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Contributions of critical and Gaussian fluctuations to the specific heat in $YBa_2Cu_3O_{7-x}$ and in $HgBa_2Ca_2Cu_3O_8$ under a magnetic field

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Abstract. The mean-field electronic specific heat C_e of a superconductor in the presence of a magnetic field is first calculated. The model contains the following as ingredients: an energy spectrum presenting saddle points in the band structure, a Josephson coupling between CuO planes and a $d_{x^2-y^2}$ gap symmetry. Superconductivity fluctuations are next extracted from published data on the specific heat of a $YBa_2Cu_3O_{7-x}$ and of an $HgBa_2Ca_2Cu_3O_8$ single crystal. Critical XY and Gaussian regimes are deduced from mean-field calculations. Magnetic field cross-overs are evaluated and physical parameters such as the Ginzburg–Landau number and the distance between CuO planes are calculated as tests.

1. Introduction

Much experimental and theoretical work pertains to the consideration of fluctuation effects on the transport and static properties of high-T_c superconductors [1]. Since high-T_c superconductors are characterized by a small coherence length and a rather high critical temperature, those fluctuations are very relevant for understanding the basis of such materials, the more so because several regimes can be observed in the magnetic field–temperature plane. Figure 1 shows the different fluctuation regimes that are thought to be observed in the B–T plane, namely critical XY, Gaussian and lowest Landau level (LLL) regimes. The dotted line represents some expected behaviour of the critical temperature T_c versus the magnetic field B. Several effects occur along such a line. In particular, for $B = 0$, the specific heat has a jump in most low- and high-T_c superconductors.

In the work reported in this paper, we have studied the behaviour of the jump of the electronic component of the specific heat as a function of the magnetic field for various high-T_c superconductors. Information will be provided here about the critical field along the dotted line in figure 1 as examples of regime cross-overs in magnetic fields.

In order to do this, fluctuation contributions to the electronic specific heat of a $YBa_2Cu_3O_{7-x}$ single crystal from [2] and for an $HgBa_2Ca_2Cu_3O_8$ single crystal from [3] should be extracted after subtraction of the phonon term and the most appropriate 'mean-field' background. Magnetic field cross-over between the XY critical and the LLL Gaussian regimes will be found, as will any dimensional

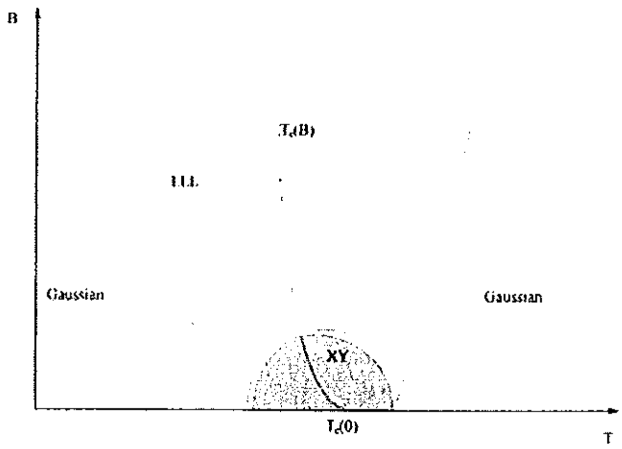

Figure 1. Schematic display of the different fluctuation regimes in the B–T plane. The dotted line corresponds to some behaviour of the critical temperature versus the magnetic field $T_c(B)$.

cross-over if it occurs. Physical parameters such as the Ginzburg–Landau ratio κ and the penetration length λ_L can be deduced and found to be in good agreement with previous results from the literature.

In section 2, the theoretical model is described. The extraction and the discussion of the fluctuation contributions are reported in section 3. Finally, conclusions are drawn in section 4.

