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Correlation between C and F Electrons in Heavy Fermion Superconductors

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ABSTRACT

The integrated s-wave and p-wave Cooper pairing in Uranium and Cerium based heavy fermion systems have been studied by analyzing the periodic Anderson model by means of the Bogoliubov-Valatin approach. The interorbital Cooper pairing between a conduction electron (c electron) and an f electron, called the "c-f pairing." S-wave and p-wave superconductivity appears to coexist with long-range antiferromagnetic order. The ground state energy was found to be 0.02eV for the Cerium based compounds while that of Uranium based compounds was 0.033eV. The value of E decreases below the transition temperature and goes to zero at zero Kelvin and this is consistent with the nature of the super-fluid state. The total energy of the system increases with increase in temperature of the system. The entropy at T_C was found as $\sim 4 \times 10^{-26} J/K$ and $\sim 1 \times 10^{-25} J/K$ for Uranium and cerium based compounds respectively. These results establish the fact that the pairing model in Uranium based heavy fermion superconductors is that of integrated s-wave and p-wave in the presence of finite Coulomb repulsion.

KEYWORDS: *Heavy fermions, Transition temperature, superconductivity, entropy*

INTRODUCTION

A remarkable variety of collective electronic phenomena have been discovered in compounds with partially filled f-orbitals where electronic correlations are dramatically enhanced [1].

In these compounds the entanglement of the rather localized f-electrons with the surrounding itinerant electrons starts at relatively high temperature leading to the development of low-energy composite quasiparticles with a heavy effective mass. The multiorbital nature of which is one of the characteristic features of HF systems, which are composed of itinerant electrons in the conduction orbitals (c electrons) and localized electrons in the f orbitals (f electrons) [2]. Due to the large Coulomb repulsion between the electrons and their strongly correlated behavior, it is expected that the pairs formed in the HF superconducting state will not be s-wave.

Instead, they are expected to pair up in the asymmetric p-wave or the anisotropic d-wave schemes in order to avoid the large spatial overlap associated with the symmetric s-wave state [5].

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) [3]. On the other hand some HF compounds such as $CeRu_2$, $CeCo_2$ and $CeCu_2Si_2$ are known to exhibit s-wave superconductivity [4].

A more sophisticated treatment is required to achieve a deeper understanding of the nature of the interorbital pairing [2].

FORMALISM

A. s-wave and p-wave pairing in heavy fermion systems

In this research we consider the correlation between c and f electron (c-f pairing) interaction as s-wave Cooper pairing and a parallel spin alignment of c-electrons making it possible to have s=1 Cooper pairs as p-wave Cooper pairing. The onsite repulsion of f-electrons is also considered and a gas of non interacting electrons in an s-band that forms the spin exchange.

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

$$H_{PAM} = H_0 + H_V, \qquad (1)$$

The Hamiltonian for this correlation is then written as

$$H = \sum_k \varepsilon_k (c_k^+ c_k + c_{-k}^+ c_{-k}) - \sum_{k\sigma} t_k (c_{k\sigma} f_{-k\sigma} - c_{-k\sigma} f_{k\sigma} + H.C) - \sum_{kk'\sigma} V_{kk'} c_{k'\bar{\sigma}}^+ c_{k'\sigma}^+ c_{i\sigma} c_{i\bar{\sigma}} + \sum_{kk'\sigma} U_{kk'} f_{k\sigma}^+ f_{-k\sigma}^+ f_{-k'\sigma} f_{k'\sigma} \quad (2)$$

Where $c_{i\sigma}^+ (f_{i\sigma}^+)$ creates an itinerant c electron (a localized f electron) with spin σ at site k. Here ε_k is the single particle energy, t_k is the hybridization between c and f states, $V_{kk'}$ is the effective attractive interaction and $U_{kk'}$ is the effective repulsive interaction.

Bogoliubov-Valatin Transformations are used to transform "(2)" by defining two new operators related to the fermion creation and annihilation operators and their conjugates.

Anticommutation laws are then used in "(2)" to give the effective quasi-particle Hamiltonian below;

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

$$+ \sum_k U_{kk'}\{(u_{k'}v_{k'}(1 - m_{-k'} - m_{k'})(u_k^2 - v_k^2)(\gamma_k^+\gamma_{-k}^+ + \gamma_{-k}\gamma_k) + u_k v_k u_{k'}v_{k'}(m_k(m_{k'} + m_{-k'} - 1) + (m_{-k} - 1)(m_{k'} + m_{-k'} - 1)\}$$

$$- \sum_k V_{kk'}\{u_k v_k u_{k'}v_{k'}\left((1 - m_{-k'} - m_{k'})(1 - m_{-k} - m_k)\right) + \text{ukvk1}-\text{m}-\text{k}'-\text{mk}'\, uk2-vk2\gamma k+\gamma-k++\gamma-k\gamma k \quad (3)$$

The BVT technique was used to diagonalize "(3)" and the ground state energy of the system is obtained as;

$E_o = (1.4\varepsilon_k + 1.8t_k + 0.2U_{kk'} - 0.2V_{kk'})$ (4)

The coefficients of the off-diagonal terms give $u_k = 0.5258$ and $v_k = 0.8506$ [1].

