Conductivity of metals with plane defects

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The conductivity components of a metal containing a system of parallel plane defects are calculated. If the scattering of the current carriers by the defects is sufficiently intense, coherent quantum effects are important, and the temperature dependence of the resistance component perpendicular to the defects is that of an insulator. The cases of strongly and weakly reflecting defects are discussed. A model is proposed to explain the temperature dependence of the transverse resistance of crystals of high-temperature superconductors.

1. INTRODUCTION

Regardless of the anisotropy of the Fermi surface, a localized Anderson transition will occur in all crystallographic directions simutaneously in a disordered metal (Refs. 1 and 2, for example). There are, on the other hand, layered materials for which the behavior of the resistance along the layers is metallic, while that across the layers corresponds to an insulator. A classic example is graphite,[3–6] in which this effect has been observed for more than 30 years, although it does not yet have a satisfactory theoretical description. The high-temperature superconductors $Y_1Ba_2Cu_3O_7$ fall in the same category.[7–9] It should be noted that the temperature dependence of the transverse resistance is not "universal" in these two compounds: There are high-quality samples in which the transverse resistance is metallic. The insulating nature of the transverse resistance is thus not an inherent property of the compounds but a consequence of the defect structure of the real crystals.

In layered materials there is a tendency toward the formation of plane defects, oriented parallel to the layers. In the superconducting cuprate $Y_1Ba_2Cu_3O_7$, for example, high-resolution electron spectroscopy has revealed twinning boundaries running parallel to the layers[10] and also some irregular alternations of Y and Ba layers[11] (the typical distance between the plane defects on a photograph shown in Ref. 11 is 100 Å). In the present paper we show that the behavior of the transverse resistance is that of an insulator when there is strong scattering of current carriers by plane defects. If the relaxation time of the transverse component of the momentum, $\tau_\perp^d$, is much smaller than the time τ_0 for departure from a state with a given energy ε and a given longitudinal momentum component $\mathbf{p}_\parallel$, then over times $\tau_\perp^d \ll t \ll \tau_0$ an electron can be scattered by plane defects many times, while the momentum $\mathbf{p}_\parallel$ is conserved. Over these times, the motion of a particle with a definite value of $\mathbf{p}_\parallel$ is essentially one-dimensional. We know that the Boltzmann equation cannot be used, regardless of the value of the parameter[1] $\varepsilon_F\tau$, for a one-dimensional disordered metal.[12,13] If no other scattering mechanisms were operating ($\tau_0 \to \infty$), the wave functions would be localized in the transverse direction, and the conductivity in this direction would vanish. Relaxation of the longitudinal component of the momentum leads to disruption of the coherence of the transverse motion and to the appearance of a finite conductivity in this direction.

Ono[14] explains the pronounced anisotropy of the resistance of graphite on the basis of scattering of current carriers by stacking faults. In Ono's paper, however, the transverse resistance was calculated by means of the Boltzmann equation, which has only a limited range of applicability for this model. In particular, the temperature dependence found for the transverse resistance by Ono was metallic.

2. WEAKLY REFLECTING PLANE DEFECTS

To calculate the transverse conductivity in the case of plane defects with a reflection coefficient $r \ll 1$, it is convenient to use a version of Berezinskiĭ's technique which was proposed by Gogolin *et al.*[15] Applying this technique to the system under consideration here requires writing the electron Green's functions in a mixed representation—the coordinate representation in the transverse direction and the momentum representation in the longitudinal direction:

$$G_\varepsilon^{\pm}(z-z', \mathbf{p}_\parallel) = (\mp i v_\perp(\varepsilon-\varepsilon_\parallel))^{-1} \exp(\pm i p_\perp(\varepsilon-\varepsilon_\parallel)|z-z'|).$$

Here the plus and minus signs specify the retarded and advanced Green's functions, respectively, and $v_\perp$ and $p_\perp$ are the transverse velocity and transverse momentum, which depend on the longitudinal momentum $\mathbf{p}_\parallel$ through the energy of the longitudinal motion, $\varepsilon_\parallel(\mathbf{p}_\parallel)$. The phonon Green's function and the impurity line must be transformed analogously. If scattering by plane defects is dominant, the technique is similar to Berezinskiĭ's technique for one-dimensional electrons with additional scattering by three-dimensional phonons.[15] The only difference is that the phonon Green's functions depend on $\mathbf{p}_\parallel$, so it is not legitimate to carry out an independent integration over the longitudinal momentum in the phonon Green's functions and in the impurity lines.

