

SPECIFIC HEAT OF THE INTEGRATED S-WAVE AND P-WAVE PAIRING IN URANIUM AND CERIUM BASED HEAVY-FERMION SUPERCONDUCTORS

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ABSTRACT

The s-wave and p-wave Cooper pairing in Uranium and Cerium based HF systems has been studied by analyzing the periodic Anderson model by means of the Bogoliubov-Valatin approach (BVT) while focusing on the interorbital Cooper pairing between a conduction electron (c electron) and an f electron, called the “c-f pairing.” It is shown that the s-wave and p-wave superconductivity appears to coexist with long-range antiferromagnetic order. Moreover, the study with different reference systems used in the BVT shows that the interorbital c-f pairing is essential for the appearance of the s-wave and p-wave superconductivity. The ground state energy (E_0) specific heat (C_v) and electronic specific heat coefficient (γ) of HF superconductors have been determined in the framework of the integrated s-wave and p-wave pairing model. The critical temperature for Uranium and Cerium based compounds is $T_C=1.8K$ and $T_C=1.2K$ respectively which are in agreement with known experimental values. The results show that uranium based compounds can be modelled for high temperature superconductivity.

Keywords: *Heavy Fermion, Specific Heat, Superconducting Transition*

INTRODUCTION

A remarkable variety of collective electronic phenomena have been discovered in compounds with partially filled f-orbitals where electronic correlations are dramatically enhanced. 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. Tuning the hybridization between f-orbitals and itinerant electrons can destabilize the heavy Fermi liquid state at low temperatures towards an antiferromagnetically ordered ground state.

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) (Keisuke & Daisuke, 2015). The correlation between c and f electrons leads to various intriguing phenomena, such as the Kondo effect (Pfeiderer *et al.*, 2009) quantum critical behavior (Shishido *et al.*, 2010) and magnetic orderings due to the Ruderman-Kittel-Kasuya-Yosida interaction (Hewson, 1997). Recently, the importance of such orbital degrees of freedom has also been recognized in the studies of superconductivity in the other strongly correlated electron systems (Keisuke & Daisuke, 2015). The multiorbital nature is considered to be the key for understanding the high- T_C superconducting properties in iron pnictides (Stewart, 2011). Previous studies Keisuke & Yamamoto (2013) suggested that the multiorbital nature can be a source of s-wave superconductivity in HF systems. Hanzawa and Yosida and Spalek (Spalek, 1988) discussed the interorbital Cooper pairing between c and f electrons, which we call the “c-f pairing,” as a possible mechanism for s-wave superconductivity.

HF materials contain elements whose f-shell electrons are strongly correlated, thus, giving rise to a large effective mass in the quasiparticles excitations. 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.

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Keisuke & Yamamoto, (2013) studied the c-f pairing for finite Coulomb repulsion, and presented a mean field phase diagram of the s-wave superconducting state. Note, however, that the mean-field approximation cannot properly describe local charge, spin, and orbital fluctuation effects, which are crucial in HF systems. Thus, more sophisticated treatment is required to achieve a deeper understanding of the nature of the interorbital pairing (Keisuke & Daisuke, 2015).

The coexistence of superconductivity and long range magnetic order was observed in several ferromagnets (UGe₂, URhGe etc) as well as antiferromagnets (UPd₂Al₃, UNi₂Al₃ etc) (Pfleiderer, 2009). On the other hand, some HF compounds such as CeRu₂, CeCo₂ and CeCu₂Si₂ are known to exhibit s-wave superconductivity (Kittaka *et al.*, 2014).

The pairing mechanism in HFSC at finite temperature is not established. Extensive experimental and theoretical studies on UPt₃, a typical HF superconductor, have been devoted in order to elucidate the pairing symmetry. Most attempts to model the properties of the heavy fermion systems on microscopic grounds make use of a somewhat modified version of the Anderson Hamiltonian.

