Prelocalization in semimetals

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The Fermi energy close to a band edge provides a conventional localization only when a one-dimensional residual resistance is large compared to $\pi\hbar/e^2$. Prior to the localization, the resistance increases first quadratically and then oscillates (between large and small values) with the length ("prelocalization"). There are several temperature regions, where the resistance may increase and decrease with temperature.

Recently it was noticed[1] that δ-function substitutional impurities at the band edge of the pure system do not give rise to the localization even in one dimension (1D). Instead, then[1] 1D residual resistance $R_r \propto L^2$, L being the length. In semimetals the Fermi energy is close to the band edge, and a direct calculation[2,3] of the localization length L_0 in a wire leads to $L_0 \sim 8k|v_a \cot k - k|S/c_1c_2v'^2$ when $|v_a| \ll k|\tan k|$. Here $v_a = v_1c_2 + v_2c_2$; $v' = v_1 - v_2$; v_1 and v_2 are the dimensionless potentials of an impurity and a basic atom; c_1 and c_2 are their concentrations ($c_1 + c_2 = 1$); k is the Fermi wave vector; S is the wire cross-section area; the interlattice spacing is 1. In semimetals (where $k \approx \pi, 2\pi, \ldots$) $|\cot k| \gg 1$. Thus, $L_0 \propto |\cot k|S$ remains large compared to the Thouless[4] inelastic diffusion length L_D down to very low temperatures. This may explain the absence of the localization in the experiments[5] on Bi.

Usually, according to the scaling theory,[6] at zero temperature the localization follows Ohm's law ($R_r \propto L$) at the dimensionless $R_r \sim 1$. In this paper I prove that in semimetals $L \sim L_0$ implies $R_r \gg 1$. Prior to the localization, the dependence of R_r on L is very special. It is characteristic of each random system (which is natural for L less than the correlation length $\sim L_0$)—see Fig. 1. The representative[6,7] ensemble average $\langle R_r \rangle$ is $\propto L$ only when L is small compared to an elastic mean free path l (if $l \sim 1$, this region is extinct). When $L > l$, but $L < L_0$, then first $\langle R_r \rangle \propto L^2$ (Fig. 2), and later *oscillates* between large values (Fig. 3). This new region, which is different from both weak and strong localization and which may exist only in semimetals, I denote as the "prelocalization." The temperature dependence of the resistance $R(T)$ in this region is also unusual (see later in this paper). I prove that $l \sim 4k^2/c_1c_2v'^2$, so $L_0 \sim lS|v_a \cot k| \gg l$. Thus, the prelocalization region where $l < L < L_0$ (and $\langle R_r \rangle \gg 1$) is rather large. To elucidate these results, consider a unity interlattice spacing and a wave vector $k = \pi$ at the band edge. Such k implies the wave-function phase shift $(n' - n)\pi$ on the way from the nth to n'th site and the phase shift $2(n' - n)\pi$ for a round trip. Since the latter phase shift is unimportant, $k = \pi$ does not "see" any randomness in the substitutional impurity positions. Thus, it does not give rise to any localization, and we find instead[1] $R_r \propto L^2$. When $k \approx \pi$ and the meaningful phase shift at an average interimpurity distance is small, then a phase-shift randomization occurs only at large distances $\propto |\pi - k|^{-1}$. Impurity position randomness is averaged out at such distances, so only impurity concentration fluctuations matter. When the single impurity scattering is weak, then the difference of the "total" phase shift $(\pi - k)L$ from an integer of 2π oscillates with L and this leads to oscillations in R_r and $\langle R_r \rangle$. When the individual scattering is strong, then a particle bounces

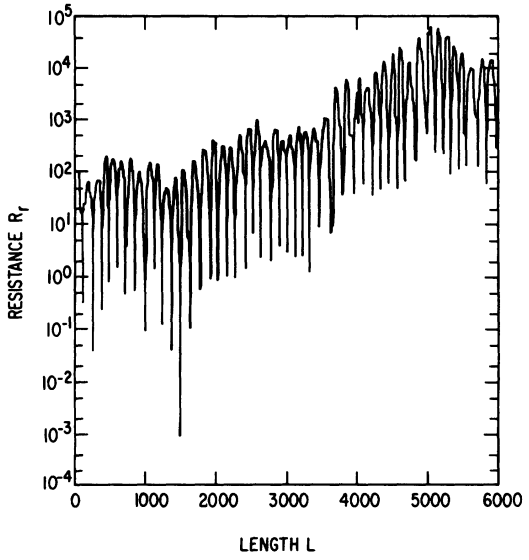

FIG. 1. Dependence of the one-dimensional (1D) residual resistance R_r on the length L. Interlattice spacing is 1, dimensionless wave vector $k = 3.14$, dimensionless impurity potentials $v_1 = 10$, $v_2 = 0$; impurity concentration $c_1 = 0.125$. Note a large scale R_r change (e.g., from 70 to 9×10^{-4} to 100 at $L \sim 1500$).

