Hopping conductivity of lightly doped compounds of the La_2CuO_4 type caused by scattering on magnons

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(Submitted 15 April 1992)
Zh. Eksp. Teor. Fiz. **102**, 1872–1881 (December 1992)

We study the two-dimensional hopping electrical conductivity caused by electron transitions between impurity states (with allowance for the presence of magnons) in lightly doped quasi-two-dimensional antiferromagnets of the La_2CuO_4 type. The probabilities of the respective elemental transitions are calculated and the temperature dependence of the hopping conductivity in various regions is established. We show that at temperatures determined by the widths of gaps in the magnon spectrum there must be a jump in the otherwise smooth variation in conductivity.

1. In connection with the problem of high-T_c superconductivity, quasi-two-dimensional systems (in the sense of their electronic and magnetic properties) have lately been widely studied. An important and interesting class of such systems consists of compounds of the La_2CuO_4 type, where the transition to the superconducting phase takes place either owing to doping by ions of bivalent elements (e.g., Ba^{2+} and Sn^{2+}) or owing to an excess of oxygen. Under light doping, so long as these compounds do not acquire superconducting properties, they are semiconducting and, being quasi-two-dimensional, conduct in the basal CuO_2 planes (see Refs. 1–3).

It is usually assumed that at low temperatures the conductivity of doped semiconductors is of a hopping nature and is related to transitions between impurity electronic states accompanied by emission or absorption of phonons. A distinctive feature of lightly doped La_2CuO_4 compounds is that at low temperatures they are quasi-two-dimensional antiferromagnets with a fairly large coupling constant $\mathcal{J}$ of the exchange interaction (on the order of 10^3 cm^{-1}) inside the plane.[1–3] Since $\mathcal{J}$ exceeds the characteristic (Debye) energy, one should expect that the main role in the hopping conductivity for such compounds is played by transitions accompanied by absorption and emission of magnons rather than of phonons. The present paper examines the two-dimensional hopping electrical conductivity caused by electron transitions between impurity states with the participation of magnons. We calculate the probabilities of the respective elementary transitions and determine the temperature dependence of the hopping conductivity in various regions. For one thing, we show that there must be jump-like variations of conductivity at temperatures determined by the widths of gaps in the magnon spectrum.

2. Current thinking views[4,5] conductivity in doped La_2CuO_4 compounds as being of a quasi-two-dimensional hole nature and taking place via oxygen ions in the basal plane (with small overlap integrals of the planes). Under light doping the holes are localized mainly at the oxygen ions in the neighborhood of impurity centers. A pure La_2CuO_4 crystal constitutes an antiferromagnet with a Néel temperature T_N of order $\mathcal{J}/\ln(J/\Delta)$, where $\Delta \ll \mathcal{J}$ is a quantity linked to the magnetic anisotropy in the basal plane resulting, as Bar'yakhtar, Loktev, and Yablonskiĭ have shown,[3] from a slight turning of the oxygen octahedrons near an ion. Under doping the Néel temperature lowers (Δ decreases) and at a certain impurity concentration the long-range magnetic order disappears in the entire temperature range. Below we consider such impurity concentrations at which the long-range magnetic order is retained in the system at $T = 0$.

The Hamiltonian describing the electron and magnon subsystems and their interaction can be written as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{imp} + \mathcal{H}_{mag} + \mathcal{H}_{int},$$

$$\mathcal{H}_0 = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}\sigma} a^+_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}, \tag{1}$$

where the Hamiltonian $\mathcal{H}_0$ describes the behavior of an unperturbed conductivity carrier (hole) in the band, where $\varepsilon_{\mathbf{k}}$ is the energy of this carrier with a wave vector k, $a^+_{\mathbf{k}\sigma}$ and $a_{\mathbf{k}\sigma}$ are the creation and annihilation operators, σ is the spin index, and $\mathcal{H}_{imp}$ and $\mathcal{H}_{mag}$ are the Hamiltonians of the impurity and magnetic subsystems, respectively. The last term in (1), H_{int}, describes the electron-magnon interaction, which we select in the form of the Shubin–Vonsovskiĭ *p-d* exchange electron-magnon interaction:[6]

$$\mathcal{H}_{int} = \mathcal{J} \sum_{\mathbf{l}} \sum_{\Delta} I_{\mathbf{l}} S_{\mathbf{l}+\Delta}, \tag{2}$$

where the vectors $\mathbf{l}$ indicate the sites where a hole can be localized, $I_{\mathbf{l}}$ is the hole spin operator, $S_{\mathbf{l}+\Delta}$ the copper spin operator, $\mathbf{l}+\Delta$ the sites in the copper sublattice closest to the oxygen site $\mathbf{l}$ ($\Delta = 1,2$), and J the coupling constant of the exchange interaction of an impurity with the matrix. The positions of copper and oxygen atoms in the CuO_2 plane and the direction of magnetization are shown in Fig. 1 (in what follows we assume that $|\mathbf{a}| = |\mathbf{b}|$ and $\mathbf{a} \perp \mathbf{b}$ hold with a fairly high accuracy).

