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Strong coupling superconductivity and Coulomb screening

Abstract

The electron-phonon coupling constant λ has been calculated for A15 compounds assuming the width of the Γ_{12} band as 80 meV. λ has been found to be inversely proportional to the molecular weight. The Coulomb pseudopotential μ* has been found to be negative for $YBa_2Cu_3O_{7-x}$. Similar analysis for U_6X superconductors showed that μ* changes sign.

Key Words

D. A15 compounds; D. HTSC; D. heavy Fermion.

Search for new superconductors has been the interest for past several decades. Such interest has led to the discovery and study of variety of superconductors. Some of these are A15 compound[1-5], heavy Fermion[6] and high-T_C superconductors[7-11] etc. Although several mechanisms for superconductivity have been proposed[7]; in many situations BCS theory has accounted for this phenomena. An improvement over the BCS theory was given by the 'strong coupling theory' which is accurate to $\sim(m_e/M)^{1/2}$. The strong coupling theory includes the effect of Coulomb screening. It appears as the Coulomb pseudopotential parameter μ* in the theory of strong coupling superconductors. In case of large effective electron mass (m^*/m_e) and reduced dimensionality the Coulomb screening can be significantly different in superconductors. Here we report the nature of μ* in HTSC and heavy Fermion superconductor on the basis of electron-phonon coupling constant estimated for A15 compounds.

The analysis is based on the empirical McMillan formula. The latter was originally derived to serve as an interpolation formula for materials where superconductivity arises from electron-phonon interaction and whose electron-phonon spectra function $\alpha^2F(\omega)$ resembles that of elemental Nb. Applying the McMillan formula to estimate coupling strengths was rather popular in the early seventies of the past century before more reliable approaches based on the solution of the (linearized) Eliashberg equations became available. One has to keep in mind that using the McMillan formula implies the assumption of a specific $\alpha^2F(\omega)$. This assumption has not been justified for the A15 superconductors. Concerning the cuprate superconductors and the heavy Fermion superconductors, it is generally agreed that superconductivity in these materials is not caused by phonons. There is no reason why the superconductivity in these materials should follow from the McMillan formula. However, there are only two types of interaction between electrons through phonons or photons and the exotic mechanisms can be assumed to originate from interaction via photons in the framework of strong coupling theory which is accurate to $\sim(m_e/M)^{1/2}$. It is therefore crucial to know the nature of Coulomb screening which occurs as μ* in the numerically derived expression for T_C. McMillan equation for T_C was obtained considering F(ω) of Nb and should be valid for other materials when structure in F(ω) is important. When the electron-phonon coupling is strong the numerically derived

McMillan equation for T_C is given by:

$$T_C=(\Theta/1.45)\ \exp[-\{1.04(1+\lambda)\}/\{\lambda-\mu^*(1+0.62\lambda)\}] \quad (1)$$

where λ is the electron-phonon coupling constant, μ^* is the Coulomb pseudopotential and Θ is the Debye temperature. The electron-phonon coupling constant λ is inversely proportional to the molecular weight M and is given by:

$$\lambda=N(0)\langle I^2\rangle/M\langle\omega^2\rangle \quad (2)$$

The Coulomb pseudopotential is given by:

$$\mu^*=\mu/[1+\mu\ln(E_B/\omega_0)] \quad (3)$$

where ω_0 is the maximum phonon frequency and E_B is an energy cut-off for screened Coulomb interaction in the theory of strong coupling superconductivity. μ^* is then calculated for A15 compounds using the band width of Γ_{12} band as 80 meV. λ was then calculated using experimentally determined values of T_C and Θ (TABLE 1). It is seen that the dependence of $\ln\lambda$ on lnM falls under two classes; Nb or V based A15 compounds. The data was least squares fitted to straight lines. The R^2 of least squares fitting was 0.76 and 0.98 for Nb based and V based A15 compounds respectively.

$$\ln(\lambda)=-0.86\ \ln M+6.12 \quad \text{for Nb type}$$
$$\ln(\lambda)=-1.09\ \ln M+6.84 \quad \text{for V type} \quad (4)$$

Therefore, λ is nearly inversely proportional to M. In order to understand the superconductivity in HTSC the $YBa_2Cu_3O_{7-x}$ is chosen which is well studied. It has a transition temperature of 92 K[8,11].

