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Fluctuation-induced diamagnetism in bulk isotropic superconductors at high reduced temperatures

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Abstract
The short-wavelength effects on the fluctuation-induced diamagnetism (FD) in bulk isotropic three-dimensional (3D) superconductors are taken into account by introducing in the Gaussian–Ginzburg–Landau approach different cut-off conditions. These calculations, which extend to the 3D case our previous results on layered superconductors, are then used to briefly analyse the FD data measured for the low-temperature superconducting alloy Pb–8 at.% In. These analyses confirm the adequacy of a total-energy cut-off for explaining, for low-temperature 3D superconductors also, the thermal fluctuation effects in the high-reduced-temperature region. These results thus provide further support to the recent proposal that, due to the localization energy, the size of the effective fluctuations cannot be appreciably smaller than the superconducting coherence length amplitude extrapolated to $T = 0$ K.

1. Introduction

Well above the superconducting transition temperature, T_{c0}, for reduced temperatures $\epsilon \equiv \ln(T/T_{c0}) \gtrsim 0.1$, the thermal fluctuations are deeply affected by the so-called short-wavelength fluctuation effects, which appear when their characteristic wavelength becomes of the order of the superconducting coherence length amplitude, $\xi(0)$ [1–4]. The behaviour of the superconducting fluctuations in this short-wavelength regime is a long-standing and still open problem, whose interest has been considerably enhanced by the discovery of the high-temperature (cuprate) superconductors (HTSC) [2, 3]. As is now well established, the properties of the HTSC in the normal state may be in some cases deeply affected by the

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superconducting fluctuations [3, 4]. But, in addition, the thermally activated Cooper pairs at high reduced temperatures may directly affect the very formation of the superconducting state in HTSC [5].

Recently, it has been shown that the thermal fluctuation effects at high reduced temperatures in the cuprate superconductor $YBa_2Cu_3O_{7-\delta}$ (Y-123) may be explained in terms of the Gaussian–Ginzburg–Landau (GGL) approach by introducing a 'total-energy' cut-off in the spectrum of the fluctuations instead of the conventional momentum cut-off always used before [6–8]. It was then proposed that such a total-energy cut-off takes into account the localization energy associated with the shrinkage of the size of the fluctuations when the reduced temperature increases [9]. This directly forbids fluctuation sizes appreciably smaller than $\xi(0)$. It will, however, be important to confirm the generality of these results by studying the superconducting fluctuations in the high-reduced-temperature region in other superconductors, in particular in the conventional (described by the BCS theory) low-temperature (metallic) superconductors (LTSC). One of the observables best suited for measuring these effects in LTSC is the fluctuation-induced diamagnetism (FD), which depends on both the superconducting coherence length and the Cooper pair's density [1]. In view of this, the main aim of this paper is to extend to bulk isotropic 3D superconductors the scenario adequate for describing most of the low-temperature metallic superconductors: our recent FD calculations under different cut-off conditions for layered superconductors [6, 7]. Let us stress immediately that such an extension requires a specific treatment of the cut-off effects in the fluctuation spectrum in the direction parallel to the applied magnetic field, which in layered superconductors is already cut off by the reduced dimensionality [6, 7]. In doing these calculations, we will clarify also the relationship between the cut-off procedures and the empirical scaling field introduced by Gollub and co-workers in their pioneering work on the FD in LTSC [10]. Although the central aim of this paper is to present a detailed account of our FD calculations for bulk isotropic 3D superconductors, we will also briefly compare these theoretical results with recent measurements on the low-temperature superconducting alloy Pb–8 at.% In (Pb–In8%). A more detailed account of these FD measurements on this and other LTSC, as well as of their analysis on the basis of our theoretical results, will be presented elsewhere [9, 11].

2. Fluctuation-induced diamagnetism in isotropic 3D superconductors under different cut-off conditions

As is well known, the fluctuation-induced magnetization, $\Delta M(\epsilon, h)$, may be defined as [1,2,12]

$$\Delta M(\epsilon, h) = -\frac{1}{\mu_0 H_{c2}(0)} \left(\frac{\partial \langle \Delta F(\epsilon, h) \rangle}{\partial h} \right)_{\epsilon} \tag{1}$$