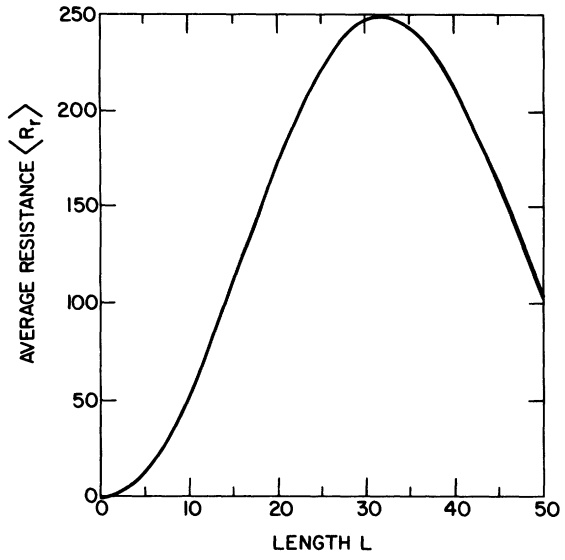

FIG. 2. 1D residual resistance $\langle R_r \rangle$, averaged over 300 samples. Impurity concentration $c_1 = 0.5$; k and v are the same as in Fig. 1.

back and forth many times between adjacent impurities, its effective path at L increases significantly, and thus the period of the oscillations of $\langle R_r \rangle$ and R_r decreases. If, for instance, $v_2 = 0$ and $v_1 > 2k \approx 2\pi$ then an individual potential v_1 implies the transmission coefficient $t \sim (1 + v_1^2/4k^2)^{-1}$, thus $\sim t^{-1}$ "bouncings" and, therefore, the period of oscillations

$$L_1 \sim t/(\pi - k) \sim 4\pi^2/v_1^2(\pi - k) \ .$$

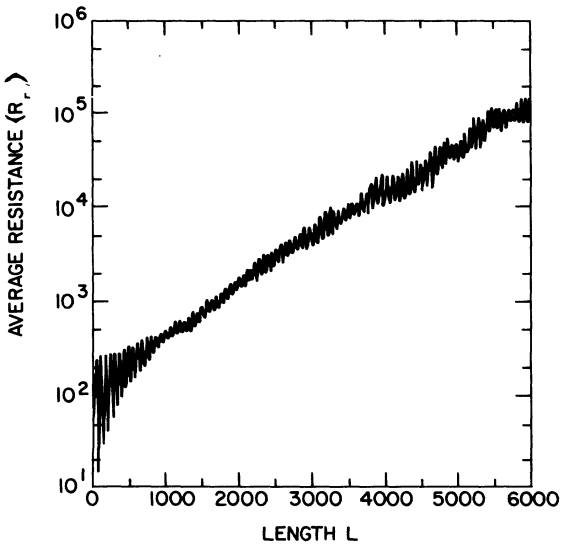

FIG. 3. Same as Fig. 2, but on a larger length L scale. Note large-scale oscillations at $L < 1000$ and a conventional localization when $\langle R \rangle > 500$.

(When $L \ll L_1$, then $\langle R_r \rangle \propto L^2$.) An elastic mean free path

$$l \sim 4k^2/v_1^2 c_1 c_2 \simeq 4\pi^2/v_1^2 c_1 c_2$$

is small compared to L_1 when $c_1, c_2 > \pi - k$, i.e., up to low impurity concentrations. The prelocalization persists until the length L becomes of order of or larger than the localization length $L_0 \sim 8\pi S/(\pi - k) c_2 v_1$. (Note that $L_0 \propto S$, while L_1 and l are independent of S.) The latter remains large compared to the inelastic diffusion length $L_D \sim \sqrt{l l_{\text{in}}}$ until an inelastic mean-free-path length l_{in} becomes

$$l_{\text{in}}^{(0)} \sim L_D^2/l \sim 16 S^2 c_1/(\pi - k)^2 c_2 \ ,$$

where S (in the dimensionless units) is the number of sites per cross section. Consider the case of $c_1 = 0.2$, $v_1 = 10$, and $\pi - k = 0.01$. Then $l \sim 2$; a "conventional" $L_0 \sim lS \sim 2S$, and $l_{\text{in}}^{(0)} \sim L_D^2/l \sim 2S^2$, while $L_1 \sim 40$, the "true" $L_0 \sim 250S$ and $l_{\text{in}}^{(0)} \sim L_D^2/l \sim 30\,000 S^2$. In a whisker 300×300 atoms in a cross section $L_0 \sim L_D$ only at the temperatures low enough to provide $l_{\text{in}}^{(0)} \sim 3 \times 10^9$ interlattice spacings, i.e., $l_{\text{in}} \sim 1$ m. Since the crucial quantity is $\pi - k$, L_D can be significantly affected by a small change in the Fermi energy ϵ_F, which may be provided by external pressure or magnetic field which leads to a paramagnetic quantization.

