Quantum Superconductor-Metal Transition in Al, C doped MgB$_2$ and overdoped Cuprates?

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We consider the realistic case of a superconductor with a nonzero density of elastic scatterers, so that the normal state conductivity is finite. The quantum superconductor-metal (QSM) transition can then be tuned by varying either the attractive electron-electron interaction, the quenched disorder, or the applied magnetic field. We explore the consistency of the associated scaling relations, $T_c \propto \lambda(0)^{-1} \propto \Delta(0) \propto \xi(0)^{-1} \propto H_{c2}(0)^{1/2}$ and $T_c(H) \propto \lambda(0, H)^{-1} \propto \Delta(0, H) \propto (H_{c2}(0) - H)^{1/2}$, valid for all dimensions $D > 2$, with experimental data, in Al, C doped MgB$_2$ and overdoped cuprates.

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Understanding the phenomenon of superconductivity, now observed in quite disparate systems, such as simple elements, fullerenes, molecular metals, cuprates, borides, etc., involves searching for universal relations between superconducting properties across different materials, which might provide hints towards a unique classification. In spite of the great impact of the BCS theory [1], the discovery of superconductivity in the cuprates in 1986 [2] made it clear that the BCS relations between the critical amplitudes of the gap ($\Delta_0$), the correlation length ($\xi_0$), the magnetic penetration depth ($\lambda_0$), the upper critical field ($H_{c2}$) and the transition temperature $T_c$, namely

$$T_c \propto \lambda_0^{-1} \propto \Delta_0^{-1} \propto \xi_0^{-1} \propto H_{c2}^{1/2},$$

(1)

Here, $\lambda(T) = \lambda_0 t^{1/2}$, $\Delta(T) = \Delta_0 t^{1/2} \simeq 1.76 \Delta(0) t^{1/2}$, $\xi(T) = \xi_0 t^{-1/2}$, and $H_{c2} = H_{c20} t$, close to the superconductor metal transition, with $t = 1 - T/T_c$ and $2\Delta(0) / (k_B T_c) \simeq 3.52$. Furthermore, there are empirical relations between $T_c$ and the zero-temperature superfluid density, $\rho_s(0)$, related to the zero-temperature magnetic field penetration depth $\lambda(0)$ in terms of $\rho_s(0) \propto \lambda^{-2}(0)$. In various families of underdoped cuprate superconductors there is the empirical relation $T_c \propto \rho_s(0) \propto \lambda^{-2}(0)$, first identified by Uemura et al. [4, 5], while in molecular superconductors, $T_c \propto \lambda^{-3}(0)$, appears to apply [6]. Both scaling forms appear to have no counterpart in the BCS scenario and even in more conventional superconductors, including Mg$_{1-x}$Al$_x$B$_2$, Mg(C$_x$B$_{1-x}$)$_2$, and MgB$_{2+x}$, such relationships remain to be explored.

According to the theory of quantum critical phenomena a power law relation between $T_c$ and $\rho_s(0) \propto \lambda^{-2}(0)$ is expected whenever there is a critical line $T_c(x)$ with a critical endpoint $x = x_c$ [7, 8, 9]. Here the transition temperature vanishes and a quantum phase transition occurs. $x$ denotes the tuning parameter of the transition. A variety of underdoped cuprate superconductors exhibits such a critical line, ending at the quantum superconductor to insulator (QSI) transition, where the materials become essentially two dimensional [10]. If the finite temperature behavior in this regime is controlled by the $3D - xy$ critical point, $T_c$ and $\rho_s(0)$ scale as

$$T_c \propto \rho_s(0)^{2/(D+z-2)}.$$

(2)

$z$ denotes the dynamic critical exponent of the quantum transition in $D$ dimensions. For $D = 2$ we recover the empirical Uemura relation, $T_c \propto \rho_s(0)$ [4, 5], irrespective of the value of $z$.

There is also considerable evidence for a critical line $T_c(x)$ in more conventional superconductors, including Mg$_{1-x}$Al$_x$B$_2$, Mg(C$_x$B$_{1-x}$)$_2$, MgB$_{2-x}$Be$_x$, and NbB$_{2+x}$, where superconductivity disappears at some critical value $x = x_c$ [11, 12, 13, 14], whereupon a quantum superconductor to metal (QSM) transition is expected to occur. To illustrate this behavior we depicted in Fig. 1 the data for $T_c$ vs. the nominal concentration $x$ for Mg$_{1-x}$Al$_x$B$_2$ and Mg(C$_x$B$_{1-x}$)$_2$ taken from Postorino et al. [11] and Gonnelli et al. [12].