where μ_0 is the vacuum magnetic permeability, $H_{c2}(0)$ is the upper critical magnetic field amplitude (extrapolated to $T = 0$ K) and $\langle \Delta F(\epsilon, h) \rangle$ is the so-called effective free energy due to fluctuations. Our main task is, therefore, to obtain $\langle \Delta F(\epsilon, h) \rangle$ in the case of bulk isotropic 3D superconductors under different cut-off conditions. Our calculations of $\langle \Delta F(\epsilon, h) \rangle$ are going to be done on the basis of the GGL approach proposed early on by Schmid to obtain $\Delta M(\epsilon, h)$ for bulk superconductors in the zero-magnetic-field limit without a cut-off [13]. Schmid's result corrected by a factor of four the pioneering BCS calculation of $\Delta M(\epsilon, h)$ done by Schmidt [14]. The GGL procedure proposed by Schmid for calculating $\Delta M(\epsilon, h)$ is now a textbook subject [1, 2, 12] and, therefore, in our extensions under different cut-off conditions we will omit the first steps and start with the expression for $\langle \Delta F(\epsilon, h)\rangle$ [12, 13]:

$$\langle \Delta F(\epsilon, h)\rangle = \frac{k_B T}{8\pi^2 \xi^2(0)} 2h \sum_{n=0}^{\infty} \int \mathrm{d}k_\parallel \left[\ln\left(n + \frac{\epsilon + h + k_\parallel^2 \xi^2(0)}{2h} \right) + \ln(2h) - \ln\left(\frac{k_B T}{2a_0} \right) \right] \tag{2}$$

where a_0 is the so-called Ginzburg–Landau normalization constant, k_B is the Boltzmann constant, $h \equiv H/H_{c2}(0)$ is the reduced magnetic field, $k_\parallel$ is the momentum of the fluctuations in the direction parallel to the applied magnetic field, and $n = 0, 1, \ldots$ is the Landau-level index.

Various comments on equation (2) are in order. Note first that, as is well known, equation (2) has an 'ultraviolet'-like divergence at all reduced temperatures and magnetic fields due to a misestimation of the contribution of the fluctuating modes with high momentum [1, 2]. The simplest way to correct this failure of the GGL approach is to restrict with a cut-off the momentum of the fluctuating modes [1, 2, 13]. The precise choice of such a cut-off becomes irrelevant for temperatures near T_{c0} and, simultaneously, low magnetic fields, when both h and ϵ are much smaller than the cut-off amplitude [1, 2, 13, 15]. In fact, in this limit the cut-off does not explicitly appear in the final expressions for the fluctuation-induced observables [1, 2]. However, it was observed early on for LTSC [16] and further confirmed for HTSC (see references [4–6, 17], and references therein) that the conventional momentum cut-off always used until recently does not explain the sharp decrease of the thermal fluctuation effects measured at high reduced temperatures, when $\xi(\epsilon)$ becomes of the order of $\xi(0)$. This has led us to propose a regularization of the GGL approach through a total-energy cut-off given by (in units of $\hbar^2/2m^*$, where $\hbar$ is the reduced Planck constant and m^* is the effective mass of the Cooper pairs) [6–8]

$$k^2 + \xi^{-2}(\epsilon) < c\xi^{-2}(0) \tag{3}$$

where k is the modulus of the momentum of each fluctuating mode, and c is a constant cut-off amplitude of the order of or less than 1. The contribution to the total energy of the fluctuating modes proportional to $\xi^{-2}(\epsilon)$ may be seen as due to the localization energy associated with the shrinkage, when the reduced temperature increases, of the superconducting wavefunction [9]. Note that by using the mean-field temperature dependence of the GL superconducting coherence length, $\xi(\epsilon) = \xi(0)\epsilon^{-1/2}$, equation (3) may be rewritten as $k^2 < (c - \epsilon)\xi^{-2}(0)$. Therefore, in the low-$\epsilon$ region (for $\epsilon \ll c$) the total-energy cut-off reduces to the conventional momentum cut-off, $k^2 < c\xi^{-2}(0)$. The differences between the two cut-off approaches appear in the high-ϵ region: equation (3) suppresses all the fluctuating modes above a well defined reduced temperature, when $\epsilon \geqslant c$. In contrast, regularization procedures which do not take into account the localization energy contribution lead to a smooth vanishing of the thermal fluctuation effects when $\epsilon \gg c$. This includes the conventional momentum cut-off and, also, the exponential weight functions which penalize the most energetic fluctuating modes used in reference [18]. Note also that in obtaining equation (2) we have neglected in the GGL free-energy functional the powers in the amplitude of the order parameter higher than two. This approach is adequate for studying the thermal fluctuations not too close to the transition [12] and, therefore, it will be particularly suitable in the high-ϵ region. Finally, in equation (2) the Landau-level index is related to the momentum of the fluctuations in the directions perpendicular to the applied magnetic field through

$$k_\perp^2 \rightarrow \frac{4e\mu_0 H}{\hbar}\left(n + \frac{1}{2} \right) \tag{4}$$

which implicitly assumes the absence of appreciably dynamic and non-local electrodynamic effects. Therefore, equation (2) does not apply when these effects become appreciable [19–21].

