

THERMODYNAMIC PROPERTIES OF HEAVY FERMION SUPERCONDUCTORS

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ABSTRACT

Certain types of interactions can lead to massive quasi-particles such that the resulting effective masses of the electrons may reach values between 100 and 1000 times the mass of the free electrons. The interactions between such heavy electrons are assumed to be singlet s-wave and triplet s-wave, and their contribution to s-wave superconductivity of heavy electrons has been studied. The effective Hamiltonian is diagonalized using the Bogoliubov-Valatin transformation, and the thermodynamic properties of such heavy fermion systems are calculated. The total energy is found to increase with temperature. There is a maximum in the specific heat at $T_C=5.2K$ suggesting a phase transition. The magnitude of specific heat is, $C_V \approx 4.8 \times 10^{-23} J/K$ at T_C . The entropy changes continuously through the transition temperature T_C . Entropy of the system is found to decrease with temperature as is conventionally the case.

Keywords: Heavy Fermions, Super Fluid, Transition Temperature

INTRODUCTION

There are experimental observations in some cases that certain types of interactions can lead, at low temperatures, to the formation of a Fermi liquid-type state with massive quasi-particles (Andrei, 2004). Depending upon the detailed characteristics for the considered systems, the resulting effective masses of the electrons may reach values between 100 and 1000 times the mass of the free electrons. Such electrons are called heavy electrons. By definition, a common and independent Fermi liquid is stable and undergoes no phase transition. Experimental evidence for magnetic or superconducting transitions in heavy-electrons systems therefore imply that residual interactions driving these transitions need to be considered.

There is a common view that in the heavy-electron systems, the correlation effects or strong interactions are the dominating reasons behind the low-temperature properties of some materials. The heavy-electron state in most cases develops smoothly within a narrow temperature range upon cooling at low temperatures. In this sense, it may be regarded as a particular state of certain metals, caused by a delicate competition of interactions between ionic moments of atoms with incompletely-filled electronic shells (favorably f electrons) and itinerant electrons. Such a state may be unstable and undergo phase transitions, either to magnetic order or superconductivity. In fact, heavy-electron system involves many-body physics that deals with strongly interacting electrons in metals.

It is well known that for the standard BCS theory the obtained value for the size of the Cooper pair is of the order of $10^3 A^\circ$ whereas the experimentally extracted value for HTSC is of the order of $10 A^\circ$ (Riseman et al., 1995; Tifrea, 2003). Hence in the conventional superconductors (BCS type), the electrons in the Cooper pairs will be weakly bound because of the large size of the Cooper pairs, whereas the electrons in the HTSC will be strongly bound in the Cooper pairs because of the smaller size of the Cooper pair. Hence strong coupling between electrons in HTSC will lead to heavy fermions being present in HTSC. It is this fact that leads to the study of thermodynamic properties of heavy fermion superconductors.

Superconducting compounds which consist of one magnetic ion with 4f and 5f electrons, (generally Ce or U) and other constituents being s, p or electron metals are known as a family of heavy-fermion superconductors. A large number of heavy fermion materials superconduct exclusively under pressure.

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The T_C values of superconducting heavy-fermions are in general very low. The first such superconductor, $CeCu_2Si_2$, was discovered in 1979 by Steglich and co-workers (Grewe and Steglich, 1991). Later the heavy-fermion phenomena was confirmed by the discovery of UBe_{12} and UPt_3 , with the critical temperatures of $T_C=0.65, 0.9$ and $0.5K$ respectively. Since the many new heavy fermion systems that super conduct at low temperatures has been found. The crystal structure of these compounds does not have a common pattern, but varies from case to case.

The superconducting states in heavy-fermions display some anomalous properties. The Sommerfeld Constant, $\gamma=C/T$, is very large and the specific heat C has a jump at the transition temperature T_C . This shows that the heavy electrons participate in superconducting pairing. Moreover the temperature dependence of C below T_C is not exponential; rather it follows a power law, indicating that the energy gap at the Fermi surface may have nodes in certain directions. This also means that the energy gap is highly anisotropic. The gap ratio for UBe_{12} is $2\Delta/K T_C \approx 6.7$ and this is much higher compared to the value of 3.5 that is obtained in the BCS theory. This indicates that the heavy fermion superconductivity is an unconventional type of superconductivity. The experimental observations in UBe_{12} indicate the existence of a d-wave energy gap, and sometimes an s-wave superconductor. Thus the pairing mechanism in heavy-fermion is not yet established properly and this is one of the most difficult problems in condensed matter physics (Allan *et al.*, 2013). Even the specific superconducting properties are not clearly understood (Keisuke & Daisuke, 2012).

As a first step in understanding the properties of heavy-fermion superconductors, it is assumed that there exists s-state singlet pairing ($^1S_0; s=0, l=0$) and s-state triplet pairing ($^3S_1; s=1, l=0$), also called the spin triplet state, simultaneously in the heavy fermion superconductor. The Hamiltonian, H , for the system will then contain the kinetic energy term, and the interaction term due to singlet and triplet pairing (Kuei *et al.*, 2014). To get the quasi-particles of the heavy-fermion superconducting state, the Hamiltonian, H , will be diagonalized using the Bogoliubov canonical transformation (Bogoliubov, 1958). The energy of the system, the specific heat C , the entropy S and the transition temperature T_C are calculated. The results are compared with whatever information is available in the literature.

