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LETTER TO THE EDITOR

On back bending of the Hall number density as a function of temperature in YBCO high-T_c superconductors

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Abstract. Experimental data for the normal state Hall number density, $n_H \propto a+bT$, in (pure and low-level Zn-doped) rather well oxygenated YBCO high-T_c superconductors show an anomalous change of slope ('back bending') above some temperature T_0 which varies from nearly 190 K to nearly 250 K depending on sample quality. A possible origin of this anomaly is discussed within a two-fluid model approach. In so doing, a semi-empirical universal relationship is established between the 'back-bending' temperature T_0, the superconducting critical temperature T_c and an 'imperfection parameter' α which reflects the role of the 'residual' contribution to the Hall number density at zero temperature. The model predictions are found to be in quite reasonable agreement with some representative experimental data on the Hall number density in high-T_c superconductors. This lends support to the proposal that the mechanism for the phenomenon has its origin in an electronic modification of the CuO_2 planes mediated by an oxygen–vacancy ordering redistribution in the basal planes.

It is now well established (e.g. see [1–5]) that in high-T_c superconductors (HTS) the Hall number density (defined as the number of carriers divided by the unit-cell volume), $n_H(T)$, shows an almost linear temperature dependence both above and below the critical temperature T_c, namely $n_H(T) = a + bT$ (except in the critical fluctuation region close to T_c), where a is the so-called 'residual' part of the Hall number density defined by extrapolation of $n_H(T)$ to zero temperature. Different explanations, both phenomenological and microscopic, for such anomalous temperature behaviour of $n_H(T)$ (as compared to that of conventional superconductors) have been proposed. An increase in the precision of the Hall effect measurements and (our) subsequent data analysis, however, reveal the existence of another peculiarity in the temperature behaviour of such data [3, 5]: namely, a change of the slope b occurs from b_- to b_+ at some temperature T_0. The latter varies from nearly 190 K (for untwinned well oxygenated YBCO single crystals) to nearly 250 K (for imperfect but well oxygenated polycrystalline YBCO). This interesting phenomenon still remains unexplained [5]. It has sometimes been interpreted as being due to some 'thermal noise' [3]. After careful examination the effect can be seen in other properties as well [6–8].

In this letter a possible origin of this change-of-slope anomaly of the normal state Hall number density, observed in different quality HTS samples and affected by imperfections, is discussed within a phenomenological two-fluid model approach for the temperature behaviour of the Hall number density. Notice that here we have used the Hall number

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density notion for representing the Hall voltage, but the same model can be used for a description of a back-bending anomaly observed in the mobility μ [5]. Since n_H and μ are directly related to each other in the specific cases treated here (i.e. where the resistivity is linear with temperature), we do not develop the case of μ further.

By analysing some representative experimental data on the Hall effect measurements in HTS, a semi-empirical relationship between the 'change-of-slope' temperature, T_0, the critical superconducting temperature, T_c, and the 'imperfection parameter' (reflecting the role of the 'residual' contribution a to the Hall number density), α, of the form $T_0 = (2+\alpha)T_c$ is established. For the best YBCO single crystals (with $\alpha \ll 1$), the model predicts that the offset 'change-of-slope' temperature, T_0, is nearly $2T_c$. This same temperature for (imperfect) polycrystalline YBCO samples is found to increase with higher 'residual' contribution. This is probably due to the oxygen-deficiency-induced inhomogeneity. Theoretical values (in particular b_-/b_+) are in rather good agreement with experimental observations on YBCO superconductors. By comparison with other experiments [9], we propose that the phenomenon originates from an electronic rearrangement in the CuO_2 planes mediated by an oxygen/defect ordering in the CuO planes [10].

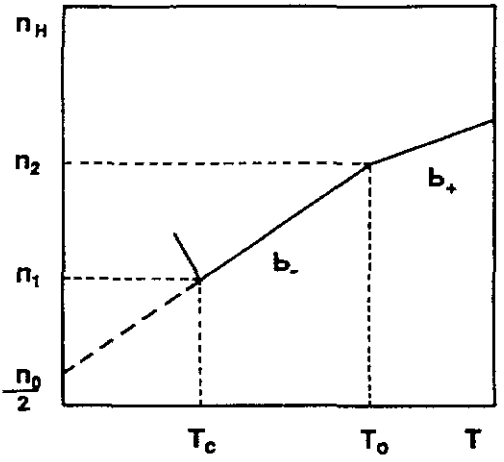

Figure 1. A sketch of the behaviour of the Hall number density as a function of temperature. Three reference number density values (n_0, n_1 and n_2) corresponding to three different temperatures ($T = 0$, $T = T_c$ and $T = T_0$) are shown.

