Two-bands effect on the superconducting fluctuating diamagnetism in MgB$_2$

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Abstract

The field dependence of the magnetization above the transition temperature $T_c$ in MgB$_2$ is shown to evidence a diamagnetic contribution consistent with superconducting fluctuations reflecting both the $\sigma$ and $\pi$ bands. In particular, the upturn field $H_{up}$ in the magnetization curve, related to the incipient effect of the magnetic field in quenching the fluctuating pairs, displays a double structure, in correspondence to two correlation lengths. The experimental findings are satisfactorily described by the extension to the diamagnetism of a recent theory for paraconductivity, in the framework of a zero-dimensional model for the fluctuating superconducting droplets above $T_c$.

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On approaching the transition temperature $T_c$ from above, superconducting fluctuations (SF) occur and, while the average order parameter is zero, one has $\langle |\psi|^2 \rangle^{1/2} \neq 0$. Therefore local pairs are generated, lacking of long-range coherence and decaying with a characteristic time which increases for $T \to T_c^+$. An interesting way to detect the SF is by means of the related magnetic screening, through a diamagnetic contribution to the magnetization. In its simplest form this contribution is written $-M_{dia}(H,T) \approx \frac{e^2}{m_c^2} n_c \xi^2(T)H$, $n_c = |\psi|^2$ being the number density of superconducting pairs and $\xi(T)$ the coherence length. On cooling towards $T_c^+$, because of the divergence of $\xi(T)$ $|M_{dia}|$ can be expected to enhance. On the other hand strong magnetic fields, comparable to the critical field $H_{c2}$, must evidently suppress the SF. Thus the isothermal magnetization curves $-M_{dia}(H,T = \text{const})$ exhibit an upturn in the field dependence. According to a model of fluctuating superconductive particles of size $d << \xi(T)$ and outside the critical region, the upturn field $H_{up}$ is about inversely proportional to the square of $\xi(T)$ \[1, 2\].

In conventional metallic BCS superconductors the diamagnetism above $T_c$ and the effect of the field in quenching the fluctuating pairs were detected a long ago, by means of magnetization measurements as a function of temperature at constant fields \[3\]. More recently, successful detection of the detailed field dependence of $M_{dia}$ has been obtained in the new superconductor MgB$_2$ \[4\].

In Fig.3 of the paper by Lascialfari et al. \[4\] an anomaly was noticeable: the curve of the reduced magnetization at $T = 39.5 K$ (while $T_c \approx 39.05 K$) showed an unexplained double structure. Later on, in view of the established two-bands character of the superconductivity in MgB$_2$ \[2\], it was suspected that the double structure in the magnetization curve could be related to the two superconducting bands in this compound. The motivation of the present letter is mainly related to this hypothesis. In the following we are going to show that the fluctuating diamagnetism (FD) above $T_c$ does reflect the presence of both the $\sigma$ and $\pi$ bands which from a variety of effects are known to occur in MgB$_2$ below $T_c$.

New magnetization measurements, with high temperature and field resolution have been carried out above $T_c = 39.1 K \pm 0.04 K$, on a high-purity sample prepared by Palenzona et al. (University of Genova). The diamagnetic contribution was obtained by subtracting from the raw data the paramagnetic contribution measured at 40K (where the SF are practically ineffective). The data obtained in a powdered sample at three representative temperatures are reported in Fig.1.
The field dependence of FD can be understood in the framework of Ginzburg-Landau (GL) theory in a simple way, by resorting to a description based on fluctuation-induced superconducting droplets of spherical shape, with diameter of the order of the coherence length. For these droplets the so-called zero-dimensional (0-D) approximation can be used, by assuming an order parameter no longer spatially dependent. Then an exact solution for the GL functional is found in closed form, valid above the critical region and for all field $H \ll H_{c2}$. This was basically the framework used in the discussion of the data in Ref. [4].

Recently, SF in the presence of two superconducting bands has been studied in regards of the paraconductivity and of the specific heat in MgB$_2$ [6]. In this work a breakdown of the GL theory is hypothesized, due to two different coherence lengths for the $\sigma$ and $\pi$ bands. In particular, the difference is relevant in the $z$-direction, i.e. $\xi_{\sigma z} \ll \xi_{\pi z}$. An effective coherence length $\tilde{\xi}_z(T)$ is introduced, with $\xi_{\sigma z} \ll \tilde{\xi}_z(T) \ll \xi_{\pi z}$, in a large temperature range where a generalized non-localized GL model can be used [6].

A system with weakly-coupled two bands labelled by 1 (in MgB$_2$ the $\sigma$ band) and 2 (in MgB$_2$ the $\pi$ band) is considered and pairs can be formed only by electrons belonging to the same band. The pairing correlation matrix contains non-diagonal terms, allowing the pair to transfer from one band to the other. Dealing with the impurity scattering, it is known that in MgB$_2$ the interband contribution is very weak, because of the different parity of the bands. Thus the transfer process can be neglected and only the scattering frequency $\nu_1$ and $\nu_2$ in the two bands is considered. The inverse of the effective coupling matrix is introduced

$$\tilde{W} = \begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{pmatrix}$$

such that $W_{11}W_{22} - W_{12}W_{21} = 0$.

