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S-wave Superconducting Model within the Finite Coulomb Regime in Cerium and Uranium Based Heavy Fermion Compounds.

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Abstract

We have studied the s-wave Cooper pairing in Uranium and Cerium based HF systems by analyzing the periodic Anderson model by means of the Bogoliubov-Valatin approach (BVT) focusing on the interorbital Cooper pairing between a conduction electron (c electron) and an f electron. The ground state energy (E_o) and entropy of this heavy superconductors have been determined. The total Energy decreases below transition temperature and goes to zero at zero Kelvin which is consistent with the nature of super-fluid state. Uranium based compounds show a system energy that is lower than that of Cerium based compounds both at low and high temperatures. Cerium based compounds show a low system energy at low temperatures and a higher one at higher temperatures which is in agreement with their atomic properties. The entropy for cerium-based compounds is higher than that of Uranium-based compounds.

KEYWORDS-*Heavy fermions, Cooper pairing, Transition , entropy*

1. Introduction

In usual heavy-fermion superconductors, the strong Coulomb repulsion between f electrons favors the nodal d-wave symmetry, which has been the subject of a number of theoretical studies [1]. In NQR measurements on $CeRu_2$ and $CeCo_2$, the spin-lattice relaxation rate exhibits an exponential decay at low temperatures and shows the Hebel-Slichter peak. Moreover, the recent photoemission spectroscopy (PES) experiment on $CeRu_2$ has shown that the density of states (DOS) has a clear superconducting gap at the Fermi level. All these results were interpreted as evidence for the fully gapped pairing state with s-wave symmetry [2]. Usually, this type of simple pairing symmetry can be understood within the framework of the conventional electron-phonon mechanism. However, it is unclear whether the electron-phonon attraction can be dominant since the Coulomb repulsion is rather strong in heavy-fermion systems [3]. The multi-orbital nature is one of the characteristic features of heavy-fermion systems, which are composed of itinerant electrons in the conduction orbitals (c electrons) and localized electrons in the f orbitals (f electrons) [4]

The correlation between c and f electrons leads to various intriguing phenomena, such as the Kondo effect [5] quantum critical behavior [6] and magnetic orderings due to the Ruderman Kittel-Kasuya-Yosida interaction [7] .The importance of such orbital degrees of freedom has also been recognized in the studies of superconductivity in the other strongly correlated electron systems. Previous studies [8] suggested that the multiorbital nature can be a source of s-wave superconductivity in heavy-fermion systems. Hanzawa and Yosida and Spalek studied the c-f pairing for finite Coulomb repulsion, and presented a mean field phase diagram of the s-wave superconducting state. However, the mean-field approximation cannot properly describe local charge, spin, and orbital fluctuation effects, which are crucial in heavy-fermion systems [2].

A more sophisticated treatment is required to achieve a deeper understanding of the nature of the interorbital pairing [4]. The advent of heavy-fermion (HF) superconductivity (SC) in $CeCu_2Si_2$ followed the discoveries of super fluidity in ^3He and HF phenomena in $CeAl_3$ [9]. Superconductivity in HF metals involves pairing order parameters which are distinct from the BCS *s*-wave type. Strong support for this is lent by the existence of multiple superconducting phases, similar to what was

observed for superfluid ^{3}He. Multiphase superconductivity was found for UPt_3 , $U_{1-x}Th_xBe_{13}$ and $PrOs_4Sb_{12}$ [10];the latter compound is unique here, since electric quadrupole fluctuations rather than magnetic dipole fluctuations, as commonly assumed for HF superconductors, are believed to mediate the Cooper pairing. Quite generally, the microscopic pairing mechanism in HF superconductors is driven by electronic interactions, contrasting SC in classical (BCS) superconductors mediated by electron-phonon coupling [10]. The coexistence of superconductivity and long range magnetic order was observed in several ferromagnets (UGe_2, URhGe etc) as well as antiferromegnets (UPd_2Al_3, UNi_2Al_3 etc) [9]

In this work we deduce the internal energy, E and the entropy, S(T) of selected heavy fermion compounds. The Uranium based HF compounds are studied and compared with Cerium based HF compounds by using the Bogoliubov-Valatin transformation technique.