TABLE 1 : Measured and calculated quantities for superconductivity in A15 compounds

A15	V_3Si	V_3Ga	V_3Pt	V_3Au	Nb_3Al	Nb_3Sn	Nb_3Pt	Nb_3Au
M	179.8	222.5	347.9	349.8	305.7	397.4	473.8	475.7
Θ (K)	431	354	346	338	310	280	267	259
T_C (K)	17.03	15.00	2.73	2.83	18.07	17.97	10.03	10.59
μ^*	0.56	0.51	0.50	0.50	0.48	0.45	0.45	0.44
λ	3.19	2.84	1.60	1.62	3.20	3.15	2.22	2.24

The calculated λ for $YBa_2Cu_3O_{7-x}$ was obtained using the least squares fitting results for A15 compounds. The μ^* is then obtained from Eq.1 using the experimentally determined values of Θ and T_C. It is seen that μ^* is negative for $YBa_2Cu_3O_{7-x}$ (TABLE 2)[12]. The positive μ^* is known to occurs for both weak and strong electron-phonon coupling in materials. However, negative μ^* in $YBa_2Cu_3O_{7-x}$ probably occurs for anomalous Coulomb screening. The effect of disorder in superconductors has been considered before. Disorder broadens the electronic band and can also enhance the Coulomb repulsion. In the case of HTSC disorder reduces T_C which can be understood in terms of reduction of density of states at ε_F or due to enhancement of Coulomb repulsion. In order to further support the existence of Coulomb screening which gives rise to $\mu^*<0$ heavy Fermion compounds such as U_6X (X≡Fe, Co, Mn and Ni) was examined along the above mentioned lines. In case of U_6X (X≡Fe, Co, Mn and Ni) the effective mass (m^*/m_e) varies from 13.5 to 23. It has been suggested from specific heat measurements that U_6X has electronic density of states similar to V_3Si. It is seen from TABLE 3 that μ^* changes sign as m^*/m_e increases. For a screened Coulomb interaction the effective mass is given by:

$$m^*/m_e = [1-0.083r_s(\ln r_s+0.2030)]^{-1} \quad (5)$$

where r_S is Coulomb screening parameter. $r_S\ln r_S$ was obtained from Eq.5 which is given in TABLE 3. It is found that for U_6X and V_3Si, μ^* varies linearly with $r_S\ln r_S$. The data could be least squares fitted to a straight line. The R^2 of the least-squares fitting was 0.96.

$$\mu^*=-0.78r_S\ln r_S+8.0 \quad (6)$$

However, $r_S\ln r_S$ versus μ^* for $YBa_2Cu_3O_{7-x}$ is found to be represented by an isolated point. In this context, it is noted that[10] from μ-spin rotation and specific heat data the extreme anisotropy of λ suggests that the carriers in $YBa_2Cu_3O_{7-x}$ belong to a relatively dense 2D Fermi liquid with effective mass $m_{ab}^*/m_e\approx10$. The isolated point for $YBa_2Cu_3O_{7-x}$ probably can be attributed to the low dimensionality.

TABLE 2 : Measured and calculated quantities for superconductivity in $YBa_2Cu_3O_7$ and U_6X

Compound	Type of λ	M	T_C (K)	Θ (K)	λ	μ^*	m^*/m_e
$YBa_2Cu_3O_7$	Nb based λ	666	92	375	3.43	-0.50	10
	V based λ				1.91	-0.68	10
U_6Ni	V based λ	1487	0.5	179	0.33	0.07	14
U_6Mn	V based λ	1483	2.19	196	0.34	1.6×10^{-3}	15
U_6Co	V based λ	1487	2.1	112	0.33	-0.05	20
U_6Fe	V based λ	1484	3.8	114	0.34	-0.1	23

TABLE 3 : μ^*, r_s and m^*/m_e for U_6X, A15 compounds and $YBa_2Cu_3O_7$

Compound	U_6Ni	U_6Mn	U_6Co	U_6Fe	V_3Si	$YBa_2Cu_3O_7$
μ^*	0.07	1.6×10^{-3}	-0.05	-0.1	0.56	-0.68
r_S	5.7373	5.7567	5.8246	5.8511	5.5417	5.6262
m^*/m_e	13.5	15	20	23	8.4	10

In conclusion, the nature of μ^* in HTSC and heavy Fermion superconductor on the basis of electron-phonon coupling constant λ estimated for A15 compounds has been reported. It is found that $\mu^*<0$ for $YBa_2Cu_3O_{7-x}$. Whereas, μ^* changes sign as m^*/m_e increases in U_6X.

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