Two-band BCS model describes well the thermodynamics of MgB$_2$

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A keen interest excited by discovery and experimental investigation of a new high $T_c$ superconductor MgB$_2$ is to a large extent associated with its dissimilarity to cuprate superconductors. The superconductivity of MgB$_2$ is definitely three-dimensional effect, whereas in cuprates it is presumably two-dimensional (2D). Nevertheless, the superconducting gap in MgB$_2$ displays strong anisotropy. The most precise tunneling measurements by Gonnelli et al. [1] give the value 2.6 for the ratio of the gaps at two conductivity bands. On the other hand, the measured gaps are the same for the tunneling in $ab$-plane and in $c$-direction, indicating that they do not depend on direction within each piece of the Fermi surface.

An important problem is how strong is the interaction in MgB$_2$. First-principles calculations [2, 3, 4] indicate that electron-phonon interaction is not weak and that Eliashberg description is appropriate. However, anisotropy and interaction were shown to influence thermodynamics oppositely. For example, the anisotropy decreases the relative discontinuity of the specific heat at the transition point [2, 3], whereas the first correction due to interaction increases it [4]. Besides, MgB$_2$ is a very hard material with high value of Debye frequency, which usually correlates with a weak coupling. Therefore it is not a priori clear what is more substantial in the case of MgB$_2$.

The purpose of our work is to demonstrate that the anisotropy effects are more substantial at least for thermodynamic measurements. We show that, as a matter of fact, the weak coupling anisotropic BCS theory describes all known thermodynamic experimental data including the temperature dependence of the energy gap and specific heat with a high precision 3–6%.

The main features of anisotropic weak coupling BCS model were elucidated in the early 1960s [2, 3, 4, 5, 11], the ultimate result being the factorization of the gap

$$\Delta(T, k) = Q(T)\chi(k),$$  

which was experimentally verified by Zavaritskii [11].

The function of angle $\chi(k)$ is the eigenfunction of the interaction operator $V(k, k')$ corresponding to the maximal eigenvalue $\lambda_+$. It satisfies linear homogeneous integral equation:

$$\int V(k, k')\chi(k')\frac{d\sigma'}{\nu_F k_F} = \lambda_+ \chi(k).$$  

Integration in Eq. (2) proceeds over the Fermi surface with $d\sigma = \frac{d^2k}{\pi^2}$ and $dS$ being a differential area of the Fermi surface; $\nu_F = \int \frac{d\sigma}{\nu_F}$ is the electron density of the state per spin at Fermi level. The function $\chi(k)$ is normalized as follows:

$$\langle \chi^2(k) \rangle = 1$$

The angular average value $\langle X \rangle$ is: $\langle X \rangle = \int X \frac{d\sigma}{\nu_F}$. The temperature dependent factor $Q(T)$ can be found from the orthogonality condition:

$$\ln \frac{Q(0)}{Q(T)} = \langle \chi^2(k) \rangle F\left(\frac{Q(T)\chi(k)}{T}\right),$$  

where

$$F(x) = \int_{-\infty}^{+\infty} \frac{du}{\sqrt{x^2 + u^2}(\exp \sqrt{x^2 + u^2} + 1)}.$$  

The value $Q(0)$ is associated with the transition temperature $T_c$ by the following relationship:

$$\frac{Q(0)}{T_c} = \frac{\pi}{\gamma} \exp\left(-\langle \chi^2(k) \rangle \ln |\chi(k)|\right),$$  

here $\gamma = e^C = 1.781072 \cdots$ and $C$ is Euler’s constants.

The specific heat $C(T)$ reads:

$$C(T) = 2\nu_F T \frac{d}{dT} \left| \Delta_k G \left(\frac{\Delta_k}{T}\right) \right|,$$  

where $G(x) = 2x \int_0^\infty \cosh(2\varphi)F(x \cosh \varphi)d\varphi$.