2. Model and Approach

A typical HF system composed of itinerant *c* electrons and nearly localized *f* electrons, which hybridize with each other is considered. Usually such a system is modeled by the periodic Anderson Hamiltonian $H_{PAM} = H_0 + H_V$, [8]

We develop a Model Hamiltonian for s-wave superconductivity in heavy fermion systems as

$$H=H_{dir}+H_{on}+H_{c\text{-}f}+H_{ee}+H_{rep} \quad (1)$$

where H_{dir} represents the hopping electrons, H_{on} represents the on-site energy of f electrons, $H_{c\text{-}f}$ represents the hybridization between the c and f states, H_{ee} represent the band occupation while H_{rep} represents the on-site coulomb repulsion in the f orbital giving rise to

$$H= \sum_k \varepsilon_k (c_k^+ c_k + c_{-k}^+ c_{-k}) + \sum_f \varepsilon_f n_{if}^f - \sum_{k\sigma} t_k (c_{k\sigma}^+ f_{-k\sigma} - c_{-k\sigma} f_{k\sigma} + H.C - \mu \sum_{i\sigma} (n_{i\sigma}^c + n_{i\sigma}^f n_{i\uparrow}^f n_{i\downarrow}^f) \quad (2)$$

where ε_k is the on-site energy of c electrons $n_{i\sigma}^f = f_{i\sigma}^+ f_{k\sigma}$ and ε_f is the on-site energy of f electrons, $c_{i\sigma}^+(f_{i\sigma}^+)$ creates an itinerant c electron (a localized f electron) with spin σ at site i and t_k is the hybridization energy between the conduction and f electron states μ is the chemical potential that determines the occupation of the band and U_k is the on-site Coulomb repulsion.

Equation (2) which is modified form of the PAM Hamiltonian is expressed in terms of creation and annihilation operators and then diagonalized to obtain the elements of the Hamiltonian that correspond to stationary states where the system is in equilibrium. Bogoliubov-Valatin Transformations are used to transform "(2)".

the inverse transformation of equations are used.

$$c_k = u_k \gamma_k + v_k \gamma_{-k}^+ \quad (3a)$$
$$c_{-k} = u_k \gamma_{-k} - v_k \gamma_k^+ \quad (3b)$$
$$c_k^+ = u_k \gamma_k^+ + v_k \gamma_{-k} \quad (3c)$$
$$c_{-k}^+ = u_k \gamma_{-k}^+ - v_k \gamma_k \quad (3d)$$

The Hamiltonian for the s-wave superconductivity model from "(2)" is

$$H = \sum_k \varepsilon_k \{2v_k^2 + (u_k^2 - v_k^2)(m_k + m_{-k}) + 2u_k v_k (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k}\gamma_k)\} - \sum_k \varepsilon_f \{2v_k^2 + (u_k^2 - v_k^2)(m_k + m_{-k}) + 2u_k v_k (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k}\gamma_k)\} - \sum_k t_k \{4u_k v_k (m_k + m_{-k} - 1) + (2u_k^2 - 2v_k^2)(\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k}\gamma_k)\} - \mu \sum_k \{2u_k^2 m_k + 2v_k^2 (1 - m_{-k}) + 2u_k v_k (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k}\gamma_k)\} + \sum_k U_k \{v_k^4 (1 - m_k)(1 - m_{-k}) + 2v_k^3 u_k (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k}\gamma_k)\} \quad (4)$$

This Hamiltonian is diagonalized by fermionic canonical transformations resulting into ground state energy of the HF system

$$E_o = 1.66\varepsilon_k + 1.66\varepsilon_f - 1.66\mu + 0.37t_k + 0.69U_k \quad (5)$$

This is based on the fact that at high temperatures most of the electrons are thermally excited to higher states and thus all the occupation numbers are equal to zero. The coefficients of the off diagonal terms gives $u_k = 0.41$and $v_k = 0.91$ [1]

The energy of the system E at any temperature is found by multiplying the ground state energy E_o by the thermal activation factor $e^{\frac{-\Delta E}{K_B T}}$ [11], where K_B is Boltzmann's constant and ΔE is the energy gap. The energy gap for superconductors is a very small quantity and it is generally 1% of the minimum energy of the system [11].Thus $\Delta E = 0.01E_o$so at any temperature T, the energy of the system is given as

$$E = E_o e^{\frac{-E_o}{100K_BT}} \quad (6)$$

Substituting equation (5) in equation (6), we obtain the magnitude of energy of the system at any given temperature as;

$$E = (1.66\varepsilon_k + 1.66\varepsilon_f - 1.66\mu + 0.37t_k + 0.69U_k) e^{\frac{-(1.66\varepsilon_k + 1.66\varepsilon_f - 1.66\mu + 0.37t_k + 0.69U_k)}{100K_BT}} \quad (7)$$

