Logarithmic divergence of normal state resistivity of bipolaronic high-$T_c$ cuprates.

A.S. Alexandrov

Department of Physics, Loughborough University, Loughborough LE11 3TU, U.K.

Abstract

The resonance Wigner scattering of charged bosons (small bipolarons) in a random potential leads to logarithmically divergent low-temperature resistivity as observed in several cuprates. Unusual temperature dependence of resistivity of $La_{2-x}Sr_xCuO_4$ as well as of the Hall effect is quantitatively described in a wide temperature range providing an evidence for $2e$ charged Bose-liquid in high-$T_c$ cuprates.

There is no need to abandon the Boltzmann kinetics to explain the linear in-plane resistivity and temperature dependent Hall effect above $T_c$ in cuprates if the bipolaron theory is applied. A fraction of the bipolarons is localised by disorder, so that the number of delocalised carriers is proportional to $T$ while the boson-boson inelastic scattering rate is proportional to $T^2$. This allows us to explain that both the in-plane resistivity and the Hall density are proportional to $T$. Recently we have extended the theory towards $c$-axis transport. The semiconductor-like temperature dependence of the $c$-axis resistivity has been understood within the Boltzmann kinetics by taking into account the contribution of thermally excited polarons to the $c$-axis transport.

In this letter the transport relaxation time of bipolarons (or any charged bosons on a lattice) is derived at low temperatures where the scattering is dominated by the elastic boson-impurity scattering and single polarons are frozen out. The temperature dependence of the resistivity appears to be in a remarkable agreement with the experimental dependence measured recently by Ando et al. in $La_{2-x}Sr_xCuO_4$ by suppressing $T_c$ down to a millikelvin.
scale with a pulsed magnetic field.

Small hole polarons are paired above \( T_c \) in the doped Mott-Hubbard insulators if the electron-phonon interaction is relatively strong \( (\lambda > 0.5) \) \[1\]. Therefore, the low-energy states of cuprates are thought to be a mixture of the intersite in-plane singlet pairs (small bipolarons) and thermally excited polarons. Above \( T_c \), which is the condensation temperature of the charged Bose-gas, these carriers are nondegenerate. Intersite singlets tunnel along the planes with an effective mass \( m^{**} \) of the order of a single-polaron mass \[5\]. Their \( c \)-axis tunneling is Josephson-like involving the simultaneous hopping of two holes. Therefore the singlet \( c \)-axis mass is strongly enhanced, \( m_{c}^{**} \gg m^{**} \), which leads to a large transport anisotropy at low temperatures when polarons are frozen out. At temperatures below the \( c \)-axis bipolaron bandwidth we expect a three-dimensional anisotropic energy spectrum and a three dimensional scattering of bipolarons dominated by the lattice defects and impurities. The number of extended bosons \( n_b(T) \) above the mobility edge is determined in the ‘single-well—single-particle’ approximation as \[2\]

\[
\frac{n_b(T)}{x} = \frac{x}{2} - n_L(T),
\]

where \( x/2 \) is the total number of pairs, and \( n_L(T) = n_L - N_L(0)k_B T \) is the number of bosons localized by the random potential with \( N_L(0) \) the density of localized states near the mobility edge. The Hall coefficient \( R_H \) measures the inverse carrier density, so that

\[
\frac{R_H}{R_{H0}} = \frac{1}{1 + T/T_L},
\]

where \( T_L = (x - 2n_L)/2k_B N_L(0) \). This simple expression fits well to the Hall coefficient temperature dependence of \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) at optimum doping \( (x = 0.15) \) \[3\] as shown in Fig.1 with \( T_L = 234K \) and the constant \( R_{H0} = 2 \times 10^{-3}cm^2/C \). If the total number of carriers \( x/2 \) is above the total number of the potential wells \( n_L \), which is assumed here, the carrier density is practically temperature independent at low temperatures \[4\]. On the other hand if \( x < 2n_L \) the re-entry effect into the normal state appears with the temperature lowering below \( T_c \) \[8\].

