Multiband superconductors close to a 3D–2D electronic topological transition

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Partial substitution of Al or Sc for Mg in the simple ceramic compound MgB2 is known to be detrimental for superconductivity. Viewed from the opposite perspective, the enhancement of $T_c$ with decreasing Al content $1-x$ in Al$_{1-x}$Mg$_x$B$_2$ from $\sim 2$ K for $x=0.5$ to $T_c=39$ K for $x=1$ has been interpreted as evidence that high-$T_c$ superconductivity in MgB$_2$ is actually driven by the interband pairing by tuning the chemical potential near a 3D–2D topological transition in one of the subbands. This tuning enhances the critical temperature by a shape resonance in ultracold atoms. In Al$_1$, which is characterized by 3D behaviour, and is almost insensitive to the ETT. This is due to a ‘shape resonance’. Moreover we have calculated a possible variation of the isotope effect on the superconducting critical temperature by tuning the chemical potential.

A 3D–2D crossover in the $\sigma$ subband can be described in terms of an electronic topological transition (ETT) of the ‘neck disruption’ kind, according to I. M. Lifshitz’s terminology (see Refs. 13, 14 for recent reviews) The ETT is associated with a 3D–2D crossover of the Fermi surface of one of the two bands: the $\sigma$ subband of the diborides. Our results agree with the observed dependence of $T_c$ on Mg content $x$ and of the isotope exponent $\alpha$. Going from $x=1$ to $x=0.5$, the $E_{2g}$ phonon mode energy $\omega_{E_{2g}}$ increases from 70 to 115 meV, while the intra and interband electron-phonon couplings are characterized by unconventional behaviours, reflecting the proximity to such a shape resonance (see Ref. 14 and refs. therein).

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FIG. 1: Typical Fermi surfaces of MgB$_2$ below (left) and above (right) the ETT. The lighter sheet refers to the $\pi$ sub-band, which is characterized by 3D behaviour, and is almost insensitive to the ETT. This darker sheet refers to the $\sigma$ sub-band, which is characterized by a 3D (left) to 2D (right) crossover, as the ETT is traversed.

Here, we consider the effect of the proximity to a 3D–2D ETT on $T_c$ and on the isotope effect of the diborides within a mean-field approach to the two-band model. The total observed isotope exponent $\alpha$ in MgB$_2$ amounts to $\sim 0.3$, which is much smaller than the value $\alpha=\frac{1}{2}$ expected for a typical BCS superconductor. This has been interpreted in terms of strong electron-phonon coupling within Migdal-Eliashberg theory, although it has been pointed out that nonadiabatic corrections may be relevant to understand this anomaly.
A value of $s \approx 1$ can be used to describe a 3D subband, while $s \ll 1$ implies small dispersion along the z direction, and can be used therefore to model a quasi-2D subband. In the following, we will specifically employ the following set of parameters: $t^{(1)} = 0.6$ eV, $s^{(1)} = 0.167$, $\epsilon^{(1)} = 0$, for the $\sigma$ subband, and $t^{(2)} = 0.9$ eV, $s^{(2)} = 1$, $\epsilon^{(2)} = 2.9$ eV, for the $\pi$ subband. Fig. 1 shows the typical Fermi surfaces, $\xi^{(i)} = 0$, for $\mu$ close to the ETT value, $\mu_c = 2.19527$ eV (cf. Ref. 23). One recovers a 3D Fermi sheet corresponding to the $\pi$ subband, almost insensitive to small changes of $\mu \sim \mu_c$, and a tubular Fermi sheet corresponding to the $\sigma$ subband. As $\mu$ increases from below to above $\mu_c$, the latter Fermi sheet undergoes a 3D to 2D ETT.