We now apply these formulas to MgB$_2$. The Fermi surface of MgB$_2$ has two $\sigma$-type 2D cylindrical hole
sheets and two \( \pi \)-type three-dimensional tubular networks.\(^{12,13,14}\) We accept a simple model introduced first by Moskalenko\(^{14}\), in which the interaction does not depend on the momentum inside each band, but only on the band index. Thus, it can be written as \( 2 \times 2 \) Hermitian matrix \( V_{ik} (i, k = \sigma, \pi) \). The order parameter (energy gap) in each band in such a model does not depend either on the momentum within each band and can be described by a 2D vector with components \( \Delta_\sigma, \Delta_\pi \). The validity of this simple model is supported by the tunneling measurements of the energy gap\(^{1}\), which displays the same values for two gaps in \( ab \)-plane and in \( c \)-direction. The normalized wave function of the Cooper pairs \( \chi_\sigma \) has the same property: \( \chi_\sigma (k) = \chi_\sigma, \chi_\pi (k) = \chi_\pi \), where \( \chi_\sigma \) and \( \chi_\pi \) are two constants. We introduce an additional simplification assuming these constants to be real. Let us denote the density of states in the \( \sigma \) and \( \pi \) bands as \( \nu_{F,\sigma} \) and \( \nu_{F,\pi} \), respectively. Then the definition of an average value \( \langle X \rangle \) for any physical value \( X \), which does not change within each band reads:

\[
\langle X \rangle = X_\sigma c_\sigma + X_\pi c_\pi ,
\]

where \( c_\sigma \) and \( c_\pi \) are statistical weights of the bands \( c_\sigma = \nu_{F,\sigma}/\nu_F \) and \( c_\pi = \nu_{F,\pi}/\nu_F \). The general normalization condition Eq. (3) for this model reads:

\[
\chi_\sigma^2 c_\sigma + \chi_\pi^2 c_\pi = 1 .
\]

Equation (3) can be written explicitly as follows:

\[
\frac{Q(0)}{T_c} = \frac{\pi}{\gamma \chi_{av}} ,
\]

where \( \chi_{av} = \chi_\sigma^2 c_\sigma + \chi_\pi^2 c_\pi \). We assume the values \( c_\sigma = 0.44 \) and \( c_\pi = 0.56 \) as found from density-functional theory calculations in Refs.\(^{12,13,15}\). The second fitting parameter is \( T_c \). There is no experimental discrepancy on this value, and it is commonly accepted to be \( T_c \approx 39 \) K. One additional fitting parameter for the two-band theory is the ratio \( \delta = \chi_\sigma/\chi_\pi \). We have extracted it from the tunneling gap measurements\(^{1}\) extrapolating them to zero temperature:

\[
\delta = \frac{\chi_\sigma}{\chi_\pi} \approx 2.54 .
\]

Equations (6) and (7) allow us to determine \( \chi_\sigma \) and \( \chi_\pi \) separately:

\[
\chi_\sigma = \frac{\delta}{\sqrt{c_\sigma \delta^2 + c_\pi}} = 1.38 ; \quad \chi_\pi = \frac{1}{\sqrt{c_\sigma \delta^2 + c_\pi}} = 0.54 .
\]

According to the weak-coupling theory, the ratio \( \delta \) must be the same at any temperature. This crucial condition is satisfied in the tunneling experiment\(^{1}\) with all experimental precision.

For the temperature dependence of the gap in the BCS two-band model, we find from Eq. (4):

\[
- \ln q = \chi_\sigma^2 F \left( \frac{\pi \chi_\sigma y}{\gamma \chi_{av} t} \right) c_\sigma + \chi_\pi^2 F \left( \frac{\pi \chi_\pi y}{\gamma \chi_{av} t} \right) c_\pi .
\]

Here \( q(t) = Q(t)/Q(0) \) and \( t = T/T_c \). The graph of the function \( q(t) \) is shown in Fig. 1 by the solid curve. The dashed curve in Fig. 1 represents experimental data by Gonnelli et al.\(^{1}\).