Gogolin *et al.*[15] showed that if the condition $\Delta\varepsilon\tau_i \gg 1$ holds ($\Delta\varepsilon$ is the typical energy transferred to a one-dimensional electron in a collision with a phonon, and τ_i is the time scale of the momentum relaxation due to collisions with impurities), the scattering by phonons affects the conductivity only to the extent that the "escape" electron relaxation time changes. An expression for the hopping conductivity in this case can be found from the expression for the complex rf conductivity through the replacement $i\omega \to 1/\tau_{ph}$. For the system under consideration here, this approximation is valid under the vastly weaker condition $v_\parallel \tau_\perp^d \Delta p_\parallel \gg 1$, where $\Delta p_\parallel$ is the typical change in the longitudinal momentum in the collisions. For scattering by impurities, this condition holds in essentially all cases, while for collisions with phonons it

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holds at temperatures $T \gg s/v_\parallel \tau_\perp^d$, where s is the sound velocity. Using the result of Ref. 15 for a one-dimensional metal, we thus find the following expression for the transverse conductivity at $\tau_\perp^d \ll \tau_0$:

$$\sigma_\perp = 4\zeta(3) N(\varepsilon_F) e^2 \langle (v_\perp \tau_\perp^d)^2/\tau_0 \rangle_{s_F}, \quad (1)$$

where $\zeta(x)$ is the Riemann function, $N(\varepsilon_F)$ is the state density, and $\langle ... \rangle_{s_F}$ means an average over the Fermi surface. Because of interference effects, the transverse conductivity differs from the classical conductivity by a factor $\tau_\perp^d/\tau_0 \ll 1$. If the escape time is determined primarily through scattering by phonons, the temperature dependence of $\sigma_\perp$ is that of an insulator.

The scattering by plane defects does not influence the longitudinal conductivity, for which we can use the usual Drude formula

$$\sigma_\parallel = e^2 N(\varepsilon_F) \langle v_\parallel^2 \tau_\parallel \rangle_{s_F}, \quad (2)$$

where $\tau_\parallel$ is the relaxation time of the longitudinal component of the momentum. This time is determined by scattering by impurities and phonons: $1/\tau_\parallel = 1/\tau_\parallel^i + 1/\tau^{ph}$. At temperatures above the Debye temperature (i.e., in a region in which the resistivity $\rho_\parallel = \sigma_\parallel^{-1}$ is a linear function of the temperature), the relaxation of $\mathbf{p}_\parallel$ is caused by scattering through large angles. In this case the times $\tau_\parallel$ and τ_0 are the same, so the product $\sigma_\perp \sigma_\parallel$ does not depend on the temperature. It is determined by the parameters of the Fermi surface and by the interaction of the carriers with plane defects.

We have assumed that the defects are infinite. For band-shaped defects with a typical width L, expression (1) remains in force if an electron over the time $L/v_\parallel$ required to cross the band, can, be scattered by impurities or phonons: $L/v_\parallel \gg \tau_0$.

At sufficiently high temperatures, the escape time τ_0 becomes comparable to the time $\tau_\perp^d$, coherent effects are suppressed, and the transverse conductivity assumes its classical value

$$\sigma_\perp^{cl} = e^2 N(\varepsilon_F) v_\perp^2 \tau_\perp.$$

Because of the scattering by plane defects, however, a specific quantum-mechanical correction to the conductivity, $\sigma_\perp^{cl} \tau_\perp \tau_0^2/(\tau_\perp^d)^3$ in order of magnitude, arises. The quantum-mechanical correction to the conductivity, $\Delta\sigma_\perp$, is determined by diagrams on which impurity lines intersect. Diagrams which contain two intersecting lines describing scattering by plane defects cancel each other out. Diagrams of the types shown in Fig. 1, a and b, in which three lines intersect, make a nonvanishing contribution (the diagrams are evaluated by the Berezinskiĭ technique). Calculations lead to the results

$$\Delta\sigma_\perp^{(a)} = -e^2 N(\varepsilon_F) \langle (v_\perp \tau_\perp \tau_0)^2/(\tau_\perp^d)^3 \rangle_{s_F}, \quad (3a)$$

$$\Delta\sigma_\perp^{(b)} = {}^1/_2 \Delta\sigma_\perp^{(a)}, \quad (3b)$$

$$\Delta\sigma_\perp = 2\Delta\sigma_\perp^{(a)} + 2\Delta\sigma_\perp^{(b)} = -3e^2 N(\varepsilon_F) \langle (v_\perp \tau_\perp \tau_0)^2/(\tau_\perp^d)^3 \rangle_{s_F}. \quad (3c)$$

In the region $\tau_\perp^d \sim \tau_\perp \sim \tau_0$ the quantum-mechanical correction $\Delta\sigma_\perp$ becomes comparable to the classical conductivity $\sigma_\perp^{cl}$, and interference effects become important in the scattering by plane defects.