Both the conventional momentum cut-off and the total-energy cut-off lead to upper limits in the sum over the Landau levels and in the integral over $k_\parallel$ in equation (2). In the case of the total-energy cut-off, by combining the relationships (3) and (4) we obtain these limits as

$$n_c = \frac{1}{2h}\,[c-\epsilon] - 1 \tag{5}$$

for the maximum Landau-level index, and

$$k_\parallel^{max} < \sqrt{c-\epsilon}\,\xi^{-1}(0) \tag{6}$$

for the upper limit in the integral over $k_\parallel$. The fluctuation-induced diamagnetism under this cut-off condition and in the so-called Prange regime [22] (i.e., for finite fields) may be now obtained by just imposing the conditions given by equations (5) and (6) in equation (2) and by then using equation (1). This gives

$$\Delta M(\epsilon,h,c)_E = -\frac{k_BT}{\pi\phi_0\xi(0)}\sqrt{2h}\int_0^{\sqrt{(c-\epsilon)/2h}} \mathrm{d}x\,\left[\frac{c-\epsilon}{2h} - \left(\frac{c}{2h}+x^2\right)\psi\left(\frac{1}{2}+\frac{c}{2h}+x^2\right)\right.$$
$$+\ \ln\Gamma\left(\frac{1}{2}+\frac{c}{2h}+x^2\right) + \left(\frac{\epsilon}{2h}+x^2\right)\psi\left(\frac{1}{2}+\frac{\epsilon}{2h}+x^2\right)$$
$$\left. -\ \ln\Gamma\left(\frac{1}{2}+\frac{\epsilon}{2h}+x^2\right)\right] \tag{7}$$

where Γ and ψ are, respectively, the Gamma and digamma functions, ϕ_0 is the magnetic flux quantum, and the dimensionless variable x is related to the out-of-plane momentum of the fluctuations through $x = \xi(0)k_\parallel/\sqrt{2h}$.

The maximum Landau-level index and the maximum wavevector in the direction parallel to the applied magnetic field taken into account by the conventional momentum cut-off may be obtained by simply changing c to $c+\epsilon$ in, respectively, equations (5) and (6). So, following the procedure described above, the fluctuation-induced diamagnetism at finite applied magnetic fields under this cut-off condition is found to be

$$\Delta M(\epsilon,h,c)_M = -\frac{k_BT}{\pi\phi_0\xi(0)}\sqrt{2h}\int_0^{\sqrt{c/2h}} \mathrm{d}x\,\left[\frac{c}{2h} - \left(\frac{c+\epsilon}{2h}+x^2\right)\psi\left(\frac{1}{2}+\frac{c+\epsilon}{2h}+x^2\right)\right.$$
$$+\ \ln\Gamma\left(\frac{1}{2}+\frac{c+\epsilon}{2h}+x^2\right) + \left(\frac{\epsilon}{2h}+x^2\right)\psi\left(\frac{1}{2}+\frac{\epsilon}{2h}+x^2\right)$$
$$\left. -\ \ln\Gamma\left(\frac{1}{2}+\frac{\epsilon}{2h}+x^2\right)\right]. \tag{8}$$

Various comments on the above cut-off-dependent expressions for ΔM are in order. Note first that when $\epsilon \ll h, c$, equations (7) and (8) reduce to the same expression:

$$\Delta M(h,c) = -\frac{k_BT}{\pi\phi_0\xi(0)}\sqrt{2h}\int_0^{\sqrt{c/2h}} \mathrm{d}x\,\left[\frac{c}{2h} - \left(\frac{c}{2h}+x^2\right)\psi\left(\frac{1}{2}+\frac{c}{2h}+x^2\right)\right.$$
$$\left. +\ \ln\Gamma\left(\frac{1}{2}+\frac{c}{2h}+x^2\right) + x^2\,\psi\left(\frac{1}{2}+x^2\right) - \ln\Gamma\left(\frac{1}{2}+x^2\right)\right]. \tag{9}$$

Therefore, as stressed above, the momentum and the total-energy cut-off conditions become equivalent in the low-reduced-temperature regime. In fact, this last conclusion remains valid for any values of h and c provided that the condition $\epsilon \ll h, c$ is obeyed. So, this confirms also in the 3D case our previous findings for layered superconductors [6, 23]: both cut-off conditions explain the short-wavelength fluctuation regime when it is accessed by increasing h, *but still in the low-reduced-temperature region*.