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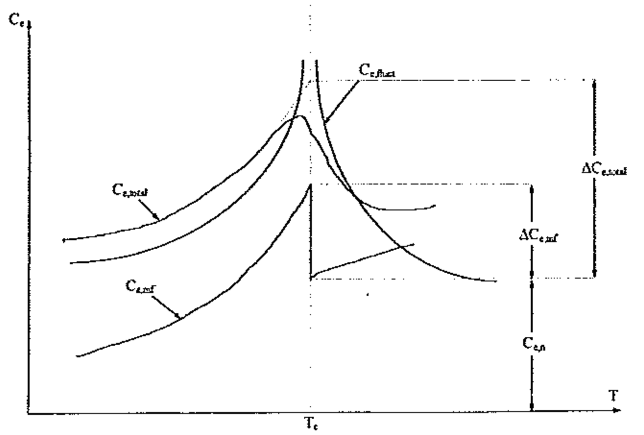

Figure 2. Sketch of the decomposition of the rough data of the electronic specific heat $C_{e.total}$ into a mean-field contribution $C_{e.mf}$ and a fluctuation contribution $C_{e.fluct}$. Other notations are readily defined.

2. Theoretical model

In figure 2, a schematic experimental result of the measurement of the electronic specific heat is presented. The electronic specific heat versus the temperature can be decomposed as

$$C_{e.total} = C_{e.mf} + C_{e.fluct} \tag{1}$$

where $C_{e.mf}$ is the so-called mean-field contribution and $C_{e.fluct}$ is the so-called fluctuation part [1]. $C_{e.total}$ is supposed to be obtained after subtraction of the phonons contribution.

Fluctuation contributions to the specific heat are known to follow a power law behaviour [4] depending on the symmetry of the order parameter and the system dimensionality. The experimental determination of the exponent will thus allow us to determine in which regime the system exists. Therefore the first part of the study of such exponents consists in calculating the mean-field contribution to the specific heat. Then the fluctuation contribution is obtained by subtracting this mean-field contribution from the global electronic specific heat.

The calculation of the field-free electronic specific heat was developed in a previous paper [5]. The electronic specific heat is found from

$$C_{e.mf} = \int E(T,k)\frac{\partial E(T,k)}{\partial T} \tag{2}$$

where $E(T,k)$ is the quasiparticle spectrum defined by

$$E(T,k) = \left\{[\epsilon(k) - \epsilon_F]^2 + \Delta^2(T,k,B)\right\}^{1/2} \tag{3}$$

where $\epsilon(k)$ is the band structure, ϵ_F is the Fermi energy and Δ the gap energy.

A 3D band structure that includes an energy coupling J between CuO_2 layers is used, namely

$$\epsilon(k) - \epsilon_F = \frac{\hbar^2}{2m^*_{ab}}k_x k_y + J\cos(k_z s) \tag{4}$$

as in the Lawrence–Doniach model [6] where m^*_{ab} is the effective mass in the plane and s the space between the copper oxide planes. The coupling energy in the z direction J is defined by

$$J = \frac{2\hbar}{s\gamma}\left(\frac{\epsilon_F}{m^*_{ab}}\right)^{1/2} \tag{5}$$

where γ is the anisotropy parameter defined by $(m^*_z/m^*_{ab})^{1/2}$ where m^*_z is the effective mass in the c direction. Therefore we can use equation (4) to describe either 3D or layered 2D compounds according to the value of J.

To take into account the magnetic field influence on the jump at T_c, namely a decrease in amplitude and a shift towards the low temperatures as observed in [2,3], the magnetic field dependence on the critical field and on the gap energy has been considered. As for the critical temperature, considering the temperature dependence of the upper critical field B_{c2} in the d-wave case [7], the following empirical formula is used:

$$T_c(B) = T_c(0)\left\{1 - \left[\frac{B}{B_{c2}(0)}\right]^{\alpha}\right\}^{\beta} \tag{6}$$

where $T_c(0)$ is the critical temperature without a field and $B_{c2}(0)$ is the upper critical field at 0 K. Our analysis of the data of [7] shows that the exponents α and β are best taken equal to 0.89 and 0.56.

