ONE-DIMENSIONAL HOPPING CONDUCTIVITY OF THE SPIN-LADDER $CaCu_2O_3$ SINGLE CRYSTALS

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Abstract

Resistivity, ρ, of the spin-ladder compound $CaCu_2O_3$ is investigated between $T \sim 130$–450 K. The ρ (T) data exhibit an activated dependence characterized by a nearest-neighbor hopping followed by a variable-range hopping (VRH) regime when T is decreased. The observed VRH conductivity on the low-temperature interval obeys the law $\ln \rho \sim T^{-3/4}$. This law can be explained and the correct matching of the characteristic energy and length scales can be found by treating $CaCu_2O_3$ as a three-dimensional array of quasi-one-dimensional electron crystals.

Spin-ladder compounds attracted much attention during recent years [1]. A typical compound, $SrCu_2O_3$ has a layered structure consisting of the linear Cu–O–Cu–O–rows ("legs") along the **b** direction and the short Cu–O–Cu "rungs" along the **a** direction, having a two-leg "ladder" structure within each layer in the (**a, b**) plane. Structure of $CaCu_2O_3$ is similar to $SrCu_2O_3$ but consists of the zigzag Cu_2O_3 chains (Cu and O atoms do not form a planar network) [1]. A strong magnetic interaction takes place along the leg, as well as the rungs, whereas the neighboring ladders are only weakly coupled. Therefore, spin-ladder compounds demonstrate interesting magnetic properties and are considered to be promising superconductive materials [1].

$CaCu_2O_3$ belonging to the ladder family, is not yet well studied. In this work a hopping conductivity of two single-crystalline $CaCu_2O_3$ samples, grown with the traveling solvent floating zone method, # 1 with **j** || **b** (along the leg) and # 2 with **j** || **a** (along the rungs) are investigated to obtain information about mechanism of the charge transfer in this material.

As can be seen from Fig. 1a the resistivity, ρ, exhibits strongly activated temperature dependence. The nearest-neighbor hopping (NNH) conductivity, $\rho(T) = \rho_{0n}\exp[E_a/(kT)]$, is observed on the high-temperature interval yielding the activation energy $E_a = 0.38$ eV and 0.40 eV for # 1 and # 2, respectively, as follows from Fig. 1b. The deviations from the NNH conductivity with lowering T are evident, too.

Therefore, the ρ (T) data have been analyzed also, first, with the d-dimensional ($d = 2, 3$) variable-range hopping (VRH) conductivity models, $\rho(T) = \rho_{0v} \exp[(T_0/T)^p]$, where T_0 is the characteristic VRH temperature and $p = 1/4$ and $1/3$ for the Mott-VRH conductivity

(non-interacting electrons, $d = 3$ and 2, respectively) or $p = 1/2$ for the Shklovskii-Efros (SE) VRH conductivity (a soft gap in the density of states, DOS, due to Coulomb interactions, $d = 2$ and 3) [3].

Approximations with the 3D Mott law, $\ln \rho \sim T^{-1/4}$ (Fig. 2a) or 2D Mott law (not shown) are rather poor, whereas the 2D or 3D SE-VRH law, $\ln \rho \sim T^{-1/2}$ (Fig. 2a, looks better).