Equation (9) may also be used to easily relate the cut-off procedures used here to the empirical scaling field, H_s, introduced by Gollub and co-workers to explain their pioneer FD results on LTSC [10]. One of the main conclusions in the studies by Gollub and co-workers was that the scaled magnetization, $\Delta M\phi_0^{3/2}/k_BT(\mu_0 H)^{1/2}$, is at $T = T_{c0}$ a universal function of H/H_s. This is fully confirmed by the behaviour of $\Delta M(h, c)$ predicted by equation (9), which at T_{c0} only depends on c/h. In fact, the relationship between c and H_s may be straightforwardly obtained from equation (9) by simply using the empirical definition of H_s, i.e., the magnetic field at which the scaled magnetization decreases to one half of its saturation value in the Prange regime without a cut-off (see below). This leads to $H_s \simeq 0.5cH_{c2}(0)$. Let us also stress here that when the dynamic and non-local electrodynamic effects are important, H_s becomes dependent on the specific characteristics of each material and much smaller than $H_{c2}(0)$ [10, 19–21]. In that case, c will also manifest this material dependence and it will be much smaller than 1.

Equations (7) and (8) also include the Prange regime without a cut-off as a particular case, that corresponds to $\epsilon, h \ll c$. Under these conditions, both equations lead to

$$\Delta M(\epsilon, h) = -\frac{k_BT}{\pi\phi_0\xi(0)}\sqrt{2h}\int_0^\infty \mathrm{d}x\,\left\{-\ln\Gamma\left(\frac{1}{2}+\frac{\epsilon}{2h}+x^2\right)+\ln\sqrt{2\pi}\right.$$
$$\left.+\left(\frac{\epsilon}{2h}+x^2\right)\left[\psi\left(\frac{1}{2}+\frac{\epsilon}{2h}+x^2\right)-1\right]\right\}. \tag{10}$$

This expression is equivalent to that previously obtained in reference [22]. In fact, both of them lead to the same saturation value of the scaled magnetization at $h \gg \epsilon$, i.e. approximately 0.324.

The above expressions for the FD in the Prange regime also include as a particular case the zero-magnetic-field limit (which may be also called the Schmidt and Schmid limit) under different cut-off conditions, which is characterized by a linear dependence of ΔM on the applied magnetic field. This implies the absence of finite-field effects (and, thus, $h \ll \epsilon$) and of dynamic and non-local electrodynamic effects (and, thus, $h \ll c$), which will introduce a non-linear dependence on H in the ΔM-behaviour. Therefore, by just imposing $h \ll \epsilon, c$ in equations (7) and (8) we obtain

$$\Delta M(\epsilon, h, c)_E = -\frac{k_BT}{6\pi\phi_0\xi(0)}h\left(\frac{\arctan\sqrt{(c-\epsilon)/\epsilon}}{\sqrt{\epsilon}}-\frac{\arctan\sqrt{(c-\epsilon)/c}}{\sqrt{c}}\right) \tag{11}$$

for the Schmidt and Schmid limit under the total-energy cut-off and

$$\Delta M(\epsilon, h, c)_M = -\frac{k_BT}{6\pi\phi_0\xi(0)}h\left(\frac{\arctan\sqrt{c/\epsilon}}{\sqrt{\epsilon}}-\frac{\arctan\sqrt{c/(\epsilon+c)}}{\sqrt{\epsilon+c}}\right) \tag{12}$$

for such a limit under the conventional momentum cut-off. These results also show that, as stressed above, the FD behaviours at high reduced temperatures predicted using the two cut-off conditions are quite different. For instance, in the case of the total-energy cut-off, equation (11) presents a singularity when $\epsilon = c$. As we have already stressed above, such a disappearance of the FD above $\epsilon = c$ is due to the fact that equation (3) forbids the existence of the superconducting fluctuations with a spatial extent much smaller than $\xi(0)$ [9]. In contrast, equation (12) does not present any singularity at a well defined temperature and it smoothly tends to zero when $\epsilon \gg c$ as

$$\Delta M(\epsilon, h, c)_M = -\frac{k_BTh}{6\pi\phi_0\xi(0)}\frac{c^{3/2}}{\epsilon^2}. \tag{13}$$