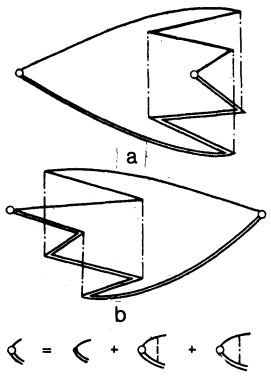

FIG. 1. Berezinskiĭ diagrams determining the quantum-mechanical correction to the conductivity in the case of a scattering by plane defects. Solid line—Retarded Green's functions; double line—advanced Green's function; dot-dashed line—line describing a scattering by plane defects; dashed line—impurity or phonon line, filled point—current vertex.

3. STRONGLY REFLECTING PLANE DEFECTS

For the scattering of electrons by plane defects with a reflection coefficient $r \lesssim 1$, the classical expression for the transverse conductivity is[14]

$$\sigma_\perp^{cl} \approx e^2 N(\varepsilon_F) v_\perp dt, \quad (4)$$

where $t = 1 - r$ is the transmission coefficient, and d is a typical distance between plane defects.

When the mean free time τ_0 becomes longer than the typical transit time $d/v_\perp$, quantum-size levels appear in each "gap" between neighboring plane defects, and the transverse momentum takes on several discrete values $p_{\perp n} = \pi n/d (n = 1,2...)$. Since d is random, the values of $p_{\perp n}$ for the neighboring gaps will generally differ. For each gap, however, a small fraction of the states are highly hybridized with a state in one of the neighboring gaps. A simple estimate shows that the highly hybridized levels are those for which the difference between the quantized values of the transverse momentum is less than $t^{1/2}/d$. The time scale for the tunneling to a neighboring gap once such a level is reached is $\tau_t \sim d/v_\perp t^{1/2}$.

Let us estimate the lifetime τ_j in a gap in a situation with scattering by impurities and phonons. If the typical transfer of longitudinal momentum in the course of a collision is $\Delta p_\parallel \gg v_\perp/v_\parallel d$, an electron will hop between quantum-size levels over a time on the order of τ_0. The electron will reach hybridized levels at a frequency $t^{1/2}/\tau_0$. The estimate of the transition time depends strongly on the ratio of the tunneling time τ_t to the lifetime in the level, τ_0.

1. In the case $\tau_0 \ll \tau_t$, the tunneling probability once a resonant level has been reached is τ_0/τ_t, and the transition time is estimated to be

$$\tau_j^{-1} \sim (t^{1/2}/\tau_0)(\tau_0/\tau_t) \sim t^{1/2}/\tau_t.$$

$$D_\perp \sim d^2/\tau_j \sim v_\perp dt,$$

and an estimate of the conductivity from Einstein's relations, $\sigma_\perp = e^2 N(\varepsilon_F) D_\perp$, again leads to the result (4).

2. In the opposite limit, $\tau_0 \gg \tau_t$, an electron goes into a neighboring gap with a probability of order unity once it reaches a resonant level. We thus find the following estimates: a transition time $\tau_j \sim \tau_0/t^{1/2}$, a diffusion coefficient

$D_\perp \sim t^{1/2} d^2/\tau_0$, and a transverse conductivity

$$\sigma_\perp \sim e^2 N(\varepsilon_F) t^{1/2} d^2/\tau_0. \quad (5)$$

If τ_0 is determined by scattering by phonons, the temperature dependence of the transverse conductivity has a plateau (4) in the interval

$$\tau_\perp^{ph} > dt/v_\perp,\ \tau_0^{ph} < d/t^{1/2} v_\perp\ \ (\tau_\perp^{ph} \geqslant \tau_0^{ph}),$$

and at $\tau_0^{ph} > d/t^{1/2} v_\perp$ this plateau gives way to insulating behavior, (5).

4. CONCLUSION

Let us examine the applicability of this model to real systems. In nearly all $Y_1Ba_2Cu_3O_7$ superconducting single crystals, the longitudinal resistance depends linearly on the temperature, so we would expect the transport time $\tau_\parallel$ and the escape time τ_0 to be comparable in order of magnitude. There are single crystals which exhibit a $\rho_\perp(T)$ behavior which is clearly of an insulating nature.[8,9] If behavior of this sort is caused by scattering of current carriers by plane defects, the product $\rho_\parallel \rho_\perp$ should be independent of the temperature. This assertion remains in force if there is an additional scattering by impurities, in which case the temperature dependence of $\rho_\parallel(T)$ takes the form $\rho_\parallel(T) = \rho_0 + Td\rho_\parallel/dT$.