The specific heat in the two-band model is given by the following equation directly stemming from Eq. (4):

\[
\frac{C(T)}{C_N(T)} = c_\sigma r_\sigma(y_\sigma) + c_\pi r_\pi(y_\pi) + \frac{12}{T \zeta(3)} \left( c_\sigma \chi_\sigma^2 r_\sigma(y_\sigma) + c_\pi \chi_\pi^2 r_\pi(y_\pi) \right)^2 ,
\]

FIG. 1: The solid curve depicts the ratio \( Q(T)/Q(0) \) vs \( t = T/T_c \) for the two-band model; the dashed curve is the same for \( \Delta_\pi \); “+” and “x” represent experimental data by Gonnelli et al.\(^{1}\).
where \( C_N(T) = \gamma T \) is the specific heat for the normal metal; \( y_a = \frac{x_b^2}{x_c^2}, y_b = \frac{x_a^2}{x_c^2} \). The functions \( r_i \) are defined by integrals \( r_i(x) = \int_{-\infty}^{\infty} g_i(\sqrt{x^2 + y^2}) dy, \) \( i = a, b, c \), where \( g_i \) read:

\[
\begin{align*}
g_a(x) &= \frac{1}{2 \cosh^2(x)}, \\
g_b(x) &= \frac{\pi^2}{14\zeta(3)} \left( \frac{\tanh x}{x} - \frac{1}{\cosh x} \right) \frac{1}{x^2}, \\
g_c(x) &= \frac{6}{\pi^2} \frac{x^2}{\cosh^2 x}.
\end{align*}
\]

(14)

For technical details related to this calculation see Mishonov et al. \[17\]; the functions \( g_i \) were introduced and graphically presented in Ref. \[18\]. The jump of the specific heat at \( T_c \) reads: cf. \[14\] \[14\]

\[
\frac{\Delta C(T_c)}{C_N(T_c)} = \frac{12}{7\zeta(3)} \frac{\left( \chi_a^2 e_\sigma + \chi_b^2 e_\pi \right)^2}{\chi_a^4 e_\sigma + \chi_b^4 e_\pi}.
\]

(15)

For the data specified earlier, we find \( \Delta C(T_c)/C_N(T_c) = 0.874 \). It agrees with the high precision measurements by Bouquet et al. \[19\] with about 3% precision. In Fig. 3 the ratio \( C(T)/C_N(T) \) vs. \( T/T_c \) is plotted. The solid curve is the prediction of the two-band weak coupling theory; the dots are experimental data by Bouquet et al. \[19\], courteously sent to us by the authors. The theoretical graph \( C(T)/C_N \) vs. \( T/T_c \) agrees well with the experimental data everywhere except of a range of low temperature \( T/T_c \leq 0.2 \). The discrepancy most probably is caused by a relatively small variation of the gap within one band. The specific heat at low temperature is proportional to \( e^{-\Delta_{min}/T} \), whereas the tunneling measurements give the value of the gap along the direction of the tunneling.

![Graph](image)

**FIG. 3:** The solid curve is the theoretical graph of the specific heat for the two band MgB\(_2\) vs. \( t = T/T_c \); the circles are the experimental data due to Bouquet et al. \[17\]; the functions \( g_i(x) \) are introduced and assumed a plausible variational procedure introduced one more parameter. As it could be expected from the results by Miranović et al., the number of parameters is too small to ensure a reasonable precision. Indeed, a satisfactory agreement with the experiment in Ref. \[23\] is reached at the expense of a rather exotic choice of parameter. Summing up, the magnetic properties can not be described by such an elementary theory as the described above two-band BCS model and require much more sophisticated approach even in the weak coupling approximation.

Given the value of discrepancy, we can estimate the variation of the gap \( \Delta - \Delta_{min} \sim 0.1-0.15 T_c \ln 2 \approx 3.3-4.2 \text{ K} \). It is about 8–12% of the value of the smaller gap.