Formalism

A. S-Wave and P-Wave Pairing in Heavy Fermion Systems

In this research we consider the interorbital Cooper pairing 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 $H_{PAM} = H_0 + H_V$, (Keisuke & Yamamoto, 2013).

$$H = H_{dir} + H_{C-f} + H_{ee(p-wave)} + H_{(f-rep)} \quad (1)$$

Where, the first term represents a gas of spin up and spin down non interacting conduction electrons while the second term describes c-f pairing orders. The Hamiltonian in Equation (1) is then written as

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

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.

Equation (2) which is modified form of the PAM 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 equation (2) by defining two new operators related to the fermion creation and annihilation operators and their conjugates. Anticommutation laws are then used in Equation (2) to give the effective quasi-particle Hamiltonian below

$$H = \sum_k \varepsilon_k \{ 2v_k^2 + (u_k^2 - v_k^2)(m_k + m_{-k}) + 2u_k v_k (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) \} - \sum_k t_k \{ (4u_k v_k ((m_k + m_{-k}) - 1)) + (2v_k^2 - 2u_k^2) (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) \} + \sum_k U_{kk'} \{ (u_k v_k (1 - m_{-k'} - m_{k'})) (u_k^2 - v_k^2) (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) + u_k v_k u_k v_k (m_k (m_{k'} + m_{-k'} - 1) + (m_{-k} - 1) (m_{k'} + m_{-k'} - 1)) \} - \sum_k V_{kk'} \{ u_k v_k u_k v_k ((1 - m_{-k'} - m_{k'}) (1 - m_{-k} - m_k)) + u_k v_k (1 - m_{-k'} - m_{k'}) (u_k^2 - v_k^2) \} \quad (3)$$

B. Diagonalization of the S-Wave and P-Wave Pairing Hamiltonian

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To diagonalize the Hamiltonian in equation (3), we put the sum of the off-diagonal terms equal to zero and simplify the resultant expression to obtain the diagonalized Hamiltonian.

$$H_{diag} = \sum_k 2v_k^2 \varepsilon_k - \sum_k t_k (4u_k v_k (m_k + m_{-k} - 1) + \sum_{kk'} U_{kk'} (u_k v_k u_{k'} v_{k'} ((m_{k'} + m_{-k'} - 1) (m_k + m_{-k} - 1)) - \sum_{kk'} V_{kk'} (u_k v_k u_{k'} v_{k'} (m_{k'} + m_{-k'} - 1) (m_k + m_{-k} - 1))) \quad (4)$$

this on subjecting it to the condition $u_k^2 + v_k^2 = 1$ gives us

$$u_k = \frac{4}{5} \text{ and } v_k = \frac{3}{5} \quad (5)$$

At the lowest energy state of this system, both m_k and m_{-k} are zero. Hence, to carry out the Bogoliubov-Valatin transformation for a superconductor in its ground state, m_k and m_{-k} are set to zero in equation (4)

$$H_{diag} = \sum_k 2v_k^2 \varepsilon_k - \sum_k t_k (4u_k v_k) + \sum_{kk'} U_{kk'} (u_k v_k u_{k'} v_{k'}) - \sum_{kk'} V_{kk'} (u_k v_k u_{k'} v_{k'}) \quad (6)$$

Using Equation (5) in Equation (6) the magnitude of the ground state energy of the system is obtained as;

$$E_0 = (0.7\varepsilon_k + 1.9t_k + 0.6U_{kk'} - 0.6V_{kk'}) \quad (7)$$

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

$$E = E_0 e^{\frac{-\Delta E}{100KT}} \quad (8)$$

$$E = (0.7\varepsilon_k + 1.9t_k + 0.6U_{kk'} - 0.6V_{kk'}) e^{\frac{-(\Delta 0.7\varepsilon_k + 1.9t_k + 0.6U_{kk'} - 0.6V_{kk'})}{100KT}} \quad (9)$$

The specific heat capacity at constant volume c_v of the system is obtained as

$$C_V = \frac{(0.7\varepsilon_k + 1.9t_k + 0.6U_{kk'} - 0.6V_{kk'})^2}{100KT^2} e^{\frac{-(\Delta 0.7\varepsilon_k + 1.9t_k + 0.6U_{kk'} - 0.6V_{kk'})}{100KT}} \quad (10)$$