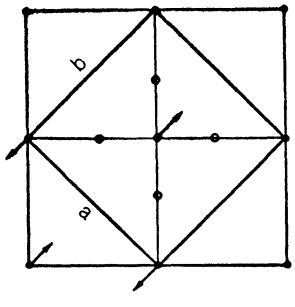

FIG. 1. Positions of copper and oxygen atoms in the basal CuO_2 plane (the ● stands for copper atoms, with the arrow denoting the direction of spin, and the O for oxygen atoms).

 0038-5646/92/121008-05$05.00

We write the Hamiltonian describing the unperturbed magnetic system as

$$\mathcal{H}_{mag} = J\sum_{\mathbf{m},\delta} S_{\mathbf{m}}S_{\mathbf{m}+\delta} - \Delta J_2 \sum_{\mathbf{m},\delta} S_{\mathbf{m}}^{y}S_{\mathbf{m}+\delta}^{y} - \Delta J_1 \sum_{\mathbf{m},\delta} S_{\mathbf{m}}^{x}S_{\mathbf{m}+\delta}^{x}, \quad J>0,$$
$$J \gg \Delta J_1, \Delta J_2 \tag{3}$$

with $J>0$, $J\gg\Delta J_1$, and $J\gg\Delta J_2$. Here $\mathbf{m}$ denote the sites of the copper sublattice, with $\mathbf{m}=\mathbf{n}j$, where $\mathbf{n}$ is the number of a magnetic cell and j the number of the sublattice; $\delta=1,\ldots,z$, with z the number of nearest neighbors in the plane; and ΔJ_1 and ΔJ_2 represent the anisotropic part of the exchange interaction, with $\Delta J_2>0$ corresponding to easy-plane anisotropy (with respect to the c_4 axis) and $\Delta J_1>0$ determining anisotropy in the basal plane. Although anisotropy in the plane is caused by the Dzyaloshinskiĭ antisymmetric exchange interaction, which is related to the slight turning of the oxygen octahedrons,[3] the observed spectrum of the antiferromagnet considered here can be obtained if one allows for the anisotropy of only the symmetric interaction, described by ΔJ_1 and ΔJ_2. The real La_2CuO_4 system is a four-sublattice antiferromagnet, but, since in what follows we do not take into account weak interplanar interactions and we consider the conductivity inside a plane, it is sufficient to allow for only two magnetic sublattices in each plane, that is, $j=1,2$.

We move on to magnon operators in Eq. (3) via the Holstein–Primakoff transformation

$$s_{n1}^{-} = (2S)^{1/2}a_n^{+}\left(1-\frac{a_n^{+}a_n}{2S}\right)^{1/2},$$
$$s_{n2}^{-} = (2S)^{1/2}\left(1-\frac{b_n^{+}b_n}{2S}\right)^{1/2} b_n, \tag{4}$$

where the operator a_n refers to the spin in sublattice *1* and b_n to the spin in sublattice *2*, and S is the atomic spin.

Next we introduce the spin-wave operators for the first and second sublattices:

$$c_{\mathbf{q}} = \frac{1}{N^{1/2}}\sum_{\mathbf{n}} e^{i\mathbf{q}\mathbf{n}}a_{\mathbf{n}}, \qquad d_{\mathbf{q}} = \frac{1}{N^{1/2}}\sum_{\mathbf{n}} e^{-i\mathbf{q}\mathbf{n}}b_{\mathbf{n}},$$

where $\mathbf{q}$ is the magnon wave vector, and N the number of magnetic cells in the crystal.

The Hamiltonian $\mathcal{H}_{mag}$ is diagonalized by the operators $\alpha_{\mathbf{q}}$ and $\beta_{\mathbf{q}}$:

$$\mathcal{H}_{mag} = \sum_{\mathbf{q}} (\varepsilon_{\alpha\mathbf{q}}\alpha_{\mathbf{q}}^{+}\alpha_{\mathbf{q}} + \varepsilon_{\beta\mathbf{q}}\beta_{\mathbf{q}}^{+}\beta_{\mathbf{q}}),$$

where $\alpha_{\mathbf{q}}$ and $\beta_{\mathbf{q}}$ are related to the operators $c_{\mathbf{q}}$ and $d_{\mathbf{q}}$ through the well-known u-v transformations (see, e.g., Refs. 7–9):

$$c_{\mathbf{q}} = u_{1\mathbf{q}}\beta_{\mathbf{q}} + v_{1\mathbf{q}}\beta_{-\mathbf{q}}^{+} + u_{2\mathbf{q}}\alpha_{\mathbf{q}} + v_{2\mathbf{q}}\alpha_{-\mathbf{q}}^{+},$$
$$d_{\mathbf{q}} = -u_{1\mathbf{q}}\beta_{\mathbf{q}} - v_{1\mathbf{q}}\beta_{\mathbf{q}}^{+} + u_{2\mathbf{q}}\alpha_{-\mathbf{q}} + v_{2\mathbf{q}}\alpha_{\mathbf{q}}^{+}. \tag{5}$$