Note finally that the Schmidt and Schmid expression for the FD in bulk isotropic superconductors in the zero-magnetic-field limit, which corresponds to simultaneously $h \ll \epsilon, c$ and $\epsilon \ll c$, is given by

$$\Delta M(\epsilon, h) = -\frac{k_B T}{12\phi_0 \xi(0)} \frac{h}{\sqrt{\epsilon}}. \tag{14}$$

This expression may be directly obtained from either of equations (11) or (12) by just imposing the condition $\epsilon \ll c$.

3. Application to Pb–8 at.% In

As an example of the usefulness of the above results, we will use them to analyse the fluctuation-induced magnetization, $\Delta M(\epsilon, h)$, measured in the zero-field limit in the LTSC alloy Pb–8 at.% In (Pb–In8%). The details of these experiments will be published elsewhere [11]. However, let us stress here that the background (or normal) contribution to the measured magnetization has been estimated by extrapolating through the transition the data measured far above T_{c0}, in the temperature region $T \gtrsim 2.5T_{c0}$ (which corresponds to $\epsilon \gtrsim 0.9$). As worked out in references [6] and [8] in the case of the HTSC, such a procedure ensures that the extraction of the FD in the high-reduced-temperature region is not appreciably affected by the choice of background.

In figure 1 we present various examples of the $\Delta M(\epsilon)_h/HT$ data measured in the ϵ-region bounded by $10^{-2} \lesssim \epsilon \lesssim 0.6$, together with their comparison with the GGL approaches in the zero-magnetic-field limit under different cut-off conditions. Note that all of these data agree with each other within the experimental uncertainties, which are well represented by the data dispersion. This clearly shows that these data correspond well to the so-called zero-magnetic-field limit, where the magnetic susceptibility becomes field independent. The solid line in this figure is the best fit to the experimental data on the FD predicted by the GGL approach in this zero-field limit and under a total-energy cut-off (equation (11)), with c as the only free parameter. In doing this comparison we have used $T_{c0} = 7.03$ K and $\mu_0 H_{c2}(0) \simeq 0.6$ T, as

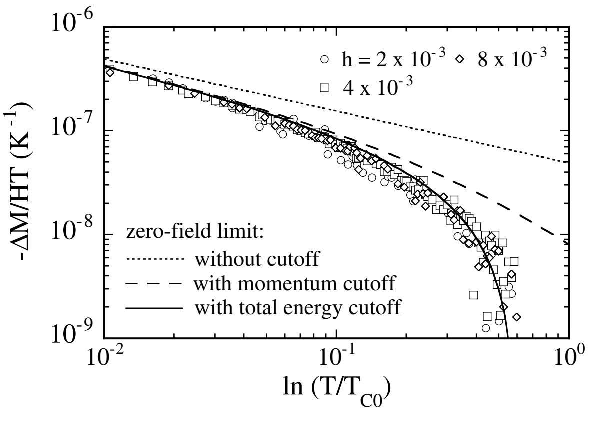

Figure 1. Various examples of the $\Delta M(\epsilon)_h/HT$ data measured at constant magnetic field, and their comparison with the predictions of the GGL approaches in the Schmidt and Schmid limit under different cut-off conditions. Note that all of these $\Delta M(\epsilon)_h/HT$ curves agree within the experimental uncertainties with each other, which clearly indicates that they correspond well to the FD in the zero-field limit. These results confirm the adequacy of the total-energy cut-off for regularizing, for 3D superconductors also, the GGL approaches.

