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Analysis of the Anomalous Temperature-Dependent Resistivity on Potassium below 1.6 K

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Recent precision measurements of the resistivity of potassium between 0.38 and 1.6 K revealed a surprising $T^{1.5}$ temperature dependence. We show that scattering of electrons by phasons—the collective excitations of an incommensurate charge-density wave—can provide an explanation.

Recent measurements by Rowlands, Duvvury, and Woods,[1] indicate the presence of an anomalous contribution to the resistivity of potassium, which, if fitted to a pure power law, varies as $T^{1.5}$. Previously proposed mechanisms that contribute to the resistivity at low temperatures, including electron-phonon and electron-electron scattering, yield curves of resistivity versus temperature that are the wrong shape to explain this high-precision data. As a resolution of this difficulty, we propose a new mechanism—scattering of electrons with phasons,[2] the collective excitations associated with phase modulation of a charge-density wave. We will see that this assumption leads to the prediction of a temperature-dependent resistivity that is in good agreement with the data.

Conventional studies of the resistivity of a metal at low temperatures yield the following contributions[3]:

$$\rho(T)=\rho_0+AT^5+BT^p\exp(-\hbar\omega_0/k_BT)+CT^2, \quad (1)$$

where ρ_0 is the residual resistivity. The term AT^5 results from normal electron-phonon scattering in the low-temperature limit. It may be greatly reduced in magnitude from the value predicted by the Bloch-Grüneisen formula if phonon-drag effects are important. Electron-phonon umklapp scattering, which is essentially unaffected by phonon drag, contributes a term at low temperatures of the form $BT^p\exp(-\hbar\omega_0/k_BT)$, where ω_0 is the frequency of the phonon with the minimum wave vector that allows participation in an umklapp process. Electron-electron scattering produces the term CT^2 at all temperatures.

The relative importance of each of these mechanisms is revealed by examining the low-temperature resistivity data in potassium. Highly accurate measurements[4,5] exhibit an exponentially decaying resistivity with decreasing temperature below about 4 K, supporting the electron-phonon umklapp scattering mechanism and lending credence to the concept of phonon drag. Below 2 K, however, significant deviations from exponential behavior have been observed, suggesting the presence of an additional scattering mechanism. In order to discover the characteristic behavior of this additional mechanism, one must first subtract the known electron-phonon umklapp contribution from the data. Unfortunately, the form of this umklapp term below 2 K is not well determined. While van Kempen *et al.*[4] have fitted

their data between 2 and 4 K with the form of the exponential term in Eq. (1) with $p=1$ and $\theta=\hbar\omega_0/k_B=19.9$, Kaveh, Leavens, and Wiser,[6] have pointed out that other values of p and θ could allow equally good fits to these data. We avoid this uncertainty by considering only data below which the electron-phonon umklapp term becomes negligible, i.e., below about 1.3 K.

We now turn to a discussion of the new anomalous temperature dependence of the resistivity, as shown by the data of Ref. 1, pictured as circles in Fig. 1, with the lowest point defining the zero of resistivity. The two highest points, above 1.3 K, are displayed to illustrate the residual influence of electron-phonon umklapp scattering on these points. The dashed arrows show the amount that one would subtract if the parameters obtained by van Kempen *et al.*[4] are used. A solid curve has been drawn through all but these two highest data points. For convenience, we will call this curve ρ(phason), with the significance of this designation becoming apparent later. There is no evidence for a T^5 contribution. Electron-electron scattering has been proposed as a possible explanation of the data,[1,4] but this must vary exactly as T^2 and does not allow for the observed dependence. This can be seen most clearly in Fig. 2, where we show the difference between the shape of the curve defined by the data and attempts to fit it with pure power laws. Because of the scatter in the data, we find it convenient to use ρ(phason) as a reference, or the horizontal line in Fig. 2, and plot $\rho-\rho$(phason), where ρ is either the data (circles) or T, $T^{1.5}$, and T^2 curves that pass through the first and last data points below 1.3 K. Clearly, the T^2 curve is the wrong shape to fit the data and describes the data as poorly as a straight line (the curve labeled T). If one desires the best-fit power law, that would be $T^{1.5}$, as was first suggested by Rowlands, Duvvury, and Woods.[1] Thus, it seems that electron-electron scattering must be ruled out, at least as the principal mechanism, and a new scattering mechanism must be invoked.