The transformation coefficients and the frequency spectrum are

$$u_{1\mathbf{q}} = \frac{1}{2\omega_\beta^{1/2}}(A_0+D_{\mathbf{q}}+\omega_\beta)^{1/2}, \qquad u_{2\mathbf{q}} = -\frac{1}{2\omega_\alpha^{1/2}}(A_0-D_{\mathbf{q}}+\omega_\alpha)^{1/2},$$
$$v_{1\mathbf{q}} = \frac{1}{2\omega_\beta^{1/2}}(A_0+D_{\mathbf{q}}-\omega_\beta)^{1/2}, \qquad v_{2\mathbf{q}} = \frac{1}{2\omega_\alpha^{1/2}}(A_0-D_{\mathbf{q}}-\omega_\alpha)^{1/2},$$
$$\omega_\alpha = [(A_0-D_{\mathbf{q}})^2-(A_{\mathbf{q}}-B_{\mathbf{q}})^2]^{1/2},$$
$$\omega_\beta = [(A_0+D_{\mathbf{q}})^2-(A_{\mathbf{q}}-B_{\mathbf{q}})^2]^{1/2}, \tag{6}$$

where

$$A_{\mathbf{q}} = \frac{1}{\hbar}2JSz\gamma_{\mathbf{q}}, \qquad B_{\mathbf{q}} = 2Sz\frac{\Delta J_1+\Delta J_2}{2},$$
$$D_{\mathbf{q}} = 2Sz\frac{\Delta J_1-\Delta J_2}{2} < 0, \qquad A_0 = 2JSz,$$
$$\gamma_{\mathbf{q}} = \frac{1}{z}\sum_{\delta} e^{i\mathbf{q}\delta} = -\gamma_{-\mathbf{q}}.$$

Since $D_{\mathbf{q}}$ is negative, ω_β is the lowest branch.

3. In studying the electron subsystem, we note that although in compounds of the La_2CuO_4 type one impurity atom perturbs several oxygen sites, below for the sake of simplicity, we employ a model in which an impurity perturbs only one site. Then the Hamiltonian $\mathcal{H}_0+\mathcal{H}_{imp}=\mathcal{H}_{el}$ assumes the form

$$\mathcal{H}_{el} = \sum_{\mathbf{k},\sigma}\varepsilon_{\mathbf{k}}a_{\mathbf{k}\sigma}^{+}a_{\mathbf{k}\sigma} + \sum_{\mathbf{p},\sigma} V_{\mathbf{p}}b_{\mathbf{p}\sigma}^{+}b_{\mathbf{p}\sigma}, \tag{7}$$

where

$$b_{l\sigma} = \frac{1}{N^{1/2}}\sum_{\mathbf{k}} a_{\mathbf{k}\sigma}e^{i\mathbf{k}\mathbf{l}}, \tag{8}$$

$\mathbf{p}$ is the oxygen site closest to the impurity, and $V_{\mathbf{p}}$ the perturbation at site $\mathbf{p}$.

Besides expanding the carrier operator in the site representation, $b_{l\sigma}$, in the electron operators of the unperturbed crystal, as was done in Eq. (8), we can also expand such operators in impurity states and the states of the continuous spectrum $\tilde{\mathbf{k}}$ perturbed by the presence of an impurity. In the simplest case, where the impurity concentration is low and the impurities affect each other very little, such an expansion can be written as

$$b_{l\sigma} = \sum_{\tilde{\mathbf{p}}} c_{l\tilde{\mathbf{p}}}a_{\tilde{\mathbf{p}}\sigma} + \sum_{\tilde{\mathbf{k}}} c_{l\tilde{\mathbf{k}}}a_{\tilde{\mathbf{k}}\sigma}, \tag{9}$$

where $\tilde{\mathbf{p}}$ defines the impurity state related to the perturbation at the impurity site $\mathbf{p}$, and $a_{\tilde{\mathbf{p}}\sigma}$ is the operator of the respective state. In the single-impurity approximation the expression for $c_{l\tilde{\mathbf{p}}}$ has the form[9]

$$c_{l\tilde{\mathbf{p}}} = \mathcal{G}_{l\mathbf{p}}\Big/\Big(\sum_{\mathbf{l}}|\mathcal{G}_{l\mathbf{p}}|^2\Big)^{1/2}, \tag{10}$$

where

$$\mathcal{G}_{l\mathbf{p}} = \frac{1}{4N}\sum_{\mathbf{k}}\frac{\exp\{i(\mathbf{l}-\mathbf{p})\mathbf{k}\}}{\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{k}}} \tag{11}$$

with $\varepsilon_{\tilde{\mathbf{p}}}<0$ being the impurity-center energy defined by the equation

$$1-V_{\mathbf{p}}\mathcal{G}_{00}(\varepsilon_{\mathbf{p}})=0, \qquad \mathcal{G}_{00}=\mathcal{G}_{\mathbf{p}\mathbf{p}}. \tag{12}$$

The vector $\mathbf{k}$ in Eq. (11) is defined in the reciprocal space corresponding to the sites of the oxygen lattice in which the number of cells is $4N$, with N the number of magnetic cells. In the reciprocal space we go over to the cell corresponding to vector $\mathbf{q}$, that is, the magnetic cell. Then we can write Eq. (11) as

$$\mathcal{G}_{\mathbf{l}} = \frac{1}{4N} \sum_{\mathbf{q},\lambda} \frac{\exp\{i(\mathbf{q}+\mathbf{Q}_\lambda)\mathbf{r}_{\mathbf{l}}\}}{\varepsilon - \varepsilon_{\mathbf{q}\lambda}}, \tag{13}$$

where $\lambda = 1,2,3,4$ numbers the four cells of the reciprocal magnetic space corresponding to a single reciprocal cell of the oxygen sublattice, and the $\mathbf{Q}_\lambda$ are the vectors in the reciprocal space that determine the positions of these cells. Among these four cells the cell singled out is the one for which $\mathbf{Q}_\lambda = 0$ and $\varepsilon_{\mathbf{q}\lambda} = \varepsilon_{\mathbf{k}}$, with $\varepsilon_{\mathbf{q}\lambda} \to 0$ as $\mathbf{q} \to 0$.