![FIG. 1: (Color online) $T_c$ vs. the nominal concentration $x$ for Mg$_{1-x}$Al$_x$B$_2$ and Mg(C$_x$B$_{1-x}$)$_2$ taken from Postorino et al. [11] and Gonnelli et al. [12].](image-url)
transition occurs in $D = 3$. Furthermore, there is considerable evidence that on increasing the Al or C content the homogeneity and the crystallographic order decrease even in segregation-free samples\cite{15, 16, 17}.

Since in these nearly isotropic materials the anisotropy does not change substantially upon substitution the QSM transition occurs in $D = 3$. Furthermore, there is considerable evidence that on increasing the Al or C content the homogeneity and the crystallographic order decrease even in segregation-free samples\cite{15, 16, 17}.

For this reason we consider the realistic case of a superconductor with a nonzero density of elastic scatterers, so that the normal state conductivity is finite. In the absence of an applied magnetic field the QSM transition can then be tuned by varying either the attractive electron-electron interaction, or the quenched disorder. In a theoretical description, quenched disorder can occur on a microscopic level, e.g., due to randomly distributed scattering centers. For such systems it was shown that the upper critical dimension $D^*_c$, above which the critical behavior is governed by a simple Gaussian fixed point (FP), is lower than that of the corresponding classical or finite temperature transition, namely $D^*_c = 2$\cite{18, 19}. For $D > 2$ the transition is then governed by a Gaussian FP with unusual properties. Since the mean-field/Gaussian theory yields the exact critical behavior at $T = 0$, all relations between observables that are derived at finite temperature within BCS theory are valid. Accordingly, the zero temperature counterpart of the scaling relation reads

$$T_c \propto \lambda(0)^{-1} \propto \Delta(0) \propto \xi(0)^{-1} \propto H_{c2}(0)^{1/2}, \quad (3)$$

while $T_c$ and the dimensionless distance from the critical point $\delta$ ($\delta < 0$ in the disordered phase) are related by \cite{18}

$$T_c \propto \exp(-1/|\delta|). \quad (4)$$

Hyperscaling is violated by the usual mechanism that is operative above an upper critical dimension. Indeed, this QSM transition occurs in $D = 3$, while the upper critical dimension of the QSM transition is $D^*_c = 2$\cite{18, 19}. For this reason the scaling relation (2), involving hyperscaling, does not apply in the present case where $z = 2$\cite{18}.

We are now prepared to confront the scaling predictions for a disorder tuned QSM transition with experiment. In Fig. 2 we show $T_c$ vs. zero-temperature muon-spin depolarization rate $\sigma(0)$ vs. $H_{c2}$ for Mg$_{1-x}$Al$_x$B$_2$ taken from Serventi et al.\cite{20}. Although the data is rather sparse, in particular close to the QSM transition, the reduction of the superfluid density $\rho_s(0) \propto \Delta(0) \propto \lambda^{-2}(0)$ with decreasing $T_c$ is clearly observed, consistent with the flow to the QSM transition where $T_c$ and $\sigma(0)$ scale as $T_c \propto 1/\lambda(0) \propto \sigma(0)^{1/2}$ (Eq. (3)).

To substantiate this supposition further, we consider the $T_c$ dependence of the gap $\Delta(0)$. In Fig. 3 we depicted the experimental data of Daghero et al.\cite{17} for the two gap superconductor Mg$_{1-x}$Al$_x$B$_2$. Although the data does not extend very close to the QSM transition, the flow to $T_c \propto \Delta(0)$ (Eq. (3)) can be anticipated.

![FIG. 2: (Color online) $T_c$ vs. zero-temperature muon-spin depolarization rate $\sigma(0)$ for Mg$_{1-x}$Al$_x$B$_2$ derived from Serventi et al.\cite{20}. The solid line is Eq. (3) in terms of $T_c = 9.7\sigma_{sc}(0)^{1/2}$.](image)

![FIG. 3: (Color online) $\Delta_s(0)$ and $\Delta_\pi(0)$ vs. $T_c$ for Mg$_{1-x}$Al$_x$B$_2$ single crystals (sc) and polycrystals (pc) taken from Daghero et al.\cite{17}. The solid and dashed lines are Eq. (3) in terms of $\Delta_s(0) = 0.22T_c$ and $\Delta_\pi(0) = 0.08T_c$.](image)

According to Fig. 3 showing $\Delta_s(0)$ and $\Delta_\pi(0)$ vs. $T_c$ for Mg$_{1-x}$Al$_x$B$_2$ single crystals taken from Gonnelli et al.\cite{17}, the flow to the QSM transition (Eq. (3)) is apparent in the $\sigma$-gap as well, while the $\pi$-gap, nearly constant down to $T_c = 19$ K, appears to merge the $\sigma$-gap below this transition temperature\cite{15}.

Next we turn to the $T_c$ dependence of the upper critical fields $H_{c2}^{\text{sc}}(0)$ and $H_{c2}^{\text{pc}}(0)$. Although the experimental
increase of the correlation lengths as the QSM transition is approached.