determined by independent magnetization measurements. As may be seen, the agreement is excellent for all of the experimentally accessible ϵ-window, and it leads to $c \simeq 0.6$. The dashed line corresponds to the Schmidt and Schmid limit under a momentum cut-off (equation (12)) with again $T_{c0} = 7.03$ K, $\mu_0 H_{c2}(0) \simeq 0.6$ T, and $c \simeq 0.6$, which only agrees with the data in the low-ϵ region, for $\epsilon \lesssim 0.1$. The differences between the experimental data and $\Delta M(\epsilon, h, c)_M$ in the high-ϵ region are well beyond the experimental uncertainties, and they cannot be overcome by using other values of c without destroying the agreement for $\epsilon \lesssim 0.1$. Note also that the Schmidt and Schmid limit without any cut-off (equation (14) again with $T_{c0} = 7.03$ K and $\mu_0 H_{c2}(0) \simeq 0.6$ T), does not agree with the data at any accessible reduced temperature, including the low-ϵ region ($\epsilon \lesssim 0.1$). This last result, which contrasts with the FD behaviour in the zero-field limit observed for HTSC [3,24], may be attributed to the importance at every reduced temperature of the short-wavelength effects in the direction parallel to the applied magnetic field in LTSC, which in layered superconductors is already cut off by the reduced dimensionality. In fact, another striking aspect of the results summarized in figure 1 is that the total-energy cut-off explains simultaneously and consistently (by using the same cut-off amplitude) the short-wavelength effects at low and high reduced temperatures.

Note that the cut-off amplitude that we have obtained for the LTSC analysed here, $c \simeq 0.6$, agrees well within the experimental uncertainties with the one that we found before when analysing, also in the high-reduced-temperature region, the in-plane paraconductivity and the FD in optimally doped Y-123 [6–8]. This finding suggests a universal origin for the total-energy cut-off condition and it supports, thus, our recent proposal that, independently of the absolute values of the GL coherence length amplitude, $\xi(0)$, the characteristic length of the fluctuations in the normal state above any superconducting transition cannot be appreciably smaller than ξ_0, the Pippard coherence length [6–9]. This last length may be seen as the effective 'size' of the Cooper pairs. In the BCS clean limit, $\xi(0) = 0.74\xi_0$. So, by using the mean-field ϵ-dependence of $\xi(\epsilon)$, the cut-off amplitude is estimated to be $c \simeq 0.55$, in excellent agreement with the experimental values found here for a moderately dirty superconducting alloy and found before for clean HTSC [6–8]. In fact, this estimate of c probably also holds at a qualitative level in dirty superconductors, because one may expect the GL coherence length and the actual superconducting coherence length at $T = 0$ K to be affected by impurities to similar extents [9, 25]. Let us, finally, stress that in addition to their interest as regards the understanding of the FD in LTSC in the high-reduced-temperature region, these results could have quite direct implications for other interesting and still open problems concerning the behaviour of the Cooper pairs above any superconducting transition. For instance, in the scenarios where the local pairing in cuprates is supposed to happen at a different temperature (T^*) to the long-range phase order (T_{c0}) [5, 26], our results suggest that $\ln(T^*/T_{c0}) \lesssim c$. It will, however, be important to probe the general applicability of these results by studying the short-wavelength regime in other LTSC and in HTSC with different dopings.

4. Conclusions

To take into account the short-wavelength effects that are mainly manifested at high reduced temperatures, the fluctuation-induced diamagnetism in bulk isotropic superconductors was calculated on the basis of the Gaussian–Ginzburg–Landau approach by introducing momentum and total-energy cut-offs. This latter cut-off takes into account the localization energy associated with the shrinkage of the size of the fluctuations when the reduced temperature increases and the Ginzburg–Landau coherence length becomes of the order of $\xi(0)$, the superconducting coherence length amplitude. These calculations extend to the 3D case our previous GGL results for layered superconductors [6–8]. In doing that, we have implemented a specific treatment of the short-wavelength effects in the fluctuation spectrum in the direction parallel to the applied magnetic field, which in layered superconductors are already cut off by the reduced dimensionality. Then, as an example of their usefulness, these theoretical results were used to briefly analyse the FD measured in the bulk isotropic low-temperature superconducting alloy Pb–8 at.% In. Our analyses fully confirm the adequacy of the total-energy cut-off for describing the FD in all of the experimentally accessible reduced temperature region, including the short-wavelength regime. In addition, the cut-off amplitude is found to be of the order of 0.6, a value similar—well within the experimental uncertainties—to those previously found for optimally doped Y-123. Although FD measurements on other LTSC and HTSC compounds are very desirable, these findings support our recent proposal that the high-reduced-temperature behaviour of the fluctuating Cooper pairs in the normal state in any superconductor is mainly dominated by the localization effects associated with the shrinkage of the superconducting wavefunction when the reduced temperature increases [6–9].

Acknowledgments

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