In what follows, when discussing conductivity we must allow for carrier hopping between a pair of impurity centers $\tilde{\mathbf{p}}$ and $\tilde{\mathbf{p}}_1$ separated by a large distance (greater than the impurity-state radius $\mathbf{r}_0$, with $r_0 \sim \sqrt{\hbar/\varepsilon_{\mathbf{p}}}$). Only two terms in Eq. (9) need to be retained to describe such hopping:

$$b_{\mathbf{l}\sigma}^{+} = c_{\mathbf{l}\tilde{\mathbf{p}}} a_{\tilde{\mathbf{p}}\sigma}^{+} + c_{\mathbf{l}\tilde{\mathbf{p}}_1} a_{\tilde{\mathbf{p}}_1\sigma}^{+}.$$

One must allow, however, for the effect of states $\tilde{\mathbf{p}}$ and $\tilde{\mathbf{p}}_1$ on each other, which must lead to the renormalization of the constants $c_{\mathbf{l}\tilde{\mathbf{p}}}$ and $c_{\mathbf{l}\tilde{\mathbf{p}}_1}$. Within the framework of the Hamiltonian (7), the interaction of impurity states takes place through states of the continuous spectrum. As a result the coefficient $c_{\mathbf{l}\tilde{\mathbf{p}}}$, for instance, assumes the form

$$c_{\mathbf{l}\tilde{\mathbf{p}}} = \frac{1}{\left(\sum_{\mathbf{l}} |\mathcal{G}_{\mathbf{lp}}|^2\right)^{1/2}} \left(\mathcal{G}_{\mathbf{lp}} + \mathcal{G}_{\mathbf{lp}_1}\mathcal{G}_{\mathbf{p}_1\mathbf{p}} \frac{V_{\mathbf{p}_1}}{(V_{\mathbf{p}} - V_{\mathbf{p}_1})\mathcal{G}_{00}}\right). \tag{14}$$

Here we have allowed only for pair interaction between centers $\tilde{\mathbf{p}}$ and $\tilde{\mathbf{p}}_1$ and ignored the interaction through intermediate impurity centers. This is possible only if

$$cr_0^3/a^3 \ll 1. \tag{15}$$

where c is the impurity center concentration, and a is the Bohr radius of a center.

We have also allowed for the fact that the spread of impurity centers in a crystal due to various imperfections of the crystal is fairly broad and exceeds the spread due to the resonant interaction between impurity states, that is,

$$(\mathcal{G}_{\mathbf{pp}_1} V_{\mathbf{p}_1} V_{\mathbf{p}} \mathcal{G}_{\mathbf{pp}_1})/\mathcal{G}_{00}(V_{\mathbf{p}} - V_{\mathbf{p}_1}) \ll 1 \tag{16}$$

for the majority of centers. As a result, the second term on the right-hand side of (13) proves to be smaller than the first (in what follows, however, the second term plays an important role).

Now we consider the interaction operator $\mathcal{H}_{\text{int}}$ specified by Eq. (2). We assume that carriers have a small effect on the magnetic subsystem, so that the latter can be described in the neighborhood of an impurity atom by an expansion in the magnon operators of the unperturbed crystal. Here, since the carriers are between two copper atoms belonging to two different magnetic sublattices, the zeroth-order terms in the magnon operators vanish (if we ignore the slight turn of the magnetic sublattice resulting from the Dzyaloshinskiĭ interaction). In what follows we retain only the terms that are linear in magnetic operators, in terms of which the operators s_{nj}^{-} and s_{nj}^{+} are expressed. Then

$$H_{\text{int}} = \mathcal{J}\left(\frac{2S}{N}\right)^{1/2} \sum_{\mathbf{q}} \sum_{\mathbf{n}} e^{i\mathbf{qn}} \sum_{\nu} I_{\mathbf{n}\nu}^{+}(c_{\mathbf{q}}^{+} + e^{i\mathbf{qt}_\nu} d_{\mathbf{q}}) + \text{H.c.}, \tag{17}$$

where $\mathbf{t}_\nu$ is the radius vector of the νth oxygen atom in a magnetic cell ($\mathbf{t}_1 = 0$, $\mathbf{t}_2 = \mathbf{a}$, $\mathbf{t}_3 = \mathbf{a} + \mathbf{b}$, and $\mathbf{t}_4 = \mathbf{b}$).

