International Journal of Modern Physics B
Vol. 27, No. 29 (2013) 1347008 (9 pages)

DOI: 10.1142/S0217979213470085



# AN ALTERNATIVE APPROACH TO MULTI-GAP SUPERCONDUCTIVITY

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Accepted 28 June 2013
Published 10 September 2013

We draw attention to a feature suggested by a widely-cited paper by Suhl, Matthias, and Walker in the context of multi-gap superconductivity that seems to have escaped serious attention: interaction parameters in a superconductor characterized by two zero-temperature gaps but a single critical temperature *must* be temperature-dependent. Guided by this cue, we have presented a plausible scenario for a quantitative explanation of the superconducting properties of $MgB_2$ via an alternative approach — the approach provided by the recently derived set of generalized-BCS equations. Attention is drawn to earlier work in diverse fields where a similar $T$-dependent approach has been fruitful.

*Keywords*: Multi-gap superconductors; multi-phonon exchanges; generalized BCS equations.

## 1. Introduction: Review of Suhl, Matthias and Walker's Approach for a Two-Gap Superconductor

The approach followed in the seminal paper by Suhl *et al.*[1] (SMW hereafter) has been invoked, albeit qualitatively, in most studies e.g., Refs. 2–6 concerned so far with multi-gap superconductors such as $MgB_2$. Salient features of this approach are: (1) It was originally given in the context of transition elements. (2) The interaction Hamiltonian in this approach comprises three pieces which correspond to

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electrons in the: (i) $s$-band with a density of states $N_s$, (ii) $d$-band with $N_d$ as the density of states, and (iii) the overlap between the $s$- and the $d$-bands. (3) Two gaps and, in general, two critical temperatures arise in this approach because the BCS interaction parameter $\lambda$ is found to be given by a quadratic equation involving $V_{ss}$, $V_{dd}$ and $V_{sd}$ which denote the interaction energies between pairs of electrons in the three pieces of the Hamiltonian. (4) It asserts that: (a) when $V_{sd} = 0$, the superconductor is characterized by two gaps and two critical temperatures; (b) when $V_{ss} = V_{dd} = 0$ and $N_s \neq N_d$, there are still two gaps with a state density $\sqrt{N_s N_d}$ and (c) when $V_{sd}$ is finite but much less than $\sqrt{V_{ss} V_{dd}}$ both the gaps close at the same temperature.

It is our purpose here to critically review these assertions and then to give a concise but complete account of the superconducting properties of $MgB_2$ via an alternative approach.

To deal with the first part, we make Eq. (4) in the SMW paper as our starting point since we have no problem up to this point in their paper:

$$\begin{aligned} A(T)[1 - V_{ss} N_s F(A,T)] &= B(T) V_{sd} N_d F(B,T)\,, \\ B(T)[1 - V_{dd} N_d F(B,T)] &= A(T) V_{sd} N_d F(A,T)\,, \end{aligned} \tag{1}$$

where $A(T)$, $B(T)$ denote the $T$-dependent gap-values and

$$F(A,T) \equiv \int_0^{\hbar\omega} d\epsilon \frac{\tanh[(\epsilon^2 + A^2)^{1/2}/2k_B T]}{(\epsilon^2 + A^2)^{1/2}}\,, \quad (k_B \equiv \text{Boltzman constant}) \tag{2}$$

while the equation for $A(T)$ is:

$$1 - \lambda_A F(A,T) = 0\,. \tag{3}$$

Thus, $F(A,T)$ is given by the inverse of the coupling constant and (3) may be used to determine $\lambda_A$ at any $T$ since $\lambda$ is independent of $T$ in the BCS theory. In particular, if $T_{c1}$ is the critical temperature for gap A, then $A(T_{c1}) = 0$ and we have $1 - \lambda_A F(0, T_{c1}) = 0$. Similarly, for gap B one has $1 - \lambda_B F(0, T_{c2}) = 0$. Note that $F(0, T_{c1}) \neq F(0, T_{c2})$.