The free energy above $T_c$ is determined by the fluctuation propagator [6]

$$F = -k_B T V \int \frac{d^3 q}{(2\pi)^3} \ln \frac{A}{\det H_{\alpha \beta}}.$$  \hspace{1cm} (1)$$

where $H_{\alpha \beta}(q)$ is the linearized GL Hamiltonian density.
\[
H_{\alpha\beta} = \begin{pmatrix}
\nu_1 (\xi_{1,a}^2 q_a^2 + W_{11} + \epsilon) & -\nu_2 W_{12} \\
-\nu_1 W_{21} & \nu_2 \left[ W_{22} + \epsilon + f (\xi_{2z}^2 q_z^2) \xi_{2x}^2 q_x^2 + g \left( \frac{2}{\pi^2} \xi_{2z}^2 q_z^2 \right) \right]
\end{pmatrix}
\]  
\tag{2}

with \( \epsilon = \frac{T - T_c}{T_c} \). Here \( g(x) = \psi(1/2 + x) - \psi(x) \) and \( f(x) = \frac{2}{\pi^2} g'(x) \), while \( \xi_{1,a}^2 q_a^2 = \xi_{1x}^2 q_x^2 + \xi_{1y}^2 q_y^2 + \xi_{1z}^2 q_z^2 \).

At a temperature close to \( T_c \), where \( \tilde{\xi}_z(T) \gg \xi_{2z}(0) \), only the long wave-length fluctuations of the order parameter can be taken into account. In this case, in the 0-D approximation and when written in terms of the effective coherence length \( \tilde{\xi}(T) \), the magnetization takes the form \[2\],

\[
M_{\text{dia}}(\epsilon, H) = -K_B T H \frac{2\pi^2 \tilde{\xi}^2 d^2 / 5\Phi_0^2}{(\epsilon + 2\pi^2 \tilde{\xi}^2 H^2 d^2 / 5\Phi_0^2)}
\]  
\tag{3}

Here \( \Phi_0 \) is the flux quantum and \( d \) the size of fluctuating droplets, that can be assumed of the order of \( \tilde{\xi}(T) \). Eq. \[3\] predicts a single upturn in the field dependence of \( M_{\text{dia}} \), at a field \( H_{\text{up}} \approx \sqrt{5\xi^2 / \pi \tilde{\xi}^2} \).

For temperatures not too close to \( T_c \), the short wave-length fluctuations are accounted for by a large value of the argument in the \( g \) and \( f \) functions in Eq. \[2\]. In order to obtain the fluctuating magnetization, the full expression of the free energy has to be derived. By assuming \( \gamma = \frac{\xi_{1z}^2}{\xi_{1x}^2} \) as a measure of the anisotropy between the plane and z-axis and neglecting the in-plane anisotropy, one writes

\[
\xi_{1,a}^2 q_a^2 = \frac{H^2}{H_{c1x}^2} \left( 1 + \frac{\gamma}{2} \sin^2 \theta \right)
\]

\[
\xi_{2x}^2 q_x^2 = \xi_{2x}^2 \left( q_x^2 + q_y^2 \right) = \frac{H^2}{H_{c2x}^2}
\]

\[
\xi_{2z}^2 q_z^2 = \frac{H^2}{H_{c2z}^2} \sin^2 \theta
\]  
\tag{4}

where \( \theta \) is the angle between \( H \) and the z-axis. In MgB\(_2\) it can be assumed \( \xi_{1x} \approx \xi_{2x} \) so that the critical fields become \( H_{c1x}^2 = H_{c2x}^2 = \frac{8\phi_0^2}{\pi^2 \xi_{1x}^2 d^2} \) and \( H_{c2z}^2 = \frac{16\phi_0^2}{\pi^2 \xi_{2z}^2 d^2} \).

From Eqs.\[1\] and \[2\] , by taking into account Eqs.\[4\], a lengthy expression for the angular-dependent diamagnetic magnetization is obtained. For external field along the z-axis no double structure in the magnetization curves is present, as it could be expected since
only one effective correlation length is involved:

\[ M_{dia}(T = \text{const}, \theta = 0, H) = -2k_B TVH \left[ \frac{1}{H_{cx}^2} \left( 1 + \frac{\pi^2}{2} \right) \epsilon + \frac{1}{H_{cx}^2} \left( W_{22} + \frac{\pi^2}{2} W_{11} \right) + \frac{\pi^2 H^2}{H_{cx}^4} \right] \] (5)