Next, allowing for the fact that the carrier spin satisfies $\sigma = 1/2$, we can write the spin operator $I_{\mathbf{n}\nu}^{+}$ in the form

$$I_{\mathbf{n}\nu}^{+} = I_{\mathbf{l}}^{+} = b_{\mathbf{l}\uparrow}^{+} b_{\mathbf{l}\downarrow}. \quad \mathbf{l} = \mathbf{n} + \mathbf{t}_\nu.$$

Finally, substituting (8) and (14) into Eq. (17), we obtain the electron-magnon interaction operator in which the small term that is the product of the second terms in (14) is discarded:

$$\begin{aligned}
\mathcal{H}_{\text{int}}^{(\tilde{\mathbf{p}}\downarrow \to \mathbf{p}_1\uparrow)} = {} & \mathcal{J}\left(\frac{2S}{N}\right)^{1/2} \frac{1}{\sum_{\mathbf{l}} |\mathcal{G}_{\mathbf{lp}}|^2} \\
& \times \sum_{\mathbf{q}} \sum_{\nu} [(u_{1\mathbf{q}} - e^{i\mathbf{qt}_\nu} v_{1\mathbf{q}}) \beta_{\mathbf{q}}^{+} \\
& + (v_{1\mathbf{q}} - e^{i\mathbf{qt}_\nu} u_{1\mathbf{q}}) \beta_{-\mathbf{q}} + (u_{2\mathbf{q}} + e^{i\mathbf{qt}_\nu} v_{2\mathbf{q}}) \alpha_{\mathbf{q}}^{+} \\
& + (v_{2\mathbf{q}} + e^{i\mathbf{qt}_\nu} u_{2\mathbf{q}}) \alpha_{-\mathbf{q}}] \\
& \times \{Y(\nu, \mathbf{p}_1, \mathbf{p}, \mathbf{q}) + \frac{\mathcal{G}_{\mathbf{pp}_1}}{(V_{\mathbf{p}} - V_{\mathbf{p}_1}) J_0} [Y(\nu, \mathbf{p}_1, \mathbf{p}, \mathbf{q}) V_{\mathbf{p}_1} \\
& - Y(\nu, \mathbf{p}, \mathbf{p}, \mathbf{q}) V_{\mathbf{p}}]\} a_{\mathbf{p}_1\uparrow}^{+} a_{\mathbf{p}\downarrow},
\end{aligned} \tag{18}$$

where

$$Y(\nu, \mathbf{p}_1, \mathbf{p}, \mathbf{q}) = \sum_{n} e^{i\mathbf{qn}} \mathcal{G}_{\mathbf{n}\nu\mathbf{p}_1} \mathcal{G}_{\mathbf{n}\nu\mathbf{p}}. \tag{19}$$

Substituting Eq. (11) into Eq. (19) yields

$$\begin{aligned}
Y(\nu, \mathbf{p}_1, \mathbf{p}, \mathbf{q}) = {} & \sum_{n} e^{i\mathbf{qn}} \frac{1}{16N^2} \sum_{\mathbf{k}\mathbf{k}_1} \\
& \frac{\exp\{i(\mathbf{n}+\boldsymbol{\nu}-\mathbf{p}_1)(\mathbf{k}_1+\mathbf{Q}_{\lambda_1})\}}{\varepsilon - \varepsilon_{\mathbf{k}_1\lambda_1}} \frac{\exp\{i(\mathbf{n}+\boldsymbol{\nu}-\mathbf{p})(\mathbf{k}+\mathbf{Q}_\lambda)\}}{\varepsilon - \varepsilon_{\mathbf{k}\lambda}} \\
\approx {} & \exp\{-i\boldsymbol{\nu}\mathbf{q} + i\mathbf{p}_1\mathbf{q}\}\chi,
\end{aligned} \tag{20}$$

$$\chi \equiv \frac{1}{16N^2} \sum_{\mathbf{k}} \frac{\exp\{i(\mathbf{p}_1 - \mathbf{p})\mathbf{k}\}}{(\varepsilon - \varepsilon_{\mathbf{k}+\mathbf{q}})(\varepsilon - \varepsilon_{\mathbf{k}})}.$$

Terms with $\lambda \neq 0$ and $\lambda_1 \neq 0$, which are small compared to the other terms, have been discarded. Combining (20) with (18), we finally get

$$\begin{aligned}
\mathcal{H}_{\text{int}}^{(\tilde{\mathbf{p}}\downarrow \to \tilde{\mathbf{p}}_1\uparrow)} = {} & \mathcal{J}\left(\frac{2S}{N}\right)^{1/2} \left(\sum_{\mathbf{l}} |\mathcal{G}_{\mathbf{lp}}|^2\right)^{-1} \sum_{\mathbf{q}} e^{i\mathbf{p}_1\mathbf{q}} \\
& \times \sum_{\nu} (u_{1\mathbf{q}} - e^{i\mathbf{qt}_\nu} v_{1\mathbf{q}}) \beta_{\mathbf{q}}^{+} \\
& + (v_{1\mathbf{q}} - e^{i\mathbf{qt}_\nu} u_{1\mathbf{q}}) \beta_{-\mathbf{q}} + (u_{2\mathbf{q}} + e^{i\mathbf{qt}_\nu} v_{2\mathbf{q}}) \alpha_{\mathbf{q}}^{+} \\
& + (v_{2\mathbf{q}} + e^{i\mathbf{qt}_\nu} u_{2\mathbf{q}}) \alpha_{-\mathbf{q}} e^{-i\nu\mathbf{q}} \\
& \times \Big| \chi(\mathbf{p} - \mathbf{p}_1, \mathbf{q}) - \chi(0, \mathbf{q}) \mathcal{G}_{\mathbf{pp}_1} \\
& \times \frac{\exp\{i(\mathbf{p} - \mathbf{p}_1)\mathbf{q}\} V_{\mathbf{p}} - V_{\mathbf{p}_1}}{\mathcal{G}_0 (V_{\mathbf{p}} - V_{\mathbf{p}_1})} \Big\} a_{\mathbf{p}_1\uparrow}^{+} a_{\mathbf{p}\downarrow}.
\end{aligned} \tag{21}$$

