Pressure and isotope effect on the anisotropy of MgB$_2$

T. Schneider$^1$ and D. Di Castro$^{1,2}$

$^{(1)}$ Physik-Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

$^{(2)}$ INFM-Coherentia and Dipartimento di Fisica, Università di Roma “La Sapienza”, P.le A. Moro 2, I-00185 Roma, Italy

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Abstract

We analyze the data for the pressure and boron isotope effect on the temperature dependence of the magnetization near $T_c$. Invoking the universal scaling relation for the magnetization at fixed magnetic field it is shown that the relative shift of $T_c$, induced by pressure or boron isotope exchange, mirrors essentially that of the anisotropy. This uncovers a novel generic property of anisotropic type II superconductors, inexistent in the isotropic case. For MgB$_2$ it implies that the renormalization of the Fermi surface topology due to pressure or isotope exchange is dominated by a mechanism controlling the anisotropy.
It is well documented that both, hydrostatic pressure\(^1\) and boron isotope exchange\(^2,3\) lead in MgB\(_2\) to a reduction of the transition temperature \(T_c\). To be specific, the dependence of \(T_c\) on hydrostatic (He-gas) pressure has been determined to 1 GPa. \(T_c\) was found to decrease linearly and reversibly under pressure at the rate \(dT_c/dP = -1.11 \pm 0.02\) K/GPa\(^1\), consistent with \(dT_c/dP = -1.24 \pm 0.05\) K/GPa reported by Di Castro et al.\(^4\). This corresponds with \(T_c = T_c(P = 0) = 39.3\) K to the relative change \(\Delta T_c/T_c \simeq -0.04\) at \(P = 1.13\) GPa. Nearly the same value, \(\Delta T_c/T_c \approx -0.03\) was derived from the change of the magnetization upon boron isotope exchange\(^2,3\). Although the anisotropy of MgB\(_2\) is moderate, the compressibility along the \(c\)-axis is significantly (64\%) larger than that along the \(a\)-axis\(^1\). Thus, the binding within the boron layers is stronger than between the layers. Reversible torque\(^5\) and magnetization measurements\(^6\) near \(T_c\) also revealed anisotropic superconducting properties characterized by \(\gamma(T_c) = \xi_a/\xi_c = \lambda_c/\lambda_a \approx 2\), where \(\xi_{a,c}\) denote the correlation lengths and \(\lambda_{a,c}\) the magnetic penetration depths along the \(a\)- and \(c\)-axis. Since in a superconductor increasing anisotropy drives a 3D to 2D crossover, enhances thermal fluctuations and reduces \(T_c\), the anisotropy is an important characteristic both for the basic understanding of superconductors and for applications. For example, Dahm and Schopohl\(^7\) calculated \(\gamma\) in the clean limit based on a detailed modelling of the electronic structure that took into account the Fermi surface topology and the two-gap nature of the mean-field order parameter. It was shown that the strong temperature dependence of the anisotropy can be understood as an interplay of the dominating gap in the \(\sigma\) band, which possesses a small \(c\)-axis component of the Fermi velocity, with the induced superconductivity on the \(\pi\)-band possessing a large \(c\)-axis component of the Fermi velocity. Furthermore, the anisotropy strongly affects the pinning and critical currents.

Here, we concentrate on the behavior near \(T_c\), where thermal fluctuations must be taken into account, as evidenced by the excess specific heat\(^8\) and the magnetoconductivity\(^9\). Noting that these fluctuations mediate universal behavior, e.g. a universal relation between magnetization, anisotropy \(\gamma\) and transition temperature \(T_c\), an analysis of the pressure and isotope effect on the magnetization should uncover the universal behavior of anisotropic superconductors and provide stringent constraints for microscopic treatments. We analyze the data for the pressure\(^4\) and boron isotope\(^2,3\) effect on the temperature dependence of the magnetization near \(T_c\). Here an effective single gap description is appropriate\(^10\). When three-dimensional (3D) Gaussian or 3D-XY thermal fluctuations dominate, the combination
\[ m(T, \delta, H) / \left( \gamma e^{3/2}(\delta) T \sqrt{H} \right) \] adopts then at \( T_c \) a fixed value \[ 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21 \]

