The upper critical field problem in MgB$_2$.

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The recent discovery of superconductivity in MgB$_2$ has initiated an immediate broad research activity due to the high transition temperature $T_c \sim 40$ K in a seemingly ordinary $s-p$ metal. The present discussions mainly focus on measured quantities $T_c$ and the gap $2\Delta$ with respect to the topics: (1) weak or strong coupling in terms of standard BCS theory, (2) its possible relationship to the superconductivity in transition metal borocarbides, (3) symmetry of the order parameter, and (4) electron-phonon (el-ph) interaction or Coulomb repulsion based mechanisms of pairing. In context of the standard phonon mechanism: (i) a dominant role of immediately coupled high-frequency boron phonons is assumed (the simple “metallic hydrogen scenario”); or (ii) a strong coupling scenario is discussed. In all those discussions, essentially the validity of the standard isotropic single band (ISB) picture is implicitly assumed. However, the low temperature value of the upper critical field $H_{c2}(0)$, the fundamental quantity of a type-II superconductor, has not analyzed so far. In this context we would like to point out an interesting puzzle: with the computed and commonly accepted average band Fermi velocity $v_F=8.9\times10^7$ cm/s and the plasma frequency $\omega_{pl}=7$ eV, the resulting clean-limit London penetration depth $\lambda_L = c/\omega_{pl}=29$ nm nearly \textit{equals} the BCS coherence length $\xi_0=0.18h v_F/k_B T_c=29$ nm while experiments on $H_c$ and $H_{c2}$ yield a Ginzburg - Landau parameter $\kappa=26$. The ISB model is the most developed \textit{part} of the theory of superconductivity. It describes \textit{quantitatively} the renormalization of the physical properties of metals due to the electron-phonon interaction. The input material parameters are the density of states at $E_F$, $N(0)$, the Fermi velocity $v_F$, the impurity scattering rate $\gamma_{imp}$, the paramagnetic impurity scattering rate $\gamma_m$, the Coulomb pseudopotential $\mu^*(\approx 0.1)$, and the electron-phonon spectral function $\alpha^2 F(\Omega)$. The temperature dependencies of physical properties are determined mainly by the first inverse moments of the spectral function - the coupling constant $\lambda=\int_0^{\infty}d\Omega\alpha^2 F(\Omega)/\Omega$ and the average boson energy $\Omega_{g0}=\exp[(2/\lambda)\int_0^{\infty}d\Omega \log(\Omega)\alpha^2 F(\Omega)]/\Omega$.

Our analysis is based on numerical calculations of $H_{c2}(T)$ solving equations first presented by Prohammer et al. In the intermediate and weak coupling cases, the clean limit value of the calculated orbital $H_{c2}(0)$ practically does not depend on the shape of the spectral function. In the spirit of Langmann the s-wave clean limit ISB-$H_{c2}(0)$ can be approximated by the following factorized formula

$$H_{c2}(0)[T] \approx 0.02T_c^2 [K](1+\lambda)^{2.4}/v_F^2 [10^7 \text{cm/s}].$$

It is convenient to express $v_F^2$ in Eq. using the related experimentally available quantities: the cell volume $V$, the Sommerfeld constant (per mole) $\gamma_S = \pi^2 k_B^2 N(0)(1+\lambda)N_A V/3$ and the bare plasma frequency $\omega_{pl}^2 = 4\pi e^2 N(0) v_F^2 / 3$

$$v_F^2 = \frac{\pi N_A V k_B^2 (1+\lambda) \omega_{pl}^2}{4\pi^2 \gamma_S}.$$
density of states (PDOS) extending to above 100 meV with main peaks at about 90, 55, 37, and 32 meV, as well as an unexpected anomalous soft mode near 17.5 meV below the maxima of acoustic modes. The measured PDOS is in agreement with $\Theta_D = 65$ meV, estimated from specific heat data [10]. The values for zone-center optical mode obtained from density-functional theory based calculations 58 meV [11], 62 meV [12], 73 meV [13] are rather similar and for our goal we adopt an Einstein spectrum with $\Omega = 60$ meV. With the standard value $\mu^* = 0.1$ at the cutoff frequency of 6(Ω) one needs $\lambda = 0.86$ to obtain $T_c = 40$ K. If the dominating coupling were that by the 17.5 meV feature $\lambda = 2.5$ would be needed.

