HEAVY FERMION MATERIAL AND IT'S SUPERCONDUCTING PROPERTY

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HEAVY FERMION MATERIAL AND IT'S SUPERCONDUCTING PROPERTY

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IN

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By

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Under the Guidance of
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BHUBANESWAR

CERTIFICATE – I

*This is to certify that the thesis entitled, " **HEAVY FERMION MATERIAL AND IT'S SUPERCONDUCTING PROPERTY** " submitted in partial fulfillment of the requirements for the award of the degree of* ***Master of Science in Physics*** *of the* ***Orissa University of Agriculture and Technology****, Bhubaneswar, is a faithful record of bona fide research work carried out by* ***Harapriya Mohanta*** *under my guidance and supervision and that no part of this thesis has been submitted for any other degree or diploma or published in any form.*

It is further certified that the help and sources of information availed of during the course of study have been duly acknowledged.

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CERTIFICATE – II

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I hereby declare that the project work entitled **"HEAVY FERMION MATERIAL AND IT'S SUPERCONDUCTING PROPERTY"** submitted by me for the partial fulfillment of the Master of Science to the **CBSH, Orissa University of Agriculture & Technology**, Bhubaneswar is my own original work and has not been submitted earlier to OUAT or to any other institution for the fulfillment of the requirement for any course of study. I also declare that no chapters of this manuscript in whole or in part in lifted and incorporated in this report from any earlier work done by me or others.

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ABSTRACT

The term “heavy fermion” was coined by Steglich et al. (1976) in the late 1970s to describe the electronic excitations in a new class of intermetallic compound with an electronic density of states as much as 1000 Times larger than ordinary metals. Since the original discovery of heavy-fermion behavior in $CeAl_3$ by Andres, Graebner and Ott (1975), a diversity of heavy-fermion compounds, including superconductors, antiferromagnets (AFMs), and insulators have been discovered. In the last10 years, these materials have become the focus of intense interest with the discovery of unconventional superconductivity in these compounds. This article is intended to be a very brief review on the most basic facts and concepts of heavy fermionphysics. Properties and conceptual understanding of this system is given in the introduction part, following with an introduction of Kondo effect. The electron-phonon interaction in the periodic Anderson model is considered. The influence of electron-phonon interaction on the phonon response of the system and on the value of the effective mass are studied. Atlast, one of the most compelling exotic properties of heavy fermions superconductivity is discussed in detailed in the third section.

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CHAPTER – 1

INTRODUCTION

1.1 HEAVY FERMION MATERIAL

Intermetallic compounds with lanthanide or actinide elements that have partially filled 4f or 5f electron shells are known as heavy fermion materials. [1] Materials having energy levels matching to energy orders several orders of magnitude smaller than in other metals are referred to as "heavy fermions." If we write energy in the form[2]

$$\boldsymbol{\varepsilon = \frac{\hbar^2 k^2}{2m^*}}$$

The effective mass (m*) must be several orders more than the mass of a free electron because the wave vector (k), which depends on the interatomic spacing, is similar to that of common metals. As a result, the term "heavy fermion" refers to how the fermion behaves as though its effective mass is greater than its rest mass.

Below a specific temperature (usually 10 K), heavy fermion systems exhibit strongly correlated electronic behaviour with conduction electron masses up to 1000 times greater than predicted by the free-electron model. [3]

Examples : CeAl3,CeCu6,CeCu2Si2,YbAl3,UBe13,UPt3,UCd11,U2Zn17.

1.2 HISTORY

In 1975, K. Andres, J.E. Graebner, and H.R. Ott identified the behaviour of heavy fermions. They noticed large heat capacity of $CeAl_3$.[4]. Frank Steglich identified the $CeCu_2Si_2$ material in 1979 as having unusual superconductivity for heavy fermion materials. [5]

1.3 PROPERTIES OF HEAVY FERMION MATERIALS

- Heavy Fermion systems maintain their usual state at room temperature or greater, but at low temperatures, several irregularities manifest. At temperatures above room temperature, the f shell electrons remain on their atomic site, and the system behaves as a weakly interacting collection of conducting electrons with ordinary masses and f-electron moments.[2][3]
- Heavy fermion compounds behave like typical metals at high temperatures, and the electrons can be thought of as a Fermi gas, where they behave as non-interacting fermions. In this instance, the interaction between the conduction electrons and the f electrons, which have a local magnetic moment, can be disregarded.[6]