The energy gap Δ is dependent on the temperature T, the momentum k and the magnetic field B. In a first approximation the energy gap can be factorized into

$$\Delta(T,k,B) = \Delta(T)\Delta(k)\Delta(B) \tag{7}$$

where $\Delta(T)$ is described by

$$\Delta(T) = \Delta(0,0)\tanh\left\{\alpha\left[\frac{T_c(B) - T}{T}\right]^{1/2}\right\} \tag{8}$$

where $\Delta(0,0)$ is the zero-temperature energy gap in absence of a field and $\alpha \cong 2.2$ [8]. $\Delta(k)$ is given by [9]

$$\Delta(k) = \hat{k}_x^2 - \hat{k}_y^2 \tag{9}$$

where $\hat{k}_x = k_x/(\pi/a)$ and $\hat{k}_y = k_y/(\pi/b)$. Finally, the magnetic field dependence of the gap energy is deduced from penetration length considerations [10] to follow

$$\Delta^d_{mag}(B) \propto 1 - \frac{B}{B_{c2}(0)}. \tag{10}$$

In the d-wave case, equations (2)–(10) together describe the theoretical mean-field approximation to $C_{e.mf}$. The physical parameters appearing in equations (2)–(10) are to be fixed to typical values found in the literature.

The statistical physics model to be used in the fluctuations regime differs according to the temperature range and the applied magnetic field value B which is considered (figure 1). In a magnetic field, Landau levels are created in the solid [11]. The energy spectrum of those levels is analogous to the solution of the harmonic oscillator [11]

$$E_n = (n + \tfrac{1}{2})\hbar\omega_c \tag{11}$$

where ω_c is the cyclotron frequency eB/m^* with m^* the effective mass. These levels are further separated with increasing field. If the temperature (k_BT) is small compared with the difference between the first and the second Landau levels ($\hbar\omega_c$), nearly all electrons are found on the lowest level. The triangular shape of the LLL regime in the B–T plane is explained by the difference between k_BT and $\hbar\omega_c$ (figure 1). The system can then be described in terms of wavefunctions corresponding to the lowest level ($n = 0$) only and fluctuations calculated with those functions in a Gaussian-like treatment of the fluctuations. At low fields, a Landau level description seems less appropriate since because of thermal fluctuations the charge carrier populations in each level interact with each other. Close to the critical temperature and for low fields, an XY critical regime is thus thought to be observable. A cross-over field should also exist between the XY critical and the Gaussian regimes [12] as indicated in figure 1.

In the Lawrence–Doniach model [6] without magnetic field, fluctuations exhibit a dimensional cross-over at a temperature $T_{3D\to 2D}$ [1]. A cross-over $B_{3D\to 2D}$ field similarly exists between the 3D and 2D regimes in a field. Below $B_{3D\to 2D}$, the 3D regime describes fluctuations associated with vortices that extend to several layers. In the 2D regime, vortices are located on one layer only. The transition from 3D to 2D corresponds to the transition between a vortex liquid and a solid lattice of vortices [13].

Cross-overs between the different regimes are thought to occur and to be detectable through electronic specific heat measurements.

Let $\Delta C_{e,total}$ be the measured jump and $\Delta C_{e,mf}$ be the calculated mean-field contribution to the jump.

In the XY regime [14], the jump $\Delta C_{e,fluct}$ due to fluctuations (figure 2) is given by

$$\Delta C_{e,fluct} = \Delta C_{e,total} - \Delta C_{e,mf} \equiv \Delta C_{XY} \propto B^{-1/2} \tag{12}$$

which exists only in 3D systems [14].

For the LLL regimes [15], the relevant value is the normalized quantity $\Delta\hat{C}_{e,fluct}$

$$\Delta\hat{C}_{e,fluct} = \frac{C_{e,fluct}}{\Delta C_{e,mf}} = \frac{C_{e,total} - C_{e,mf}}{\Delta C_{e,mf}}. \tag{13}$$

This ratio depends on the magnetic field in different ways according to the dimensionality of the system [15], namely

$$\Delta\hat{C}_{3DL} \propto B^{-1/2} \tag{14}$$

and

$$\Delta\hat{C}_{2DL} \propto B^{-1} \tag{15}$$

in the 3D LLL and 2D LLL cases respectively. Notice the different power laws.