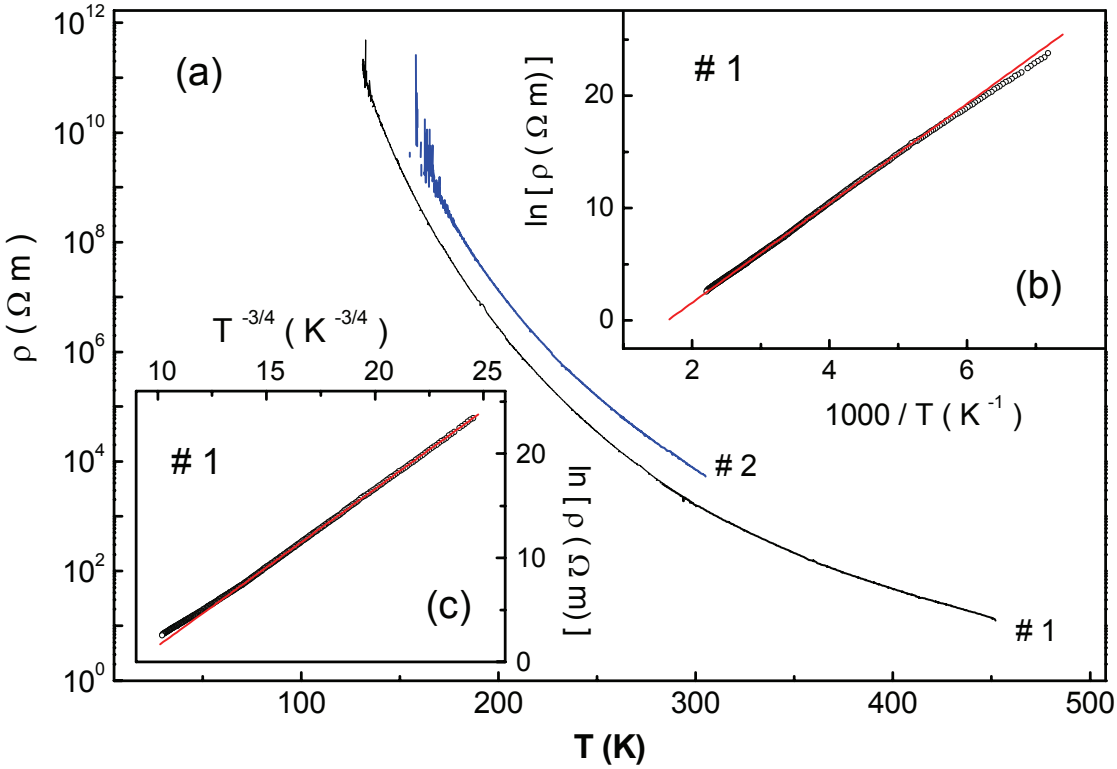

Fig. 1. The dependence of ρ on T (a) and the plots of ln ρ vs. T^{-1} (b) and ln ρ vs. $T^{-3/4}$ (c).

However, neither model with $d > 1$ can describe our ρ (T) data satisfactorily, taking into account the values of the typical energy and length scales. Indeed, from the explicit analysis with the Mott law we obtain the DOS width $\Delta E \approx 1.5 - 1.6$ eV ($d = 3$) or 1.1 eV ($d = 2$), exceeding considerably $E_a = 0.38 - 0.40$ eV, which contradicts the expected relation $\Delta E \approx E_a$. Applying the SE model we obtain the width of the Coulomb gap $\Delta_{CG} \approx 0.37 - 0.39$ eV $\approx E_a$, contradicting the expected relation $\Delta_{CG} < E_a$, and the unphysical value of the localization radius $\xi < 0.1$ Å.

Since in $CaCu_2O_3$ the electron transfer integral is strongly anisotropic, $t_{leg} : t_{rung} : t_{inter} \approx 5 : 2 : 1$ [2], the one-dimensional (1D) transport can be expected. Therefore, for the next we apply two 1D models for the analysis. Both of them predict the dependence of ρ (T) similar with that of the SE-VRH model, i. e. $\ln \rho \sim T^{-1/2}$, which can fit our data on the low-temperature interval (Fig. 2a). The first model proposed by Yu et al. [4] dealing with non-interacting electrons in isolated disordered 1D structures like macromolecules, yields the values of the 1D electron band $\Delta E \approx 0.38$ eV and 0.40 eV coinciding with E_a. However, for the localization radius we obtain the unrealistic value of $\xi \approx 0.3$ Å again.

