MASTER

COO/2315-11

THEORY OF ELECTRON-PHONON SCATTERING EFFECTS IN METALS

Progress Report

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Dec. 1, 1976 - Nov. 30, 1977

Prepared for the U. S. Energy Research and Development Administration under Grant No. EY-76-S-02-2315.002

ABSTRACT

This progress report describes the scope of our investigations and briefly discusses significant results obtained during the past year. The general areas in which the investigations were carried out are transport properties and quasiparticle lifetimes in normal metals and superconductors. The more specific research projects upon which progress is reported are a) the calculation of order parameter relaxation times in aluminum, b) transport coefficients of the noble metals (emphasizing deviations from Matthiessen's rule), c) variational transport calculations for a superconductor, d) some general results on quasiparticle relaxation time anisotropy in polyvalent metals, and e) a clarification of the roles of electron-electron and electron-phonon scattering in simple metals at low temperatures.

I. INTRODUCTION AND SCOPE

During the past year this group has undertaken investigations in the area of nonequilibrium phenomena in normal and superconducting metals. The properties studied specifically are quasiparticle lifetimes and transport coefficients, with emphasis on the anisotropy and its consequences, such as deviations from Matthiessen's rule (DMR). We are primarily interested in the electron-phonon interaction, but have studied electron-electron scattering as well and, to a lesser extent, electron-impurity scattering since this enters the DMR.

In the next section I review the status of each member of our research group, and briefly describe his activities for the past year. Finally in Sec. III, specific results are reported for the various projects underway.

II. PERSONNEL

There have been three graduate students and one undergraduate (recently graduated) associated with this program during the past year. Two of the graduate students are currently being supported by Grant funds.

Bill Jumper is beginning his fourth year with the group (fifth year at Dartmouth) and has recently obtained results on deviations from Matthiessen's rule in the noble metals. Bill is expected to complete his doctoral thesis this summer; it will be based on his DMR calculations for potassium[1] completed a year ago, as well as the current work on the noble metals and its extensions. Bill has been supported on the G.I. bill since June. This support extends only through February, and so I shall propose that Bill be supported by this grant, starting from that time through the summer.

Eusebio Garate is beginning his third year with the group, and has continued his general studies of superconductivity, including gap anisotropy and non-equilibrium phenomena. Recently, in order to focus his effort, he has applied the variational method to the calculation of thermal conductivity. He has obtained new results (as described later) and we are encouraged to apply his method to other nonequilibrium phenomena. We do not plan to publish the results until these additional studies are completed. We expect Eusebio will complete his degree work by next fall.

Lee Cole is beginning his second year with the group, and has recently completed a program for calculating the temperature-dependent anisotropic quasi-particle lifetime for a simple metal. We shall be making use of this program to calculate quantities of interest in particular experimental situations.

Rob Duncan graduated with a bachelor's degree last June, and has remained at Dartmouth to continue his research with our group. Rob wrote an excellent Senior Honors Thesis on the microscopic theory of superconductivity, and has since been developing his ideas further. The work involves an alternate formulation of BCS theory which has considerable pedagogical value, in addition to its more direct impact on our other superconductivity work. Rob and I will prepare our work for publication this summer.

III. TOPICAL REPORTS

Significant results have been obtained in a number of projects, most of which are as yet incomplete. This section is used to briefly describe these results and to review the status of the projects underway.

A) Order Parameter Relaxation in Aluminum

Dr. A.B. Meador and I have used previously-developed programs[2] in order to complete a detailed calculation of the phonon-limited anisotropic quasiparticle lifetimes in aluminum, and to perform the appropriate Fermi surface average[3] for the superconducting-phase lifetimes recently measured.[4,5] A separate preprint of this work is enclosed, and so it will not be discussed in detail here. The paper is important in two respects: i) the calculation may be used as a vehicle to compare the normal and superconducting-phase lifetimes, and ii) the method used is accurate in the limit of zero temperature (see ref. 2), as required for the superconductor.

B) Deviations from Matthiessen's Rule

Mr. Jumper has calculated the electrical and thermal resistivities of copper as functions of temperature and impurity concentration (residual resistivity). He has used 2-OPW electron states[6] and the Moriarty pseudopotential[7] for the electron-phonon interaction; phonon modes are fit to inelastic neutron scattering data. He plans to do similar calculations for silver. The reason for our pseudopotential treatment of electronic structure is that we believe the DMR mechanism is the same for both the noble and simple polyvalent metals.