As an explanation of this anomalous temperature dependence of the resistivity, we suggest the mechanism of electrons scattering from phasons, collective excitations corresponding to phase modulation of a charge-density wave (CDW). The proposal of a CDW ground state in potassium has provided successful and consistent explanations of other anomalies, which have recently

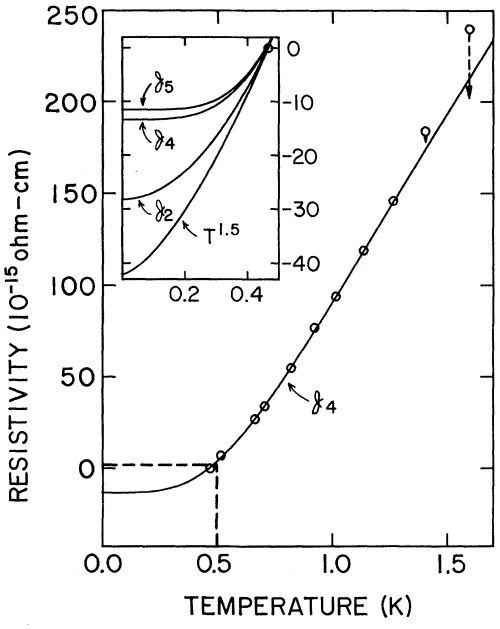

FIG. 1. Plot of resistivity vs temperature for the data of simple K2C of Rowlands, Duvvury, and Woods (Ref. 1), indicted by circles. The dashed box has been enlarged and foreshortened in the inset. The curves and arrows are described in the text.

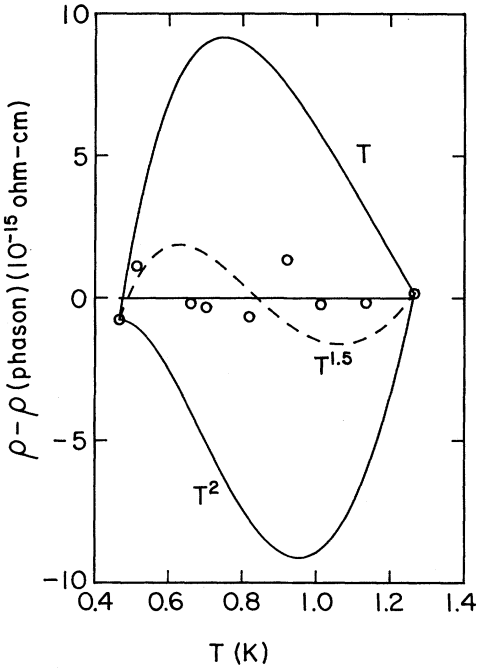

FIG. 2. Plot of resistivity subtracted from ρ(phason), the smooth curve through the data in Fig. 1. The data of Fig. 1 are shown as circles scattered about the horizontal line ρ(phason). Curves labeled T, $T^{1.5}$, and T^2 are the corresponding pure power laws that pass through the first and last data points below 1.3 K.

been reviewed.[7] Phasons have been considered in other contexts and several of their properties have been described.[2,8-10] Of particular interest here, the electron-phason interaction has been derived to be of the form[9]

$$V_{e\varphi}=\tfrac{1}{2}G\sum_{\vec{q}}\varphi_{\vec{q}}\{\cos[(\vec{Q}+\vec{q})\cdot\vec{r}-\omega_{\vec{q}}t]-\cos[(\vec{Q}-\vec{q})\cdot\vec{r}-\omega_{\vec{q}}t]\}, \tag{2}$$

where $G\cos(\vec{Q}\cdot\vec{r})$ is the total self-consistent potential and $\vec{Q}$ the wave vector of the static CDW. $\varphi_{\vec{q}}$, $\omega_{\vec{q}}$, and $\vec{q}$ are the magnitude, frequency, and wave vector of the phason, respectively.

A phason is actually a normal mode of the lattice whose frequency is zero at the point $\vec{Q}$ in the Brillouin zone and varies linearly with $\vec{q}$ away from that point, with the velocity in the direction of $\vec{Q}$ much greater than that perpendicular to $\vec{Q}$. For simplicity, we assume a Debye-like model and choose a cutoff that reflects the anisotropy of the phason spectrum such that the occupied phason space is small compared to the Brillouin zone. In addition, we assume extreme anisotropy of the phason spectrum, postponing the more general case to a longer, more extended paper. We thus define a phason frequency and temperature as

$$\omega_{\vec{q}}=c_{\parallel}q_{\parallel}, \quad \Theta_{\varphi}=\hbar c_{\parallel}q_{\varphi}/k_{B}, \tag{3}$$

where $c_{\parallel}$ and $q_{\parallel}$ are the phason velocity and wave vector parallel to $\vec{Q}$. Here, the phason space is approximated by a pillbox of width q_{φ} along $\vec{Q}$.