Consider now the case when $V_{sd} = 0$. In this case we have from (1)

$$A(T)[1 - V_{ss} N_s F(A,T)] = 0\,,$$

$$B(T)[1 - V_{dd} N_d F(B,T)] = 0\,.$$

In general therefore, when $A(T) \neq B(T) \neq 0$ we have:

$$[1 - V_{ss} N_s F(A,T)] = 0\,,$$

$$[1 - V_{dd} N_d F(B,T)] = 0$$

and, in particular

$$[1 - V_{ss} N_s F(A, T_{c1})] = 0\,,$$

$$[1 - V_{dd} N_d F(B, T_{c2})] = 0\,.$$

These equations are independent of each other and lead to two unequal gaps and the associated $T_c s$. Hence we agree with the SMW assertion 4(a) in the first paragraph.

Let us now consider the two equations in (1) when $V_{ss} = V_{dd} = 0$. Multiplying the two equations, we have:

$$F(A,T)F(B,T) = 1/V_{sd}^2 N_s N_d \equiv 1/\lambda_{\text{eff}}^2$$

or

$$\lambda_{\text{eff}} = +V_{sd}\sqrt{N_s N_d}$$

since $\lambda_{\text{eff}}$ must be positive. So, there is *only one gap* — not two as stated in 4(b).

We now consider the case when $V_{sd} \neq 0$. The values of the gaps corresponding to $V_{sd} = 0$ were designated as $A$, $B$, respectively. Let their values be $A'$, $B'$ when $V_{sd} \neq 0$. Equations (1) now are:

$$A'(T)[1 - V_{ss}N_s F(A',T)] = B'(T)V_{sd}N_d F(B',T)\,,$$

$$B'(T)[1 - V_{dd}N_d F(B',T)] = A'(T)V_{sd}N_s F(A',T)\,.$$

With the definitions:

$$\lambda_s \equiv V_{ss}N_s\,, \quad \lambda_d \equiv V_{dd}N_d\,, \quad \alpha \equiv V_{ss}^2/V_{ss}V_{dd}\,,$$
$$F(A',T) \equiv 1/\lambda_1\,, \quad F(B',T) \equiv 1/\lambda_2 \tag{4}$$

these may be written as:

$$A'(T)(1 - \lambda_s/\lambda_1) = B'(T)V_{sd}N_d/\lambda_2\,,$$

$$B'(T)(1 - \lambda_d/\lambda_2) = A'(T)V_{sd}N_s/\lambda_1\,.$$

Multiplying these together, we obtain:

$$(1 - \lambda_s/\lambda_1)(1 - \lambda_d/\lambda_2) = \alpha\lambda_s\lambda_d/\lambda_1\lambda_2\,, \tag{5}$$

where we have used (4) to write $N_s N_d = \lambda_s\lambda_d/V_{ss}V_{dd}$.

Note that for any assigned value of $\alpha$, the single Eq. (5) cannot determine the two unknowns $\lambda_1$ and $\lambda_2$; also that one may not use $\lambda_2 = \lambda_d$ or $\lambda_1 = \lambda_s$ as a first approximation because it causes the LHS of (5) to vanish.

If we now assume that:

$$F(A' = 0, T_c) = F(B' = 0, T_c) = 1/\lambda \tag{6}$$

and recall from above that we had two distinct gaps in the absence of the inter-band interaction, then (6) is *tantamount to demanding* that these gaps close at the same $T_c$ when such an interaction is switched on. Equation (5) now becomes:

$$\lambda^2 - (\lambda_s + \lambda_d)\lambda + (1-\alpha)\lambda_s\lambda_d = 0\,, \tag{7}$$

solutions of which are:

$$\lambda_{1,2} = \frac{\lambda_s + \lambda_d \pm \sqrt{(\lambda_s - \lambda_d)^2 + 4\alpha\lambda_s\lambda_d}}{2}\,. \tag{8}$$

In the SMW paper, the equation for $F(0)$ is

$$[V_{sd} + N_d(V_{sd}^2 - V_{ss}V_{dd})F(0)][V_{dd} + N_s(V_{sd}^2 - V_{ss}V_{dd})F(0)] = V_{sd}^2 \tag{9}$$

the solutions of which are:

$$\begin{aligned} F(0) &= \frac{1}{\lambda_{1,2}} \\ &= \frac{\pm\left[V_{sd}^2/N_sN_d + \frac{1}{4}(V_{dd}/N_s - V_{ss}/N_d)^2\right]^{1/2} - \frac{1}{2}(V_{dd}/N_s + V_{ss}/N_d)}{V_{sd}^2 - V_{ss}V_{dd}}\,. \end{aligned} \tag{10}$$

This expression has been used by SMW in the BCS equation for $T_c$ — without the $\pm$ signs which seems to be an inadvertent omission. It is straightforward to check, *by rationalizing the expression for* $1/F(0)$ that, in terms of $\lambda_S$, $\lambda_d$ and $\alpha$ defined in (4), the solutions in (10) are **identical** with those given in (8). It follows therefore that in obtaining (10) SMW have made the assumption stated in (6).

