An alternative normal state c-axis resistivity model for high-$T_c$ superconductors

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An alternative model for c-axis resistivity in layered high-$T_c$ crystalline superconductors is proposed and has been characterized as an essentially two-dimensional Fermi liquid. Average ionization energy is included as additional parameter that determines the concentration of tunnelling electrons between Cu-O$_2$ layers. This model agrees well quantitatively with the Bi2212 and Y123 single crystals, and qualitatively with the pure 1212 phase polycrystals.

Keywords: Normal state c-axis and a-b plane resistivity, Fermi-Dirac statistics and ionization energy

1. Introduction

The out-of-plane conduction mechanism in the normal state of high-$T_c$ superconductors is intriguing. In the early stages, facts were pointed out how anomalous various normal state properties were in the simple framework of Fermi liquid \cite{1}. This Fermi liquid predicted large Fermi surface whereas small Fermi surface was expected from the strong correlation models where the normal state transport properties favored the latter. Further studies revealed that the conventional field theoretic many-body treatment does not seem to lead to the non-Fermi liquid behavior either \cite{2}. Apart from that, according to RVB theory, the normal state of high-$T_c$ superconductors is all metals in the Cu-O$_2$ planes and is semiconductor-like for conduction between those planes \cite{3}. In addition, Anderson and Zou suggested that both the a-b plane and c-axis resistivities can be fitted very accurately by $\rho = A/T + BT$. It is also believed that there is a gap induced by the localization of carriers along c direction, which acts as an anomalous constraint of c-axis hopping rate \cite{4}. Parallel to this, the c-axis normal state resistivity of high-$T_c$ superconductors were derived via Fermi-Dirac statistics assuming the only object that were allowed to tunnel through the Cu-O$_2$ layers are the real electrons as required by the RVB theory. This phenomenological model is also used to fit the a-b plane resistivity. Furthermore, the estimation of resistivity transition such as from metallic to semiconductor or vice versa upon substitution in the pure 1212 phase polycrystals is also reported.

2. The model

The tunnelling electron’s distribution can be derived using Fermi-Dirac statistics and ionization energy as an anomalous constraint. This derivation involves two restrictive conditions: i) the total number of electrons in a given system is constant and ii) the total energy of $n$ electrons in that system is also constant. Both conditions are as given below

$$
\sum_i dn_i = 0.
$$

(1)

$$
\sum_i (E_{\text{electron}}) dn_i = 0.
$$

(2)

In condition (2) however, the ionization energy, $E_I$ will be included as an additional constraint where $E_{\text{electron}} = E_{\text{initial state}} + E_I$. This is to justify that an electron to occupy a higher state N from the initial state M is more probable than from state L if the condition $E_I(M) < E_I(L)$ at certain temperature, $T$ is satisfied. Thus, condition (2) is rewritten as

$$
\sum_i (E_{\text{initial state}} + E_I) dn_i = 0.
$$

(3)

The importance of this inclusion is that it can be interpreted as a gap and also, particularly the $E_I$ can be used to estimate the resistivity transition upon substitution of different valence state ions. Finally, the probability of an electron to occupy an energy level $E$ is given by

$$
f_e \approx e^{-\mu - \lambda(E+E_I)},
$$

(4)

if $e^{\mu + \lambda(E+E_I)} \gg 1$. Note that the distribution (4) can be reduced to the standard Fermi-Dirac distribution if $E_I \rightarrow 0$. The concentration of electrons is given by

$$
n = \int_0^\infty f_e(E) N_e(E)dE,
$$

(5)

where $\mu = -E_F/kT$, $\lambda = 1/kT$ and $N_e(E)$ is the two dimensional density of states that was derived from the Schrodinger equation. The solution of integral (5) gives the concentration of tunnelling electrons between Cu-O$_2$ layers for high-$T_c$ superconductor as

$$
n = \frac{m^*kT}{\pi \hbar^2} \exp \left[ \frac{E_F - E_I}{kT} \right].
$$

(6)
This concentration is expressed in term of ionization energy and $k$ is the Boltzmann constant. $m^*_e$ is the effective electron mass and $E_F$ is the Fermi level. It is well known that the scattering among Fermions gives $1/\tau \propto T^2$ and $\rho \propto T^2$ from the empirical rule [2,3,4]. According to the elementary metal theory, the resistivity of metal is given by $\rho = \frac{m^*_e}{e^2}\tau$ where $e$ and $\tau$ are the electron’s charge and the mean scattering free time, respectively [3]. Therefore, the phenomenological model of c-axis normal state resistivity can be written in the form

$$\rho_c(T, E_f) = A \frac{\pi \hbar^2}{e^2 k^2} T \exp \left[ \frac{E_f - E_{F_c}}{kT} \right], \quad (7)$$

Where $A$ is independent of temperature. This model is comparable with the form given in Ref. [4] where in the exponential term, the gap, $\delta$ is used instead of the term $(E_f - E_{F_c})$ as an anomalous constraint of c-axis hopping rate between Cu-O$_2$ layers. It shows that this exponential term has a similar meaning to this gap.

