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A new look at the high T_c superconductors using BCS-theory

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Abstract. Using the conventional phonon-exchange mechanism of superconductivity we have succeeded in reproducing the transition temperature T_c of a large number of newly discovered high T_c superconductors by introducing a certain modification to the well-known BCS-formula for T_c.

Keywords. Phonon exchange mechanism; modified BCS formula.

1. Introduction

After the discovery of the high transition temperature (T_c) superconductors (Bednorz and Müller 1986; Wu *et al* 1987) there have been a great interest in understanding the true mechanism responsible for superconductivity in these systems. The main obstacle against accepting the conventional BCS-theory (Bardeen *et al* 1957) for these high T_c oxide superconductors is that there is an absence of the isotope effect in some of the compounds like $YBa_2Cu_3O_7$ and $EuBa_2Cu_3O_7$ (Batlogg *et al* 1987; Bourne *et al* 1987) whose transition temperatures T_c are around 90 K. A complete absence of the isotope effects in any superconductor implies that the force responsible for binding a pair of electrons may not be produced by the exchange of a phonon. Subsequent measurement of the isotope effect in the material $La_{1\cdot 85}Ba(Sr)_{0\cdot 15}CuO_4$ (Batlogg *et al* 1987; Faltens *et al* 1987) having a transition temperature of ≈ 40 K has, on the other hand, shown a non-zero isotope shift, thereby justifying in favour of the phonon-mediated coupling and the BCS-theory operating in this system. To verify the situation in $YBa_2Cu_3O_{7-\delta}$, later on, a precise measurement of the isotope effect was again made (Leary *et al* 1987; Katayama-Yashida *et al* 1988; Batlogg *et al* 1988). These measurements demonstrated a non-zero isotope shift in T_c which was much smaller than the value to be predicted by the phonon-exchange mechanism. A much more recent data on the isotope effects in $Ba_{1-x}K_xBiO_3$ (Loong *et al* 1989), which is known to be a high temperature superconductor having a $T_c \approx 30$ K (Mattheiss *et al* 1988; Cava *et al* 1988), further indicated a substantial shift in T_c. One of the remarkable differences between the Bi and Cu systems is that the charge carriers of the former are the electrons, while those of the latter are the holes. It is thus clear that the BCS-pairing mechanism among the carriers cannot be ruled out in all these high T_c systems. In view of this, we have tried to see how for the phonon mediated BCS theory is applicable to these high T_c superconducting compounds. Our analysis shows that by introducing a suitable modification to the BCS-formulae for T_c it is possible to explain the transition temperature of a large number of high T_c superconducting compounds.

2. Derivation of the modified BCS-formula for T

We start our discussion with the two familiar equations, one for the superconducting energy gap parameter $\Delta_0(0)$, and the other for the transition temperature T_c of the BCS-theory, which are given as (Animalu 1978)

$$\Delta_0(0) = \hbar\omega_D/\sin h\left[\frac{1}{N(0)V}\right], \tag{1}$$

and

$$(1/N(0)V) = \int_0^{\hbar\omega_D} \frac{dx}{x} \tan h\left(\frac{x}{2k_\beta T_c}\right). \tag{2}$$

For metals like Al and Cd etc where the transition temperature is very low (Tilley and Tilley 1986), we take the experimental value of their Debye frequency, $\hbar\omega_D$, known from the phonon dispersion measurements and the value of the energy gap parameter at zero temperature, $\Delta_0(0)$, known from the tunnelling measurements. With the help of (1) the value of the strength parameter $g = [N(0)V]$ is determined for both the cases. After this, we proceed to evaluate the integral on the right hand side of (2) by keeping both T_c and $\hbar\omega_D$ constant. With this, one notices that the value of g is immediately reproduced. It has been found out that this is true in all the cases of low T_c-superconductors. When this procedure is adopted for high T_c-materials, we observe that it is not possible to obtain the same g from both (1) and (2) by maintaining T_c and θ_D constant. To show this explicitly, we classify the newly discovered high T_c-materials into two groups, one with T_c around 90 K and the other around 30 K. We consider the fact that the former are characterized by $(2\Delta_0(0)/k_\beta T_c) = 5{\cdot}5$ (Tsai *et al* 1988; Phillips 1989) and the latter are characterized by $(2\Delta_0(0)/k_\beta T_c) = 4{\cdot}5$ (Kirtly *et al* 1987). We regard $YBa_2Cu_3O_{7-\delta}$ as the reference system; as such, its Debye temperature $\theta_D(\hbar\omega_D = k_\beta\theta_D)$ is supposed to be fairly accurately known. Since θ_D of this system has not been accurately known, we have chosen its $\theta_D = 582$ K. Such a choice of θ_D by us is only a matter of convenience which may not look unreasonable from the point of view of fitting the high temperature specific heat data (Henry *et al* 1988) for $YBa_2Cu_3O_{7-\delta}$ with a $\theta_D = 500$ K. Thus, for the reference system having its $\theta_D = 582$ K and $(2\Delta_0(0)/k_\beta T_c = 5{\cdot}5)$, we first determine the value of parameter g from (1) and then try to reproduce its value from (2) by evaluating the integral on the right side of (2) without changing its $k\omega_D$ and T_c. It is found that for $T_c = 92$ K and $\theta_D = 582$ K, the value of g is never reproduced from (2). In order to get back the value of g from (2), θ_D (equivalently $\hbar\omega_D$) is now varied. It is seen that the value of θ_D required to reproduce g is less than 582 K, which we denote by $\theta_D^{(c)}$, meaning thereby that it is the value of θ_D at $T = T_c$. This being the case, we feel that θ_D used in (1) to calculate g is the value at zero temperature. Thus, it looks from our calculation that for all high T_c superconductors, the value of the Debye temperature θ_D at $T = T_c$ is different from the value at $T = 0$ K. Such temperature variation of θ_D has been known for metallic systems like Al and Mg (Grimvall 1986). Now in order to account for the temperature variation of θ_D, we assume that