Several facets of the problem have been explored, with the following results: i) the calculated DMR are large (of the same order as the observed ones) and depend quite strongly on the anisotropy of the electron-impurity scattering rates, ii) angular-dependence of the nonequilibrium distribution is more important than energy-dependence for determining DMR (in contrast with what we found in potassium[1]), and iii) we examined the effect of departures from cubic symmetry in the relaxation time,[8] and found these to be small. This finding will be of considerable value in simplifying future computations.

Following further study of the electron-impurity aspect of the problem, and the completion of a similar calculation for silver, the results will be submitted for publication. We are hoping to complete this project in about three months.

C) Transport in Superconductors

Mr. Garate is applying the variational technique to a calculation of the thermal conductivity in a superconductor. Earlier attempts reported in the literature[9] were frustrated, and it now appears that this may have been the result of the choice of trial function. Mr. Garate's improved trial function seems to reproduce the results of numerical solution of the Boltzmann equation,[10] and to have the added flexibility to treat combined scattering mechanisms (electron-phonon and electron-impurity) relatively easily.

The calculation will be tested against thermal conductivities measured[11] in samples of varying purity, and if the method proves successful, it will be applied to other nonequilibrium properties.

D) Quasiparticle Relaxation Rates

Mr. Cole and I have studied the quasiparticle relaxation time $\tau(\hat{k},T)$ as a function of position $\hat{k}$ on the Fermi surface and temperature T within the two-OPW model, in an attempt to obtain some general understanding of its behavior in simple metals. The important metal parameters upon which τ depends are the electron-ion form factor V_G and its derivative V_G', evaluated at the reciprocal lattice point $\vec{G}$; V_G determines the wavefunctions and Fermi surface shape near the zone boundary (G), and both parameters enter the electron-phonon matrix elements. If we consider the relaxation rate as a function of these two variables in addition to $\hat{k}$ and T, and recognize that τ depends on $\hat{k}$ only through its perpendicular distance k_G from (G), (and possibly on a band index) then we can prove the homogeneity property

$$\tau^{-1}(\alpha k_G, \alpha T; \alpha V_G, V_G') = \alpha^3 \tau^{-1}(k_G, T; V_G, V_G')$$

This means that we may express τ as a function of k_G and T through their ratios to V_G:

$$\tau^{-1}(k_G, T; V_G, V_G') = T^3 f(k_G/V_G, T/V_G; V_g').$$

This "scaling function" f depends only on three variables; both the wavevector scale and the temperature scale are determined by V_G. An immediate and surprising corollary of this theorem is that, in the regime where $\tau^{-1} \sim T^3$, it must be <u>independent</u> of V_G.

Mr. Cole has examined all of these dependences numerically, and found that the two-OPW model is capable of the richness of behavior found in more specific detailed calculations.[2] In particular, the parameter V_G' is chiefly responsible for the asymmetry of τ between different bands near the same zone boundary. It appears that the minimum values of τ across a ridge may differ by factors of three or four depending upon whether $\hat{k}$ is on the "upper" or "lower" band. We are hoping to complete and publish this phase of our study in the next four months.

E) Electron-Electron Scattering

In a recent conference paper,[12] I reviewed some known results[13] for the electron-electron contributions to transport coefficients and quasiparticle scattering rates in the simple metals. In order to test the feasibility of observing these effects experimentally, however, these contributions must be weighed against the electron-phonon ones which are dominant at all but the lowest temperatures. I made this comparison using our as yet unpublished results for the electron-phonon contributions in the low-temperature limit.

The conclusions drawn from the comparison are that the electrical resistivity is most favorable for observing electron-electron scattering; even here, measurements must be made near or below 1K (except perhaps in the noble metals[14]). In the thermal resistivity or in quasiparticle lifetime measurements, even lower temperatures would be required; this coupled with the relatively lower precision attained in these measurements tends to argue against their use. Of course the thermal resistivity has been shown to be useful at high temperatures,[15] and these measurements should be pursued further.

Level of Activity

There is no significant difference between the level of activity actually performed and that contemplated in the Contract. The principal investigator spent one-third time on the program during the first two quarters (spring and summer) of the Contract year, and will devote full time during each of the last two quarters.

Travel Performed

The principal investigator used alloted funds for travel to the March 1977 meeting of the American Physical Society. He also traveled to Cavtat, Yugoslavia, to deliver an invited paper (Ref. 12) at the European Physical Society Conference held there in May 1977. A combination of personal funds and Dartmouth funds was used for this travel.

see COO-2315-12

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