Theoretical Formulation

The superconducting electron system is considered as being in some condensed phase and the scattered pairs of electrons are in s-state singlet pairing and s-state triplet pairing. The electrons are paired so as to minimize the ground state energy. With this assumption the Hamiltonian for the singlet and triplet pairing is written as,

$$H = K.E + P.E \text{ (Singlet pairing)} + P.E \text{ (Triplet pairing)}. \quad (1)$$

where the pairing superconducting states are considered to be both singlet ($s=0, l=0$) and triplet ($s=1, l=0$). The Hamiltonian in Eq (1) is then written as

$$H = \sum_k \epsilon_k (c_k^+ c_k + c_{-k}^+ c_{-k}) - \sum_{kk'} V_{kk'} c_k^+ c_{k'}^+ c_{-k} c_{-k'} + \sum_{kk'} U_{kk'} c_k^+ c_{k'}^+ c_{-k} c_{-k'} \quad (2)$$

Eq (2) will be expressed in terms of the new 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 Eq (2). This is achieved by defining two new operators that are related to the old fermion creation and annihilation operators such that,

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

Their conjugates are

$$\gamma_k^+ = u_k c_k^+ - v_k c_{-k} \quad \gamma_{-k}^+ = u_k c_{-k}^+ + v_k c_k \quad (4)$$

In order to write the Hamiltonian in Eq (2) in terms of the new operators, the inverse transformation of Eq (3) and (4) are used. The inverse transformations of (3) and (4) are

$$\begin{aligned} c_k &= u_k \gamma_k + v_k \gamma_{-k}^+ & c_{-k} &= u_k \gamma_{-k} - v_k \gamma_k^+ \\ c_k^+ &= u_k \gamma_k^+ + v_k \gamma_{-k} & c_{-k}^+ &= u_k \gamma_{-k}^+ - v_k \gamma_k \end{aligned} \quad (5)$$

The Hamiltonian expressed in terms of new operators will have three parts namely the Kinetic, Potential (Singlet) and Potential (Triplet) parts which are then diagonalized as explained in each step below.

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Kinetic Energy

Eq (5) are used in Eq (2) to express the K.E of the Hamiltonian in terms of the new operators. Substituting the creation and annihilation operators using Eq (5) we get,

$$H_{K.E} = \sum_k \epsilon_k \left(u_k^2 \gamma_k^+ \gamma_k + u_k v_k \gamma_k^+ \gamma_{-k}^+ + u_k v_k \gamma_{-k} \gamma_k + v_k^2 \gamma_{-k} \gamma_{-k}^+ + u_k^2 \gamma_{-k}^+ \gamma_{-k} - u_k v_k \gamma_k^+ \gamma_{-k}^+ - u_k v_k \gamma_{-k} \gamma_k + v_k^2 \gamma_k \gamma_k^+ \right) \quad (6)$$

Introducing particle number operators m_k that represent cases when particles are created we write,

$$\begin{aligned} m_k &\equiv \gamma_k^+ \gamma_k & 1-m_k &\equiv \gamma_k \gamma_k^+ \\ m_{-k} &\equiv \gamma_{-k}^+ \gamma_{-k} & 1-m_{-k} &\equiv \gamma_{-k} \gamma_{-k}^+ \end{aligned} \quad (7)$$

Eq (8) are used in Eq (7) to get

$$H_{K.E} = \sum_k \epsilon_k \left(u_k^2 m_k + v_k^2 (1-m_k) + v_k^2 (1-m_{-k}) + u_k^2 m_{-k} + u_k v_k \gamma_k^+ \gamma_{-k}^+ + u_k v_k \gamma_{-k} \gamma_k + u_k v_k \gamma_k^+ \gamma_{-k}^+ + u_k v_k \gamma_{-k} \gamma_k \right) \quad (8)$$

Using the relations,

$$\gamma_k^+ \gamma_{-k}^+ = -\gamma_{-k}^+ \gamma_k^+ \quad \text{and} \quad \gamma_{-k} \gamma_k = -\gamma_k \gamma_{-k} \quad (9)$$

We get,

$$H_{K.E} = \sum_k \epsilon_k \left\{ 2v_k^2 + (u_k^2 - v_k^2)(m_k + m_{-k}) + 2u_k v_k (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) \right\} \quad (10)$$

The first term of equation (11) is a constant, the terms with m_k and m_{-k} generate particles and are called diagonal terms bearing $\gamma_k^+ \gamma_k$, $\gamma_k \gamma_k^+$ operators, the third term is off-diagonal i.e. bearing $\gamma_k^+ \gamma_{-k}^+$ and $\gamma_{-k} \gamma_k$ operators. They are without m_k and m_{-k} .

Eq (10) is the transformed form of the Kinetic Energy part.