A crucial point in all this reasoning is that the impurities are vacancies or δ-function substitutions. A general case will be considered elsewhere.

According to Ref. 2, the residual resistance R_r for a potential $V = \sum_{n=1}^{L} v_n \delta(x - n)$, where v_n is randomly chosen to be v_1 (with the probability c_1) or v_2 (with the probability c_2), equals

$$R_r = [\exp(G_L^{(+)}) + \exp(G_L^{(-)}) - 2]/4 \ , \tag{1}$$

$$G_L^{(\pm)} = \sum_{n=1}^{L} \ln \left[\frac{(1 + X_n^{(\pm)2})}{(\omega_{n-1} + \omega_{n-1}^{-1} X_n^{(\pm)2})} \right] \ , \tag{2}$$

where

$$X_{n+1} = \omega_n (X_n - r_n)/(1 + r_n X_n) \ ,$$

$$\omega_n = \tan^2(h_n/2 + \pi/2) \ ,$$

$$r_n = \tan[k - (h_n + h_{n-1})/2] \ ,$$

$$h_n = \arctan(v_n/2k), \quad h_0 = 0; \quad X_1^{(\pm)} = \pm 1 \ .$$

Equations (1) and (2) lead to the plots in Figs. 1–5. The approach is readily applicable to any sequence of arbitrary and arbitrarily located nonoverlapping potentials. In Figs. 1–5 holes localized by impurity potenital barriers were considered. According to the above recurrence relations, electron (with $k > \pi$) scattering at impurity potential wells is similar. The energy of electrons between potential barriers and holes between potential wells lies either in the gap or

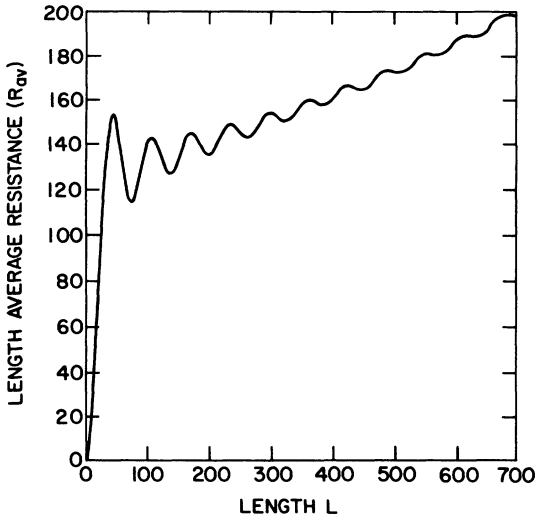

FIG. 4. Residual resistance R_{av}, averaged over 9000 samples and the length; c,k,v are the same as in Fig. 2.

close to an energy gap of the average potential. In this case their localization differs less from the conventional picture. The scattering of small k's is the strongest because an electron with a small velocity proportional to k spends a large time proportional to $1/k$ near an impurity. Its localization differs from a conventional one only in the case of a weak well scattering.

In semimetals, conductivities of electrons and holes add up, so the larger conductivity dominates. When electrons are in the first band ($k \approx 0$), the dominant hole conductivity is very different for impurity potential barriers and wells.

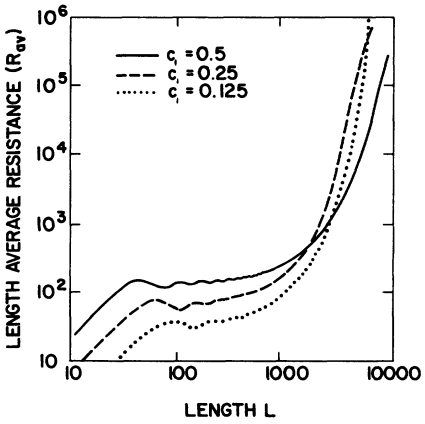

FIG. 5. Residual resistance R_{av}, averaged over 300 samples and the length, for impurity concentrations $c_1 = 0.125$, 0.25, 0.5; k and v are the same as in Fig. 1. Note that at $L > 9000$ resistance *decreases* when impurity concentration *increases,* in agreement with Ref. 2.

A large magnetic field, which essentially alters the distance between the Fermi energy and a band edge and thus L_0, may change the resistance by orders of magnitude in the strong localization case.