- One distinguishing characteristic of heavy fermion materials is that they exhibit strongly correlated quantum fluctuations in the magnetic and electronic degrees, which can result in a variety of unusual behaviours.[3]
- They are on the verge of a magnetic instability, which will eventually give way to a long-range magnetic order produced by interactions between the 4f or 5f magnetic moments via conduction electrons.[2][3]
- Several members of the group of heavy fermion materials become superconducting below a critical temperature. Here the superconductivity is unconventional.[6]

Specific heat of heavy fermion materials :

Heavy fermion materials have a linear term for their low-temperature specific heat that is up to 1000 times greater than what is predicted by the free electron model.[6]

For normal metals , at low temperature the specific heat $\boldsymbol{C}_P$ consists of the specific heat of the electrons $C_{p,el}$ which depends linearly on temperature T and of the specific heat of the crystal lattice vibrations (phonons) $C_{p,ph}$ which depends cubically on temperature.

$$\mathbf{C_p=C_{p,el}+C_{p,ph}=\gamma\, T+}\beta \boldsymbol{T}^3$$

with proportionality constants **γ** and β .

The majority of the specific heat at low temperatures comes from the electronic contribution. Providing the electronic specific heat are,

$$\boldsymbol{C_{p,el}=\gamma T=\frac{\pi^2}{2}\frac{k_B^2}{\epsilon_F}nT}$$

with Boltzmann constant $\boldsymbol{k}_B$, the electron density n and the Fermi energy ε_F . The proportionality constant **γ** is called the Sommerfeld Coefficient.

Relation between heat capacity and "thermal effective mass" :

The extremely high specific heat Cp of the heavy fermion system at low temperatures serves as evidence for the extremely large effective mass of the conduction electron..[6]

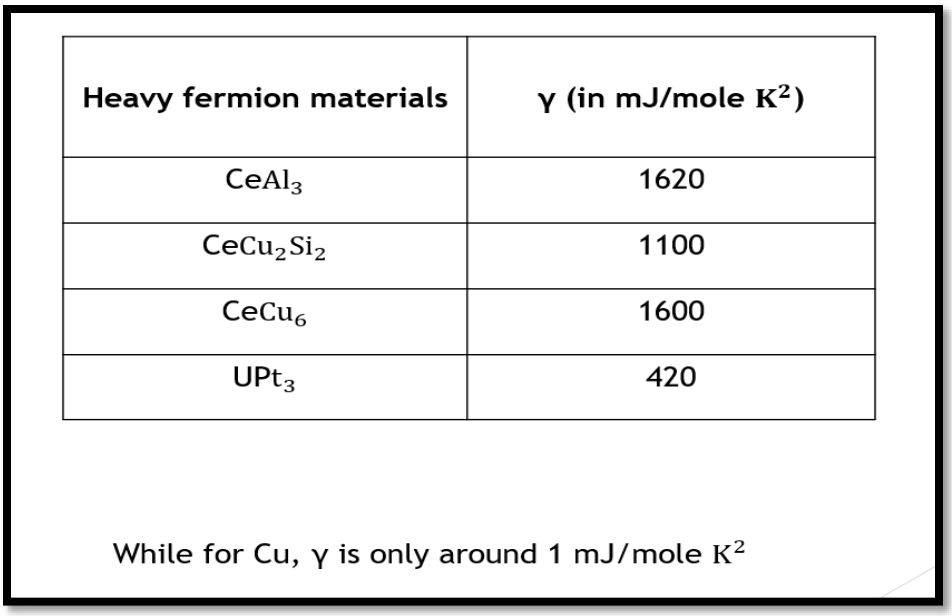
The Fermi energy ε_F inversely proportional to the particle's mass :

$$\boldsymbol{\varepsilon_F=\frac{\hbar^2k_F^2}{2m}}$$

where $\boldsymbol{k}_F$ stands for the Fermi wave number that depends on the electron density and is the absolute value of the wave number of the highest occupied electron state. Thus, because the Sommerfeld Parameter γ is inversely proportional to ε_F, γ is proportional to the particle's mass and for high values of γ, the metal behaves as a Fermi gas in which the conduction electrons have a high effective mass.