Potential Energy for Singlet Pairing

Eq (5) are used to express the P.E of the singlet part of the Hamiltonian in terms of the new operators. From Eq(2)

$$H_{P.E(S)} = - \sum_{kk'} V_{kk'} c_k^+ c_{k'}^+ c_{-k} c_{-k'} \quad (11)$$

Using Eq (5) , Eq (11) and later transformed. The P.E Part thus becomes

$$H_{P.E(S)} = - \sum_{kk'} V_{kk'} \left\{ \left(u_k^2 \gamma_k^+ \gamma_{k'}^+ - u_k v_k \gamma_k^+ \gamma_{k'} + u_k v_k \gamma_{-k'} \gamma_k^+ - v_k^2 \gamma_{-k'} \gamma_k \right) \left(u_k^2 \gamma_{-k} \gamma_{-k'} + u_k v_k \gamma_{-k} \gamma_{-k'}^+ - u_k v_k \gamma_k^+ \gamma_{-k'} - v_k^2 \gamma_k^+ \gamma_{-k'}^+ \right) \right\} \quad (12)$$

Introducing particle number operators we write

$$\begin{aligned} 1-m_{k'} &\equiv \gamma_{k'} \gamma_{k'}^+ & m_k &\equiv \gamma_k^+ \gamma_k & 1-m_k &\equiv \gamma_k \gamma_k^+ & 1-m_{-k'} &\equiv \gamma_{-k'} \gamma_{-k'}^+ \\ m_{-k} &\equiv \gamma_{-k}^+ \gamma_{-k} & 1-m_{-k} &\equiv \gamma_{-k} \gamma_{-k}^+ & m_{k'} &\equiv \gamma_{k'}^+ \gamma_{k'} & m_{-k'} &\equiv \gamma_{-k'}^+ \gamma_{-k'} \end{aligned} \quad (13)$$

Eq (13) are used to represent Eq (12) in terms of number operators. Thus

$$H_{P.E(S)} = - \sum_{kk'} V_{kk'} \left\{ \left(u_k^2 \gamma_k^+ \gamma_{k'}^+ - v_k^2 \gamma_{-k'} \gamma_k + u_k v_k m_{k'} + u_k v_k (1-m_{-k'}) \right) \left(u_k^2 \gamma_{-k} \gamma_{-k'} - v_k^2 \gamma_k^+ \gamma_{-k'}^+ + u_k v_k (1-m_{-k}) - u_k v_k m_k \right) \right\} \quad (14)$$

we get

$$H_{P.E(S)} = - \sum_{kk'} V_{kk'} \left\{ u_k v_k u_k v_k \left((1-m_{k'} - m_{k'}) (1-m_{-k} - m_{-k}) \right) + u_k v_{k'} (1-m_{k'} - m_{k'}) (u_k^2 - v_k^2) (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) \right\} + 4OT \quad (15)$$

where 4OT stands for "fourth order terms". The third term is an off-diagonal term which shall be considered later so as to leave a system of independent fermions.

Potential Energy for Triplet Pairing

From equation (2) we write

$$H_{P.E(T)} = \sum_{kk'} U_{kk'} c_k^+ c_{k'}^+ c_{-k} c_{-k'} \quad (16)$$

Eq (5) are used to transform equation (16). The P.E (triplet) part thus becomes

$$H_{P.E(T)} = \sum_{kk'} U_{kk'} \left\{ \left(u_k \gamma_k^+ + v_k \gamma_{-k} \right) \left(u_k \gamma_{-k}^+ - v_k \gamma_k \right) \left(u_{k'} \gamma_{k'} - v_{k'} \gamma_{k'}^+ \right) \left(u_{k'} \gamma_{k'}^+ + v_{k'} \gamma_{-k'} \right) \right\} \quad (17)$$

or

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$$H_{P,E(T)} = \sum_{kk'} U_{kk'} \left\{ \left(u_k^2 \gamma_k^+ \gamma_{-k}^+ - u_k v_k \gamma_k^+ \gamma_{-k} + u_k v_k \gamma_{-k} \gamma_k^+ - v_k^2 \gamma_{-k} \gamma_k \right) \left(u_{k'}^2 \gamma_{-k'} \gamma_{k'}^+ + u_{k'} v_{k'} \gamma_{-k'} \gamma_{k'}^+ - u_{k'} v_{k'} \gamma_{k'}^+ \gamma_{-k'} - v_{k'}^2 \gamma_{k'}^+ \gamma_{-k'} \right) \right\} \quad (18)$$

The particle number operators in Eq(13) are then used in Eq (18) to get

$$H_{P,E(T)} = \sum_{kk'} U_{kk'} \left\{ \left(u_k^2 u_{k'} v_{k'} (1-m_{-k'}) \gamma_k^+ \gamma_{-k}^+ - u_k^2 u_{k'} v_{k'} m_{k'} \gamma_k^+ \gamma_{-k}^+ - v_k^2 u_{k'} v_{k'} (1-m_{-k'}) \gamma_{-k} \gamma_k + v_k^2 u_{k'} v_{k'} m_{k'} \gamma_{-k} \gamma_k \right. \right. \\ \left. \left. + v_k^2 u_{k'} v_{k'} m_{k'} \gamma_k^+ \gamma_{-k}^+ - v_k^2 u_{k'} v_{k'} (1-m_{-k'}) \gamma_k^+ \gamma_{-k}^+ + u_k^2 u_{k'} v_{k'} (1-m_{-k'}) \gamma_{-k} \gamma_{k'} - u_k^2 u_{k'} v_{k'} m_{k'} \gamma_{-k} \gamma_{k'} \right. \right. \\ \left. \left. + u_k v_{k'} u_{k'} v_{k'} m_{k'} m_{k'} - u_k v_{k'} u_{k'} v_{k'} m_{k'} (1-m_{-k'}) + u_k v_{k'} u_{k'} v_{k'} (1-m_{-k'}) (1-m_{-k'}) - u_k v_{k'} u_{k'} v_{k'} m_{k'} (1-m_{-k'}) \right\} + 4OT \quad (19)$$

or

$$H_{P,E(T)} = \sum_{kk'} U_{kk'} \left\{ u_k v_k u_{k'} v_{k'} ((m_{k'} + m_{-k'} - 1)(m_k + m_{-k} - 1) + u_{k'} v_{k'} (1-m_{-k'} - m_{k'})) (u_k^2 (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) - \gamma_{-k} \gamma_k) \right. \\ \left. + u_k v_k (m_k - 1 + m_{-k}) (v_{k'}^2 (\gamma_{k'}^+ \gamma_{-k'}^+ + \gamma_{-k'} \gamma_{k'}) - \gamma_{-k'} \gamma_{k'}) \right\} \quad (20)$$

