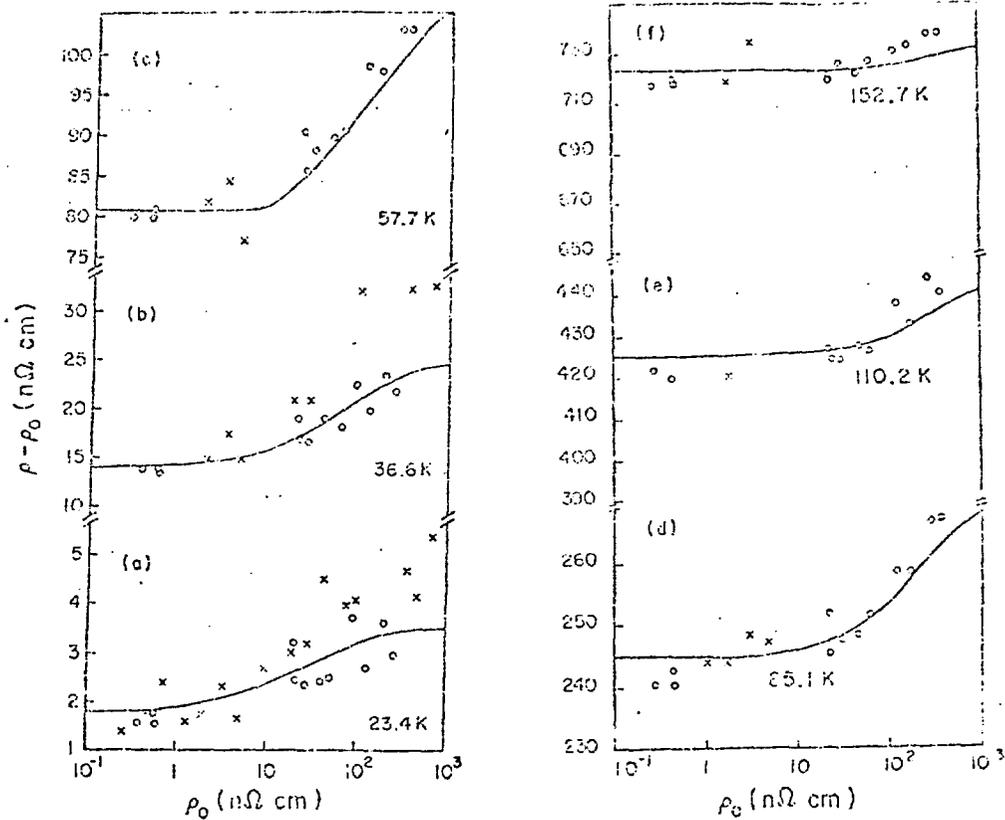


Fig. 4.  $\rho(T) - \rho_0$  plotted versus  $\rho_0$ . Mattheissen's rule says the data should be on a horizontal line. In cases (a,b,c) the theory has not been adjusted. In cases (d,e,f) the theory has been shifted upwards by a constant correction of (4%, 7%, 8%). This shift compensates for a slight discrepancy between  $\rho_{\text{pure}}(T)$  and experiment seen in fig. 2 at  $T \gtrsim 80\text{K}$ . Data are from refs. 15(0) and 16(x).

species of impurity. Again, only trivial adjustments were made in the theory and the agreement with experiment is quite spectacular. This strongly suggests that the finer details of Bloch-Boltzmann theory are indeed meaningful, that band theory does justice to transport at a detailed level, and that our computational algorithms are adequate.

## 6. THERMAL CONDUCTIVITY

Although we have made calculations for Nb, Ta, and Pd as well, only results for Cu are discussed here. Figure 5 shows that once again close agreement with experiment is found. Corrections to the lowest order approximation are particularly important in  $\kappa(T)$  at low  $T$ , because the  $\epsilon$ -dependence of  $\delta$  plays a special role in heat conduction. The Wiedemann-Franz law is accurately obeyed for  $T \gtrsim \Theta_D$  but not at low  $T$ .

## 7. MAGNETOTRANSPORT

The regime of weak applied magnetic fields is defined by  $\omega_c \tau \ll 1$ . Here the current can be written

$$j_\alpha = c_{\alpha\beta}^{(0)} E_\beta + \sigma_{\alpha\beta\gamma}^{(1)} E_\beta H_\gamma + \sigma_{\alpha\beta\gamma\delta}^{(2)} E_\beta H_\gamma H_\delta + \dots \quad (10)$$

In a cubic crystal the term linear in  $H$ , a third rank tensor, is determined by a single number, the Hall coefficient ( $R_H$ ), while the quadratic part, a

*Greek kappa*

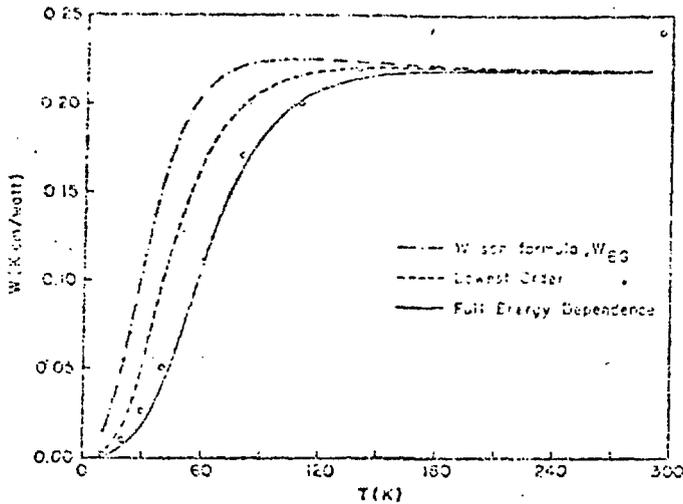


Fig. 5. Thermal resistance of Cu. Data are from ref. 13.