We can express the energy of the system at any temperature, E as a function of temperature by multiplying the ground-state energy, E_0 by the thermal activation factor, $e^{\frac{-\Delta E}{KT}}$ to give;

$$E_o = \left(1.4\varepsilon_k + 1.8t_k + 0.2U_{kk'} - 0.2V_{kk'}\right) e^{\frac{-\left(1.4\varepsilon_k + 1.8t_k + 0.2U_{kk'} - 0.2V_{kk'}\right)}{100K}} \quad (5)$$

The superconducting entropy by this model is given as;

$$s = m\left(\frac{\left(1.4\varepsilon_k + 1.8t_k + 0.2U_{kk'} - 0.2V_{kk'}\right)}{100K}\right)\left(\frac{K}{10^{-2}TE_0} + \frac{3K^2}{10^{-4}TE_0^2} + \frac{6K^3T}{10^{-4}TE_0^3} + \frac{6K^4T^2}{10^{-8}TE_0^4}\right) e^{\frac{-0.01E_0}{KT}} \quad (6)$$

Results and Discussion

At zero temperature the energy corresponds to the lowest energy level of the system in the ground state as seen from figure 1.0. The value of E decreases below T_C (K) and becomes 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. 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 the energy of interaction between Cooper pair is a stretched sigmoid shaped curve. Similar shapes of curves relating to energy and temperature has been noted by other scientists [6]. The rate of increase of energy with temperature for Uranium is lower than that of Cerium in the temperature range of 0K-2.2K. However, at high temperatures (T>2.20K) the trend is reversed with Cerium showing a lower rate of change of system energy. High-T_c superconductivity, being a low-energy process requires that the system energy should be kept as low as possible. Thus Uranium based compounds would be a better candidate for the construction of a room-temperature superconductor.

A comparison of the Uranium based compounds and Cerium based compounds ground state energy reveals that the ground state energy of the Cerium based compounds (0.02eV) is lower than the ground state energy of the Uranium based compounds system (0.033eV). This is best thought of as an atomic property of the material. [6].

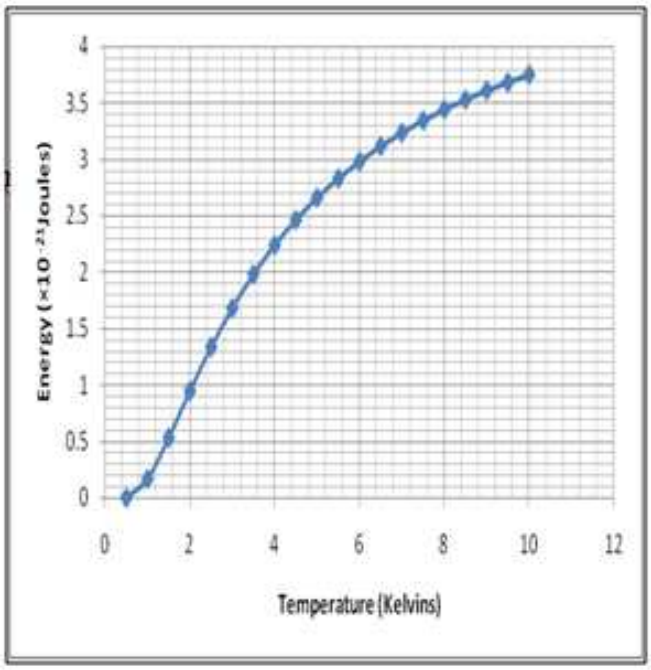

Fig 1.0: Variation of internal energy and temperature for **Cerium based compounds.**