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The normal state of the bipolaronic superconductor is reminiscent to that of a non-degenerate semiconductor. The characteristic kinetic energy of carriers appears to be of the order of the temperature rather than of the Fermi energy of usual metals. The most effective scattering at low temperatures is then caused by the attractive shallow potential wells which for slow particles is described by the familiar Wigner resonance cross-section

$$\sigma(E) = \frac{2\pi\hbar^2}{m} \frac{1}{E + |\epsilon|}. \quad (3)$$

Here

$$\epsilon = -\frac{\pi^2}{16} U_{\text{min}} \left( \frac{U}{U_{\text{min}}} - 1 \right)^2 \quad (4)$$

is the energy of a shallow virtual ($U < U_{\text{min}}$) or real ($U > U_{\text{min}}$) localised level, $U$ the well depth and $U_{\text{min}} = \pi^2 \hbar^2 / 8ma^2$ with the well size $a$. In the non-crossing approximation, which describes the essential physics, the transport relaxation rate is the sum of the scattering cross-sections from different potential wells within the unit volume multiplied by the velocity $v = \sqrt{2E/m}$. There is a wide distribution of potential wells with respect to both $U$ and $a$ in real cuprates. Therefore, one has to integrate the Wigner cross-section, Eq.(3), over $U$ and over $a$. By doing the integration over $U$ we take into account only shallow wells with $U < U_{\text{min}}$ because the deeper wells are occupied by localised carriers and cannot yield a resonant scattering. The result is

$$\langle \sigma(E) \rangle \equiv \gamma^{-1} \int_0^{U_{\text{min}}} \sigma(E) dU = \frac{4\pi\hbar^3}{m\gamma a\sqrt{2mE}} \tan^{-1} \left( \frac{\pi^2\hbar}{8a\sqrt{2mE}} \right), \quad (5)$$

where the width of the $U$-distribution $\gamma$ is supposed to be large compared with $U_{\text{min}}$. By doing the integration over size $a$ one has to take into account the fact that the Wigner formula, Eq.(3) is applied to slow particles with $a \leq \hbar \sqrt{2mE}$. However, because the $U$-averaged cross-section, Eq.(5) behaves like $1/a^2$ at large $a$ one can extend the integration over $a$ up to infinity to obtain the inverse mean free path as

$$l^{-1}(E) = \frac{n_L}{A} \int_{a_{\text{min}}}^{\infty} \langle \sigma(E) \rangle da \simeq \frac{\pi^2\hbar^3 N_L(0)}{mA\sqrt{2mE}} \ln \frac{E_0}{E}. \quad (6)$$
for $E \ll E_0$. Here $A$ is the width of the size distribution of the random potential, $N_L(0) = n_L/\gamma$, $E_0 = \pi^4 h^2/128 ma_{min}^2$ and $a_{min}$ is the minimum size. We expect a very large value of $A$ of order of a few tens $\AA$ due to the twin boundaries and impurity clusters in real cuprates which are not screened. On the other hand, single impurities are screened. A simple estimate of the screening radius by the use of the classical expression, $r_D = \sqrt{k_B T \epsilon/16 \pi n_B e^2}$ yields a value of $a_{min}$ of the order or even less than the interatomic spacing ($\sim 1.9 \AA$), which corresponds to a quite large $E_0/k_B = 1500K$ if $m = 10m_e$. As a result, in a wide temperature range we arrive at the logarithmic transport relaxation rate as

$$1/\tau \equiv v l^{-1}(E) = 1/\tau_0 \ln \frac{E_0}{E},$$

where $\tau_0 = m^2 A/\pi^2 h^2 N_L(0)$ is a constant. The above formula is applied to the isotropic s-scattering of slow particles with an isotropic 3D energy spectrum described by the effective mass $m$. However, assuming that the attractive field scales as $U(r) = U(x^2 + y^2 + z^2 m^*_c/m^{**})$ one obtains the same result for the anisotropic spectrum as well, if $m = m^{**}$. Because the Wigner formula, Eq.(3) is somewhat more general than the assumption made in its derivation $[9]$ we expect that the obtained logarithmic dependence, Eq.(7) is not changed if the attraction potential $U(r)$ is modified.