Now we are in a position to apply our $Q$-test to selected superconductors. The results are presented in Table 1 [4]. For the weakly anisotropic transition metal Nb it is approximately fulfilled, whereas strong deviations do occur both for the transition metal borocarbide YNi$_2$B$_2$C and for MgB$_2$ under consideration. The latter one is checked in the weak and as well as in the strong coupling cases.

These difficulties can be resolved in the framework of a more complex effective $N$-band model. For an anisotropic system it is obtained by dividing the Fermi surface into $N$ parts and approximating the $k$-dependent quantities in each part by their mean values [4]. The input material parameters of such a model are the densities of states at $E_F$ $N_i(0)$, the Fermi velocities $v_F,i$, the impurity scattering rates $\gamma_{imp,i,j}$, the Coulomb pseudopotentials $\mu^*_i(\approx 0.1)$, and the electron-phonon spectral functions $\alpha^2_{j,i}F(\omega)$. For the sake of simplicity, as a first step, we consider here such effects in the frame of an effective two-band model. Recently it was successfully applied to transition metal borocarbides in a combined study of Eliashberg theory and de Haas van Alphen effect [7]. Unfortunately, due to the lack of single crystals, at present there is no available experimental information on the electronic structure near the Fermi surface of MgB$_2$. For this reason, we performed electronic structure calculations on a very dense $k$-mesh using the full-potential nonorthogonal local-orbital minimum-basis scheme [9]. Thus we get more detailed information on the Fermi velocities compared with published data [10].

The Fermi surface of MgB$_2$ (see Fig. 1) consists of four disjoint sheets: two hexagonal heavy hole tubes around the $\Gamma - A$ line and a light hole and an electron honeycomb. In the spirit of a two-band model we divide the quasiparticles into subgroups with approximately similar material parameters. We choose the heavy-hole tube as the first effective band (central blue piece in the middle of Fig. 1). Its DOS contribution $N_h(0) = N_i(0)$ is about a third of the total DOS: $N(0)/N_h(0) \approx 3$ and we adopt $N_2(0)/N_1(0) = 2$. The average Fermi velocity over this hole tube is $v_{F1} = 4.5 \times 10^7$ cm/s while for the remaining fast Fermi surface sheets we choose $v_{F2} = 11 \times 10^7$ cm/s. In the clean limit the scattering rates $\gamma_{imp,i,j}$ can be set to 0. Let's start with weak-coupling scenario. If one could ignore the fast quasiparticles entirely, one would return to the ISB case, considered above, with $\lambda = 0.8$ and $v_F = 4.5 \times 10^7$. From Eq.1 one then gets $H_{c2}(0) = 6.5$ T which is still much smaller than the experimental value. Moreover, within a consequent isotropic coupling scenario the interband coupling cannot be ignored. As a result, we arrive at 2T, only (see Fig. 2). For comparison the ISB case for the same $\lambda$ and $v_F = 8.9 \times 10^7$ cm/s is shown, too. For this moderate anisotropy of $v_F$, the two-band effect is practically unimportant. Hence, to describe $H_{c2}(T)$ quantitatively, an enhanced coupling of the heavy holes would be needed. Deformation potential calculations provide support for such an enhancement for the larger heavy-hole tube [11].