4. The probability of carrier hopping accompanied by the creation of a magnon is

$$w^{(p\downarrow\to p_1\uparrow)}=\frac{2\pi}{\hbar}\mathcal{J}^2(2S)\chi^{-2}(0,\mathbf{q})\frac{1}{N}\sum_{\mathbf{q}}\{X^2+Y^2$$
$$+2XY\cos[(\mathbf{p}-\mathbf{p}_1,\mathbf{q})]\}\mathcal{L}_{q\beta}(n_{q\beta}+1)\delta(\varepsilon_{pp_1}-\varepsilon_{q\beta})$$
$$+\mathcal{L}_{q\alpha}(n_{q\alpha}+1)\delta(\varepsilon_{pp_1}-\varepsilon_{q\alpha}), \qquad (22)$$

where

$$\varepsilon_{pp_1}=\varepsilon_p-\varepsilon_{p_1},$$
$$X=\chi(\mathbf{p}_1-\mathbf{p},\mathbf{q})+\chi(0,\mathbf{q})\frac{V_{p_1}\mathcal{G}_{pp_1}}{\mathcal{G}_0(V_p-V_{p_1})},$$
$$Y=-\chi(0,\mathbf{q})\frac{V_p\mathcal{G}_{pp_1}}{\mathcal{G}_0(V_p-V_{p_1})}, \qquad (23)$$
$$\mathcal{L}_{q\beta}=\left|\sum_\nu(u_{1q}-e^{iqt_\nu}v_{1q})e^{-iv\mathbf{q}}\right|^2,$$
$$\mathcal{L}_{q\alpha}=\left|\sum_\nu(u_{2q}+e^{iqt_\nu}v_{2q})e^{iv\mathbf{q}}\right|^2.$$

When calculating the quantities in (22) and (23), we make certain simplifying assumptions. The magnon wave vector is assumed to be small in comparison with the characteristic wave vector of a carrier, or $|\mathbf{q}|\ll|\mathbf{k}_0|$ (here $k_0=1/r_0$, with $r_0=d/\alpha$ the radius of the electronic state), and the carrier dispersion law is assumed to be parabolic, or $\varepsilon(\mathbf{k})=\varepsilon_0(dk)^2$, where it is convenient to select d^2 as the area of a magnetic cell.

Since in the formula for χ in Eq. (20) the principal contribution is provided by the small-$\mathbf{k}$ region, summation over reciprocal magnetic cells can be replaced by integration over the entire $\mathbf{k}$-space. We then get

$$\chi(\mathbf{p}_1-\mathbf{p})\equiv\chi_1=\frac{1}{16(2\pi)^2}\frac{(p_1-p)/d}{\varepsilon_0^{3/2}(-\varepsilon_p)^{1/2}}K_1\left(\alpha\frac{p_1-p}{d}\right), \qquad (24)$$

with $\alpha=|\varepsilon_p|/\varepsilon_0$ and $K_1(x)$ a cylinder function, and

$$\chi(0)\equiv\chi_2=\sum_1|\mathcal{G}_{1p}|^2=\frac{1}{16\pi\varepsilon_0|\varepsilon_p|}. \qquad (25)$$

In the two-dimensional case considered here, $\mathcal{J}_{pp_1}$ in Eq. (14) has the form

$$\mathcal{G}_{pp_1}=\frac{1}{8\pi\varepsilon_0}K_0\left(\alpha\frac{p_1-p}{d}\right), \quad \frac{p_1-p}{d}\gg1, \qquad (26)$$

where $K_0(x)$ a modified Bessel function. An estimate of Y_{00} yields

$$\mathcal{G}_0=\mathcal{G}_{pp}\approx\mathcal{G}_{p_1p_1}|_{|p-p_1|\approx d}=\frac{1}{8\pi\varepsilon_0}\cdot\zeta,$$

where $\zeta\approx\ln(k_m/k_0)\gg1$, where $k_m/k_0\gg1$ and k_m is a quantity of the order of the maximum wave vector in the Brillouin zone.

When calculating the sum over ν (over oxygen sites) in (23), we assume $\mathbf{q}$ small and retain only the principal terms in the expansion. This yields, for instance, the following expression for $L_{q\beta}$:

$$\mathcal{L}_{q\beta}=\sum_{\nu,\nu'}\{(u_{1q}-v_{1q})^2+(\mathbf{q}t_\nu)(\mathbf{q}t_{\nu'})v_{1q}^2\}$$
$$=16(u_{1q}-v_{1q})^2+4v_{1q}^2(\mathbf{q}(\mathbf{a}+\mathbf{b}))^2. \qquad (27)$$

Assuming that B_q, $|D_q|\ll A_0,A_q$, we have the following expressions for u_{1q} and v_{1q}:

$$(u_{1q}-v_{1q})^2=\frac{\omega_{\beta q}}{A_0}, \quad v_{1q}^2=\left(\frac{A_0}{\omega_{\beta q}}-1\right), \quad \omega_{\beta q}^2=\omega_{0\beta}^2+\zeta q^2, \qquad (28)$$

$$\omega_{0\beta}^2=2A_0(B_0-D_0), \quad \zeta=\frac{A_0^2d^2}{2}, \quad B_0=B_{q=0}, \quad D_0=D_{q=0};$$

where $\omega_{0\beta}$ and $\omega_{0\alpha}$ are the cutoff frequencies in the spin excitation spectrum of the antiferromagnet.