Eq (20) is the transformed form of the Potential Energy of the triplet pairing. The last two terms are the off-diagonal terms.

Effective Hamiltonian

The effective Hamiltonian $H = H_{K,E} + H_{P,E(S)} + H_{P,E(T)}$ is written by adding equations (10), (15) and (20) with the approximation that the 4OT can be neglected being negligible higher order terms i.e.

$$H = H_{K,E} + H_{P,E(S)} + H_{P,E(T)} \\ H = \sum_k \epsilon_k \left\{ 2v_k^2 + (u_k^2 - v_k^2)(m_k + m_{-k}) + 2u_k v_k (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) \right\} \\ - \sum_{kk'} V_{kk'} \left\{ u_{k'} v_{k'} u_k v_k ((1-m_{-k'} - m_{k'})(1-m_{-k} - m_k)) + u_{k'} v_{k'} (1-m_{-k'} - m_{k'}) (u_k^2 - v_k^2) (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) \right\} \\ + \sum_{kk'} U_{kk'} \left\{ u_k v_k u_{k'} v_{k'} ((m_{k'} + m_{-k'} - 1)(m_k + m_{-k} - 1) + u_{k'} v_{k'} (1-m_{-k'} - m_{k'})) (u_k^2 (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) - \gamma_{-k} \gamma_k) \right. \\ \left. + u_k v_k (m_k - 1 + m_{-k}) (v_{k'}^2 (\gamma_{k'}^+ \gamma_{-k'}^+ + \gamma_{-k'} \gamma_{k'}) - \gamma_{-k'} \gamma_{k'}) \right\} \quad (21)$$

Parametric Expressions for u_k and v_k for the Singlet State

A system of independent fermions is determined on the assumption that the off-diagonals terms of Eq (10), (15) and (20) vanish. 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 Eq (10) and (15) and the 4OT neglected since the non-diagonal terms vanish. The modified form of combining equations (10) and (15) then gives

$$\sum_k 2\epsilon_k u_k v_k (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) - \sum_{kk'} V_{kk'} (u_k^2 - v_k^2) (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) = 0 \quad (22)$$

When the non-diagonal terms vanish Eq (22) becomes

$$2\epsilon_k u_k v_k - (u_k^2 - v_k^2) \sum_{k'} V_{kk'} u_{k'} v_{k'} = 0 \quad (23)$$

The condition $u_k^2 + v_k^2 = 1$ is used to express u_k and v_k in the form of a single variable χ such that

$$u_k^2 = \frac{1}{2} - \chi_k \quad v_k^2 = \frac{1}{2} + \chi_k \quad (24)$$

and when used in Eq (23) gives

$$2\epsilon_k \sqrt{\frac{1}{4} - \chi_k^2} + 2\chi_k \sum_{k'} V_{kk'} \sqrt{\frac{1}{4} - \chi_{k'}^2} = 0 \quad (25)$$

The quantity, Δ_k , is expressed as

$$\Delta_k \equiv \sum_{k'} V_{kk'} \sqrt{\frac{1}{4} - \chi_{k'}^2} \quad (26)$$

Hence on solving equation (25)

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$$\chi_k = \pm \frac{\epsilon_k}{2\sqrt{\epsilon_k^2 + \Delta_k^2}} \quad (27)$$

Quasi particle Spectrum for the Singlet State

Using Eq (27) in Eq (24) gives

$$u_k^2 = \frac{1}{2} \left(1 + \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta_k^2}} \right) \quad (28)$$

$$v_k^2 = \frac{1}{2} \left(1 - \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta_k^2}} \right) \quad (29)$$

The Hamiltonian consisting of diagonal terms is used to determine the quasi particle energy because the diagonal terms correspond to stationary states when the system is in equilibrium.

The quasiparticles energy is found using equation (28) and equation (29).

The Energy E_{ks} necessary to create a quasi particle excitation will be obtained from the diagonal terms of the Hamiltonian $H_D = \sum_k \epsilon_k (2v_k^2 + (u_k^2 - v_k^2)(m_k + m_{-k})) - \sum_{kk'} V_{kk'} (u_k v_k u_{k'} v_{k'} ((1 - m_{-k'} - m_{k'})(1 - m_{-k} - m_k)))$ (30)

Now,

$$E_{ks} = \frac{\partial \langle H_D \rangle}{\partial \langle m_k \rangle} \quad (31)$$

$$E_{ks} = \epsilon_k (u_k^2 - v_k^2) + 2u_k v_k \sum_{kk'} V_{kk'} u_{k'} v_{k'} (1 - m_{-k'} - m_{k'}) \quad (32)$$

$$\text{Approximating } \Delta_k \approx \sum_{kk'} V_{kk'} u_{k'} v_{k'} (1 - m_{-k'} - m_{k'})$$

Equation (32) becomes

$$E_{ks} = \epsilon_k (u_k^2 - v_k^2) + 2u_k v_k \Delta_k \quad (33)$$

Eq (28) and (29) are substituted in Eq (35) to obtain the quasi particle energy for the singlet pairing.

$$E_{ks} = \sqrt{\epsilon_k^2 + \Delta_k^2} \quad (34)$$

Equation (34) is the quasiparticles energy spectrum of the singlet state.