## 2. Application of SMW Approach to $MgB_2$

We now attempt to apply the SMW formalism to the concrete example of $MgB_2$ the two gaps of which have been reported[7] to close at the same $T_c$. Relevant superconducting features of $MgB_2$ are[8]:

$$\Delta_{01} = 2.1 \text{ meV}\,, \quad \Delta_{02} = 6.2 \text{ meV}\,; \quad T_c = 39 \text{ K}\,; \quad \Theta_D = 815 \text{ K}\,, \tag{11}$$

where the Debye temperature $\Theta_D$ has been taken to be the mean of 750 K and 880 K. In view of remark 4(a) in the opening paragraph, we are induced to attribute the values of the two zero-temperature gaps in (11) to $\alpha = 0$ in (8) and $\lambda_S$ calculated via

$$\lambda(0) = \frac{1}{\operatorname{arcsinh}(k_B\Theta_D/\Delta_0)}\,. \tag{12}$$

Thus

$$\lambda_1 = \lambda_d = 0.238\,, \quad \lambda_2 = \lambda_s = 0.32\,. \tag{13}$$

We note that the $T_c s$ corresponding to these $\lambda_S$ are 13.9 K and 40.9 K, respectively. On the other hand, $\lambda$ corresponding to the empirical[8] $T_c = 39$ K calculated via

$$\lambda(T_c) = \frac{-1}{\ln(T_c/1.14\Theta_D)} \tag{14}$$

is found to be,

$$\lambda(39 \text{ K}) = 0.315\,. \tag{15}$$

Comparing this value with the second of the two values in (13), it is seen that $\lambda(0) > \lambda(39 \text{ K})$. This inequality will be further discussed.

We now seek to find if a small positive value of $\alpha$ (which we recall denotes $V_{sd}^2/V_{ss}V_{dd}$) can bring about closure of the two gaps at the higher $T_c$ in accord with the assertion by SMW. To this end we successively put $\alpha = 0.01$, 0.02 and 0.03 in (8) and determine the values of $\lambda_{1,2}$ that they lead to, and find that:

$$\begin{aligned}\lambda_{1,2} &= 0.230, 0.328 \quad (\alpha = 0.01)\\ &= 0.222, 0.336 \quad (\alpha = 0.02)\\ &= 0.216, 0.342 \quad (\alpha = 0.03)\,. \end{aligned} \tag{16}$$

As a matter of fact, the smaller the value of $\alpha$, the closer are the $\lambda_{1,2}$-values to the original values in (13) that one had with $\alpha = 0$. It is easy to see that the following inferences drawn from the above considerations are not dependent on the particular values of $\lambda_S$ invoked in (13): (a) If experiment dictates that an SC has *two zero-$T$* gaps $\Delta_0$ but only one $T_c$, then we need two $\lambda_S$ at $T = 0$ which must converge to the same value as $T_c$ is approached. This requirement cannot be met by the SMW approach because any real, finite (nonzero) positive value of $\alpha$ in this approach causes the *greater* of the two $\lambda_S$ in the theory to *increase* and the smaller one to decrease: this is transparent from (8) above which as already noted is identical with (10). (b) Even if one assumes that a suitable value of $\alpha$ due to the inter-band interactions could meet the requirement under consideration, the fact would remain that a $\lambda$ at $T = 0$ goes over to another value as $T_c$ is approached. So either $\lambda_S$ or $\lambda_d$, or both of them must have a rather complicated T-dependence (due to itinerancy?) if one is to realize the broken curve in Fig. 2 of SMW. (c) The assertion about the nature of $T$-dependence of the $\lambda_S$ follows from the fact the figure under consideration shows a change in the curvature of the plot of $\Delta(T)/\Delta_0$ against $T$ near the higher $T_c$. Finally, (d) if one follows this plot backwards to $T = 0$, one finds a *third* value for $\Delta_0$.