Another group of available experimental thermodynamic data relates to magnetic properties: the energy gaps in external magnetic field \[24\] and the dependence of the second critical field on temperature \[21\]. The dependence of \( H_{c2} \) on temperature was considered theoretically in the framework of anisotropic BCS model by two groups of authors \[22, 22\], based on classical approach by Helfand and Wertheimer \[24\]. Unfortunately, a consistent solution of these problems at any temperature between 0 and \( T_c \) requires much more detailed knowledge about the Fermi surface. For example, to reach a satisfactory convergence Miranović et al. \[22\] were forced to introduce 11 different parameters characterizing the Fermi surface and electron interaction. It is clear, that our real knowledge of the Fermi surface is too poor for such a sophistication. Dahm and Schopohl \[23\] applied a simplified model of the Fermi surface as consisting of a torus and cylinder characterized by 4 parameters only and assumed a plausible variational procedure introducing one more parameter. As it could be expected from the results by Miranović et al., the number of parameters is too small to ensure a reasonable precision. Indeed, a satisfactory agreement with the experiment in Ref. \[23\] is reached at the expense of a rather exotic choice of parameter. Summing up, the magnetic properties can not be described by such an elementary theory as the described above two-band BCS model and require much more sophisticated approach even in the weak coupling approximation.

Let us discuss why this simplified theory works so well. Let us start from the assumption supported by experiments that the gap does not vary within each band. The in-band isotropy of the gap could be a result of sufficiently strong in-band scattering. At the scattering time \( \tau \sim 10^{-14} \text{ s} \), i.e. at the residual resistance larger than \( 10^{-5} \Omega \text{cm} \), the energy gap becomes isotropic. However, the ratio of the gaps for different bands still remains bigger than 2 indicating that the inter-band scattering must be much weaker. It should be emphasized that it is the density of states which becomes isotropic, whereas the order parameter remains anisotropic unless the Ioffe-Regel limit \( \tau \epsilon_F \sim 1 \) of scattering rate is reached \[24\]. The tunnelling experiment measures just the density of state.

Second question is why the weak-coupling model gives so high accuracy. Two different aspects must be enlightened. First, the separability of variables for the order parameter, even in the framework of the weak-coupling approximation, has the precision of of the weak coupling constant, i.e. \( (\ln \frac{\Delta}{\omega_D})^{-1} \sim 0.3 \). For the case of the two-band model such a crude estimate can be checked more accurately by a direct solution of the nonlinear matrix
equation for the energy gap. It has a following form:
\[
\Delta_i = \sum_j V_{ij} \Delta_j \left( \frac{1}{\lambda_\pi} - f(\beta \Delta_j) \right) \Delta_j , \tag{16}
\]
where \(i, j\) take values \(\sigma, \pi\) and \(f(x) = \int_{-\infty}^{\infty} \left( \tanh \frac{u}{2} - \tanh \sqrt{\omega^2 - x^2} \right) du\). Its solution can be found as a superposition of two normalized eigenstates of the corresponding linear equation: \(\Delta_j = Q_+ \Psi_{+j} + Q_- \Psi_{-j}\). In our calculations we used only one of them, \(\Psi_+\) corresponding to the larger eigenvalue \(\lambda_+\). Such an approximation is justified when the second eigenvalue \(\lambda_-\) is much less than \(\lambda_+\), even if \(\lambda_+\) is not very small. Indeed, the symmetrized matrix \(\tilde{V}\) with matrix elements \(\tilde{V}_{ij} = \sqrt{\omega_\pi} V_{ij}\) can be represented as \(\tilde{V} = \lambda_+ |+\rangle\langle+| + \lambda_- |-\rangle\langle-|\). This representation shows that, at \(\lambda_- = 0\) the operator \(\tilde{V}\) is separable, and the solution of non-linear equation (16) is factorizable: \(\Delta = Q(T)\Psi_+\). The equation \(\lambda_- = 0\) is equivalent to \(\text{Det} \tilde{V} = V_{\sigma \pi} V_{\pi \sigma} - V_{\sigma \sigma}^2 = 0\). Though such a fine tuning of parameters seems improbable, our numerical calculations demonstrate that the ratio \(\lambda_-/\lambda_+\) and the thermal variation of of the ratio \(\Delta_-/\Delta_\pi\) remain small (about 3%) even at \(\Delta(T)\) by \(3\%\). We thank to Dr. A. Junod and to Dr. R. Gonnelli for sending us our original experimental data of their works. This work was supported by NSF under the grants DMR-0321572 and DMR 0103455.

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