It was shown above, that at given $T_c = 40$ K and el-ph interaction with high-frequency phonons, only, the coupling constant cannot exceed unity and $H_{c2}(0)$ doesn’t exceed several Tesla at most. To increase the coupling constant, we are forced to adopt strong coupling to low-frequency mode(s). Hence, we adopt a two-peak spectral function containing for instance a low-frequency peak at 17.5 meV as well as an effective high-frequency peak at 60 meV with comparable spectral weights. We adopt $\lambda_{60_{meV}}/\lambda_{17.5_{meV}} = 0.33$. Then reasonable agreement with available experimental data for $H_{c2}(T)$ [6,17] can be achieved with $\lambda_{11} = 1.5$, $\lambda_{22} = 0.4$ and $\lambda_{21} = 0.5$ (see Fig. 2). With the bare band value $N(0) = 1.7$ mJ/mol K$^2$ [11] we arrive at $\gamma_S = 4.1$ mJ/mol K$^2$ and $\omega_{pl} = 7.5$ eV in accord with experimental data [10,13,4]. The calculated gap values $2\Delta_1 = 5k_BT_c$ and $2\Delta_2 = 3k_BT_c$ above and below the BCS value $3.5k_BT_c$, respectively, can be compared with the experimental values taken from tunneling ($3.4k_BT_c$, $4.83k_BT_c$) [18,20] and specific heat ($2.4k_BT_c$) [18] and NMR data ($2.5k_BT_c$, $5.6k_BT_c$) [21,22].

It is interesting to realize, that switching off the soft mode at fixed remaining parameters results in $T_{c,hard} \approx 7K$, only. However, switching off instead the high-frequency modes, we would arrive at $T_{c,soft} \approx 20K$ at least. Alternatively, if the spectral functions differ significantly for various Fermi surface sheets, the contribution of the high-frequency modes to $T_c$ can enhanced up to about 20 K. Anyhow, this means, that the “medium” high $T_c$ superconductivity of MgB$_2$ within our model is not provided by a simple “hydrogen-like” scenario as frequently discussed in the literature, but by a more complex scenario, where both $T_c$ and $H_{c2}(0)$ do depend very sensitively on the coupling with the soft-mode. A somewhat similar interplay of high- and low-frequency phonons occurs in the well-known PdH(D) palladium hydrides (deuterides).

The strong coupling in the heavy-hole band due to interaction with the soft mode needs some interpretation and discussion. A simple down-tuning of the calculated $E_{2g}$-mode frequency from 58.5 meV [14] to 17.5 meV, preserving thereby the harmonic approximation, would result in large zero-point fluctuations amplitudes for which there is not enough space in a real crystal. In addition we would arrive at an unrealistic super strong coupling limit: $\lambda_1 = 10.4$ adopting the estimated Hopfield parame-
ter $\eta_1 = 8.2$eV/Å$^2$ [11]. These difficulties can be resolved adopting an anharmonic model for the lattice vibrations. Within its extreme anharmonic two-level system approximation (deep double- or multiple wells) \textsuperscript{23,24} the corresponding anharmonic electron-boson coupling constant reads

$$\lambda_1(T) = \frac{2}{3} \eta_1 d_0^2 \tanh(\hbar \omega_1/2k_B T)/\hbar \omega_1,$$ \hspace{1cm} (4)

where $d_0 \sim 0.1$ Å is a typical double-well distance. It is sizable and at the same time not too large: thus we arrive at $\lambda_1=2$ in accord with $\lambda_{11} + \lambda_{12}$ obtained above phenomenologically. Quite interestingly, in this limit the boson frequency remains constant whereas the intensity of its spectral density increases with decreasing $T$ like in the experimental neutron data \textsuperscript{11} until saturation at low $T$ is achieved. For the adopted value of $\omega_1=17.5$ meV this occurs below 50 K, i.e. only slightly above $T_c$. Alternatively, in principle, a softening of other modes than the $E_{2g}$ mode should be considered, too. Guided by the experience obtained from the somewhat related transition metal borocarbides (see below), a softening of the acoustic modes \textsuperscript{23} is worthy to be considered. On the other hand, despite the soft mode the general features of the phonon density of states till 60 meV are reasonably well described by the model \textsuperscript{13}.