Thus,

$$\mathcal{L}_{q\beta}\approx\frac{16}{A_0}\omega_{\beta q}+4\frac{A_0}{\omega_{\beta q}}(\mathbf{q}(\mathbf{a}+\mathbf{b}))^2. \qquad (29)$$

Combining Eqs. (24)–(29), we can transform (22) into

$$w^{(p\downarrow\to p_1\uparrow)}=4S\frac{\mathcal{J}^2}{\hbar^3A_0^2}\varepsilon_{pp_1}[n(\mathbf{q}_{0\beta})+1]\chi_2^{-2}\cdot$$
$$\times\left\{(X^2+Y^2)\left[\frac{8\varepsilon_{pp_1}}{A_0\hbar}+\frac{2A_0\hbar}{\varepsilon_{pp_1}}q_0^2|\mathbf{a}+\mathbf{b}|^2\right]\right.$$
$$+2XY\left[\frac{8\varepsilon_{pp_1}}{A_0\hbar}J_0(rq_{0\beta})+\frac{2A_0\hbar}{\varepsilon_{pp_1}}q_{0\beta}^2|\mathbf{a}+\mathbf{b}|^2\right]$$
$$\left.\times\left[\cos^2\varphi_0J_0(rq_{0\beta})+(\sin^2\varphi_0-\cos^2\varphi_0)\frac{1}{rq_{0\beta}}J_1(rq_{0\beta})\right]\right\}$$
$$\times\theta(\varepsilon_{pp_1}-\hbar\omega_{0\beta}), \qquad (30)$$

where $\mathbf{r}=\mathbf{p}-\mathbf{p}_1$, φ_0 is the angle between vectors $\mathbf{r}$ and $\mathbf{a}+\mathbf{b}$, $J_0(x)$ and $J_1(x)$ are the Bessel functions of the respective orders, $\theta(x)$ is the unit-step function (equal to 1 if $x>0$ and 0 if $x<0$), and

$$q_{0\beta}=\frac{2^{1/2}}{A_0d}\left[\frac{\varepsilon_{pp_1}^2}{\hbar^2}-\omega_{0\beta}^2\right]^{1/2}. \qquad (31)$$

For simplicity, only the expressions for the probability of carrier hopping with the participation of the lower branch of the magnon spectrum are given in (30) and (31).

Simpler results follow from Eq. (30) for $rq_{0i}\gg1$ and $rq_{0i}\ll1$, where $i=\alpha,\beta$; it is assumed that in these two limiting cases we have $r/r_0\gg1$.

Aside from this, at low temperatures, a range of extreme interest to the processes considered here, we can ignore the magnon occupation numbers. Then the probability of magnon-initiated carrier transitions between the localized states $\mathbf{p}$ and $\mathbf{p}_1$ is

$$w^{(p\downarrow\to p_1\uparrow)}=\frac{2S}{\pi^2}\frac{\mathcal{J}^2}{\hbar^4A_0^3}\varepsilon_{pp_1}^2\frac{r}{r_0}[(1-\delta_\beta)\theta(\varepsilon_{pp_1}-\hbar\omega_{0\beta})$$
$$+(1-\delta_\alpha)\theta(\varepsilon_{pp_1}-\hbar\omega_\alpha)]e^{-2r/r_0}, \quad \delta_i=\omega_{0i}^2\hbar^2/2\varepsilon_{pp_1}^2; \qquad (32)$$

with $\delta_i=\omega_{0i}^2\hbar^2/2\varepsilon_{pp_1}^2$, when $rq_{0i}\ll1$, and

$$w^{(p\downarrow\to p_1\uparrow)}=(z\nu_0)^2(2S)\frac{\mathcal{J}^2}{\hbar^4A_0^3}\varepsilon_p^2\frac{r_0}{r}[\theta(\varepsilon_{pp_1}-\hbar\omega_{0\beta})$$
$$+\theta(\varepsilon_{pp_1}-\hbar\omega_{0\alpha})]e^{-2r/r_0}, \qquad (33)$$

when $rq_{0i}\gg1$.

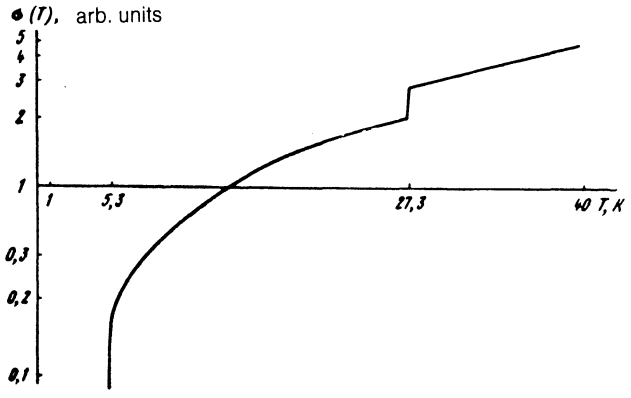

FIG. 2. The temperature dependence of conductivity ($T_0 = 100$ K, $\hbar\omega_{0\beta}/k = 14$ K, and $\hbar\omega_{0\alpha}/k = 42$ K).