Parametric expressions for u_k and v_k for the Triplet state

To carry out the Bogoliubov-Valatin transformation for a superconductor in its ground state, the m_k , m_{-k} are set equal to zero in Eq (10) and (20) and the 4OT neglected since the non-diagonal terms vanish.

The modified form of combining equations (10) and (20) then gives

$$\sum_k 2\epsilon_k u_k v_k (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) + \sum_{kk'} U_{kk'} (u_k^2 u_{k'} v_{k'} (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k)) = 0 \quad (35)$$

or

$$2\epsilon_k u_k v_k + u_k^2 \sum_{k'} U_{kk'} u_{k'} v_{k'} = 0 \quad (36)$$

Eq (36) is solved using Eq (26) to get

$$2\epsilon_k \left(\frac{1}{4} - X_k^2 \right)^{\frac{1}{2}} + \left(\frac{1}{2} - X_k \right) \sum_{k'} U_{kk'} \left(\frac{1}{4} - X_k^2 \right)^{\frac{1}{2}} = 0 \quad (37)$$

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We now define a new quantity Δ as,

$$\Delta = \sum_{k'} U_{kk'} \left(\frac{1}{4} - X_k^2 \right)^{\frac{1}{2}} \quad (38)$$

Eq (37) then becomes

$$2\varepsilon_k \left(\frac{1}{2} - X_k \right)^{\frac{1}{2}} \left(\frac{1}{2} + X_k \right)^{\frac{1}{2}} + \left(\frac{1}{2} - X_k \right) \Delta = 0 \quad (39)$$

or

$$X_k = \frac{1}{2} \left(\frac{\Delta^2 - 4\varepsilon_k^2}{4\varepsilon_k^2 + \Delta^2} \right) \quad (40)$$

The parametric expressions for u_k and v_k are obtained by substitution of Eq (40).

Using Eq (24) and (40) we obtain

$$u_k = \pm \frac{2\varepsilon_k}{\sqrt{4\varepsilon_k^2 + \Delta^2}} \quad \text{and} \quad v_k = \pm \frac{\Delta}{\sqrt{4\varepsilon_k^2 + \Delta^2}} \quad (41)$$

Quasi particle Spectrum of the Triplet State

The Hamiltonian consisting of diagonal terms is used to determine the quasi particle energy because the diagonal terms correspond to stationary states when the system is in equilibrium. The quasiparticles energy is found using Eq (41).

The Energy E_{kT} necessary to create a quasi particle excitation will be obtained from the diagonal terms of the Hamiltonian

$$H_d = \sum_k 2\varepsilon_k v_k^2 + \sum_k \varepsilon_k (u_k^2 - v_k^2)(m_k + m_{-k}) + \sum_{kk'} U_{kk'} u_k v_k u_{k'} v_{k'} ((m_{k'} + m_{-k'}) - 1)(m_k + m_{-k} - 1) \quad (42)$$

Now

$$E_{kT} = \frac{\partial \langle H_d \rangle}{\partial \langle m_k \rangle}$$

Approximating $\Delta \approx \sum_{k'} U_{kk'} u_{k'} v_{k'} ((m_{k'} + m_{-k'}) - 1)$ gives

$$E_{kT} = \varepsilon_k (u_k^2 - v_k^2) + 2u_k v_k \Delta \quad (43)$$

Eq (41) are substituted in Eq (43) to get

$$E_{kT} = \varepsilon_k \left(\frac{4\varepsilon_k^2}{4\varepsilon_k^2 + \Delta^2} - \frac{\Delta^2}{4\varepsilon_k^2 + \Delta^2} \right) + 2 \left(\frac{2\varepsilon_k}{\sqrt{4\varepsilon_k^2 + \Delta^2}} \frac{\Delta}{\sqrt{4\varepsilon_k^2 + \Delta^2}} \right) \Delta$$

$$E_{kT} = \frac{4\varepsilon_k^3 + 3\varepsilon_k \Delta^2}{4\varepsilon_k^2 + \Delta^2} \quad (44)$$

Eq (44) is the quasi particle energy for the triplet pairing.

Energy of the Assembly

The effective Hamiltonian given by Eq (2) is considered by summing the diagonal and non-diagonal parts of the various components of the Hamiltonian with the condition that the non-diagonal parts are set equal to zero or vanish whereas the 4OT are neglected i.e.