Despite some of the above, rather ambiguous, features of the SMW approach, it provides one with an important clue for dealing with a superconductor that is characterized by two $\Delta_0 s$ and one $T_c$, which is: consider the possibility of the $\lambda_S$ in the theory to be $T$-dependent. This is the feature of their approach that seems to us to have escaped serious attention and which we follow up.

Even if the SMW approach is assumed to work for closure of both the gaps of a CS at the same $T_c$, it cannot account for such high-$T_c s$ as have been observed. This is so simply because that approach is based on the *single*-phonon exchange dynamics for the formation of Cooper pairs. We now invoke multi-phonon exchanges via the generalized-BCS equations (GBCSEs) to address the observed (high) $T_c$ and the two gaps of $MgB_2$.

## 3. Quantitative Study of $MgB_2$ via Generalized-BCS Equations

It seems pertinent first of all to investigate if a $T$-dependence of $\lambda$ is also a feature of elemental superconductors. To this end we calculated $\lambda(T = 0)$ via (6) and $\lambda(T_c)$ via (7) for seven selected elements: Cd, Pb, Hg, Sn, In, Tl and Nb. Interestingly, as shown,[9] we found that for all of these:

$$\lambda(0) > \lambda(T_c)\,. \tag{17}$$

Additionally, the difference between these two $\lambda_S$ is significant for Pb and Hg, whereas for the other five elements it is marginal. Therefore, while for the latter five elements $\lambda$ may be eliminated between (12) and (14) leading approximately to the well-known BCS value of 3.53 for the gap-to-$T_c$ ratio $2\Delta_0/k_BT_c$ one cannot do so for Pb and Hg, the so-called "bad actors". A $T$-dependence of $\lambda$ is thus seen to shed light on the violation of the alleged universal gap-to-$T_c$ ratio in BCS theory.

With the clue provided by SMW, and the feature of elemental superconductors noted above in view, we now give a concise but complete account of the superconducting features of $MgB_2$ via the alternative approach provided by the GBCSEs. We recall[10–12] that these equations constitute a generalization of the BCS equations because: (a) they incorporate the mechanism of multi-phonon exchanges for the formation of Cooper pairs in addition to the usual one-phonon exchange mechanism and (b) they invoke more than one Debye temperature in order to take into account the anisotropy of a composite (i.e., nonelemental) superconductor. The GBCSEs for the two gaps are:

$$1 = \lambda_1^c(T)\int_{|W_1|/2}^{k_B\Theta_1^c+|W_1|/2} dx\frac{\tanh(x/2k_BT)}{x}\,, \tag{18}$$

$$\begin{aligned}1 = \lambda_1^c(T)&\int_{|W_2|/2}^{k_B\Theta_1^c+|W_2|/2} dx\frac{\tanh(x/2k_BT)}{x}\\ &+\lambda_2^c(T)\int_{|W_2|/2}^{k_B\Theta_2^c+|W_2|/2} dx\frac{\tanh(x/2k_BT)}{x}\,,\end{aligned} \tag{19}$$

where,

$$\lambda_1^c(T) = \lambda_1^c(0) + \alpha_1 T\,;\quad \lambda_1^c(0) = 0.2216\,,\quad \alpha_1 = 1.7923\times10^{-3}\ \mathrm{K}^{-1},\quad \Theta_1^c = 1062\ \mathrm{K}$$

$$\lambda_2^c(T) = \lambda_2^c(0) + \alpha_2 T\,;\quad \lambda_2^c(0) = 0.1073\,,\quad \alpha_2 = -2.749\times10^{-3}\ \mathrm{K}^{-1},\quad \Theta_2^c = 322\ \mathrm{K}$$

$$|W_1| = \Delta_1\,,\quad |W_2| = \Delta_2\,.$$

The equation for the higher $T_c$ follows from (19) by putting $|W_2| = 0$, giving

$$1 = \lambda_1^c(T)\int_0^{k_B\Theta_1^c} dx\frac{\tanh(x/2k_BT)}{x} + \lambda_2^c(T)\int_0^{k_B\Theta_2^c} dx\frac{\tanh(x/2k_BT)}{x}\,. \tag{20}$$