5. At low temperatures the conductivity of this two-dimension La_2CuO_4 system with a low dopant concentration is of a hopping nature. The prevailing conductivity here is the one with varying hopping length. The respective expression for the specific resistance of two-dimensional systems, $\rho(T)$, has the form[10,11]

$$\rho(T) = \rho_0 \exp \zeta_c,$$
$$\zeta_c = (T_0/T)^{1/3},$$

where $T_0 = \beta/kg(\mu)r_0^2$, with $g(\mu)$ the density of states at the Fermi surface (depending on the impurity concentration and also caused by the spread in the impurity levels), and the numerical factor $\beta \approx 13.8$ within the framework of percolation theory.

According to Shklovskiĭ and Éfros,[11] the pre-exponential factor ρ_0 has the form $\rho_0 = L_0 R_0$, where

$$\rho_0 = (kT/e^2 w_c) L_0,$$
$$w_0 = w^{(p_i \to p_i')}|_{\varepsilon_{pp'} = \varepsilon_0,\ r=\bar{r}}; \qquad (34)$$
$$\varepsilon_0 = kT\zeta_c, \quad \bar{r} = r_0\zeta_c/2,$$

and L_0 is the characteristic correlation range. Estimates of L_0 yield $L_0 = r_0 \zeta_c^{1+\nu}$, with $\nu \approx 1.34$ the critical index of the correlation range.[12]

Noting that $r = \bar{r}$ and $\varepsilon_{pp'} = \varepsilon_0$ are given by (34), we find that the characteristic parameter $q_{0i}r$ determining the form of the expression for the transition probability [Eqs. (32) and (33)] is

$$q_{0i}\bar{r} \equiv x = \frac{1}{2^{1/3}A_0}\frac{r_0}{d}\zeta_c\left[\left(\frac{kT\zeta_c}{\hbar^2}\right)^2 - \omega_{0i}^2\right]^{1/3}, \quad i = \alpha, \beta.$$

with $i = \alpha,\beta$. Let us write the expression for ρ_0 in the two limiting cases in x:

$$\rho_0 = \frac{r_0 T_0^{(\nu-2)/3}}{e^2}\left\{\left[\frac{2S}{2\pi^2}\frac{\mathcal{J}^2}{\hbar^4}\frac{k}{A_0^3}\right]\sum_i \theta(y_i)(1-\delta_{0i})\right\}^{-1} T^{-(\nu+1)/3},$$
$$x \ll 1; \qquad y = kT\zeta_c - \hbar\omega_{0i}, \quad \delta_{0i} = \omega_{0i}^2\hbar^2/2\varepsilon_0^2; \qquad (35)$$

$$\rho_0 = \frac{r_0 T_0^{(\nu+2)/3}}{e^2}\left\{\left[(2\pi)^2 2S\frac{\mathcal{J}^2}{\hbar^4 k}\frac{\varepsilon_p^2}{A_0^3}\right] \times \sum_i \theta(y_i)(1-\delta_{0i})\right\}^{-1} T^{(1-\nu)/3}, \quad x \gg 1, \qquad (36)$$

with $y_i = kT\zeta_c - \hbar\omega_{0i}$ and $\delta_{0i} = \omega_{0i}^2\hbar^2/2\varepsilon_0^2$.

We see that the temperature dependence of the pre-exponential factor differs considerably in the limiting cases $x \ll 1$ and $x \gg 1$, but in both cases ρ_0 diminishes as T grows. We especially note that because of the unit-step functions in (35) and (36) ρ experiences two jumps at temperatures T_{0i} defined by

$$kT_{0i} = (\hbar\omega_{0i})^{1/3}/(kT_0)^{1/3}. \qquad (37)$$

Since near a jump $x \to 0$ holds, we must use Eq. (35) when studying the behavior of ρ_0 in this region. Since $\hbar\omega_{0i} \ll kT_0$, the temperature T_0 of the jump determined by (36) proves to be essentially smaller than the existing energy gap in the spectrum of the ferromagnet. The temperature dependence of σ obtained via Eq. (35) is depicted in Fig. 2.

This discussion and the resulting jump in conductivity are, of coures, idealized. In reality, owing to the spread in energy levels, even at temperatures below the jump there are states that lead to a finite value of conductivity. As a result, in the jump region one should observe a change in the temperature dependence of conductivity. Moreover, the resistance caused by carrier hopping with a fixed hopping length becomes essential. A detailed analysis of the transition from the temperature behavior of conductivity considered here to the one in the case of $T \lesssim T_{0i}$ requires special treatment.

Note that the characteristic variation in the temperature behavior of conductivity in La_2CuO_4 compounds in the low-temperature range and the transition from conductivity with a varying hopping length to conductivity of the activation type, which corresponds to a constant hopping length, have been observed in experiments,[13,14] and the transition temperature in such experiments is, apparently, commensurate with the temperature T_{0i} defined by Eq. (37), which corresponds to a higher branch of spin excitations.

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Translated by Eugene Yankovsky