$E_K = E + \text{Singlet} + \text{Triplet}$

$$E_K = \sum_k \varepsilon_k \left\{ 2v_k^2 + (u_k^2 - v_k^2)(m_k + m_{-k}) + 2u_k v_k (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) \right\}$$

$$- \sum_{kk'} V_{kk'} \left\{ u_k v_{k'} u_{k'} v_k ((1 - m_{-k'} - m_{k'})(1 - m_{-k} - m_k)) + u_k v_{k'} (1 - m_{-k'} - m_{k'}) (u_k^2 - v_k^2) (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) \right\}$$

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$$+ \sum_{kk'} U_{kk'} \left\{ u_k v_k u_{k'} v_{k'} ((m_{k'} + m_{-k'} - 1)(m_k + m_{-k} - 1) + u_{k'} v_{k'} (1 - m_{k'} - m_{k'})) (u_k^2 (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k) - \gamma_{-k} \gamma_k) \right. \\ \left. + u_k v_k (m_k - 1 + m_{-k}) (v_{k'}^2 (\gamma_{k'}^+ \gamma_{-k'}^+ + \gamma_{-k'} \gamma_{k'}) - \gamma_{-k'} \gamma_{k'}) \right\} \quad (45)$$

The diagonal parts of Eq (45) correspond to quasi-particle states when the system is in equilibrium i.e

$$E_k = \sum_k 2\varepsilon_k v_k^2 + (u_k^2 - v_k^2)(m_k + m_{-k}) - \sum_{kk'} V_{kk'} u_{k'} v_{k'} u_k v_k ((1 - m_{k'} - m_{k'}) (1 - m_k - m_k)) + \sum_{kk'} U_{kk'} u_{k'} v_{k'} u_k v_k \quad (46)$$

The particle number operators $m_k = m_{-k} = 0$ (This means the quasi-particles represented by the operators γ 's are few in number or do not exist). Eq (46) then becomes

$$E_k = 2\varepsilon_k v_k^2 - u_k v_k \sum_{k'} V_{kk'} u_{k'} v_{k'} + u_k v_k \sum_{k'} U_{kk'} u_{k'} v_{k'} \quad (47)$$

The singlet and triplet gaps are represented by

$$\Delta_v = \sum_{k'} V_{kk'} u_{k'} v_{k'} \quad (48)$$

$$\Delta_u = \sum_{k'} U_{kk'} u_{k'} v_{k'} \quad (49)$$

Eq (47) is then by substitution written as

$$E_k = 2\varepsilon_k v_k^2 - u_k v_k \Delta_v + u_k v_k \Delta_u \quad (50)$$

To study the temperature dependence of the system the total energy E_τ is found by multiplying energy of states E_k by the thermal activation factor $e^{\frac{-E_k}{K_B T}}$. Hence

$$E_\tau = E_k e^{\frac{-E_k}{K_B T}} \quad (51)$$

Equation (50) is used in Eq (51) thus

$$E_\tau = (2\varepsilon_k v_k^2 + u_k v_k (\Delta_u - \Delta_v)) e^{\frac{-E_k}{K_B T}} \quad (52)$$

Eq (52) is the total energy of the assembly with the triplet and singlet contributions.

Specific Heat Capacity

The specific heat capacity is determined using the following relation

$$C = \frac{\partial E_\tau}{\partial T} \quad (53)$$

and hence

$$C = \frac{(2E_k \varepsilon_k v_k^2 + E_k u_k v_k (\Delta_u - \Delta_v))}{K_B T^2} e^{\frac{-E_k}{K_B T}} \quad (54)$$

Eq (54) is the Specific heat Capacity equation for heavy fermion systems.

Transition Temperature

The transition temperature of the system is obtained by witing

$$\left(\frac{\partial C}{\partial T} \right)_{T=T_c} = 0 \quad (55)$$

To simplify equation (54) the larger terms are then represented by letting

$$\rho = \frac{(2E_k \varepsilon_k v_k^2 + E_k u_k v_k (\Delta_u - \Delta_v))}{K_B} \text{ and } \left(\frac{E_k}{K_B} \right) = \beta. \quad (56)$$

Then Eq (54) can be expressed as

$$C = \frac{\rho e^{\frac{-\beta}{T}}}{T^2} \quad (57)$$

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Thus we get

$$\left(-\frac{2\rho}{T^3} e^{-\left(\frac{\beta}{T}\right)} + \frac{\beta\rho}{T^4} e^{-\left(\frac{\beta}{T}\right)} \right)_{T=T_c} = 0 \quad (58)$$

or

$$T_c = \frac{\beta}{2} = \frac{E_K}{2K_B} \quad (59)$$

Entropy

The entropy of a system is determined from the relation

$$S_2 - S_1 = \int_1^2 ds = \int_1^2 \frac{dQ}{T} = \int_1^2 \frac{mCdT}{T} \quad (60)$$

The equation for entropy from equation (60) then becomes

$$S = m \left(\frac{2E_K \epsilon_k v_k^2 + E_K u_k v_k (\Delta_u - \Delta_v)}{K_B} \right) \left(\frac{K_B}{TE_K} e^{-\frac{E_K}{K_B T}} + \frac{3K_B^2}{E_K^2} e^{-\frac{E_K}{K_B T}} + \frac{6K_B^3 T}{E_K^3} e^{-\frac{E_K}{K_B T}} + \frac{6K_B^4 T^2}{E_K^4} e^{-\frac{E_K}{K_B T}} \right) \quad (61)$$

where $m \approx 100m_e$.

Essential Parameters

The following values for different physical quantities have been used.