Different criteria exist in order to separate the different regimes, namely the critical and the Gaussian regions and the 3D and 2D regimes. First let us recall the Ginzburg–Levanyuk number G_i [1] given by

$$G_i = \frac{1}{2}\gamma^2\left[\frac{k_BT_c(0)}{H_c^2(0)\xi^3(0)}\right]^2 \tag{16}$$

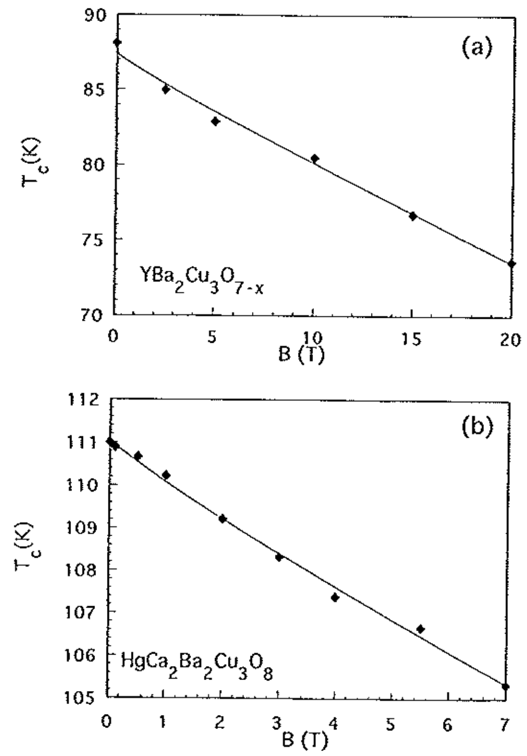

Figure 3. Experimental data of the magnetic field B dependence of the critical temperature T_c ♦ (*a*) in $YBa_2Cu_3O_{7-x}$ [2] and (*b*) in $HgBa_2Ca_2Cu_3O_8$ [3]. The full lines represent the fit with equation (6).

where $H_c(0)$ is the thermodynamic field separating the critical temperature regime from the Gaussian regime. The cross-over field $B_{XY\to Gaussian}$ between critical and Gaussian regimes is similarly defined as equal to $B_{c2}G_i$.

Klemm [13] has found a dimensional cross-over for a magnetic field $B_{3D\to 2D}$ given by

$$B_{3D\to 2D} = \frac{\zeta^2\Phi_0}{4\pi s^2} \tag{17}$$

where $\zeta = 0.345\,89/0.091\,33\gamma$, s and γ have been defined for equation (4) and equation (5) and $\Phi_0 = hc/2e$ is the flux quantum.

3. Discussion of experimental data

The physical parameters generally found in the literature for $YBa_2Cu_3O_{7-x}$ and $HgBa_2Ca_2Cu_3O_8$ are given in table 1, and J is calculated from equation (5). $T_c(0)$ and $B_{c2}(0)$ have been found by fitting the experimental curve of $T_c(B)$ with equation (6) (see figure 3). The fitting parameters are displayed in table 2. As the Hg-1223 is not fully oxygenated [3], some uncertainty remains about the value of the gap amplitude $\Delta(0, 0)$. The well-oxygenated compound should have a 48 meV gap [16]. The values that we have chosen are near 20 meV. They are those which best fit the high-field data so that the experimental and the

Table 1. Physical parameters of a fully oxygenated $YBa_2Cu_3O_{7-x}$ and a $HgBa_2Ca_2Cu_3O_8$ compound. The interplane exchange energy J is calculated from equation (5).