On the contrary for field in the \( ab \)-plane the magnetization turns out

\[ M_{dia}(T = \text{const}, \theta = \frac{\pi}{2}, H) = -\frac{\pi k_B T d^3 H}{3S(H)} \left[ \frac{1}{H_{cx}^2} \left( 1 + \frac{1}{2} \gamma \right) + f \left( \frac{\pi^2}{2} t \right) + H^2 f' + H^2 g' \right] \frac{\epsilon}{H_{cx}^2} \] (6)

where \( t = \frac{2}{\pi^2 \epsilon^2 H_{cx}^2} \) and \( g' \) and \( f' \) are the derivative of \( g \) and \( f \) functions with respect to \( H^2 \). In Eq.(6) the function \( S(H) \) takes the form

\[ S(H) = W_{11} + W_{22} + \frac{H^2}{H_{cx}^2} \left( 1 + \frac{1}{2} \gamma \right) \left[ f \left( \frac{\pi^2}{2} t \right) + H^2 g \right] \epsilon + \frac{H^2}{H_{cx}^2} \left[ W_{11} + \frac{H^2}{H_{cx}^2} \left( 1 + \frac{1}{2} \gamma \right) \right] \] (7)

In Fig.2 the theoretical magnetization resulting from this equation is reported for a representative value of the reduced temperature \( \epsilon \) and compared with the one derived for single band, for the effective correlation length. It is noticeable how the shape of the magnetization curve is affected by the two bands, displaying a double structure which resembles two upturn fields.

Single crystals of MgB\(_2\) large enough to yield a size of diamagnetic signal above \( T_c \) are not available and therefore our measurements have been carried out in powders. Thus the data reported in Fig.1 can be considered approximately correspondent to the theoretical case of \( \theta \approx \frac{\pi}{2} \). From the inset in Fig.1 it is noted that for \( T \) close to \( T_c \) one has a magnetization curve similar to the dashed one in Fig.2. This type of field dependence, with a single upturn field, can be considered a signature of the validity of the GL regime, for \( \epsilon \approx 3 \times 10^{-3} \). Eq. (8)
gives a satisfactory fitting of the data in correspondence to a value $\tilde{\xi} = 22\, \text{nm}$, compatible with the coherence length (see Ref. [7]).

For $T$ not too close to $T_c$, $M_{dia}$ should be discussed in terms of the angular dependent full expression (not reported here), by averaging over $\theta$. By using for a qualitative illustration the form of the magnetization pertaining to $\theta = \frac{\pi}{2}$ a reasonable fit of the data is obtained (Fig.3). In the fit we have used $\gamma \simeq 0.02$. The critical fields turn out $H_{c1x} = 9.8 \times 10^4\, \text{Oe}$ and $H_{c2z} = 11.5 \times 10^2\, \text{Oe}$, dependent on temperature through $d = \tilde{\xi}(T) = \tilde{\xi}(0)\varepsilon^{-1/2}$. $W_{11}$ and $W_{22}$ depend on temperature. Far from $T_c$ the superconductive coupling in the $\pi$ band is weak and this corresponds to a large $W_{22}$. In the inset of Fig.3 the ratio $W_{11}/W_{22}$ is plotted as a function of the reduced temperature, showing a dependence of the form $W_{11}/W_{22} \sim \varepsilon^2$. The ratio of the magnetization values at the upturn fields $M_{up1}/M_{up2}$ shows the same temperature dependence. This evidences that the SF involving the $\pi$ band are supressed at a field smaller than the ones related to the $\sigma$ band. By increasing the temperature the decrease of the coupling in the $\pi$ band produces a reduced contribution to the fluctuating magnetization.

By summarizing, in this work we have shown that the presence of the two SC $\sigma$ and $\pi$ bands in MgB$_2$ has a noticeable effect also in the fluctuating diamagnetism above $T_c$. By adapting to the fluctuating diamagnetism the approach recently developed for the paraconductivity, a model extending the Ginzburg-Landau formalism to include the effect of non-evanescent magnetic field has been developed. In particular, by relying on the zero-dimensional approximation for the superconducting droplets the model has been proved to account for the basic aspects of the experimental findings.

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Captions for figures

Fig.1 Diamagnetic contribution $M_{dia}$ to the magnetization in MgB$_2$ as a function of the magnetic field $H$ (after zero field cooling), for three temperatures above $T_c = 39.1 \pm 0.04\, K$. No difference was observed for the magnetization in field-cooled condition at the
same temperature (data not reported). In the inset the data for $M_{dia}$ at a temperature close to $T_c$ are reported, showing that for $H$ smaller than the upturn field $H_{up}$ the GL law in finite field, namely $M_{dia}(H,T \approx T_c) \propto -\sqrt{H}$ (solid line), is well obeyed.

Fig.2 Comparison of the field dependence of the fluctuating magnetization above $T_c$, for reduced temperature $\epsilon = 8 \times 10^{-3}$, in the case of a single superconducting band (dashed lines) and for the $\sigma$ and $\pi$ bands (solid line).

Fig.3 Fits of the magnetization curves at two representative temperatures above $T_c$ in powered MgB$_2$ (see Fig.1) on the basis of the theoretical expression (Eq. (6)) in the text, according to the generalized, non-local GL functional. In the inset the temperature dependence of the ratios $\frac{W_{11}}{W_{22}}$ and $\frac{M_{dia}(H_{up}^1,T)}{M_{dia}(H_{up}^2,T)}$ are reported. The departure between the theoretical prediction and the experimental data for $H \to 0$ is likely to be due to the subtraction procedure. In fact a very small amount of ferromagnetic impurities could enhance the paramagnetic term for small fields.

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Fig. 1