Since γ is very large for heavy fermion materials , so the effective mass is larger.

In heavy fermion compounds ,the electronic specific heat coefficient(γ) is much larger than normal metals .



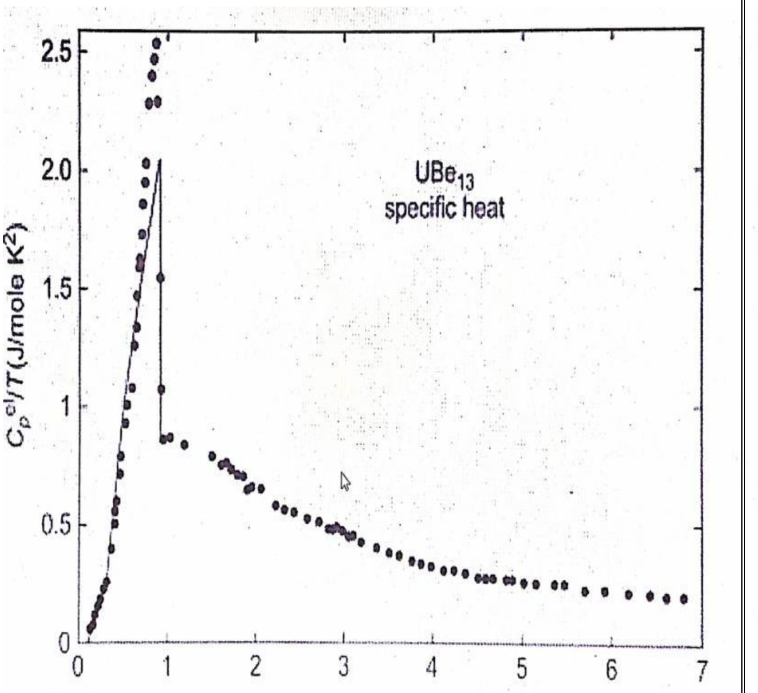
Heavy fermion materials	γ (in mJ/mole K^2)
$CeAl_3$	1620
$CeCu_2Si_2$	1100
$CeCu_6$	1600
UPt_3	420

While for Cu, γ is only around 1 mJ/mole K^2

(Table 1 : γ value of some heavy fermion materials) [3]

Example : UBe_{13} at low temperature

The heavy fermion compound UBe_{13} has a peak in its specific heat at a temperature of about 0.75 K, which drops rapidly to zero as the temperature approaches 0 K. Due to this peak, the γ factor in this temperature range is significantly higher than the free electron model. [6]



(Fig. 1 : Electronic specific heat of UBe_{13} below 7°K)[7]

First, we need to grasp the so-called Kondo effect in order to comprehend heavy fermion systems.[8][9]

1.4 KONDO EFFECT

The Kondo effect is a description of how magnetic impurities in a metal scatter conduction electrons, changing electrical resistance with temperature. [10] The mechanism by which a free magnetic impurity ion is "screened" by the spins of the electrons at low temperatures and low magnetic fields leads in this effect, which refers to an unconventional phenomenon. The conductivity reduces as the impurity ion is screened because some conduction electrons are bound to it. The electronic resistivity, which is caused by impurities scattering conduction electrons, typically decreases monotonically with decreasing temperature. Consequently, the two effective methods will result in a low resistivity at low temperatures. Kondo provided this justification in 1963 for the puzzling "minimum conductivity" that had been identified 30 years before.[11]

The interaction between the localised magnetic moment and the itinerant electrons is referred to as coupling in the Kondo problem.