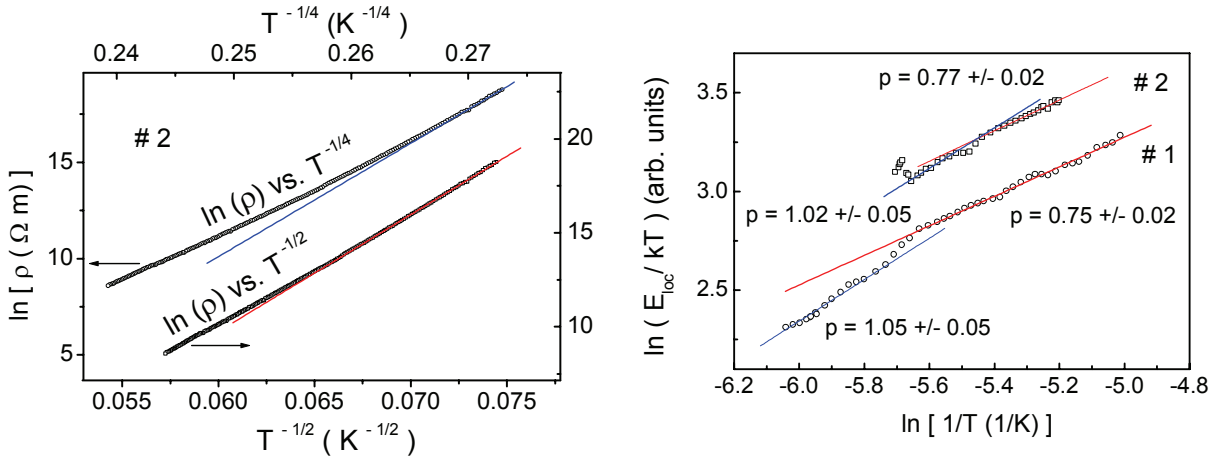

Fig. 2. The plots of ln ρ vs. $T^{-1/4}$ and ln ρ vs. $T^{-1/2}$ (a) and the temperature dependence of E_{loc} (b).

Serota et al. [5] proposed a percolation model of 1D VRH conductivity, which takes into account a finite length, L, of a 1D chain. No electron correlations have been suggested, as well. With this model we obtain $\xi \approx 1.4 - 1.7$ Å from the value of the characteristic VRH temperature contradicting drastically to $\xi \approx 5.6 - 6.8$ Å following from the onset temperature of the VRH conductivity. In addition, the values of $\Delta E \approx 0.75 - 0.80$ eV are much higher than E_a.

Hence, the 1D models [4, 5] above cannot explain our data, too. Another weak point showing their inapplicability is the explicit $\rho(T)$ dependence determined below. Analysis of the *local activation energy*, $E_{loc} \equiv d\ ln\ \rho\ /\ d\ (kT)^{-1}$ [3], can give the accurate value of p in the VRH conductivity law above, which can be presented as $\ln [E_{loc} / (kT)] = \ln p + p \ln T_0 + p \ln (1/T)$ (where the prefactor ρ_{0v} is taken constant). As can be seen from Fig. 2b, the value of $p \approx 1$ corresponds to the NNH conductivity on the high-temperature interval, in agreement with Fig. 1b, whereas on the low-temperature interval we have $p \approx 3/4$. Also Fig. 1c presents the best linearization of $\rho\ (T)$ in coordinates ln ρ, $T^{-3/4}$ (cf. Fig. 2a).

The law $\ln \rho \sim T^{-3/4}$ is the most important disagreement with the 1D models above [4, 5] which deal with the true 1D structures or single isolated 1D chains. Instead, in $CaCu_2O_3$ we have an array of quasi-1D chains, which fill in the 3D space of the crystal. This is just a case discussed by Fogler, Teber, and Shklovskii (FTS) [6]. The main idea of their approach is that they describe such structures as *the 3D array of quasi-1D electron crystals*. The 1D chains are divided by impurities into the segments (rods). The conductivity is metallic inside a rod, whereas hopping charge transfer sets in due to tunneling of the electrons between different rods along the same chain. At high T they found the conventional NNH conductivity. At low T the Coulomb interactions between the electrons and/or different rods in the transversal direction are important. The VRH conductivity law at low T depends on the dimensionality of hopping (tunneling) $d = 1$, 2, or 3 and on the character of the Coulomb interactions in the system, which governs the DOS, $g(\varepsilon)$, of charge excitations along the chains, having the form $g(\varepsilon) \sim |\varepsilon|^{\mu}$, where $\mu = 0$, 1, or 2. The general result of the FTS concept is that $p = (\mu + 1)/(\mu + d)$. Hence, for $d = 1$ and $\mu = 2$ we have $p = 3/4$, coinciding with the values of p found above from the analysis of the local activation energy (Fig. 2b). The law $g\ (\varepsilon) \sim \varepsilon^2$ means existence of the soft parabolic Coulomb gap Δ near the Fermi energy, like, e.g., in the 3D doped semiconductors [3]. Within the FTS model we obtain the values of $\Delta_{CG} \approx 0.26$ eV and 0.27 eV; this means that the Coulomb gap lies entirely inside the electron band $\Delta E \approx E_a =$

0.38 eV and 0.40 eV for # 1 and # 2, respectively, and the contradictions like those arising from applications of the 3D and 2D Mott and SE VRH conductivity models (see above), in the FTS model do not exist. Also the correct matching of the length scales can be found within the FTS model [6].

To conclude, the hopping conductivity of the spin-ladder $CaCu_2O_3$ has been investigated, exhibiting behavior typical of a 3D array of the quasi-1D electron crystals.

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