The solid line is Eq. (3) in terms of $\Delta c(0) = 0.18T_c$.

data for Mg$_{1-x}$Al$_x$B$_2$ single crystals taken from Klein et al. [16] and Kim et al. [21] shown in Fig. 5 is rather sparse, consistency towards QSM scaling behavior $H_{c2}^{ab,c}(0) \propto T_c^2$ (Eq. (4)), indicated by the solid and dashed lines, can be anticipated. From these lines we deduce for the zero temperature anisotropy the estimate $\gamma(0) = (H_{c2}^a(0) / H_{c2}^{ab}(0))^{1/2} = \xi_{ab}(0) / \xi_c(0) \approx 1.9$. Because $H_{c2}^{ab}(0) \propto \xi_c(0)^{-2} \propto T_c^2$ and $H_{c2}^a(0) \propto \xi_{ab}(0)^{-2} \propto T_c^2$ the reduction of the upper critical fields mirrors the increase of the correlation lengths as the QSM transition is approached.

Finally we consider the magnetic field tuned QSM transition for fixed $x$. Noting that the correlation length and the magnetic field scale as $\xi(0)^2 (H_{c2}(0, x) - H) \propto \Phi_0$, together with Eq. (4), the zero temperature gap scales then close to the QSM transition as

$$\Delta(0, x) \propto (H_{c2}(0, x) - H)^{1/2}. \quad (5)$$

Here the critical line $T_c(x, H)$ ends at $H_{c2}(T = 0, x)$. In Fig. 6 we depicted $\Delta \pi (T = 6.5 K)$ vs. $H$ applied along the $c$-axis of a Mg$_{1-x}$Al$_x$B$_2$ single crystals with $x = 0.2$ ($T_c \approx 24 K$) taken from Giubileo et al. [22]. Although Eq. (5) represents the asymptotic behavior we observe remarkable agreement with the local tunneling data over the entire magnetic field range. Clearly, the occurrence of the magnetic field tuned QSM transition is not restricted to the gap. From Eqs. (3) and (5) we deduce

$$T_c(x, H) \propto \lambda(0, x, H)^{-1} \propto \Delta(0, x, H) \propto (H_{c2}(0, x) - H)^{1/2}, \quad (6)$$

which remains to be tested experimentally.

FIG. 6: (Color online) $\Delta \pi (T = 6.5 K, x = 0.2)$ vs. $H$ applied along the $c$-axis of Mg$_{1-x}$Al$_x$B$_2$ single crystals taken from Giubileo et al. [22]. The solid line is Eq. (3) in terms of $H_{c2}^{ab}(0) = 0.0085T_c^2$ and $H_{c2}^a(0) = 0.003T_c^2$.

The corresponding schematic phase diagram is shown in Fig. 7. As the substituent concentration or the magnetic field is increased $T_c$ is suppressed and driven all the way to zero, where along the line $H_{c2}(T = 0, x)$ the QSM transition, characterized by the scaling relations (3) and (6) occurs.

These scaling relations also imply that close to the QSM transition the isotope and pressure effects on these observables are not independent of one another. From Eqs. (3) and (6) we deduce for the relative changes upon isotope substitution or applied pressure the relations

$$\frac{\Delta T_c}{T_c} = \frac{\Delta a}{a} - \frac{\Delta \lambda(0)}{\lambda(0)} = \frac{\Delta b}{b} + \frac{\Delta \Delta(0)}{\Delta(0)} = \frac{\Delta c}{c} + \frac{\Delta H_{c2}(0)}{2H_{c2}(0)}. \quad (7)$$
where \( T_c = a/\lambda(0) = b\Delta(0) = cH_{c2}(0)^{1/2} \) and

\[
\frac{\Delta T_c(x, H)}{T_c(x, H)} = \frac{\Delta d}{d} - \frac{\Delta \lambda(0, x, H)}{\lambda(0, x, H)} = \frac{\Delta e}{e} + \frac{\Delta \Delta(0, x, H)}{\Delta(0, x, H)}
\]

\[
= \frac{\Delta f}{f} + \frac{\Delta H_{c2}(0, x)}{2H_{c2}(0, x)}
\]