We recall that the Debye temperature is just another way to specify the Debye *frequency* — two such temperatures arise for a binary because of the difference in the masses of the vibrating ions that constitute its lattice. A virtue of GBCSEs is: Given any two of the triplet of the BCS quantities $\{\Delta_{01}, \Delta_{02}, T_c\}$, they enable one to calculate the third, which is an extension of what the normal BCS equations achieve for elemental superconductors. For a detailed account of the values of $\lambda_1^c(0)$,

$\lambda_2^c(0)$, $\Theta_1^c$ and $\Theta_2^c$ quoted above, we refer the reader to Ref. 11. It is easy to verify that the GBCSEs given above can quantitatively account for not only the two zero-temperature gaps and the $T_c$ of $MgB_2$, but also closure of the gaps at the higher $T_c$ in accord with experiment. In addition, one is enabled to tackle other problems such as the thermal conductivity of this SC via, e.g., the Geilikman–Kresin/BRT theories.[13–15]

We now address a question that cannot have escaped the cognoscenti: How is it that the set of GBCSEs above for a two-gapped SC has two interaction parameters whereas the SMW approach has three such parameters? We note that while the physical origin of multiple gaps in the approach delineated above is different from the one in SMW, *effectively*, it nonetheless has three interaction parameters for a two-gapped SC. Symbolically, these are

$$(\lambda_1^c, \Theta_1^c)\,, \tag{21}$$

$$(\lambda_2^c, \Theta_2^c)\,, \tag{22}$$

$$(\lambda_1^c, \Theta_1^c) + (\lambda_2^c, \Theta_2^c) \tag{23}$$

It has been shown in Refs. 11 and 12 that we are led via (23) to the larger gap and via (21) or (22) to the smaller gap in $MgB_2$, YBCO, etc — in agreement with experiment. If the parameters in (21) lead to the observed smaller gap, then a natural question to ask is: What about another small gap led to by the parameters in (22)? In our work in references just cited, we had remarked that it is "too small to be observed." It turns out that precisely such gaps have recently been reported[16–18] for the iron-pnictide SCs. For a detailed account via GBCSEs of the gaps and the $T_c$ of the prominent member $Ba_{0.6}K_{0.4}Fe_2As_2$ of the iron-pnictide family we refer the reader to Ref. 19.

## 4. Some Remarks about T-Dependent Hamiltonians

Indeed, the above considerations have willy-nilly led us to the not-very-familiar territory of $T$-dependent Hamiltonians because the effect of temperature on any property of the system is usually taken into account by averaging over the Boltzmann-weighted $T$-independent energy eigenvalues. Nonetheless, it is not the first time that such territory has been reached, as evidenced by the employment of $T$-dependent dynamics in the context of:

(1) Superconductivity in the work of Bogoliubov, Zubarev and Tserkovnikov, as discussed by Blatt[20];
(2) An explanation[21] of the empirical law: $H_c(T) = H_c(0)[1 - (T/T_c)^2]$, where $H_c(T)$ is the critical field at $T$;
(3) Finite-temperature behaviour[22–25] of a class of relativistic field theories (RFTs) to address the question of restoration of a symmetry which at $T = 0$ is broken either dynamically or spontaneously;
(4) Wick–Cutkosky model[26] in an RFT;

(5) The legions of unidentified solar emission lines[27];
(6) QCD to explain[28,29] the masses of different quarkonium families and their deconfinement temperatures, and most recently in
(7) A comparative study[30] of the experimental features of the Bose–Einstein condensates in clouds of $^{7}$Li,$^{23}$Na, $^{41}$Ca, $^{85}$Rb, $^{87}$Rb and $^{133}$Cs atomic gases.

## 5. Conclusions

We have pointed out that in a situation envisaged by SMW in the framework of the BCS theory, the interaction parameters must be $T$-dependent. Acting on this cue, we have presented a plausible scenario for a quantitative understanding of the superconducting properties of $MgB_2$ via the set of GBCSEs. Finally, we have drawn attention to the similarity of the $T$-dependent approach followed here with earlier such studies in diverse fields.



## Acknowledgments

GPM thanks Ms. Amudhakumari for an interesting discussion about the contents herein during the conference EUROQUAM2010. He also thanks S. R. Choudhary for valuable e-exchanges concerned with this submission. MdeLl thanks UNAM-DGAPA-PAPIIT (México) for partial support from grant IN102011 and J. E. Hirsch for a brief consultation.

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