Figure 2 shows plots of $(\rho_\parallel \rho_\perp)^{1/2}$ for single crystals 1, 2, and 3 of Ref. 8 (these crystals exhibited a superconducting transition at $T \sim 90$ K). We see that for all three crystals there is a plateau on the plot. For crystal 2, for example, the value of $(\rho_\parallel \rho_\perp)^{1/2}$ varies within 6% limits between 100 and 250 K. The increase in $(\rho_\parallel \rho_\perp)^{1/2}$ with increasing temperature is naturally linked with a transition of $\rho_\perp$ to a classical regime. In certain single crystals, there is a large region of residual resistance on the $\rho_\perp(T)$ curve; this region gives way to an insulating behavior as the temperature is lowered.[7,8] As was shown in Sec. 3, this behavior occurs in the scattering of carriers by plane defects with a small transmission coefficient ($t \ll 1$). From (2), (4) and (5) we find the relation

$$\frac{(\rho_\parallel \rho_\perp)^{1/2}_{T<T_0}}{(\rho_\perp)_{T>T_0}} \sim \frac{v_\perp}{v_\parallel} t^{3/4}, \quad (6)$$

where T_0 is the temperature at which the dependence $\rho_\perp(T)$ becomes that of an insulator. Relation (6) can be used to estimate the typical transmission coefficient t. Using the estimate $v_\parallel/v_\perp \sim 5$, which follows from measurements of the anisotropy of the field H_{c2} in these materials, we find $t \sim 0.2$ for single crystal 1 of Ref. 8. At such transmission coefficients,

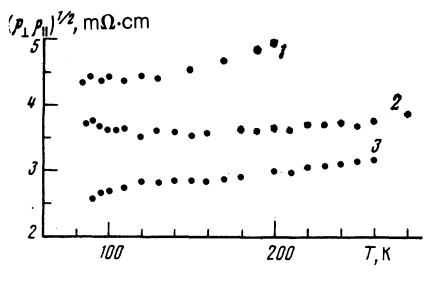

FIG. 2. Temperature dependence of $(\rho_\perp \rho_\parallel)^{1/2}$ for single crystals 1, 2, and 3 of Ref. 8.

the temperature dependence $\rho_\perp(T)$ becomes that of an insulator when the mean free path across the layers, $l_\perp$, becomes comparable in magnitude to the typical distance between plane defects, d. Taking $d \sim 100$ Å, we can find an estimate of the mean free path along the layers, $l_\parallel$, at the temperature at which the insulating behavior sets in:

$$l_\parallel \sim v_\parallel d/v_\perp \sim 500 \text{ Å}.$$

This estimate is more than an order of magnitude greater than estimates of $l_\parallel$ made in Refs. 16 and 17. Note, however, that the estimates of Refs. 16 and 17 were afflicted by a large uncertainty because of the absence of reliable measurements of the band parameters (the effective mass and Fermi velocity) of the high-temperature superconductors. Anderson and Zou[18] and Xing *et al.*[19] believe that the insulating behavior of $\rho_\perp(T)$ is an internal property of the compounds. That assumption contradicts the fact that the $\rho_\perp(T)$ behavior varies wildly from one sample to another.

In most of the papers on graphite (e.g., Refs. 3–6), the temperature dependence of the resistance components has been reported over the temperature range $0 < T < 300$ K. In this range the functional dependence $\rho_\parallel(T)$ is nonlinear, so there is no reason to believe that the times $\tau_\parallel$ and τ_0 are the same. As a rule, $1/\rho_\perp$ falls off more rapidly than $\rho_\parallel$ with decreasing temperature. On the basis of the model proposed here, this behavior can be explained if the inequality $\tau_\parallel^{ph} \gtrsim \tau_\parallel^i \gg \tau_0^{ph}$ holds for the impurity time $\tau_\parallel^i$. In this case, $1/\rho_\perp \sim 1/\tau_0^{ph}$ would vary more rapidly than the longitudinal component of the resistance, $\rho_\parallel \sim 1/\tau_\parallel^i + 1/\tau_\parallel^{ph}$, with decreasing temperature.

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[1)] We are using a system of units with $\hbar = k = 1$.

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