where \( m = M/V \) is the magnetization per unit volume, \( C \) a constant adopting for Gaussian and 3D-XY fluctuations distinct universal values. Furthermore, \( \epsilon(\delta) = \left( \cos^2(\delta) + \sin^2(\delta)/\gamma^2 \right)^{1/2} \), where \( \delta \) is the angle between the applied magnetic field \( H \) and the \( c \)-axis, \( \Phi_0 \) the flux quantum, and \( k_B \) the Boltzmann constant. Thus, plotting \( m(T) / \left( \gamma e^{3/2}(\delta) \sqrt{H} \right) \) vs. \( T \), the data taken in different fields cross at \( T_c \). In powder samples this relation reduces to

\[ m(T_c) \sqrt{H} f(\gamma(T_c)) = -k_B C \Phi_0^{3/2}, \quad f(\gamma(T_c)) = \left[ \gamma \left( e^{3/2}(\gamma, \delta) \right) \right]_{T_c}. \]  

As the isotope and pressure effect on the magnetization at fixed magnetic field is concerned it implies that the relative shifts of magnetization per unit volume \( m \), anisotropy \( \gamma \) and \( T_c \) are not independent but related by

\[ \Delta m(T_c) / m(T_c) = \Delta M(T_c) / M(T_c) - \Delta V(T_c) / V(T_c) = \Delta f(\gamma(T_c)) / f(\gamma(T_c)) + \Delta T_c / T_c. \]  

On that condition it is impossible to extract these changes from the temperature dependence of the magnetization. However, supposing that close to criticality the magnetization data scale within experimental error as

\[ iM(T) = jM(aT), \]  

where \( i \neq j \) \( M \) denotes the magnetization for different isotopes or taken at different pressures, the universal relation \( \text{(4)} \) reduces to

\[ -\frac{\Delta T_c}{T_c} = \Delta V(T_c) / V(T_c) + \frac{\Delta f(\gamma(T_c))}{f(\gamma(T_c))} = 1 - a. \]  

Hence, when Eq.\( \text{(4)} \) holds true, the pressure and isotope effect on \( T_c \) mirrors that of the anisotropy \( \gamma = \xi_{ab}/\xi_c = \lambda_{ab}/\lambda_c \) and of the volume. In particular, when \( \gamma(T_c) >> 1, \) \( f(\gamma(T_c)) \rightarrow 0.556\gamma(T_c) \) and with that \( -\Delta T_c / T_c = \Delta V(T_c) / V(T_c) + \Delta \gamma / \gamma. \)

We are now prepared to analyze the experimental data for the pressure and isotope effect on the magnetization of MgB\(_2\). While the volume change upon isotope exchange is negligible, it can be appreciable by applying pressure. In terms of the bulk modulus \( B \approx 147.2 \text{ GPa} \)
FIG. 1: Field cooled (0.5mT) magnetization of a MgB$_2$ powder sample vs. $T$ near $T_c$ for $P = 0.15$ and $P = 1.13$ GPa taken from Di Castro et al. [4]. The dots are the $P = 0.15$ data rescaled according to Eq.(4) with $a = 0.968$.

it is given by $\Delta V/V = -\Delta P/B$ so that for $\Delta P \simeq 1$ GPa, $\Delta V/V \simeq -0.007$. In Fig[1] we displayed the field cooled (0.5mT) magnetization of a MgB$_2$ powder sample vs. $T$ near $T_c$ for $P = 0.15$ and $P = 1.13$ GPa taken from Di Castro et al. [4]. The dots are the $P = 0.15$ data rescaled according to Eq.(4) with $a = 0.968$. Noting that the rescaled $P = 0.15$ data collapse near $T_c$ within experimental error onto the $P = 1.13$ GP data, $\Delta M/M \simeq 0$ follows and Eq.(5) applies as

$$-\frac{\Delta T_c}{T_c} = \frac{\Delta V(T_c)}{V(T_c)} + \frac{\Delta f(\gamma(T_c))}{f(\gamma(T_c))} = 1 - a \simeq 0.032.$$  \hspace{1cm} (6)

To check the scaling analysis we note that the pressure dependence of $\Delta T_c/T_c = (T_c(P) - T_c(0))/T_c(0)$ is well described by $\Delta T_c/T_c = -0.032P$ with $P$ in GPa[4], yielding for $\Delta P = 0.98$ GPa the value $\Delta T_c/T_c = -0.032$, in excellent agreement with our estimate. In addition to it, the scaling analysis reveals that the pressure induced reduction of $T_c$ is mainly due to the anisotropy. Indeed, since $\Delta T_c/T_c \simeq 4.5\Delta V(T_c)/V(T_c) \simeq -0.032$, there is a significantly larger and positive anisotropy contribution $\Delta f(\gamma(T_c))/f(\gamma(T_c)) \simeq 0.04$. Noting that $f(\gamma)$, displayed in Fig[2] increases with $\gamma$ the anisotropy is found to increase with pressure.