The system entropy is determined to be;

$$S=m\left(\frac{(1.66\varepsilon_k + 1.66\varepsilon_f - 1.66\mu + 0.37t_k + 0.69U)^2}{K_B}\right)$$

$$\left(\frac{K}{10^{-2}TE_o} e^{-\frac{0.01E_o}{KT}} + \frac{3K^2}{10^{-4}E_o^2} e^{-\frac{0.01E_o}{KT}} + \frac{6K^3T}{10^{-6}E_o^3} e^{-\frac{0.01E_o}{KT}} + \frac{6K^4T^2}{10^{-8}E_o^4} e^{-\frac{0.01E_o}{KT}} \right) \quad (8)$$

3. Results and Discussion

The value of E decreases below T_C (K) and goes to zero at T=0 K and this is consistent with the nature of super-fluid state. The total energy of the system increases with increase in temperature of the system. The Uranium based compounds show a system energy that is lower than that of Cerium based compounds both at low and high temperatures. Cerium based compounds show a low system energy at low temperatures and a higher one at higher temperatures which is in agreement with their atomic properties [12] when the two compounds are studied comparatively as seen in fig 1.0 and fig 2.0.

There exists an exponential increase in the energy of the system as the temperature increases approaching a plateau like state dependent on type of the material. It was noted that energy of interaction between Cooper pair is a stretched sigmoid shaped curve. Similar shapes of curves relating energy and temperature were noted by other scientists [13], [14] and [26]. The rate of increase of energy with temperature for Uranium is lower than that of Cerium. Both compounds show very low energy at T_C.

A graph depicting the variation of energy versus temperature is as shown in fig 1.0

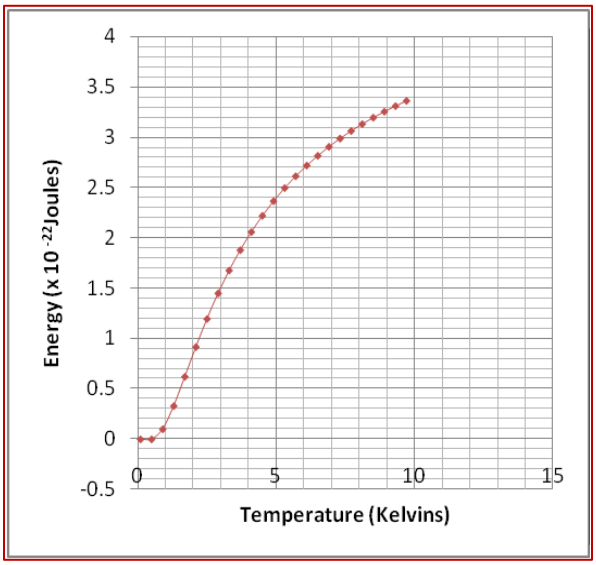

Figure 1.0; **Variation of System Energy against Temperature for Uranium compounds.**
for Uranium compounds E_k=0.1eV,E_f= -3eV,μ= -0.52eV t_k= -0.43 eV, U=6 eV[16].

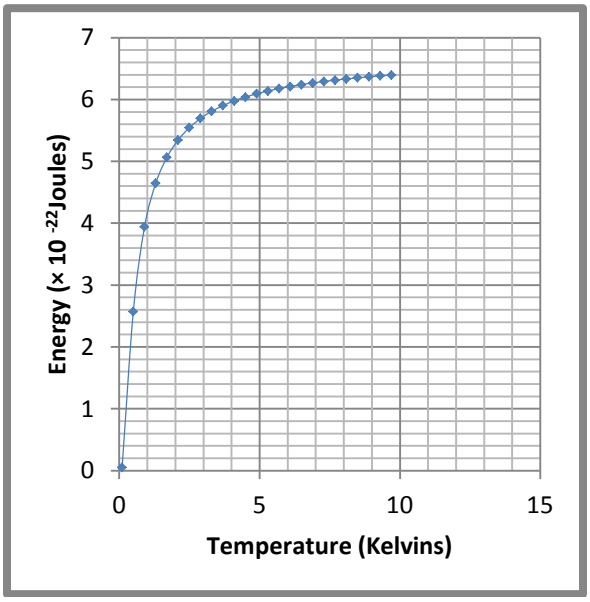

Figure 2.0 **Variation of System Energy against Temperature for Cerium compounds.**
Experimental parameters used for Cerium compounds are E_k=0.1eV,E_f= -3eV,μ= -0.52eV t_k= -0.4 eV, U=6 eV [16].

