Sign and temperature dependence of the Hall effect of $Bi_2Sr_2YCu_2O_8$ single crystals at compositions below that for metallic conduction

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LETTER TO THE EDITOR

Sign and temperature dependence of the Hall effect of $Bi_2Sr_2YCu_2O_8$ single crystals at compositions below that for metallic conduction

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Abstract. In $Ba_2Sr_2YCu_2O_8$ single crystals at compositions below that for metallic conduction, the electrical resistivity decreases with increasing temperature, while the Hall coefficient is temperature independent and of positive sign. These features are explained in terms of hopping of hole-like bipolarons in the CuO_2 planes.

In the cuprate superconductors at compositions below that for metallic conduction, it has been proposed that the preformed bosons due to holes in the oxygen 2p band are localized by disorder and move by thermally activated hopping [1]. Experimental data by Forro [2] on $Bi_2Sr_2YCuO_8$ single crystals gives a resistivity decreasing with increasing temperature, and a Hall coefficient R_H which is temperature independent and whose sign is positive. This is reminiscent of the behaviour of the p type amorphous chalcogenide glasses [3] As_2Te_3 and $As_2Se_xTe_{3-x}$ which show a mildly thermally activated Hall mobility, but with, however, an anomalous negative sign. In the present letter, we propose and explanation of both the normal sign and the temperature dependence of the Hall effect of $Bi_2Sr_2YCu_2O_8$ single crystals.

It was shown by Holstein [4] that the sign of the Hall effect for holes (missing electrons) relative to that for electrons in the same energy band, is given by the factor $(-1)^{n+1}$, where n is the number of sites in a closed path determined by the local site geometry and lattice structure. More completely, Emin [5] showed that the absolute sign of the Hall angle is given by

$$\mathrm{sgn}(\theta_H) = (\mathrm{sgn}(\epsilon)^{n+1}(-q)(-1)^n \prod_i J_{i,i+1}) \tag{1}$$

(The Hall angle is conventionally positive for electrons and negative for holes.) This explains the n-signed Hall effect in the As based chalcogenide glasses quoted above: specifically, $n = 3$ since the structure is composed of three-fold coordinated As atoms. Then with the product of transfer integrals having a negative sign, $J_{i,i+1}$ usually being negative, equation (1) predicts $\mathrm{sgn}(\theta_H) > 0$, a negatively signed Hall effect. Here, $(\epsilon)^{n+1} = +1$ with $\epsilon = -1$ corresponding to an unoccupied state (hole) and $q < 0$, since electrons are the bona fide charge carriers.

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In the present case, the CuO_2 planes are perfectly cubic and we have hole bipolarons moving about a four-site closed path; the Hall mobility of the small polaron for this case has been derived [6]. Here, the product of transfer integrals is positive regardless of the sign of J, $q < 0$ as above, and $(\epsilon)^{n+1} = -1$, so that $\mathrm{sgn}(\theta_H) < 0$; a normal p type Hall effect observed by Forro [2]. The normal sign would also be compatible with extended state motion, but the temperature dependence would not be; this is discussed below.

As stated above, the experimental data shows a thermally activated electrical conductivity, and a Hall coefficient which is temperature dependent. Now the electrical conductivity and the magnitude of the Hall coefficient are given by

$$\begin{aligned} \sigma &= pq\mu_c \\ |R_H| &= (1/p\,|\,q\,|)(\mu_H/\mu_c) \end{aligned} \tag{2}$$

where p is the carrier (bipolaron) concentration, $q = 2e$, and μ_c and μ_H are the conductivity (drift) and Hall mobilities, respectively. With these formulae we can consider alternative transport mechanisms. For the random-phase model [7] one would have temperature-independent mobilities but a thermally activated carrier concentration. In addition to the activated conductivity, this would also yield an activated Hall coefficient, contrary to the measured constant Hall coefficient [2]. Another possibility, suggested by Dr A S Alexandrov, is that the constant R_H is due to itinerant bipolarons, if the density of states at the mobility edge is sufficiently low that their number is essentially temperature independent, while the thermally activated resistivity is due to activated hopping in the localized regime; we do not think this dual possibility likely. Here we consider thermally activated hopping of bipolarons localized by disorder, and propose that the data can be explained by p being temperature independent and μ_c and μ_H having equal activations energies. We will now give physical arguments that this is physically plausible.