	$\Delta(0,0)$ (meV)	s (nm)	γ	$m^*_{ab}(m_e)$	J (meV)	T_c (K)
$YBa_2Cu_3O_{7-x}$	25 [16]	0.6 [17]	5 [18]	12 [18]	20	90 [18]
$HgBa_2Ca_2Cu_3O_8$	48 [16]	1.6 [19]	16 [20]	≈4	3.5	134 [16]

Table 2. Critical temperature T_c and upper critical field B_{c2} of the $YBa_2Cu_3O_{7-x}$ compound from [2] and the $HgBa_2Ca_2Cu_3O_8$ compound from [3] as obtained by a fit of the experimental data with equation (6).

	T_c (K)	B_{c2} (T)
$YBa_2Cu_3O_{7-x}$ [2]	87	87
$HgBa_2Ca_2Cu_3O_8$ [3]	111	101.8

mean-field contributions in the high-field range have the same asymptotic behaviour and value.

Let us define the normalized specific heat jump

$$\Delta C_{e.n} = \Delta C_{e.total}/C_{e.n}(T_c) \tag{18}$$

and the mean-field normalized jump

$$\Delta C_{e.mf}/C_{e.n}(T_c) \tag{19}$$

where $C_{e.n}$ is the non-superconducting specific heat just above T_c (figure 2). In figure 4, the experimental data (circles) for $\Delta C_{e.n}$ are compared with the mean-field normalized jump $\Delta C_{e.mf}/C_{e.n}$ (broken line) versus the magnetic field. The full line is an arbitrary interpolation through the experimental points as a guide to the eye. The $YBa_2Cu_3O_{7-x}$ case is considered in figure 4(a). The data of figure 4(b) from the Hg-1223 compound is compared with two different mean-field backgrounds, namely for $\Delta(0,0)$, see equation (8), equals 20 meV and 21 meV (figure 4(b)) to take into account some material content uncertainties [3] as indicated above.

Under a magnetic field, the fluctuation contribution to the electronic specific heat can be rather huge as compared with the field-free mean-field jump. In fact, several authors neglect this mean-field part of the electronic specific heat. However, the mean-field specific heat cannot be neglected: it is about 60% for a 3D compound such as $YBa_2Cu_3O_{7-x}$ (figure 4(a)). In 2D compounds such as Hg-1223, the mean-field specific heat is about 20% of the total specific heat (figure 4(b)).

After the mean-field magnetic-field-dependent background is taken into account, fluctuations can be better extracted. The fluctuation contribution to the jump $\Delta C_{e.fluct}$, see equation (12), and the normalized fluctuation contribution $\Delta\hat{C}_{e.fluct}$, see equation (13), versus the magnetic field are represented in a log–log plot so as to study the critical exponents in a classical way [4].

These results are shown in figures 5–7 for the $YBa_2Cu_3O_{7-x}$ and the $HgBa_2Ca_2Cu_3O_8$ compound with $\Delta(0,0) = 20$ meV and $\Delta(0,0) = 21$ meV respectively. The full circles and squares represent the data and the opened ones the interpolation resulting from the