where \( T_c(x, H) = d/\lambda(0) = e\Delta(0, x, H) = fH_{c2}(0, x)^{1/2} \). \( a \) to \( f \) are non-universal coefficients. We sketched, following Kirkpatrick and Belitz [18] the scaling relations of a quantum superconductor to metal (QSM) transition for nearly isotropic three dimensional systems, considering the realistic case of a superconductor with a nonzero density of elastic scatterers, so that the normal state conductivity is finite. The QSM transition can then be tuned by varying either the attractive electron-electron interaction, the quenched disorder, or the applied magnetic field. We have shown that Mg\(_{1-x}\)Al\(_x\)B\(_2\) and Mg(B\(_{1-x}\)C\(_x\))\(_2\), where increasing Al or C enhances the disorder even in segregation-free samples [15, 16, 17], are potential candidates to observe this QSM transition, characterized by the scaling relations [3], [6], [7], and [8]. Indeed, as a whole, the spare experimental data points to this QSM transition, but more extended experimental data are needed to confirm this characteristic scaling relation unambiguously. Indeed, based on band structure calculations and the Eliashberg theory, it was argued that the observed decrease of \( T_c \) of Al and C doped MgB\(_2\) samples can be understood mainly in terms of a band filling effect due to the electron doping by Al and C [23, 24]. Finally we note that NbB\(_{2+x}\) [14, 25, 26], Nb\(_{1-x}\)B\(_2\) [27], MgB\(_{2-x}\)Be\(_x\) [13] are additional potential candidates, as well as overdoped cuprates [28, 29, 30]. In particular, evidence for \( 1/\lambda(0)^2 \propto T_c^2 \) emerges for NbB\(_{2+x}\) from the muon-spin rotation study of Khasanov et al. [20]. Moreover, based on our analysis, a plot of \( T_c \) vs. \( 1/\lambda(0)^2 \) of cuprate superconductors should rise more steeply in the underdoped limit (\( T_c \propto 1/\lambda(0)^2 \)) than in the overdoped limit (\( T_c \propto 1/\lambda(0)^2 \)). Various experiments appear to support this behavior qualitatively [1]–[3] but more data are necessary to confirm it quantitatively. On the other hand, there is considerable experimental evidence [31] that for overdoped cuprates the zero temperature gap is proportional to \( T_c \) (Eq. [3]).

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[1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. 108, 1175 (1957).
[2] J. G. Bednorz, K. A. Müller, Z. Phys. B 64, 189 (1986).
[3] J. B. Ketterson and S. N. Song, Superconductivity, (Cambridge University Press, Cambridge 1999).
[4] Y.J. Uemura et al., Phys. Rev. Lett. 62, 2317 (1989).
[5] Y.J. Uemura et al., Phys. Rev. Lett. 66, 2665 (1991).
[6] F. L. Pratt, and S. J. Blundell, Phys. Rev. Lett. 94, 097006 (2005).
[7] K. Kim and P. B. Weichman, Phys. Rev. B 43, 13583 (1991).
[8] T. Schneider and J. M. Singer, Phase Transition Approach to High Temperature Superconductivity (Imperial College Press, London, 2000).
[9] T. Schneider, in The Physics of Superconductors (edited by K. H. Bennemann and J. B. Ketterson, Springer, Berlin, 2004).
[10] T. Schneider, Physica B 326, 289 (2003).
[11] P. Postorino et al., Phys. Rev. B 65, 020507 (2001).
[12] R.S. Gonnelli et al., J. of Physics and Chemistry of Solids 67, 360 (2006).
[13] J. S. Ahn, Young-Jin Kim, M.-S. Kim, S.-I. Lee, and E. J. Choi, Phys. Rev. B 65, 172503 (2002).
[14] R. Escamilla and L. Huerta, Supercond. Sci. Technol. 19, 623 (2006).
[15] R.S. Gonnelli et al., Phys. Rev. B 71, 060503(R) (2005).
[16] T. Klein et al., Phys. Rev. B 73, 224528 (2006).
[17] D. Daghero et al., cond-mat/0608020.
[18] T. R. Kirkpatrick and D. Belitz, Phys. Rev. Lett. 79, 3042 (1997).
[19] Lubo Zhou and T. R. Kirkpatrick, Phys. Rev. B 72, 024514 (2005).
[20] S. Serventi et al., Phys. Rev. Lett. 93, 217003 (2004).
[21] Heon-Jung Kim et al., Phys. Rev. B 73, 064520 (2006).
[22] F. Giubileo et al., cond-mat/0604354
[23] O. de la Peña, A. Aguayo, and R. de Coss, Phys. Rev. B 66, 012511 (2002).
[24] J. Kortus, O. V. Dolgov, and R. K. Kremer, Phys. Rev. Lett. 94, 027002 (2005).
[25] H. Takagiwa et al., J. Phys. Soc. Jpn. 73, 2631 (2004).
[26] R. Khasanov et al., unpublished.
[27] A. Yamamoto, C. Takao, T. Masui, M. Izumi, and S. Tajima, Physica C 383, 197 (2002).
[28] C. Niedermayer et al., Phys. Rev. Lett. 71, 1764 (1993).
[29] Y. J. Uemura et al., Nature 364, 605 (1993).
[30] C. Bernhard et al., Phys. Rev. B 52, 10488 (1995).
[31] D. C. Peets et al., cond-mat/0609250.