Typical temperature behaviour of the Hall number density, $n_H(T)$, deduced from the experimental data on the Hall effect in HTS [1–5] is shown schematically in figure 1. To analyse a possible origin of the 'change-of-slope' anomaly in the behaviour of the $n_H(T)$ as a function of temperature, it is convenient to introduce the following notation for the Hall number densities at three markedly different reference temperatures, $T = 0$, $T = T_c$ and $T = T_0$: n_0 is related to the 'residual' value of the Hall number density which is defined in the usual way as the extrapolation of $n_H(T)$ to zero temperature (see figure 1); $n_1 = n_H(T_c)$ is the (interpolated) value of the Hall number density at $T = T_c$, and $n_2 = n_H(T_0)$ is the corresponding value at $T = T_0$, where T_0 is the 'back-bending' temperature, i.e. the temperature above which the Hall number density changes its slope (see figure 1). Some representative data concerning the value of the previously introduced reference points, n_0, n_1 and n_2, deduced from the Hall effect measurements in HTS are presented in table 1. We

have taken care to use only such data for which the signal to noise ratio is approximately greater than 5, hence omitting a few data points near T_c and room temperature. We thus reduce the likelihood of 'thermal noise' and 'fluctuations' as the source of the anomaly. As is clearly seen from table 1, all the experimental data roughly obey a semi-empirical relation, $n_1 \simeq n_2/2$. At the same time, the 'residual' value of the Hall number density, $n_0/2$, varies rather strongly, from nearly zero (for the well oxygenated untwinned YBCO single crystal with a high T_c) to nearly 60% of n_1 for polycrystalline YBCO (with a 'low' T_c).

Table 1. Estimates of the Hall number densities (n_0, n_1 and n_2), critical temperature (T_c), 'change-of-slope' temperature (T_0^{exp}) and slope ratio of $(b_-/b_+)^{exp}$, deduced from some experimental data [1–5], versus theoretical predictions for T_0^{th} (see equation (2)) and $(b_-/b_+)^{th}$ (see equation (5)). The first column, δ, indicates either an approximate value of the oxygen deficiency estimated from the corresponding value of the critical temperature (T_c) or as mentioned in the appropriate reference, or just refers to a particular type of sample.

δ	T_c	$n_0/2$	n_1	n_2	T_0^{exp}	T_0^{th}	α	$(b_-/b_+)^{exp}$	$(b_-/b_+)^{th}$	Ref.
0	94.5	0.074	0.725	1.62	200	199.7	0.114	1.31	1.054	[1]
#1	90	0.194	0.83	1.82	230	207.5	0.305	1.62	1.132	[3]
0	88.3	0.31	0.768	1.40	210	236.4	0.677	1.17	1.253	[4]
0.1	89.4	0.215	0.577	1.04	205	231.9	0.591	1.12	1.229	[4]
0.15	88.8	0.16	0.483	0.87	195	221.0	0.495	1.19	1.198	[4]
0%Zn	90	0.36	1.062	2.24	240	226.2	0.513	1.56	1.204	[5]
2%Zn	89	0.41	1.006	1.95	235	239.2	0.688	1.97	1.256	[5]
4%Zn	70	0.415	0.796	1.70	235	216.2	1.089	1.64	1.352	[5]

Turning to the temperature behaviour of the Hall number density both above and below T_c (see figure 1), we notice its striking resemblance [11] to the well known prediction of the two-fluid model for the thermal balance between the normal, $n_n(T)$, and superfluid, $n_s(T)$, components, namely

$$n_H(T) = n_n(T) + n_s(T) = n_1\left(\frac{T}{T_c}\right) + \frac{n_0}{2}\left(1 - \frac{T}{T_c}\right). \tag{1}$$

Formally, equation (1) is valid both above and below T_c (but outside the critical fluctuation region near T_c where $n_H(T)$ strongly deviates from a simple linear law). In this letter, however, we shall consider the normal state properties of the Hall number density only. So, in what follows, the above equation will be used for temperatures $T > T_c$. In this case, the 'residual' contribution, $n_0/2$, is defined as a zero-temperature extrapolation of the Hall number density, $n_H(T)$ (figure 1).