3. Discussion

The experimental $\rho_c$ plots of doping dependent Bi2212 and Y123 single crystals were best fitted quantitatively with the phenomenological model (7). The Bi2212 samples, 1a and 1b were annealed at 10 and 10$^{-3}$ atm respectively to control the oxygen content [4]. In contrast, all the Y123 samples have the same composition, which is YBa$_2$Cu$_3$O$_7$, except for the volume of the unit cell which are 630 $\times$ 640 $\times$ 75 and 390 $\times$ 400 $\times$ 25 $\mu$m$^3$ for samples B and C respectively [9].

The experimental plots and the calculated curves of $\rho_c(T, E_f)$ versus $T$ for Bi2212 are shown in Fig. 1a and b. Both the experimental and the calculated plot in Fig. 1a can be separated into two regions: (i) $E_f - E_{F_c}$ (110K) < $kT$ (metallic-like behavior at $T$ > 110K) and (ii) $E_f - E_{F_c}$ (110k) > $kT$ (semiconductor-like behavior at $T$ < 110K). That is, $\rho_c(T, E_f)$ property changes from metallic-like behavior at high temperatures to semiconductor behavior at low temperatures. $\rho_c \propto \rho_{ab}$, suggesting that scattering or fluctuations in the Cu-O$_2$ planes may dominate the linear term of $\rho_c$ [3,4]. In addition, the thermal energy, $kT$ is higher than the constraint, $E_f - E_{F_c}$ above 110K which give rise to the conductivity of tunnelling electrons. At low temperatures however, $\rho_c$ is incoherent and can be interpreted as an indication of a low thermal energy as $T$ goes below 110K.

Similarly, the experimental and the calculated resistivity curves for Y123 samples B and C as shown in Fig. 2a also indicates the same characteristics, where the metallic-like behavior occurs when $E_f - E_{F_c}$ (155.7K) < $kT$ for sample B and $E_f - E_{F_c}$ (139.8K) < $kT$ for sample C. The resistivity for both B and C increases with temperature at $T < 155.7$K and $T < 139.8$K respectively suggesting the semiconductor-like region starts below those temperatures. The calculated $\rho_{ab}$ from model (7) for samples B and C as shown in Fig. 2b were also in good agreement with the experimental data. However, the $E_f - E_{F_c}$ parameter has a much lower value as expected compared to $c$-axis which can be due to the low spin fluctuations in the Cu-O=2 planes. There is no significant differences in $A$ and $E_f - E_{F_c}$ parameters between sample B and C for both the $a-b$ plane and $c$-axis although the ratio $a/c$ differs in large magnitude, which are approximately 8 for B and 16 for C.

The resistivity transition from sample 1a to 1b as the O$_2$ content decreases in Bi$_2$Sr$_2$CaCu$_2$O$_y$ is due to the transition of $E_f - E_{F_c}$ (110K) < $kT_r$ to $E_f - E_{F_c}$ (390K) > $kT_r$. $T_r$ is the room temperature. Therefore, the concentration of electrons, $n$ between layers in sample 1b is small due to insufficient thermal energy since $kT_r$ < 390K. Table 1 lists $A$ and $E_f - E_{F_c}$ parameters in detail for the calculated curves. In the $\rho(T)$ transition estimation, Ti-Sr-(Y$_{1-f}$X$_f$)-Cu-O system is considered for an example where the average $E_f$ for X$^{2+}$ and Y$^{A+}$ ions in that system can be calculated using