The s-wave superconducting model reveals qualitatively both HF compounds. An exponential growth of entropy for both compounds is noted at lower temperatures as in fig 3.0 and 4.0. The entropy curves agree with the ones obtained by [17]. The rate of increase of entropy with temperature of the Cerium based compounds is higher than that of Uranium based compounds. The entropy at T_C for both compounds is very low. The superconducting phase appears below T_C because the free energy of the superconducting phase becomes less than the free energy of the normal phase for all temperatures below T_C . The state of disorder diminishes with decrease in internal energy of the system (particles settle and interact less as the system liberates energy) [15].

Our results point out that the entropy in the SC state is less than that in the normal state for all temperatures below T_C showing that SC is more ordered than the normal state. These results are in total agreement with other theoretical studies as reported by [15].

These results establish the fact that the pairing model in Cerium based HF superconductors is that of s-wave symmetry in the presence of finite Coulomb repulsion which is in agreement with experimental results [17].

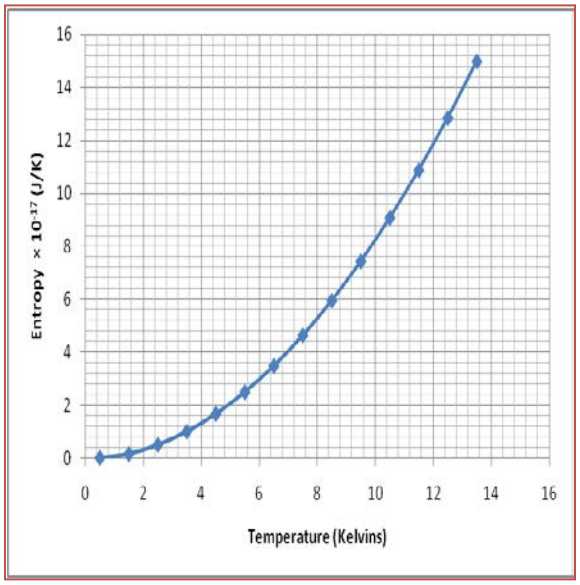

Figure 3.0; **Variation of System Entropy against Temperature for Cerium compounds.**
Experimental parameters used for Cerium compounds are E_k=0.1eV,E_f= -3eV,μ= -0.52eV t_k= -0.4 eV, U=6 eV, V_{kk}=0.7 eV. [16].

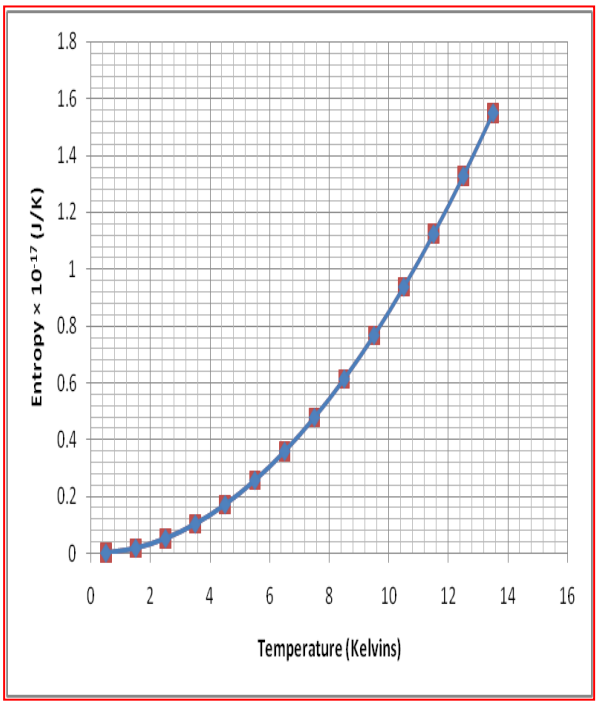

Figure 4.0; **Variation of System Entropy against Temperature for Uranium compounds.**
Experimental parameters used for Uranium compounds E_k=0.1eV,E_f= -3eV,μ= -0.52eV t_k= -0.43 eV, U=6 eV, V_{kk}=0.7 eV. [16]

4. Conclusions

We have been able to modify and diagonalize the s-wave superconducting model using BVT technique. Further we examined the internal energy and hence the entropy of the HF system within the finite coulomb regime. We deduce that superconductivity is a low energy process and hence, Uranium is projected to be the likely suitable material for the construction of room temperature superconductors. Our results point out that the entropy in the SC state is less than that in the normal state for all temperatures below T_C . Entropy at T_C of the Uranium based compounds is lower than of Cerium based compounds i.e. $4 \times 10^{-19} JKg^{-1}$ and $3.8 \times 10^{-18} JKg^{-1}$ respectively.

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