Taking into account the above-mentioned semi-empirical relation ($2n_1 \simeq n_2$) between $n_1 = n_H(T_c)$, the Hall number density at $T = T_c$ and $n_2 = n_H(T_0)$, the Hall number density at $T = T_0$, equation (1) predicts the following form of the 'change-of-slope' temperature:

$$T_0 = (2 + \alpha)T_c \tag{2}$$

where

$$\alpha \equiv n_0/(2n_1 - n_0). \tag{3}$$

Surprisingly, according to equation (2), the temperature T_0 (above which the 'normal state' Hall number density changes its slope) turns out to be related rather simply to the

superconducting temperature T_c. This means that the so-called 'normal state' properties of the Hall effect are essentially influenced by the superconducting correlations up to more than $2T_c$. This was already hinted at in [8] for the electrical resistivity. Taking into account the values of the 'imperfection' parameter α (which is related to the experimentally deduced values, n_0 and n_1, of the Hall number density; see equation (3)) and the critical temperature T_c we calculate according to equation (2) the value of the 'change-of-slope' temperature T_0 and compare it with the corresponding experimental value as found from the same experimental data. The results are collected in table 1, and show a quite reasonable agreement between the experimental (T_0^{exp}) and the calculated (T_0^{th}, see equation (3)) values.

Furthermore, due to equations (2) and (3), we can rewrite equation (1) in the form

$$n_H(T) = 2n_1\left(\frac{T}{T_0}\right) + \frac{n_0}{2}\left(1 - \frac{T}{T_0}\right). \tag{4}$$

It follows from equation (4) that at $T_c < T < T_0$ the second term in the RHS of this equation (which is due to the 'residual' contribution) adds a positive correction to the leading term, while above T_0 the situation changes qualitatively since *the second term starts to increase negatively*, thus reducing the value of the $n_H(T)$ slope. This means that below T_0 (but above T_c), $n_H(T) = a + b_-T$, where $b_- = 2n_1/T_0$. Above T_0, equation (4) predicts for the slope b the value $b_+ = 2n_1(1 - n_0/4n_1)/T_0$, that is (see equation (3))

$$b_-/b_+ = 2(1+\alpha)/(2+\alpha). \tag{5}$$

In table 1, the comparison of the experimentally found ratios of slopes $(b_-/b_+)^{exp}$ and those calculated (according to equation (5) by using the experimental values of the 'imperfection' parameter, α, see above) $(b_-/b_+)^{th}$ are presented for some YBCO samples. The agreement is quite satisfactory (a factor of about 1.5) considering the uncertainties in the experimental values.

It is worth mentioning that the 'imperfection' parameter, α (see equation (3)), can be related to the so-called 'electron–hole asymmetry' parameter discussed by Ullah and Dorsey [12] and by Rice *et al* [1]. The latter authors have argued that in their untwinned and well oxygenated single crystals (with negligibly small 'residual' parts of the Hall number density, $n_0 \ll 1$, and the normal state resistivity, $\rho_0 \ll 1$) α was found to be much less than unity, reflecting a nearly ideal symmetry between electrons and holes in their high-quality sample. At the same time, ultrasonic investigations [6] and neutron diffraction studies [7] allow us to conclude that the previously mentioned anomaly can be also attributed to the structural phase transition (so-called 'cell doubling', within the CuO plane due to oxygen rearrangement) in HTS oxides.

In conclusion, the phenomenon [3,5] appears to be due to some physical effect. Also, the change in slope temperature corresponds to that at which fluctuations disappear in the electrical resistivity data [8]. One possible reason is similar to what is seen in La cuprates [9] where due to oxygen diffusion at moderate temperature a new electronic periodicity occurs which is unfavourable for the superconducting order parameter and its phase coherence. In fact, such an anomalous oxygen/vacancy diffusion has just been observed in simulation studies [10]. Therefore our investigation provides some evidence in favour of the mechanism in which oxygen/vacancy diffusion in the CuO planes induces a preferred charge transfer (or polarization) in the CuO_2 planes resulting in superconductivity even at such a 'high' temperature.

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