$$E_f[X^{z+}] = \sum_{i=1}^{z} \frac{E_{fi}}{z} \quad (8)$$

and

$$E_f[Y^{A+}] = \sum_{i=1}^{A} \frac{E_{fi}}{A}. \quad (9)$$

$i = 1, 2,...z$ and $i = 1, 2,...A$. $z^+$ and $A^+$ is the valence state of X and Y respectively. If $E_f[X^{z+}] < E_f[Y^{A+}]$ then the substitution of Y with X will reduce $E_f - E_{F_c}$ parameter thus, reduces $\rho_c(T)$ as the curves in Fig. 3 shows. Furthermore, the $\rho_c(T)$ rises rapidly with $E_f - E_{F_c}$ for 100K compared to 300K due to the low tunnelling electron’s concentration. This figure also reveals that the room temperature c-axis resistivity increases exponentially with the systematic substitution of different valence state ions. Table 2 summaries the estimated $\rho(T)$ for single and double substituted polycrystalline high-$T_c$ of pure 1212 phase superconductors. Substitution of Sr$^{2+}$, Er$^{3+}$, Pr$^{3+}$ and Y$^{3+}$ with Ba$^{2+}$, Sr$^{2+}$, Sr$^{2+}$ and Ca$^{2+}$ respectively reduces $\rho(T)$ since the ionization energies of the latter is lower than the former. On the other hand, the substitution of Sr$^{2+}$ with Tm$^{2+}$, Sm$^{2+}$, Eu$^{2+}$ and Dy$^{2+}$ increases $E_f$ hence, $\rho(T)$, therefore the metallic to semiconductor-like transition can be expected and vice versa for the former. Here, $\rho_c(T)$ is assumed to be roughly $\rho(T)$ due to polycrystallinity of the samples.
Figure 1: Temperature dependence of the $c$-axis resistivities of Bi2212 single crystals annealed at a) 10 and b) $10^{-3}$ atm.

Figure 2: Experimental (dotted) and calculated (solid line) plots for YBa$_2$Cu$_2$O$_7$ single crystals. a) $c$-axis and b) $a-b$ plane resistivities.

4. Conclusions

Ionization energy has been used in the Fermi-Dirac statistics as an additional restrictive condition. The calculation for the tunnelling electron’s concentration was done by employing the two-dimensional Fermion characteristics. The proposed model (7) agrees well quantitatively with the experimental $\rho_c(T)$ of Bi2212 and Y123 single crystals and also predicts the resistivity will increase with the average ionization energy. In addition, both the experimental data of $\rho_c(T)$ and $\rho_{ab}(T)$ can be fitted with the proposed model. Besides that, the estimated $\rho(T)$ transition upon substitution of ions with larger or smaller ionization energies also agrees well with the pure 1212 phase polycrystals.

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| Samples | $A$ (ms\(^{-1}\) K\(^{-1}\)) | $E_{I-E_{F}}$ (J) |
|---------|----------------|----------------|
| 1a      | $1.4 \times 10^{-3}$ | 110 K          |
| 1b      | $6.117 \times 10^{-3}$ | 390 K          |
| $B_{ab}$| $5.707 \times 10^{-3}$ | 36.6 K         |
| $C_{ab}$| $4.636 \times 10^{-3}$ | 38.6 K         |
| $B_{c}$ | $2.12 \times 10^{-5}$  | 155.7 K        |
| $C_{c}$ | $2.832 \times 10^{-5}$  | 139.8 K        |
| System                                                                 | Average $E_1$ (KJ mol$^{-1}$)     | Estimated (Increasing $y$) 1212 | Experimental (Increasing $y$) 1212 |
|-----------------------------------------------------------------------|-----------------------------------|---------------------------------|-----------------------------------|
| $(Pb_{0.2}Cu_{0.8})(Sr_{1-y}Ba_y)_{2}YCu_2O_7$ [10]                  | $Sr^{2+}:807$, $Ba^{2+}:734$      | Decreasing $\rho(T)$            | Decreasing $\rho(T)$             |
| TlSr$_2$(Er$_{1-y}$Sr$_y$)Cu$_2$O$_7$ [11]                            | $Sr^{2+}:807$, $Er^{3+}:1315$     |                                 |                                   |
| TlSr$_2$(Pr$_{1-y}$Sr$_y$)Cu$_2$O$_7$ [12]                             | $Ca^{2+}:807$, $Pr^{3+}:1210$     |                                 |                                   |
| GaSr$_2$(Y$_{1-y}$Ca$_y$)Cu$_2$O$_7$ [13]                              | $Ca^{2+}:867$, $Y^{3+}:1260$      |                                 |                                   |
| TlSr$_2$(Tm$_{1-y}$Sr$_y$)Cu$_2$O$_7$ [14]                             | $Sr^{2+}:807$, $Tm^{2+}:880$      | Increasing $\rho(T)$            | Increasing $\rho(T)$             |
| TlSr$_2$(Sr$_{2-y}$Sm$_y$)Cu$_2$O$_7$ [15]                             | $Sr^{2+}:807$, $Sm^{3+}:1299$     |                                 |                                   |
| TlSr$_2$(Sr$_{2-y}$Eu$_y$)Cu$_2$O$_7$ [15]                              | $Sr^{2+}:807$, $Eu^{2+}:817$      |                                 |                                   |
| TlSr$_2$(Sr$_{2-y}$Dy$_y$)Cu$_2$O$_7$ [15]                              | $Sr^{2+}:807$, $Dy^{2+}:849$      |                                 |                                   |