The right-side diagram displays a schematic of a weakly coupled high temperature situation in which the magnetic moments of the metal's conduction electrons pass by the magnetic moment of an impurity at the Fermi velocity with only a slight antiferromagnetic correlation. However, at low temperatures, an overall nonmagnetic state is created by a strong binding between one conduction electron moment and the impurity magnetic moment. [13]

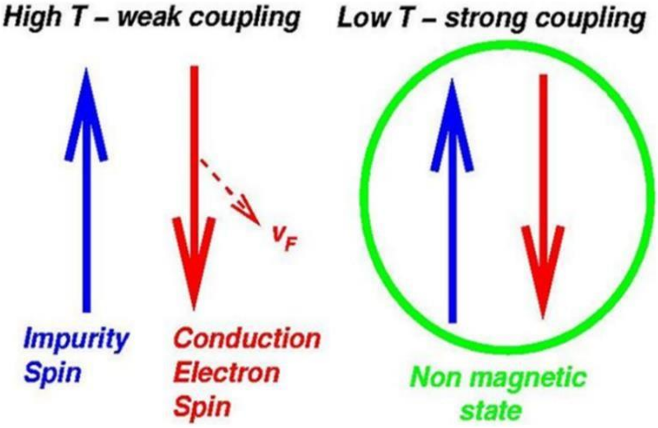


Fig.2 : coupling of impurity spin and conduction electron spin[13]

According to Kondo's model, the rate at which conduction electrons scatter off the magnetic impurity should diverge as the temperature approaches 0K..[12] The creation of heavy fermions and Kondo insulators in intermetallic compounds, particularly those combining rare earth elements like cerium, praseodymium, and ytterbium and actinide elements like uranium, is likely explained by the Kondo effect when extended to a lattice of magnetic impurities.[13]

As well as taking into account the Kondo effect, the resistivity's dependence on temperature is expressed as

$$\rho(t) = \rho_0 + aT^2 + c_m ln \frac{\mu}{T} + bT^5$$

The term aT^2 illustrates the contribution from the Fermi liquid characteristics, while the term bT^5 is from the lattice vibrations, where ρ_0 is the residual resistivity. a , b, c_m and μ are constants. By using the Anderson model, which assumes that a spin already has a local magnetic moment associated with it and is related to the conduction electrons via an exchange interaction J, Kondo was able to determine the third term of the logarithmic dependency on temperature.

CHAPTER - 2

EFFECT OF CORRELATION ON THE ELECTRON PHONON INTERACTION

2.1 INFLUENCE OF ELECTRON-PHONON INTERACTION ON PHONON SOFTENING

It is possible to explain all of the heavy fermions' anomalous characteristics by considering how strongly the correlated f-electrons hybridised with those in the conduction band close to the Fermi level.

Many have emphasised the importance of the electron-phonon interaction, in particular the physical characteristics related to the observed magneto-elastic effect (coupling of phonon to the f-electrons), anisotropic Fermi surface, and the manifestation of the deformation potential (the coupling of phonons to the conduction electrons). [15][16] to explain some of the low temperature behaviour.

Although in these systems inelastic neutron scattering or Raman investigations rarely yield direct experimental evidence for phonon anomaly, studies on elastic constant and ultrasonic attenuation have instead provided indirect evidence of strong electron-phonon coupling.

The softening of the elastic constants is the most obvious of these. Strong phonon anomalies have been clearly observed in the elastic constant measurements at low temperatures in $CeAl_3$, $CeCu_6$, UPt_3, Ube_{13} and few others which give an indirect evidence of the electron–phonon coupling in these systems.[16-18]

The features of the HF systems are largely explained by the intra-atomic Coulomb interaction between the f -electrons.

Taking into account the effect of finite band width, Lee et al [20] have established that when electron-phonon coupling is strongly correlated, the coupling constant dominates for nearly filled bands.The study of Miyake et al[21][22] and Min et al[23] have concluded through their calculations that superconductivity of the BCS type may be mediated by phonons in HF systems.

The results of further research also showed that the Coulomb correlation causes the phonon to get harder and the electron-phonon coupling constant to become stronger.By computing the phonon response function as a function of temperature, it is possible to analyse the significant impact that the electron correlation has on various phonon anomalies

Here, under the framework of the periodic Anderson model, we investigate two distinct electron-phonon coupling mechanisms (PAM)[19]. These are (i) the typical interaction in the f -bands between the phonons and the electrons and

(ii) the electron–phonon interaction arising from hybridization term of the (PAM).[24]

Here, in the presence of the onsite Coulomb repulsion, we will assess the contribution to the phonon self-energy from the mixing of the f and conduction electrons as well as the f electrons alone.