We introduce $X_n \equiv \tan[\pm\pi/4-(n-1)k+b_n^{\pm}]$, where $b_1^{\pm}=0$, and derive the recurrence for $b_n^{\pm}$. When $h_n \ll 1$, we determine $b_n^{\pm}$ in a linear approximation in h_n and evaluate R_r by Eqs. (1) and (2). After simple algebraic transformations one obtains

$$R_r \approx \left[\sum_{n=1}^{L} h_n \cos(2nk)\right]^2 + \left[\sum_{n=1}^{L} h_n \sin(2nk)\right]^2 . \quad (3)$$

Then by Eq. (3),

$$\langle R_r \rangle \approx L\Delta h^2 + \langle h \rangle^2 \sin^2(kL)/\sin^2 k \ , \quad (4)$$

where $\Delta h^2 = \langle h^2 \rangle - \langle h \rangle^2$, and where triangular brackets denote ensemble average.

In the general case in the prelocalization region $\langle R_r \rangle$ can be evaluated following the approach of Refs. 2 and 8. In the localization region a representative R_r and L_0 were evaluated in Ref. 2.

In Ref. 3 the calculation of the resistance of a wire was mapped on that of a 1D random potential. The latter equals the wire impurity potential averaged over all possible cross-section impurity positions. The resulting equation, replacing Eq. (4), reads

$$\langle R_r \rangle \sim L/Sl + v_{av}^2 \sin^2(kL)/4k^2 \sin^2 k \ . \quad (5)$$

The first term is the classical Ohmic term with the elastic mean free path $l \sim 4k^2/c_1 c_2 v'^2$.

At finite temperature T, when the inelastic diffusion length L_D (i.e., the direct distance between two consecutive inelastic collisions, $L_D \propto \tau_{in}^{1/2}$, τ_{in} being an inelastic mean-free-path time) is small compared to L_0, then one should average over all lengths L of the order of L_D, and the conductivity proportional to L is obtained in the leading approximation for $L \gg L_D$.

Therefore a resistance $R(T)$ is related to

$$R_{av}(L) \equiv L^{-1} \sum_{L'=1}^{L} \langle R_r(L') \rangle$$

by the equation $R(T) \sim R_{av}(L_D)(L/L_D)$.

According to Eq. (4), when $L < 1/|\pi - k|$, then $R_{av} \propto L^2$, while $L \gg 1/|\pi - k|$ leads to

$$R_{av}(L) \sim L/2Sl + v_{av}^2/8k^2 \sin^2 k \equiv A + BL \ . \quad (6)$$

Weak oscillations, provided by Eq. (4), are neglected in Eq. (5). The numerical calculation of $R_{av}(L)$, according to Eqs. (1) and (2), is presented in Fig. 4 and, for different impurity concentrations, in Fig. 5.

When the temperature T decreases, $R(T) \propto \tau_{in}^{-1}$ and decreases with T (the "classical" temperature dependence), if $L_D < l$. Then, when $l < L < 1/|\pi - k|$ and $R_{av}(L) \propto L^2$, a prelocalization regime starts: $R(T) \propto \tau_{in}^{1/2}$ and increases with T. Then, when $R_{av}(L) \simeq A + BL$; $R(T) \simeq \tau_{in}^{-1/2}$ and decreases

with T. This decrease continues as long as R_{av}/L decreases, i.e., until a straight line from $L=0$ to a given L becomes tangent to $R_{av}(L)$. Weak $R(T)$ oscillations with T, related to R_{av} oscillations with L, may also be possible in the prelocalization region. Finally, $R(T)$ gives rise to the Thouless regime[4]: $R(T) \propto \tau_{in}^{-1}$ when $L_D > L_0$ and $\ln R(T) \propto T^{-1}$ at very low temperatures. Usually even at high temperatures $L_D \gg 1/|\pi - k|, l$; this may extinguish the first two regions [$R(T) \propto \tau_{in}^{-1}$ and $R(T) \propto \tau_{in}^{1/2}$], unless a certain pressure, and/or magnetic field, and/or impurity concentration provide $|\pi - k| < 1/L_D$ and/or $L_D < l$. Since the prelocalization region persists up to very large values of R_{av}, the $R(T)$ decrease with T persists up to extremely low temperatures. This was actually observed in experiments[5] on Bi.

In this calculation T has everywhere been assumed to be small compared to the Fermi energy ϵ_F and thus it does not affect available values of $|\pi - k|$. The increase in $T \gtrsim \epsilon_F$ would decrease the available values of $|\pi - k|$ and thus decrease the corresponding resistance.

Since L_0 is very different for electrons and holes in semimetals,[2] at low temperatures electrons may be localized while holes are not, or the other way around. This may be verified in a strong magnetic field H, because then the effective electron and hole densities are no longer compensated, and $R \propto H^2$ should be replaced by the $R(H)$ dependence, which exhibits saturation.

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