The numerical values of C_v are obtained using the condition $u_k^2 + v_k^2 = 1$

$$u_k = \frac{1}{\sqrt{2}}, \quad v_k = \frac{1}{\sqrt{2}}$$

According to the experimental works of (Allan, et al., 2013) on heavy fermions

Single particle energy, $\epsilon_k = \hbar\omega_D = 300\mu\text{eV} = 4.8 \times 10^{-23} \text{J}$

The triplet and singlet energy gaps are given by the relation $\Delta_v \approx 0.05\Delta_u$ according to (Khanna, 2008).

The heavy fermion superconductivity energy window is equivalent to $-600\mu\text{eV} < E < 600\mu\text{eV}$ according to (Allan, et al., 2013)

Energy gap for the triplet $\Delta_u = 9.6 \times 10^{-23} \text{J}$ and $E_{KS} = \sqrt{(\epsilon_k^2 + \Delta_k^2)}$

$E_{KS} = 4.8239402 \times 10^{-23} \text{J}$, $E_{KT} = 9.6 \times 10^{-23} \text{J}$ and $E_K = 1.44239 \times 10^{-23} \text{J}$

Boltzmann constant $K_B = 1.3806488 \times 10^{-23} \text{JK}^{-1}$

RESULTS AND DISCUSSION

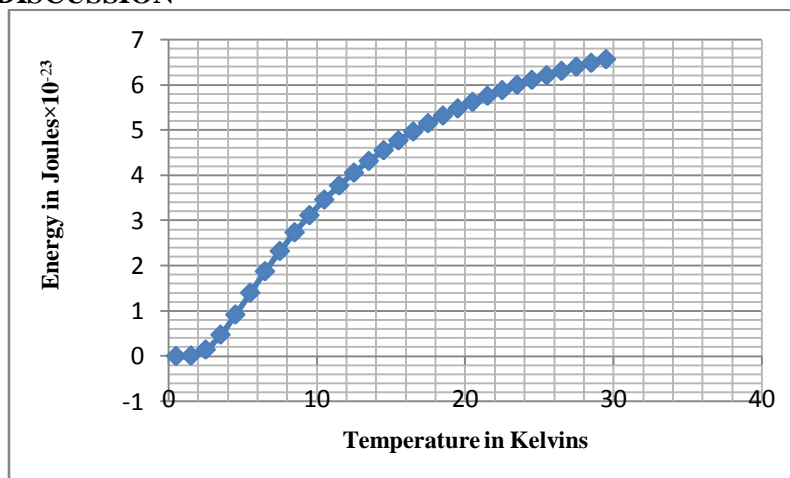


Figure 1: Variation of Total Energy against Temperature

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Eq (52) was used to compute the values of quasi-particle energy against changes in the temperature. A graph depicting the variation of quasi-particle energy versus temperature is shown in figure 1.

Eq (54) is used to compute the values of specific heat against temperature changes

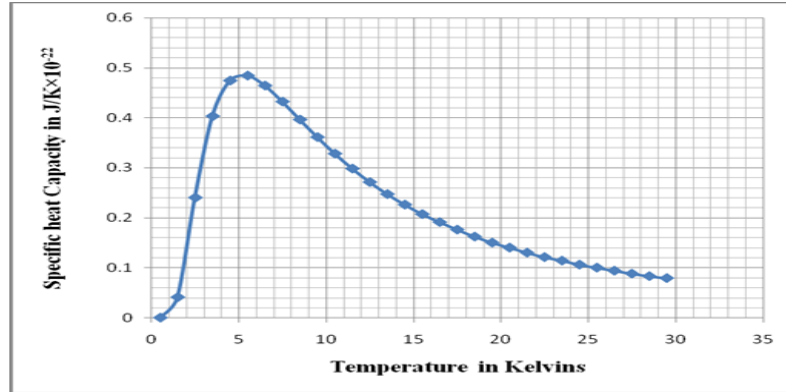


Figure 2: The graph of specific heat against temperature.

The shape of the specific heat curve is similar to the specific heat curve of UBe_{13} (Ott H.R.,1992). The curve shows a turning point at $T_C=5.2\text{K}$.

Equation (61) gives the variation of Entropy with temperature

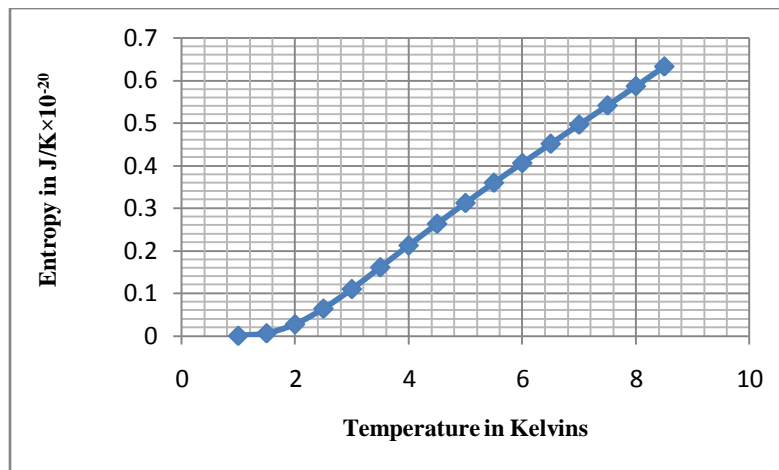


Figure 3: Variation of Entropy against Temperature

Discussion

The value of E decreases below T_C (5.2K) and becomes zero at $T=0$ K 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.