The temperature-dependent resistivity due to electron-phason scattering along each principal axis was calculated with "golden-rule" perturbation theory using the potential of Eq. (2). Results were obtained via a variational solution of the Boltzmann equation, assuming the Fermi surface to be rigidly displaced in $\vec{k}$ space by the electric field.[11] For the simple model described above, the resistivity can be expressed in terms of Bloch-Grüneisen functions $\mathcal{G}_n(x)$ as

$$\rho_{e\varphi}(T)=A[(\sqrt{2}T/\Theta_{\varphi})]^5\mathcal{G}_5(\Theta_{\varphi}/\sqrt{2}T)+B(T/\Theta_{\varphi})^4\mathcal{G}_4(\Theta_{\varphi}/T)+C(T/\Theta_{\varphi})^2\mathcal{G}_2(\Theta_{\varphi}/T), \tag{4}$$

where

$$\mathcal{G}_n(x)=\int_0^x \frac{z^n dz}{(e^z-1)(1-e^{-z})}. \tag{5}$$

The expressions for the three coefficients in Eq. (4) are complicated and their magnitudes depend on the phason anisotropy, as well as on the distribution of $\vec{Q}$ domains throughout the sample. In fact, the magnitude of the observed anomalous temperature dependence of the resistivity varies from run to run and sample to sample and seems to be related to the magnitude of the residual resistivity, which also depends on $\vec{Q}$-domain structure.[11] For this reason, we defer discussion of these coefficients to a more extended paper and direct our attention here only to the shape of the resistivity curve as a function of temperature. For this reason, we have fit the data in Fig. 1 separately with each of the three terms in Eq. (1), e.g., using the form $\rho_0+\beta(T/\Theta_{\varphi})^4\mathcal{G}_4(\Theta_{\varphi}/T)$. Each term individually fits the data as well as the other two, but with different parameters. The excellence of the fit can be seen in Fig. 1, where the smooth curve through the data can now be identified with the result of fitting with the $\mathcal{G}_4$ term.

Results for the $\mathcal{G}_2$ and $\mathcal{G}_5$ terms would be indistinguishable in Fig. 1 from the $\mathcal{G}_4$ curve in the regions of the data, but their extrapolations to lower temperatures differ. These are shown in the inset of Fig. 1, along with the extrapolation of the pure power law $T^{1.5}$ identified in Fig. 2. The phason temperatures needed for the fit are $\Theta_{\varphi}=3.43$ K for $\mathcal{G}_4$, $\Theta_{\varphi}=4.58$ K for $\mathcal{G}_5$, and $\Theta_{\varphi}=4.85$ K for $\mathcal{G}_2$. The phason temperature and extrapolation below the lowest data point for the true combination of terms in Eq. (4) would lie between the values for the separate terms. On the other hand, the $T^{1.5}$ curve lies well below these other curves in the ultralow-temperature region. Therefore, it is extremely important that ultralow-temperature resistivity measurements be done in order to determine the precise shape of the curve. If the data would fall on the $T^{1.5}$ curve, this would eliminate electron-phason scattering as the explanation for the anomalous contribution to the resistivity. On the other hand, if the data would lie in the region of the graph between the $\mathcal{G}_5$ and $\mathcal{G}_2$ curves, further information could be obtained about the values of the phason temperature Θ_{φ} and the phason cutoff q_{φ}. This information could be coupled with determinations from specific-heat experiments if the predicted signature of

phasons[10] is observed there, and a more complete picture of phasons in potassium would be possible.

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Self-Scattering Path-Variable Formulation of High-Field, Time-Dependent, Quantum Kinetic Equations for Semiconductor Transport in the Finite-Collision-Duration Regime

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Quantum kinetic equations for describing transport in submicron semiconducting devices in the finite collision duration regime are developed which are nonlocal in time and momentum. Utilizing a projected self-scattering formulation, a retarded path-integral equation is obtained. Quantum kinetic equations are usually exceedingly difficult to solve. The formulation found here presents a powerful technique to achieve these solutions even in the case where nonlocal effects are important.

The Boltzmann transport equation (BTE) has long been the basis for semiclassical transport studies in semiconductors and other materials. Its utility also stems from the fact that it is readily transformable into a path variable form which can be adapted to numerical solutions for complicated energy-dependent scattering processes.[1-3] In this form, the BTE is often referred to as the Chambers-Rees path-integral equation, and serves as the basis for Monte Carlo[4-6] and iterative[7-9] calculations of transport. However, the BTE is valid only in the weak-coupling limit under the assumptions that the electric field is weak and slowly varying at most, the collisions are independent, and the collisions occur *instantaneously* in space and time. Each of these approximations can be expected to be violated in future submicron-dimensioned semiconductor devices. We have previously shown that in such devices, the time scales are such that collision durations are no longer negligible when compared to the relevant time scale upon which transport through the device occurs.[10,11] In this situation, even for time-independent fields, the quantum kinetic equations are nonlocal in time and momentum. It may be recalled that the BTE can be rigorously derived from the density-matrix Liouville-equation formulation of quantum transport.[12,13] Here, we draw upon that formulation for a retarded-time kinetic equation, which replaces the BTE, and show that by introducing a projected self-scattering process, a retarded path integral can be developed. The power of this technique allows a single path integral to be used, rather than the expected multiple retarded path integrals.

If the instantaneous collision approximation is relaxed, an additional field contribution appears as a differential superoperator term in the collision integrals evaluated in the momentum repre-