In the hopping regime, the site-jump events contributing to conduction or to the Hall effect require the energetic coincidence of two or more sites. Specifically, conduction requires the energetic coincidence of two sites, while the Hall effect requires the coincidence of three or four sites. For a single polaron, the local displacement coordinate of the initially occupied site is $x^{(0)}$ and the binding energy is E_b. For the two-site coincidence event, assuming an electron–lattice interaction which is linear in the local coordinate, the displacement of the initial site reduces to $(1/2)x^{(0)}$ and that of the final site increases to the same value. The elastic energy of each site in excess of E_b is $(1/4)E_b$, so that the two-site activation energy is $\epsilon_2 = (1/2)E_b$. For the three-site coincidence [8] operative for the three-site Hall effect, the initial displacement decreases to $(2/3)x^{(0)}$ while the other two-displacements increase to $(2/3)x^{(0)}$, the three-site activation energy being $\epsilon_3 = (4/3)\epsilon_2$. Similarly, the four-site activation energy appropriate to a quadruple coincidence is $\epsilon_4 = \epsilon_3/6 = (3/2)\epsilon_2$. (In this case, the three-site coincidence determine the Hall mobility, the fourth site being non-coincident; four-site coincidences come into play only at very high temperatures [6].) It is seen that the difference in activations energies successively decrease basically because the higher-order coincidence event is 'partially prepared' by the lower-order event, since the displacements are correlated.

For the intersite bipolaron, two holes are common to two sites and $x^{(0)bi}$ is the change in intersite separation (see figure 1). Bipolaron motion again requires that $x^{(0)bi}$ of the two initial state reduces by 1/2 while the intersite separation of the final pair of sites increases to $(1/2)x^{(0)bi}$. However, this case differs from the above in that the displacements are not at a given site but involve pairs of sites, and the orthogonal displacements in the

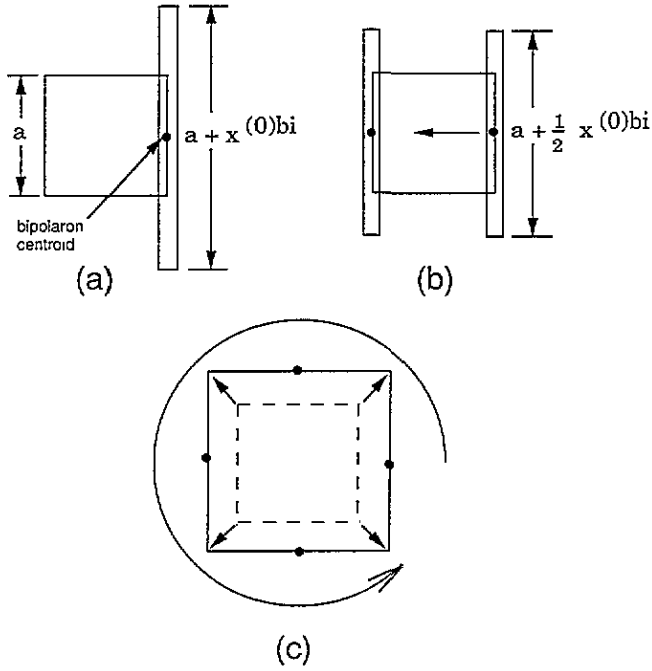

Figure 1. (a) Self-trapped configuration for small polaron. (b) Activated configuration for two-site jump rate w_2. (c) Activated configuration for magnetic-field-dependent four-site jump rate w_4.

two-dimensional geometry are not correlated. Local modes to which the bipolaron couple have been suggested by experiment [9]. Let us, however, assume a local symmetrical displacement. As is clear from examination of figure 1, the elastic energy required is twice that of the above coincidence event. Thus, $\epsilon_4 = 2\epsilon_2$, yielding a activation energy of ϵ_2 for μ_H, since $\mu_H \propto w_4/w_2$, where w_2 and w_4 are the two-and four-site jump rates, respectively. Thus, according to equation (2), a zero activation is obtained for the Hall coefficient R_H.

Finally, we point out that the thermopower measured by Ferro [2] is positive in sign, between 100 and 200 μV K^{-1} in magnitude, and increases with increasing temperature. These features are consistent with bipolaronic hopping transport [10].

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