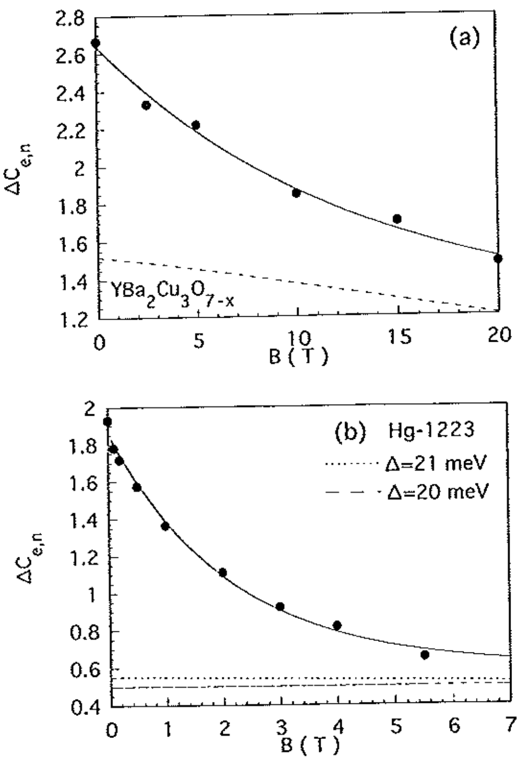

Figure 4. Comparison between the experimental normalized specific heat jump $\Delta C_{e.n} = \Delta C_{e.total}/C_{e.n}$ and the mean-field normalized jump (a) in the $YBa_2Cu_3O_{7-x}$ and (b) in $HgBa_2Ca_2Cu_3O_8$ for different mean-field backgrounds, i.e. either with $\Delta(0,0) = 20$ meV or with $\Delta(0,0) = 21$ meV as indicated. The full circles are the experimental data, the broken lines represent the mean-field behaviours and the full lines the fit of the experimental data with an exponential law.

experimental data. The circles refer to equation (12) and the left-hand scale on figures 5–7. The squares result from equation (13) and are linked to the right-hand scales on figures 5–7.

In figure 5, a straight line with slope −0.5 is found in the magnetic field range between 3 T to 7.7 T for $\Delta C_{e.fluct}$ in the $YBa_2Cu_3O_{7-x}$ sample. This is characteristic of a critical regime as described by equation (12). The exponent −0.5 is also observed from 7.7 T to 14 T for $\Delta\hat{C}_{e.fluct}$ relevant to a 3D LLL behaviour as described by equation (14). That means that the fluctuation contribution cross-over between a 3D XY and a 3D LLL regime occurs for a critical field $B_{XY\rightarrow Gaussian}$ equal to 7.7 T.

For the Hg-1223 sample, figure 6 presents the

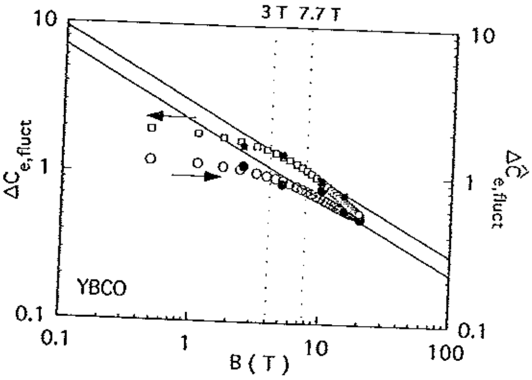

Figure 5. Fluctuation contribution to the jump $\Delta C_{e,fluct}$ and fluctuation contribution to the jump divided by the mean-field contribution to the jump $\Delta \hat{C}_{e,fluct}$ versus the magnetic field in a log–log graph for the $YBa_2Cu_3O_{7-x}$ sample [2].

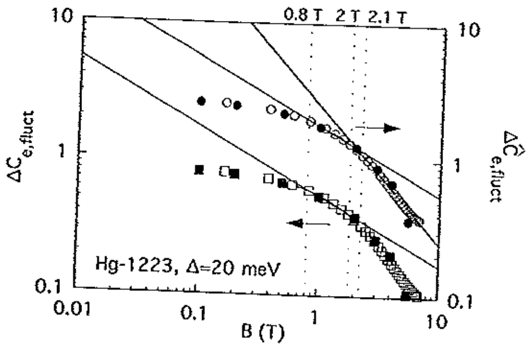

Figure 6. Fluctuation contribution to the jump $\Delta C_{e,fluct}$ and fluctuation contribution to the jump divided by the mean-field contribution to the jump $\Delta \hat{C}_{e,fluct}$ versus the magnetic field for the $HgBa_2Ca_2Cu_3O_8$ sample [3] with a mean-field background with $\Delta(0,0) = 20$ meV.

fluctuations relative to a background taken with $\Delta(0,0) = 20$ meV. An exponent −0.5 is found for $\Delta C_{e,fluct}$ between 0.7 T and 2 T. On the other hand, a power law with an exponent −0.5 fits the interpolated experimental curve for $\Delta \hat{C}_{e,fluct}$ in the range between 0.8 T and 2.1 T. The exponent −1 is also observed for fields greater than 2.1 T in $\Delta \hat{C}_{e,fluct}$. Thus from equations (12)–(15), a cross-over between a 3D XY regime and a 3D LLL regime occurs at 2 T and another one between a 3D LLL and a 2D LLL regime at 2.1 T. To sum up, the system which is 3D XY at low field becomes 3D LLL at 2 T and crosses over to a 2D LLL regime at 2.1 T.