There is an interesting similarity between the picture we arrived at above for MgB$_2$ and the picture based on the present knowledge on transition metal borocarbides such as YNi$_2$B$_2$C. The latter exhibit pronounced nesting properties of a rather complex Fermi surface (FS). There the strongly coupled slow electrons stem from the nested parts of the FS. The anisotropy of the FS in borocarbides is somewhat larger than in the present case but the anisotropy of the coupling in MgB$_2$ seems to be larger. In this context the $q$-dependent measurement of the soft phonon near 17 meV in the superconducting state is of great interest. Analogous behavior as for the anomalously small 7 meV mode for YNi$_2$B$_2$C \textsuperscript{25} might be expected. The $H_{c2}(0)$, the positive curvature of $H_{c2}(T)$ near $T_c$, and the sizeable deviations of the shape of $H_{c2}(T)$ at low $T$ from the parabolic WHH (Werthamer-Helfand-Hohenberg) - shape in both systems can be ascribed to the interband coupling with the remaining weakly coupled fast quasiparticles.

In conclusion, the proposed ISB criterion excludes the applicability of the frequently used isotropic single band model. The shape and the magnitude of the upper critical field in MgB$_2$ can be successfully described within a multi-band Eliashberg model with two options. Provided the modern band structure calculations describe correctly the electronic structure near the Fermi surface, then there should be a sizeable coupling to some soft bosonic modes, not necessarily phonon-like, not predicted by harmonic phonon calculations but seen possibly in the neutron data. Otherwise the bare quasiparticle Fermi velocities should be considerably smaller than the band structure predictions.

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TABLE I. ISB check for selected superconductors. Input quantities: $\omega_{pl}$ in eV, $H_{c2}(0)$ in Tesla, cell volume $V$ in $\text{Å}^3$, Sommerfeld constant $\gamma_S$ in mJ/mol K$^2$, $T_c$ in K, coupling constant $\lambda$, and the ISB parameter $Q$ (Eq. (1)). Row 3: weak coupling, $\langle \Omega \rangle = 60$ meV; row 4: strong coupling $\langle \Omega \rangle = 17.5$ meV.

|       | $\omega_{pl}$ | $H_{c2}(0)$ | $V$ | $\gamma_S$ | $T_c$ | $\lambda$ | $Q$ |
|-------|---------------|-------------|-----|-------------|-------|-----------|-----|
| Nb    | 9.9           | 0.35        | 18  | 7.8         | 9.3   | 0.9       | 1.4 |
| YNi$_2$B$_2$C | 4.0   | 10          | 64  | 19          | 15    | 0.7       | 4.1 |
| MgB$_2$  | 7.0           | 18          | 29  | 3.0         | 40    | 0.8       | 8.4 |
| MgB$_2$  | 7.0           | 18          | 29  | 3.0         | 40    | 2.5       | 3.3 |

*Ref. [26,27] and references therein.
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*Refs. [13,10,16], weak coupling scenario, $\langle \Omega \rangle = 60$ meV
*Ibid, strong coupling scenario, $\langle \Omega \rangle = 17.5$ meV

FIG. 1. (Color) The Fermi surface of MgB$_2$ in the full Brillouin-zone. The $\Gamma$-point is the midpoint of the hexagonal prisma and the $A$-point(s) are the midpoints of the hexagons at the top and the bottom of the prisma, respectively. Light-hole tube (upper panel); Heavy-hole tube inside the hole honeycomb (middle panel); Electron honeycomb (lower panel). The Fermi velocities are measured in units of $10^7$ cm/s presented by different colors shown at the bottom of the figure.
FIG. 2. Experimental data for $H_{c2}(T)$ of MgB$_2$ compared with the theoretical curve of the two-band model for both anisotropic coupling and Fermi velocities (full line). Parameter set see text. For comparison the case of a complete isotropic single band model (ISB) (dashed) and the two-$v_F$-band model with isotropic coupling (dotted line) are shown, too.