Transition temperature of the superconducting state, T_c is calculated to be

$$T_C = \frac{0.7\varepsilon_k + 1.9t_k + 0.6U_{kk'} - 0.6V_{kk'}}{200K} \quad (11)$$

The electronic specific heat coefficient which is basically the ratio of C and T is computed to be

$$\gamma = \frac{(E_0)^2 e^{\frac{-E_0}{100KT}}}{100KT^3} \quad (12)$$

RESULTS AND DISCUSSION

Essential Parameters

The following values for different physical quantities have been used

For Cerium compounds $E_k=0.1\text{eV}$, $t_k= -0.5 \text{ eV}$, $U_{kk}=6 \text{ eV}$, $V_{kk}=1.5 \text{ eV}$

For Uranium compounds $E_k=0.1\text{eV}$, $t_k= -0.43 \text{ eV}$, $U_{kk}=4 \text{ eV}$, $V_{kk}=0.7 \text{ eV}$ (Chen & Wang, 2016)

A. Energy

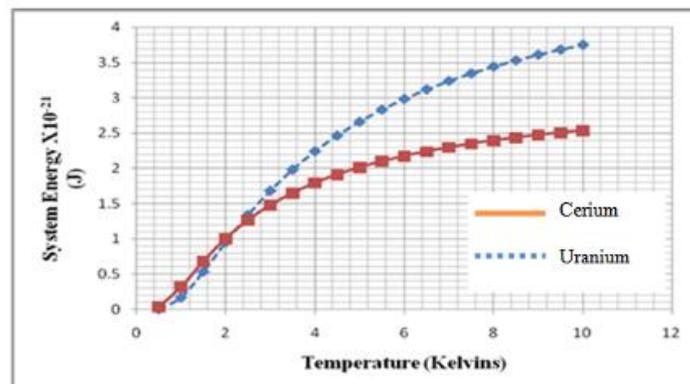


Figure 1: Variation of System Energy against Temperature

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When the temperature is zero the energy corresponds to the lowest energy level of the system in the ground state as seen from figure 1. 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 energy of interaction between Cooper pair is a stretched sigmoid shaped curve. Similar shapes of curves relating energy and temperature has been noted by other scientists (Rapando *et al.*, 2015; Sakwa *et al.*, 2013 and Odhiambo *et al.*, 2016). 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 ($T > 2.20$ K) 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.

At about 2.20K, both Cerium and Uranium have common system energy of 0.008eV. Beyond this point both graphs begin to flatten with Cerium approaching a constant value of energy or leveling faster than Uranium.

There exists a certain 'plateau' or cross-over energy of 0.008eV common to all superconductors beyond which the rate of increase of energy with temperature diminishes. A quick 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 (Butcher *et al.*, 1994).

B. Specific Heat

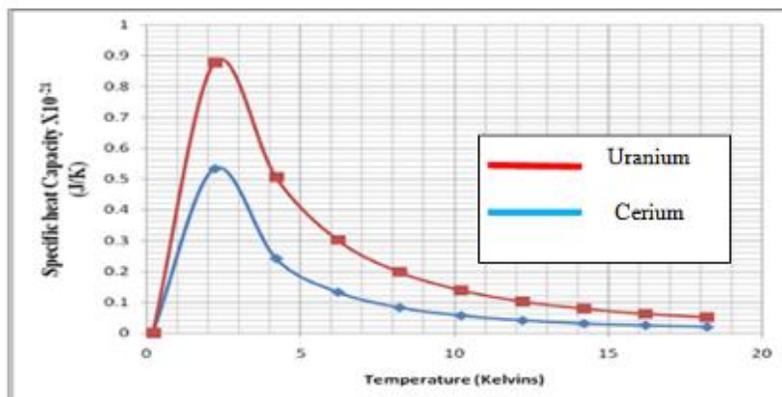


Figure 2: The Graph of Specific Heat against Temperature

From the graph of specific heat in figure 2, Gaussian shaped curves relating specific heat for Cerium and Uranium based compounds is noted. This type of shape was observed by other scientists (Rapando *et al.*, 2015; Sakwa *et al.*, 2013 and Odhiambo *et al.*, 2016).