Next we turn to the boron isotope effect. In Fig[3] we show the normalized zero field cooled magnetization data vs. $T$ near $T_c$ of a Mg$^{10}$B$_2$ and Mg$^{11}$B$_2$ powder samples taken from Hinks et al. [2] (Fig[3a]) and Di Castro et al. [3] (Fig[3b]). The dots are the Mg$^{10}$B$_2$ data rescaled according to Eq.(4) with $a = 0.972$ (Fig[3a]) and $a = 0.974$ (Fig[3b]). Apparently,
FIG. 2: \( f(\gamma) = \gamma \langle \varepsilon(\gamma)^{3/2} \rangle \) vs. \( \gamma \). The straight line indicates the asymptotic behavior in the limit \( \gamma \to \infty \), where \( f(\gamma) = \gamma \langle |\cos(\delta)|^3 \rangle \approx 0.556\gamma \).

\[ \Delta M/M \approx 0 \text{ within experimental error. Thus} \]

\[ -\frac{\Delta T_c}{T_c} = \frac{\Delta V(T_c)}{V(T_c)} + \frac{\Delta f(\gamma(T_c))}{f(\gamma(T_c))} = 1 - a \approx 0.028, 0.026, \quad (7) \]

close to the value emerging from the pressure effect at 1.13 GPa (Eq. (6)) and the estimate of Hinks et al.\[2\]. Since there is no conclusive evidence for any significant lattice constant change for this isotope exchange\[23\], the volume change appears to be negligibly small so that \( |\Delta V(T_c)/V(T_c)| \ll \Delta f(\gamma(T_c))/f(\gamma(T_c)) \) holds. Hence, in analogy to the pressure effect, the reduction of \( T_c \) reflects essentially an increase of the anisotropy and with \( \Delta \gamma(T_c)/\gamma(T_c) = \Delta \lambda_c(T_c)/\lambda_c(T_c) - \Delta \lambda_a(T_c)/\lambda_a(T_c) \) a change of the \( c \)-axis and / or in-plane magnetic penetration depths. Within the microscopic mean-field scenario\[7, 24, 25\], it implies a renormalization of the Fermi surface topology due to thermal fluctuations modified by isotope exchange or applied pressure.

To summarize, we have shown that in the two-band superconductor MgB\(_2\) the relative change of the transition temperature upon Boron isotope exchange or applied pressure mirrors near \( T_c \) essentially that of the anisotropy. Because this property stems from 3D-Gaussian or 3D-XY thermal fluctuations and the experimental fact that close to \( T_c \) the magnetization scales within experimental error as \( i M(T) = \bar{j} M(\bar{a}T) \), where \( i \neq j \) \( M \) denotes the magnetization for different isotopes or taken at different pressures, it appears to be a universal property of anisotropic type II superconductors. Indeed, in a variety of cuprate
FIG. 3: Zero field cooled magnetization data at fixed magnetic field vs. $T$ near $T_c$ of a Mg$^{10}$B$_2$ and Mg$^{11}$B$_2$ powder samples taken from Hinks et al. [2] (Fig. 3a) and Di Castro et al. [3] (Fig. 3b). The open circles are the Mg$^{10}$B$_2$ data rescaled according to Eq.(4) with $a = 0.972$ (Fig. 3a) and $a = 0.974$ (Fig. 3b).

superconductors the relative change of $T_c$ upon isotope exchange was also found to mirror that of the anisotropy [21]. Thus, in anisotropic type II superconductors the pressure or isotope exchange induced variation of $T_c$ does not single out the mechanism mediating superconductivity but mirrors predominantly the change of the anisotropy, which puts a stringent constraint on microscopic treatments.

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[⁎] Corresponding author: T.Schneider

Email address: toni.schneider@swissonline.ch

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