As far as the background with $\Delta(0,0) = 21$ meV is concerned (figure 7), the exponent of the power law is −0.5 for $\Delta C_{e,fluct}$ in the range 0.6–1.9 T. A cross-over between exponents −0.5 and −1 occurs at 1.9 T for $\Delta \hat{C}_{e,fluct}$. Therefore the 3D LLL zone does not seem to exist and the system directly passes from a 3D XY to a 2D LLL at 1.9 T.

Thus, the critical fields between the critical and

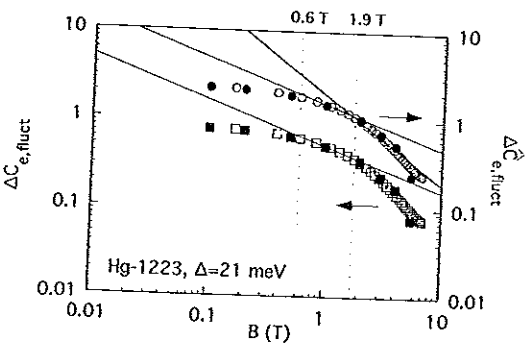

Figure 7. Fluctuation contribution to the jump $\Delta C_{e,fluct}$ and fluctuation contribution to the jump divided by the mean-field contribution to the jump $\Delta \hat{C}_{e,fluct}$ versus the magnetic field for the $HgBa_2Ca_2Cu_3O_8$ sample [3] with a mean-field background calculated for $\Delta(0,0) = 21$ meV.

Gaussian fluctuations and between 3D and 2D systems are very close to one another in this $\Delta(0,0) = 21$ meV case.

The Ginzburg–Landau factor can be deduced from cross-over fields from equation (16) and is found to be $\kappa = 139.64$ in the $YBa_2Cu_3O_{7-x}$ case, thereby giving a London penetration depth equal to 181.5 nm for $\xi(0) = 1.3$ nm [21].

For a critical 2 T field, from equation (16), κ becomes 49.11 and $\lambda_L = 785.77$ nm for $\xi(0) = 16$ nm [19] in the $HgBa_2Ca_2Cu_3O_8$ case. Using equation (17), the space s between the CuO_2 planes is calculated and is found to be equal to 2.1 nm.

The values of κ, λ_L and s are close to the values found in the literature in both high-T_c superconductor cases, recalling that the examined Hg-1223 compound was not well oxygenated.

4. Conclusions

After subtraction of the theoretical values of the mean-field contribution calculated for a high-T_c superconductor model considering saddle point singularities near the Fermi level and a d-wave gap parameter, superconducting fluctuations have been extracted and different regimes have been observed as a function of the magnetic field in the electronic specific heat of a $YBa_2Cu_3O_{7-x}$ and an $HgBa_2Ca_2Cu_3O_8$ single crystal.

In the $YBa_2Cu_3O_{7-x}$ case, the fluctuation contribution exhibits a 3D behaviour at low field while a cross-over occurs for $B_{XY \to Gaussian}$ at 7.7 T. The 2D LLL is not observed in the studied range of magnetic field.

For the $HgBa_2Ca_2Cu_3O_8$, we cannot determine whether a 3D LLL regime exists. However, the range of B where the 3D LLL regime could occur is likely to be small. The 2D LLL regime is well observed above 2.1 T. More and better data concerning the jump of the specific heat would be of interest here.

Physical parameters deduced in the above are in good agreement with other results found into the literature and confirm the goodness of the data analysis method.

The above considerations should of course be corroborated by other data, on other samples, but also on other properties such as the thermal conductivity [22] or the electrothermal conductivity in a magnetic field [23].

Acknowledgments

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