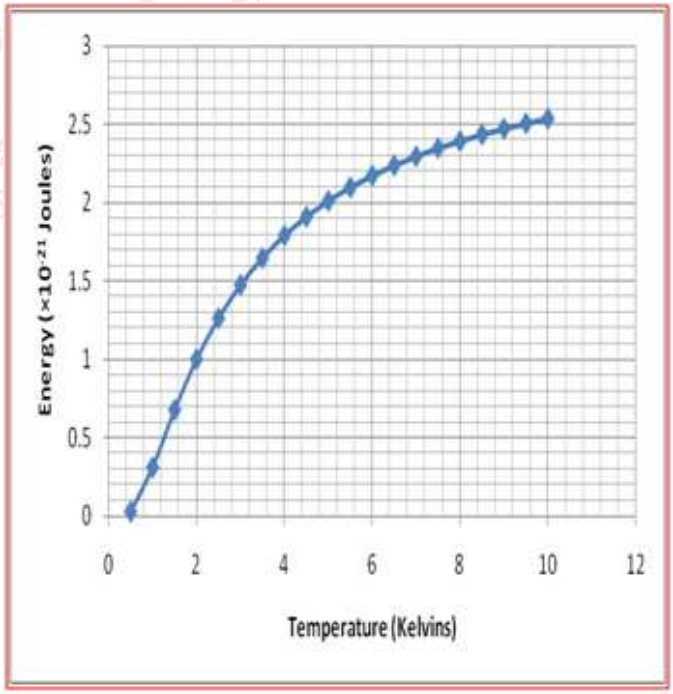

Fig 1.1: Variation of internal energy with temperature for Uranium based compounds.

Experimental parameters For Cerium compounds E_k=0.1eV, t_k= -0.4 eV, U_{kk}=4 eV V_{kk}=1.0 eV and Uranium compounds E_k=0.1eV, ,t_k= -0.43 eV, U_{kk}=4 eV, V_{kk}=0.7 eV [9].

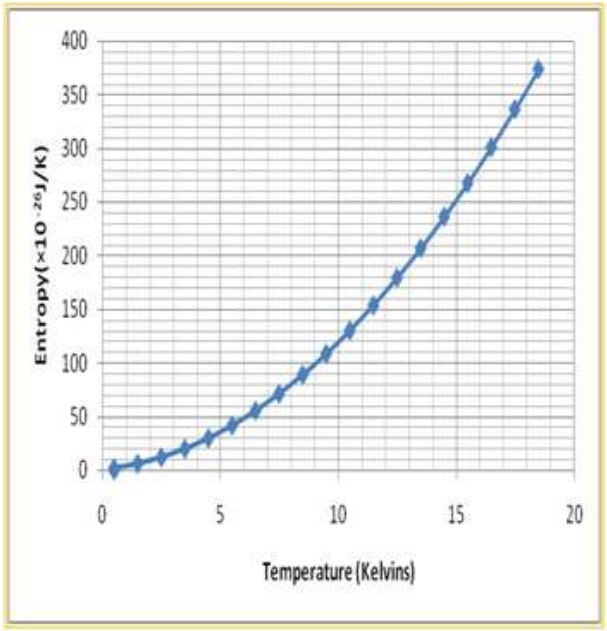

Fig 1.2: Variation of entropy with temperature for Cerium based compounds

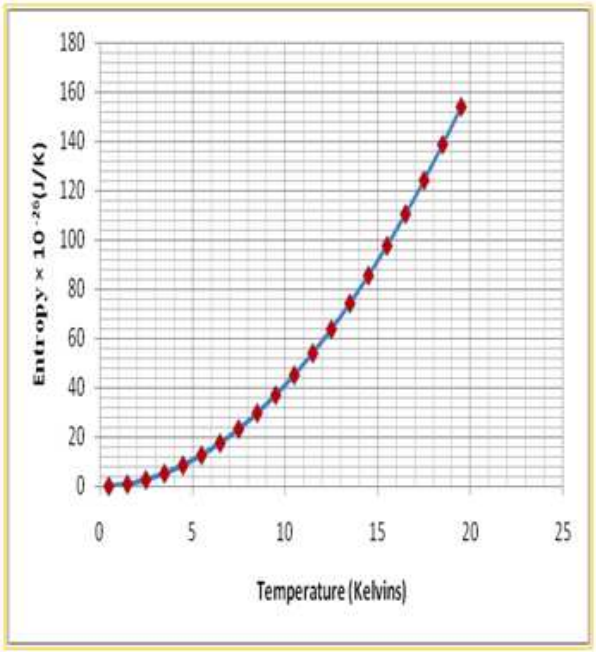

Fig 1.3: Variation of entropy with temperature for Uranium based compounds.

The s-wave and p-wave superconducting model reveals qualitatively both HF compounds. The exponential growth of entropy for both compounds is noted at lower temperatures as in figures (1.2) and (1.3). The entropy curves agree with the ones obtained by [7]. The rate of increase of entropy with the 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 a decrease in internal energy of the system (particles settle and interact less as the system liberates energy) [8].

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 [8].

CONCLUSION

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. $4 \times 10^{-26} JKg^{-1}$ and $1 \times 10^{-18} JKg^{-1}$ respectively.

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