The maximum value of specific heat capacity for the Uranium-based compounds is maintained at 0.006eV/K and 0.003eV/K for Cerium based compounds.

The specific heat jump of these compounds is strongly influenced by the presence of magnetic impurities. The reduction of the specific heat jump corresponds to pair breaking situations. The jump corresponds to T_c . At $T \gg T_c$ the impurity spin is essentially free to fluctuate driven by thermal agitation; the strongly temperature dependent pair breaking mechanism acts upon the system in the superconducting state and leads to the strong reduction of the specific heat jump. At $T \ll T_c$ the impurity spin is locked into a singlet bound state and no longer takes part in dynamics.

There is unusual temperature dependence of the specific heats below 10K showing the possibility of p-wave pairing of superconducting electrons (Chung *et al.*, 2015). There exists power law temperature dependence below T_c . The low temperature specific heat in both Cerium and Uranium compounds

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includes T^2 as seen from equation (10) terms consistent with the presence of nodes in the superconducting energy gap. Clearly, T_c for Uranium-based compounds is approximately 1.75K and 1.2K for Cerium based compounds which is approximately equal to the experimental value of 2.0 K by Chen & Wang, (2016). Several values of U varying between 1 and 4 eV can be used to analyze the effect of f -electron correlation in HF compounds (Wang *et al.*, 2002).

C. Electronic Specific Heat Coefficient

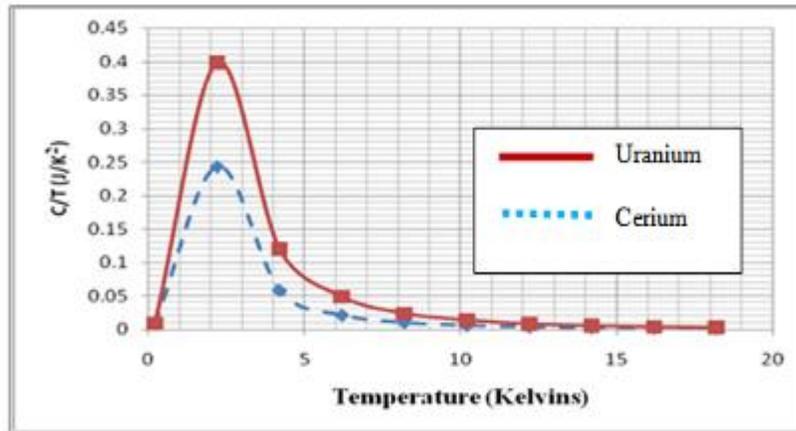


Figure 3: The Graph of Specific Heat Divided by Temperature against Temperature

Electronic specific heat coefficient is defined by the ratio of specific heat to temperature. It majorly gives the electronic contribution to the specific heat at any given moment. It is a measure of the temperature dependent electronic density of states near the Fermi surface, and below 10K is some two or more orders of magnitude in excess of that observed in ordinary metals.

From the graph Electronic specific heat coefficient figure 3 the electronic specific heat coefficient γ is determined. For Cerium based heavy-fermion systems the γ -value is $0.25 \times 10^{-21} \text{J/K}^2$ and $0.4 \times 10^{-21} \text{J/K}^2$ for Uranium based HF systems, this is larger. For an ordinary metal the γ -value is of the order of 1-10 mJ/K'mol. Such a large γ -value is usually explained by the existence of heavy electrons or quasiparticles at the Fermi surface. From these observations the jump in the specific heat $C(T)/T$ at $T_c \approx 2.2 \text{ K}$ is of the same gigantic order. It is concluded that the heavy-mass charge carriers make up the Cooper pairs. These results are in good agreement with Steglich *et al.*, (1979). Similar conclusions were drawn for a few Uranium based HF superconductors discovered in the mid 1980ies, i.e., UBe_{13} , UPt_3 and URu_2Si_2 (Schlabitz *et al.*, 1984).

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