The densities of states (DOS) $N_i(\xi)$ corresponding to the model dispersion relations, Eqs. 1, have been derived by several authors (see e.g. Ref. 24), also including a next-nearest neighbour hopping term, which is here neglected for the sake of simplicity. In the limit $s = 0$, $N_i(\xi)$ can be expressed analytically in terms of elliptic integrals, and is characterized by a logarithmic, Van Hove singularity at $\xi = 0$. While the $\pi$ subband has an almost constant DOS around the ETT, due to its 3D character, the DOS corresponding to the $\sigma$ subband displays a pronounced kink at $\mu = \mu_c$, which is where the Fermi surface changes its topology from 3D to 2D (Fig. 1). To avoid confusion, it should be emphasized that the quasi-Van Hove peak at $\mu = 0$, which is a consequence of the small value of $s^{(1)}$, will not be addressed by the present discussion. The almost singular behaviour at $\mu = 0$ is related to another ETT (corresponding to a change from hole- to particle-like character in the Fermi surface), whose relevance for the high-$T_c$ cuprates has been emphasized elsewhere (see e.g. Refs. 15, 16, and refs. therein).

Within the two-band model of superconductivity, the equation for $T_c$ (essentially, the linearized BCS gap equations for a two-band system) reads

$$-1 + V_{11} F_1^c + V_{22} F_2^c + (V_{12}^2 - V_{11} V_{22}) F_1^c F_2^c = 0, \quad (2)$$

with $\omega_D$ denoting the Debye frequency, and $\chi_c(\xi) = (2\xi)^{-1} \tanh(\beta_c \xi/2)$ the pairing susceptibility at the inverse critical temperature $\beta_c = (k_B T_c)^{-1}$. In the absence of interband coupling ($V_{12} = 0$), Eq. 2 factorizes into two equations, and the critical temperature is then the larger onset temperature of superconductivity in each band. In order to describe the superconducting diborides via the two-band model, a nonzero value of the interband coupling is therefore important to guarantee two separate gaps, while retaining a single $T_c$, as evidenced by first-principle calculations and observed e.g. by point contact spectroscopy.

We started by numerically evaluating $T_c$ within the two-band model of Eq. 2, as a function of the proximity to the ETT, $\mu - \mu_c$. We employed $V_{11} = 0.2$, $V_{22} = 0.1$, $V_{12} = 2$, while $\omega_D = 70 - 115$ meV (see Ref. 3 and refs. therein). Within a rigid band approximation, a change in the Al/Mg content in Al$_{1-x}$Mg$_x$B$_2$ is here parametrized by a change in the chemical potential $\mu$. The actual relation between $x$ and $\mu$ is expected to be nonlinear, and has been studied to some extent in Ref. 4. Therefore, we have neglected an explicit dependence of the coupling constants and of the Debye frequency on $\mu$, which may be in principle derived by combining the results of Refs. 4 and 8. However, we do not expect that our results would be changed much, at least qualitatively. Our results are therefore in agreement with Fig. 1 of Ref. 4, showing the experimental variation of $T_c$ in Al$_{1-x}$Mg$_x$B$_2$ as a function of Mg content $x$. In particular, we find a monotonic increase of $T_c$ when the ETT is traversed so that the $\sigma$ subband undergoes a 3D to 2D crossover. Exactly at the
ETT, \( T_c = T_c(\mu) \) is characterized by a shoulder, which corresponds to the kink at \( x = 0.66 \) in the experimental \( T_c = T_c(x) \) of Ref. 4.

In order to extract the isotope coefficient \( \alpha = (1/2)(\partial \log T_c/\partial \log \omega_D) \), we have evaluated \( \partial T_c/\partial \omega_D \) at fixed \( \mu \) by differentiating Eq. 2 (see e.g. Refs. 22, 23). Specifically, we find downward deviations from the BCS value \( \alpha = \frac{1}{2} \), with a minimum at the ETT. Such a minimum is more pronounced for larger values of the Debye frequency \( \omega_D \).

This is not surprising, as has been emphasized in connection with the role of a logarithmic Van Hove singularity for the anomalous isotope effect of the cuprates\(^\text{25,32}\). A generic feature of a non-constant DOS is that of providing deviations (even divergences, when logarithmic singularities are present) of \( \alpha \) from its standard BCS value\(^\text{29}\). This is a consequence of the asymmetry of the DOS, which has to be evaluated at \( \xi = \pm \omega_D \) in the expression for \( \alpha \). Such an asymmetry is more pronounced in the proximity to an ETT, where the DOS for the \( \sigma \) subband displays a kink.