fourth rank tensor, contains three distinct numbers. We have calculated all four of these numbers as a function of temperature for Cu. The results for the Hall coefficient are shown in fig. 6. The common belief that

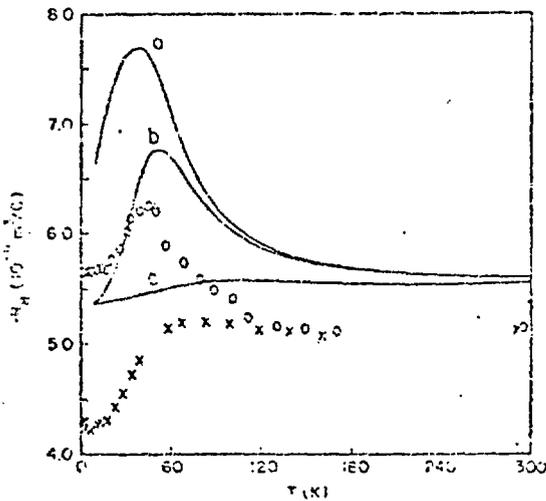


Fig. 6. Hall coefficient in Cu. Curves (a,b,c) are calculated with resistance ratios (RRR) of (38500, 70,4). The data, from ref. 17, are for Ni impurities with RRR=110 (O) and Au impurities with RRR=27 (X).

$R_H = 1/nq$  and measure the carrier concentration and sign is actually correct only for elastic scattering around an ellipsoidal energy surface, a good approximation in many semiconductors, but meaningless for transition metals. The lowest order trial solution has a Fermi distribution which is shifted first by an amount  $a = -eE/\hbar$  in the direction of the E field and then by an amount  $b E \times H$  in the direction of the Lorentz force, where b must be determined from the Boltzmann equation. Unfortunately there is no variational principle for the Hall coefficient to guarantee that errors in  $R_H$  are higher order than errors in the distribution.

In relaxation time approximation the formula for the Hall coefficient is

$$R_H = (6\pi\hbar)^{-1} \sum_k v_k^3 \kappa_k \tau_k^2 (-\partial f / \partial \epsilon_k) / [\sum_k v_k^2 \tau_k (-\partial f / \partial \epsilon_k)]^2 \quad (10)$$

where  $\kappa_k$  is the Gaussian curvature of the Fermi surface at point  $k$ . If  $\tau_k = \tau$  is independent of  $k$ , it cancels from eq. (10) so that  $R_H$  is a purely geometrical object, independent of  $T$ , measuring a complicated average of curvature times velocity to the third power. This is understandable because in regions of large velocity and curvature, the Lorentz force can give a large redirection of the current. The lowest order trial solution reproduces this geometric answer. As can be seen in fig. 6, there is a large  $T$ -dependent correction for  $T < 100K$ , but at higher  $T$ , both theory and experiment give a  $T$ -independent value of  $R_H$ . At lower  $T$  the absence of a variational principle makes  $R_H$  difficult to compute, and agreement with experiment is only semi-quantitative. As in the DMR calculations, no effort was made to account for the anisotropy of the impurity scattering. The large difference between Ni and Au impurities shows the need for a more sophisticated treatment.

The lowest order  $T$ -Independent theory does quite well for many transition metals at high  $T$ . This is illustrated in table III. The palladium

Table III. Hall coefficients calculated in lowest order and expressed as  $Z_{\text{eff}} = -(\rho_{\text{cell}} / R_H e)$

	$Z_{\text{eff}}^{\text{theory}}$	$Z_{\text{eff}}^{\text{expt}}$
Cu	1.39	1.42
Nb	-1.50	-1.28
Pd <sub>I</sub>	0.53	1.23
Pd <sub>II</sub>	0.69	

results are off by a factor of 2 however, and show a significant dependence on the band structure (illustrated by calculations which used two different Mattheiss-prescription potentials, from relativistic (II) and non-relativistic (I) atomic charge calculations.) The factor of 2 discrepancy has been analyzed in paper G2 of table IV, and arises from the very large curvature anisotropy on the central portion of the Pd Fermi surface, which makes the result peculiarly sensitive to scattering anisotropy omitted in lowest order.

Finally the magnetoresistance calculations for Cu in paper G3 of table IV merit a comment. All three coefficients agree nicely with the available low  $T$  single crystal data. An as yet unchecked prediction was made, namely that the "Seitz coefficients," defined such that  $T$ -dependence cancels in lowest order, should actually exhibit a fairly strong  $T$ -dependence in the temperature interval  $20K \leq T \leq 100K$ . We hope this prediction will be checked.

## 8. CONCLUSION

When this work was started 8 years ago, it was not completely obvious that the Bloch-Boltzmann theory would work in detail for transition metals. The lesson to be drawn from our calculations is that accurate band theory combined with the Bloch-Boltzmann theory is spectacularly successful at accounting for a wide range of effects. Although there are important unresolved questions<sup>2</sup> in the distinction between quasiparticles and density functional energy bands, there is no evidence that LDA bands fail to describe

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See also papers C2, C3, and E2.

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