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Is MgB₂ a BCS-like charged superfluid?

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Letter

Is $MgB₂$ a BCS-like charged superfluid?

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Two complementary mechanisms have been proposed for relatively high temperature superconductor MgB_2 . While the first is the electron–phonon mechanism of BCS theory, advocated strongly by Pickett and co-workers, the second, by Bianconi et al., invokes Feshbach shape resonances. While we cannot presently discount the second mechanism, and while both proposals exploit the multiband nature of the electronic structure of $MgB₂$, we show here that five body-centred cubic (bcc) transition metals, whose superconducting transition temperature correlate intimately with elastic constants and therefore are plainly BCS-like in character, lie on a curve which has $MgB₂$ at the high T_c end. Any alternative mechanism to electron–phonon interaction in $MgB₂$ will need to account quantitatively for this circumstance.

Keywords: Electron–phonon mechanism; Superfluid MgB_2

In a recent study [1], we have related the superconducting transition temperature T_c of five body-centred cubic (bcc) transition metals to elastic constants and especially to the so-called Cauchy deviation (see figure 1). Here, we want to relate such results for these BCS-like transition metals to recent work on $MgB₂$, with a relatively high transition temperature $T_c = 39$ K [2].

To do this, we show in figure 2, for comparison with figure 1, the five bcc metals on a conventional BCS plot in which the transition temperature T_c is scaled with the Debye temperature Θ_{D} [3]. Unlike figure 1, where the five bcc metals are ordered via the elastic constants precisely with their transition temperatures, figure 2 has a less simple ordering, even though these five metals lie on a (scaled) BCS-like plot.

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Figure 1. Critical temperature T_c of five bcc transition metals, correlated with Cauchy deviation $C^* = (C_{12} - C_{44})/(C_{12} + C_{44})$, C_{ij} being elastic constants. Redrawn after Ref. [1].

Figure 2. Critical temperature T_c scaled with Debye temperature Θ_D vs. $\lambda N(E_F)$, for five bcc superconducting elements, and MgB₂. Filled circles are data as collected by Sun et al. (see Ref. [8], and refs. therein, including Kotegawa et al. [13] for MgB_2). Filled triangle is directly constructed from data by Kotegawa et al. [8] (notice discrepancy with datum for MgB₂ as reported by Sun et al. [8]). Open circles refer to $Mg_{1-x}Al_xB_2$ ($x = 0.00 - 0.50$), with T_c taken from figure 1 of Ref. [12], $\Theta_D \propto \omega_{E_{2g}}$ taken from figure 3 of Ref. [12], and $\lambda N(E_F)$ identified with $\lambda_{\sigma\sigma}$ as plotted in figure 4 of Ref. [12]. The error bars have been constructed only for the two end points at $x = 0.00$ (MgB₂) and $x = 0.50$ (Mg_{0.5}Al_{0.5}B₂, the latter error bar being almost invisible on the present scale). Dashed line is McMillan's formula, equation (1), valid for $\lambda N(E_F) \leq 1$, while solid line is a strong-coupling generalization thereof, due to Sun *et al.* [8]. Dashed-dotted line is a guide to the eye, referred to in the text.

The main focus of this article is to examine how $MgB₂$ relates to these five bcc metals from the point of view of the BCS mechanism of electron–phonon interaction. This mechanism has been strongly advocated by Pickett and co-workers [4,5], though the electron–phonon interaction has to be surprisingly strong to yield the measured transition temperature $T_c = 39.4 \text{ K}$. However, we have added to the BCS-like plot in figure 2 this material $MgB₂$, and this lies on the scaled BCS-like curve, both within McMillan's approximation [6,7]

$$
T_{\rm c} = 1.14\Theta_{\rm D} \exp \frac{-1.04[1 + \lambda N(E_{\rm F})]}{\lambda N(E_{\rm F}) - \mu^* [1 + 0.62\lambda N(E_{\rm F})]},\tag{1}
$$

with Coulomb pseudopotential $\mu^* = 0.1$, and within a recent strong-coupling generalization thereof, due to Sun *et al.* [8] (see also Ref. [9]). In figure 2, we have used the quantity $\lambda N(E_F)$, where λ measures the strength of the electron–phonon interaction and $N(E_F)$ represents the density of states at the Fermi energy E_F . This supports the view of Pickett and co-workers that $MgB₂$ is a BCS-like superfluid.

We note here the interesting proposal of Bianconi and co-workers, where T_c is correlated crucially with features of the band structure of the layered material $MgB₂$ [10,11]. This is proposed as a complementary mechanism to that of Pickett and co-workers. That, we feel, would require to attribute to 'an accident' the correlation shown in figure 2 in which MgB₂ indeed fits smoothly on the BCS-like curves of T_c/Θ_D versus $\lambda N(E_{\rm F})$.

While, because of comparison between the BCS mechanism and that proposed by Bianconi et al. [10], we have added cases for $Mg_{1-x}Al_xB_2$ to figure 2 (see Ref. [12] and refs. therein), we must stress that the five bcc metals plus $MgB₂$ are ordered crystals. With doping, disorder will affect the nature of electron states with precursor effects reflecting a tendency towards Anderson localization. The five bcc ordered crystals lie well on a curve with $MgB₂$ (dashed-dotted line in figure 2), taking account of the 'scatter' between the data for MgB_2 of Sun *et al.* [8] and of Kotegawa *et al.* [13].

To conclude, it is important to add that Feshbach resonances have been proposed by Bianconi and co-workers [10] as a complementary mechanism to that of An and Pickett [4,5]. Both references [10] and [11] invoke the multiband nature of the electronic structure of MgB2. Though the Feshbach resonance proposal cannot be discounted as a possible alternative to the electron–phonon mechanism advocated by An and Pickett $[4,5]$ and other authors, the proximity of $MgB₂$ to the curve containing the five bcc transition metals shown in figure 2, which materials are manifestly superconducting due to an electron–phonon mechanism from figure 1, would have to be accounted for by any such alternative mechanism as put forward by Bianconi et al. [10].

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