The low temperature resistivity is now derived by the use of Boltzmann theory as

$$\rho(T) = \rho_0 \ln \frac{\omega_0}{T},$$

where $\rho_0^{-1} = 2(x - 2n_L)e^2 \tau_0/m$ and $\omega_0 = E_0/k_B$. At high temperatures the inelastic scattering of extended bosons by localised bosons becomes important as discussed in ref. $[2]$ so that

$$1/\tau = \alpha T^2$$

with the constant, $\alpha$, proportional to the density of states at the mobility edge, $N_L(0)$ squared. Combining both elastic, Eq.(7), and inelastic, Eq.(9), scattering, and taking into account the temperature dependence of the extended boson density $n_B(T)$, Eq.(1), we arrive at
\[
\frac{\rho(T)}{\rho_0} = \ln\left(\frac{\omega_0}{T}\right) + \left(\frac{T}{T_B}\right)^2 \frac{1}{1 + T/T_L},
\]

with the constant \(T_B = 1/\sqrt{\alpha\tau_0}\). The solid line in Figs.2,3 is a fit to the experimental data with \(\rho_0 = 7.2 \times 10^{-5}\Omega cm\), \(\omega_0 = 1900K\) \(^4\) and \(T_B = 62K\) which appears to be remarkably good. The value of \(\omega_0\) agrees well with the estimate above. In the underdoped samples the effective mass of bipolarons as well as the screening radius significantly increases \(^4\), so \(\omega_0\) might be less about one order of magnitude. On the other hand, the logarithmic dependence derived above is well verified in the temperature range \(\hbar^2/2mA^2 < k_BT < \hbar^2/2ma^2_{min}\). With increasing doping the screening becomes more efficient and potential wells of a large size \(A\) are less probable. Hence, the temperature interval for the logarithmic dependence is less, and its disappearance in overdoped samples is expected. Because the bipolaron energy spectrum is three dimensional at low temperatures, there is no temperature dependence of the anisotropy \(\rho_c/\rho_{ab}\) at low \(T\) as observed \(^4\).

A simple estimate of the polaronic level shift in \textit{LSCO} shows that the electron-phonon coupling is more than sufficient to bind two polarons into a small bipolaron. For the Fröhlich interaction the polaron level shift is given by \(^5\)

\[
E_p \simeq \frac{q_D e^2}{\pi} (\epsilon^{-1} - \epsilon_0^{-1}),
\]

where \(q_d = (6\pi^2/\Omega)^{1/3}\) is the Debye momentum, \(\Omega\) the unit cell volume. With the static and high frequency dielectric constants \(\epsilon_0 >> \epsilon \simeq 5\) and \(q_D \simeq 0.7\AA^{-1}\) one obtains \(E_p \simeq 0.64eV\). As a result, there is a large attraction between two polarons of the order of \(2E_p \simeq 1eV\). At the same time the band mass enhancement is less than one order of magnitude because of the phonon dispersion as shown in ref. \(^5\). This is in contrast with some assessments of the electron-phonon interaction and the bipolaronic mechanism of high-\(T_c\) superconductivity based on the incorrect estimate of the coupling constant and of the effective mass. The hole-hole coupling via phonons, Eq.(11), is at least four times stronger than the magnetic coupling, determined by the exchange \(J \simeq 0.15eV\), which makes any model of high-\(T_c\) without phonons highly unrealistic (see also ref. \(^11\)). A large isotope effect on both \(T_c\)
and on the Néel temperature $T_N$ \cite{12} in LSCO confirms this conclusion. The pair-distribution analysis of neutron scattering \cite{13} suggests that the ‘spin-gap’ is consistent with the formation of a bipolaronic local singlet state as we predicted well before high-$T_c$ cuprates were discovered \cite{14}. We believe that the normal state ‘pseudogap’ observed with magnetic, kinetic, thermodynamic and ARPES measurements has the same origin \cite{3,1}, and a so-called ‘pairing without phase coherence’ \cite{15} is none other than the bipolaron formation.

In conclusion, the bipolaron kinetics remarkably well describes the unusual logarithmic divergence of the low-temperature resistivity as well as the high-temperature resistivity and the Hall effect observed in several high-$T_c$ cuprates, in particular, in the reference system $La_{2-x}Sr_xCuO_4$ \cite{4}. The logarithmic divergence is caused by the resonance Wigner scattering of slow nondegenerate carriers (bipolarons) scattered by the attractive random potential in the 3$D$ doped insulators.

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FIGURES

The Hall effect in $La_{2-x}Sr_xCuO_4$ (triangles) described by the theory (solid line) for $x = 0.15$.

The ‘ab’ resistivity of $La_{2-x}Sr_xCuO_4$ with $x = 0.13$ (diamonds) described by Eq.(7) in a wide temperature range (solid line).

The same as in Fig.2 at low temperatures.