However, although the proximity to the ETT tends to decrease the value of the isotope exponent \( \alpha \), the model is not able to recover the anomalously low isotope effect observed experimentally in the diborides. This is probably due to the oversimplification of the model, which does not take into account strong-coupling effects\(^\text{21}\), the nonlinear electron-phonon coupling in the \( E_{2g} \) mode\(^\text{33}\), and, to a less extent, the unconventional doping dependence of the electron-phonon couplings and of the phonon energy\(^\text{4}\).

For the sake of completeness, we have numerically studied \( T_c \) as a function of \( \mu \) around the ETT varying the other relevant parameters, \textit{i.e.} \( \omega_D \) and \( V_{12} \). Fig. 2 shows the \( \mu \)-dependence of the adimensional ratio \( k_B T_c/\hbar \omega_D \) for fixed \( V_{12} = 2 \) and increasing \( \omega_D = 70 \) – \( 115 \) meV and \( \omega_D = 200 \) – \( 600 \) meV. One may conclude that the relative enhancement of \( T_c \) near the ETT is greater for smaller \( \omega_D \). This is to be expected, since in this case the integral in Eq. 3 selects a shorter energy ‘window’ around the Fermi level, thus increasing the importance of the ETT. On the other hand, Fig. 4 shows the \( \mu \)-dependence of \( T_c \) for increasing \( \omega_D = 100 \) – \( 500 \) meV, with decreasing \( V_{12} \), so to keep \( T_c(\mu = 2 \text{ eV}) \approx \text{const} \).

In order to compare with the experimental dependence of \( T_c \) on Al content \( x \) in \( \text{Al}_{1-x}\text{Mg}_x\text{B}_2\text{H}_6 \), we can estimate the dependence of effective couplings \( \lambda_{ij} \) (\( i, j = 1, 2 \)) and of the Debye frequency \( \omega_D \) of the \( E_{2g} \) phonon mode on the proximity \( \mu - \mu_c \) of the chemical potential from the ETT by combining the results of Refs. 22, 23 as is shown in Fig. 3. Then, we can estimate the effective coupling constants in Eq. 2 from \( \lambda_{ij} = V_{ij} \sqrt{\mu_p n_i} \), where \( n_i \) is the partial DOS associated with the \( i \)-th band. Fig. 4 then shows our results for the critical temperature \( T_c \) and the isotope coefficient \( \alpha \) as a function of \( \mu - \mu_c \). Indeed, one finds a steeper dependence of \( T_c \) close to the ETT, in qualitative agreement with the experimental results in Al-doped MgB\(_2\).

In conclusion, within the two-band model of superconductivity, we have studied the effect of the proximity to a 3D–2D crossover (electronic topological transition) on the doping dependence of the critical temperature and of the isotope effect. The proximity to the ETT correctly takes into account, both quantitatively and qualitatively, for the enhancement of \( T_c \) as a consequence of a quantum interference effect between the two electronic bands.
characterizing the diborides.