$$\theta_D(T) = \theta_D^{(0)}\left[1 - \gamma\frac{T}{\theta_D^{(0)}}\right] \quad \text{for } T \leqslant T_c, \tag{3}$$

where the value of γ (an adjustable parameter) is determined by knowing $\theta_D^{(c)}$ and $\theta_D^{(0)}$. For our reference system $YBa_2Cu_3O_{7-\delta}$, it is found that $\theta_D^{(c)} = 388$ K. This enables us to have $\gamma = 2{\cdot}11$. We now look at the BCS-formulae for T_c which in the weak coupling limit is given as

$$T_c = 1{\cdot}14\,\theta_D \exp[-1/g]. \tag{4}$$

Table 1. Determination of the value of the Debye temperature at $T = 0\,K$ and $T = T_c$.

$La_{1.85}Sr_{0.15}CuO_4$ $T_c = 35\,K$				$Tl_2Ba_2CaCu_2O_8 (T_c = 110\,K)$			
$\theta_D^{(0)}$	g	$\theta_D^{(c)}$	γ	$\theta_D^{(0)}$	g	$\theta_D^{(c)}$	γ
380	0·43906	301	2·257	730	0·61938	485	2·23
370	0·44415	293	2·200	700	0·63457	466	2·13
365	0·44679	289	2·171	695	0·63723	463	2·11
358	0·45060	284	2·110	690	0·63993	460	2·09
350	0·45512	278	2·060	680	0·64544	454	2·065

Table 2. Evaluation of the transition temperature using modified BCS formula

System	Expt T_c(K)	$\theta_D^{(0)}(K)$	g	$\theta_D^{(c)}(K)$	γ	T_c[MBCS]
$Ba_{0.7}K_{0.75}BiO_3$	29.35	300	0·45073	238	2·11	29·48
$La_{1.85}Sr_{0.15}CuO_4$	35	358	0·45060	284	2·11	35·16
$Ba_{1.5}Sr_{0.5}YCu_3O_{6.7}$	87	552	0·63567	368	2·11	87·07
$YBa_2Cu_3O_{7-\delta}$	92	582	0·63677	388	2·11	91·97
$Ba_2La_{0.9}Y_{0.1}Cu_3O_{6.7}$	94·5	600	0·63541	400	2·11	94·60
$Tl_2Ba_2CaCu_2O_8$	110	695	0·63723	463	2·11	109·91

In this equation if θ_D is assumed to be $\theta_D^{(c)}$, then we obtain $T_c = 91{\cdot}98\,K$, corresponding to a value of $g = 0{\cdot}63677$ for the compound $YBa_2Cu_3O_{7-\delta}$. The actual T_c for the system being 92 K, we conclude that the BCS weak coupling formula for T_c is also applicable for the high T_c superconducting materials. With the help of (3), the BCS-formula (4) may be modified to be written in the form:

$$T_c^{[\mathrm{MBCS}]} = \left[\frac{1{\cdot}14\theta_D^{(0)}\exp\left[-\frac{1}{g}\right]}{1 + 1{\cdot}14\gamma\exp\left[-\frac{1}{g}\right]}\right]. \tag{5}$$

We have repeated this calculation for several systems (with T_c between 35 K and 120 K) by varying the values of $\theta_D^{(0)}$. It is noted that in all cases, $\gamma = 2{\cdot}11$, corresponding to a specific choice of $\theta_D^{(0)}$ only. This has been shown in table 1 for two systems. Using the values of $\theta_D^{(0)}$ and g for several systems we have calculated their T_c's using the modified BCS-formulae (5). This is shown in table 2.

3. Conclusion

In the present calculation we have been able to obtain the transition temperature of a variety of high T_c superconducting materials by suitably modifying the well-known BCS formula for T_c. Our calculation shows that the conventional phonon-mediated pairing mechanism among the carriers may be valid even for high T_c superconductors.

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