In figure 1, it is observed that at $T=0$, $E=0$ which implies that the states below the superconducting gap are filled and the states above the superconducting gap are empty. Now it is much harder for impurities to scatter the pair of electrons because they need a finite amount of energy. If there is not enough energy to get to an unoccupied state, then the electron does not change its state, there is no dissipation, and hence there is no electrical resistance. To get across the superconducting gap requires a minimum amount of energy of about $1.2 \times 10^{-23}\text{J}$. The gap doesn't appear suddenly at T_C (5.2K); it opens up gradually as T decreases below T_C , just like the order parameter. When the temperature increases, the energy is observed to increase. This implies thermal fluctuations will populate the f-level by conduction electrons, thereby increasing the f-electron number. This will involve the breaking of Cooper pairs and hence the

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suppression of the superconducting gap. At high temperatures the f -electrons are localized on their atomic sites and do not contribute to conduction.

Superconductivity is a true reversible thermodynamic state and in moving from the normal to the superconducting state, a material undergoes a thermodynamic phase transition. In order for this to happen, the overall free energy must be lower in the superconducting state than in the normal state as seen in figure 1 and this energy difference, which depends on the temperature, is known as the condensation energy. At high temperatures heavy fermion compounds behave like normal metals and the electrons can be described as Fermi gas, in which the electrons are assumed to be non-interacting fermions. The specific heat capacity of heavy fermion superconductors jumps at T_C , but the scale remains set by the large effective mass of the quasiparticles (Coleman, 2007). If the superconducting state did not have heavy fermion properties, the specific heat below the jump would be much smaller (Coleman, 2007).

In figure 2, the graph of specific heat assumes nearly perfect Gaussian shape. A peak in specific heat occurs at about 5.2K. At this point the system is unstable and there is a second order phase transition from a normal metal into a superconducting state that is much like the super fluid transition. At T_C , there is a phase transition, the fermions pair up and the specific heat depicting a second order transition meaning there is no latent heat.

The weak interaction of fermions is mediated by the lattice and approaches zero at absolute zero. Super fluidity in fermions is exhibited on the basis of interaction and is a phenomenon that is realized at any temperature below a finite transition temperature. At room temperatures, the f -electrons of the magnetic ions behave as localized spins; the conduction electrons are the s , p or d electrons and have quite ordinary effective masses. As the temperature is lowered, the f -electrons begin to couple to the conduction electrons, resulting in very large effective masses for the hybridized carriers (Andrei, 2004). At low temperatures the electronic specific heat shows a continuous increase until superconductivity sets in at $T_C = 5.2K$.

Furthermore, the temperature dependence of the heat capacity below T_C is not exponential. Instead, it follows a power law, as seen from figure 2 indicating that the energy gap at the Fermi surface has nodes in certain directions. Thus, the energy gap is highly anisotropic (Andrei, 2004).

However, contrary to conventional materials, some of the f -electrons become itinerant at low temperatures. Crudely speaking, it is these itinerant f -electrons that lead to the uncommon behaviors of heavy fermion materials at low temperatures (Hua, 2008).

The large magnitude of the specific heat jump ($4.8 \times 10^{-23} J/K$) that occurs at the superconducting transition temperature, T_C , shows that the electrons that take part in the formation of the heavy-fermion state form the Cooper pairs.

In figure 3 shown above, entropy increases continuously with increase in temperature. This shows excitation of the particles in the system. The entropy approaches zero at $T \rightarrow 0$, as it should.

The gradient dS/dT goes to zero sharply as $T=0K$. The rate of change dS/dT (gradient of the graph) consistently decreases at temperatures below $T_C=5.2K$ and becomes zero from $T=1.5K$ i.e. system becomes more orderly. When molecules are cooled their total energy decreases resulting into less and less vigorous molecules.

The entropy of the system at T_C is $3.5 \times 10^{-21} J/K$. The graph confirms this observation by depicting that entropy decreases with decrease in temperature. At extremely low temperatures as the entropy of the material drops, an electron passing by lattices in the crystal will cause an electron-electron interaction making efforts to form Cooper pairs and at a particular temperature i.e. T_C the material changes electric state. This is when the material becomes superconducting. But if a field is applied, the electrons would have some component counteracting the electron-electron interaction and decreases entropy. At $T=0$, $S=0$, it seems reasonable to regard this entropy as being carried by a set of localized f spins which emerge above temperatures. To ensure that $S = 0$ at $T = 0$, localized spins order magnetically due to spin-spin interaction. Similarly, a system with the fermion condensate must experience some sort of a low-temperature phase transition eliminating the excessive entropy S . Particle disorder decreases with decrease in the total energy of the system.

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Conclusion

Figure 3 suggests that particles settle and interact less as the system gives out energy. This is in agreement with conventional knowledge and concurs with (Khanna *et al.*, 2010). It is also in good agreement with (Ayodo, 2008), (Ayodo *et al.*, 2010) on low temperature statistical thermodynamics of binary bose-fermi system. Entropy is a measure of molecular disorder (Ayodo, 2008) when the system cools, the internal energy of the particles decreases resulting in less and less particle motion. The graph in figure 3, confirms this observation by predicting that entropy decreases with decrease in temperature even for a system of heavy fermions

ACKNOWLEDGEMENT

We appreciate our Universities who have given us platforms to share our talents and skills as their dedicated employees.

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