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1 J. S. Slusky, N. Rogado, K. A. Regan, M. A. Hayward, P. Khalifah, T. He, K. Inumaru, S. Loureiro, M. K. Haas, and H. W. Zandbergen, Nature (London) 410, 343 (2001).
2 S. Agrestini, C. Metallo, M. Filippi, L. Simonelli, G. Campi, C. Sanipoli, E. Liarokapis, S. D. Negri, M. Giovannini, A. Saccone, A. Latini, and A. Bianconi, Phys. Rev. B 70, 134514 (2004).
3 A. Bussmann-Holder and A. Bianconi, Phys. Rev. B 67, 132509 (2003).
4 A. Bianconi, S. Agrestini, D. D. Castro, G. Campi, G. Zangari, N. L. Saini, A. Saccone, S. D. Negri, and M. Giovannini, G. Profeta, A. Continenza, G. Satta, S. Massidda, A. Cassetta, A. Pifferi, and M. Colapietro, Phys. Rev. B 65, 174515 (2002).
5 A. Bianconi, Solid State Commun. 89, 933 (1994).
6 A. Perali, A. Bianconi, A. Lanzara, and N. L. Saini, Solid State Commun. 100, 181 (1996).
7 A. Bianconi, D. D. Castro, S. Agrestini, G. Campi, N. L. Saini, A. Saccone, S. D. Negri, and M. Giovannini, J. Phys.: Condens. Matter 13, 7383 (2001).
8 J. M. Blatt and C. J. Thompson, Phys. Rev. Lett. 10, 332 (1963).
9 C. J. Thompson and J. M. Blatt, Phys. Lett. 5, 6 (1963).
10 A. Valletta, A. Bianconi, A. Perali, and N. L. Saini, Z. Phys. B 104, 707 (1997).
11 A. Bianconi, A. Valletta, A. Perali, and N. L. Saini, Physica C 296, 269 (1998).
12 I. M. Lifshitz, Sov. Phys. JETP 11, 1130 (1960). [Zh. Eksp. Teor. Fiz. 38, 1569 (1960)].
13 A. A. Varlamov, V. S. Egorov, and A. V. Pantsulaya, Adv. Phys. 38, 469 (1989).
14 Ya. M. Blanter, M. I. Kaganov, A. V. Pantsulaya, and A. A. Varlamov, Phys. Rep. 245, 159 (1994).
15 G. G. N. Angilella, E. Piegari, and A. A. Varlamov, Phys. Rev. B 66, 014501 (2002).
16 G. G. N. Angilella, G. Balestrino, P. Cermelli, P. Podio-Guidugli, and A. A. Varlamov, Eur. Phys. J. B 26, 67 (2002).
17 G. G. N. Angilella, R. Pucci, A. A. Varlamov, and F. Onufrieva, Phys. Rev. B 67, 134525 (2003).
18 H. Suhl, B. T. Matthias, and L. R. Walker, Phys. Rev. Lett. 3, 552 (1959).
19 S. L. Bud’ko, G. Lapertot, C. Petrovic, C. E. Cunningham, N. Anderson, and P. C. Canfield, Phys. Rev. Lett. 86, 1877 (2001).
20 D. G. Hinks, H. Claus, and J. D. Jorgensen, Nature (London) 411, 457 (2001).
21 G. A. Ummarino, R. S. Gonnelli, S. Massidda, and A. Bianconi, Physica C 407, 121 (2004).
22 E. Cappelluti, S. Ciuchi, C. Grimaldi, L. Pietronero, and S. Strassler, Phys. Rev. Lett. 88, 117003 (2002).
23 J. Kurtus, I. I. Mazin, K. D. Belashchenko, V. P. Antropov, and L. L. Boyer, Phys. Rev. Lett. 86, 4656 (2001).
24 P. de la Mora, M. Castro, and G. Tavizon, ..., ..., (2004), preprint cond-mat/0405238.
25 D. Y. Xing, M. Liu, and C. D. Gong, Phys. Rev. B 44, 12525 (1991).
26 A. Ino, C. Kim, M. Nakamura, T. Yoshida, T. Mizokawa, Z. Shen, A. Fujimori, T. Kakeshita, H. Eisaki, and S. Uchida, Phys. Rev. B 65, 094504 (2002).
27 A. Y. Liu, I. I. Mazin, and J. Kurtus, Phys. Rev. Lett. 87, 087005 (2001).
28 R. S. Gonnelli, D. Daghero, G. A. Ummarino, V. A. Stepanov, J. Jun, S. M. Kazakov, and J. Karpinski, Phys. Rev. Lett. 89, 247004 (2002).
29 R. Combescot and J. Labbe, Phys. Rev. B 38, 262 (1988).
30 J. J. Rodriguez-Núñez and A. A. Schmidt, Phys. Rev. B 68, 224512 (2003).
31 R. Combescot, Phys. Rev. Lett. 68, 1089 (1992).
32 C. C. Tsuei, D. M. Newns, C. C. Chi, and P. C. Pattnaik, Phys. Rev. Lett. 65, 2724 (1990).
33 B. Renker, K. B. Bohnen, R. Heid, D. Ernst, H. Schober, M. Koza, P. Adelmann, P. Schweiss, and T. Wolf, Phys. Rev. Lett. 88, 067001 (2002).
34 A. Bianconi, S. Agrestini, and A. Bussmann-Holder, J. Supercond. 17, 205 (2004).