To study phonon anomalies in the HF system we will require a total Hamiltonian

$H = H_0 + H_{e-p} + H_p$ (1)

which consists of three terms: (i) the electronic Hamiltonian H_0, (ii) the Hamiltonian for the phonons H_p and (iii) the electron–phonon interaction term H_{e-p}. The electronic Hamiltonian H_0 correspond to that of the PAM and is given by

$$H_0 = \sum_{k\sigma} \varepsilon_k C^+_{k\sigma} C_{k\sigma} + E'_0 \sum_{k\sigma} f^+_{k\sigma} f_{k\sigma} + \gamma_0 \sum_{k\sigma} (f^+_{k\sigma} C_{k\sigma} + C^+_{k\sigma} f_{k\sigma})$$
$$+ (U/2) \sum_{i\sigma} n^f_{i\sigma} n^f_{i-\sigma}, \tag{2a}$$

where $C^+_{k\sigma}(C_{k\sigma})$ and $f^+_{k\sigma}(f_{k\sigma})$ are the creation and annihilation operators for conduction and f-electrons with momentum k and spin σ respectively, ε_k is the energy of electron in the conduction band, E'_0 is the position of f-level, $n_\sigma = f^+_{i\sigma} f_{i\sigma}$ is the number operator for f electrons, γ_0 represent the strength of the hybridization between the f-electrons and the conduction electrons and U is the onsite Coulomb repulsion between the f-electrons of opposite spin. [26]

Considering the importance of the lanthanide contraction in these systems, the phonons are assumed to interact predominantly with the f-electrons. While the interaction of the phonons with the conduction electrons is neglected, it has been argued by Fulde that their interaction with the hybridization term can contribute substantially to the phonon anomalies. Thus the electron–phonon interaction Hamiltonian is given by

$$H_{e-p} = \sum_{kq\sigma} \Big[f_1(q)(f^+_{k+q,\sigma} C_{k,\sigma} + C^+_{k+q,\sigma} f_{k,\sigma})$$
$$+ f_2(q) f^+_{k+q,\sigma} f_{k,\sigma} \Big] \left[b_q + b^+_{-q} \right], \tag{2b}$$

where $f_1(q)$ and $f_2(q)$ are the coupling constants, the former corresponds to the interaction arising between phonons with the hybridization terms and the latter corresponds to the strength of interaction with the f-electrons. Finally the Hamiltonian for the phonons is given by

$$H_p = \sum_q \omega_q b^+_q b_q, \tag{2c}$$

$b^+_q(b_q)$ being the creation (annihilation) operator for the phonons with the wave vector q and frequency ω_q.

Following the standard technique of Zubarev[25] the different correlation functions involved in these equations are evaluated.

These computations take into account a variety of dimensionless characteristics, including the ratio of the two electron-phonon interaction strengths r = $f_2(0) / f_1(0)$; the dimensionless coupling constant g = N(0) $f^2(0)/\omega_0$, N(0) being the density of states at the Fermi level.[26]

All the energies in the system are measured with respect to the strength of the hybridization (γ_0) which is the single dominant parameter, e.g., the position of the f -level is given by d = E'_0/γ_0 , the coulomb repulsion U'=U/γ_0 , the band width W'=W/γ_0 and the inverse of the temperature by b= γ_0/2KT . Similarly the variable band energies are denoted by y = ε_k/γ_0 and the renormalized phonon frequency $\tilde{\omega} = \omega/\omega 0$ is measured with respect to the frequency (ω_0) of the bare phonon. The value of r is always kept less than one so as to make $f_1(0)$ more stronger than $f_2(0)$. Since the Fermi level is set to zero, the value of d is negative if the f-level is below it and positive if it is above it. The fluctuation of reduced phonon frequency($\tilde{\omega}$) with inverse temperature (b) for various values of the parameters r, g, and d is depicted in the figures with the Coulomb correlation U' = 0

Figure 3 shows the variation of the reduced phonon frequency with inverse temperature for several values of r at g=0.003 and d=-4.0. We can observe that phonon softening is decreased when r is changed from 0.1 to 0.001. Further, it is found that r decreases above 0.005 have little impact on phonon energy; for instance, the two curves coincide at r=0.005 and 0.001, with only a slight departure from the fluctuation at r=0.01 [26]

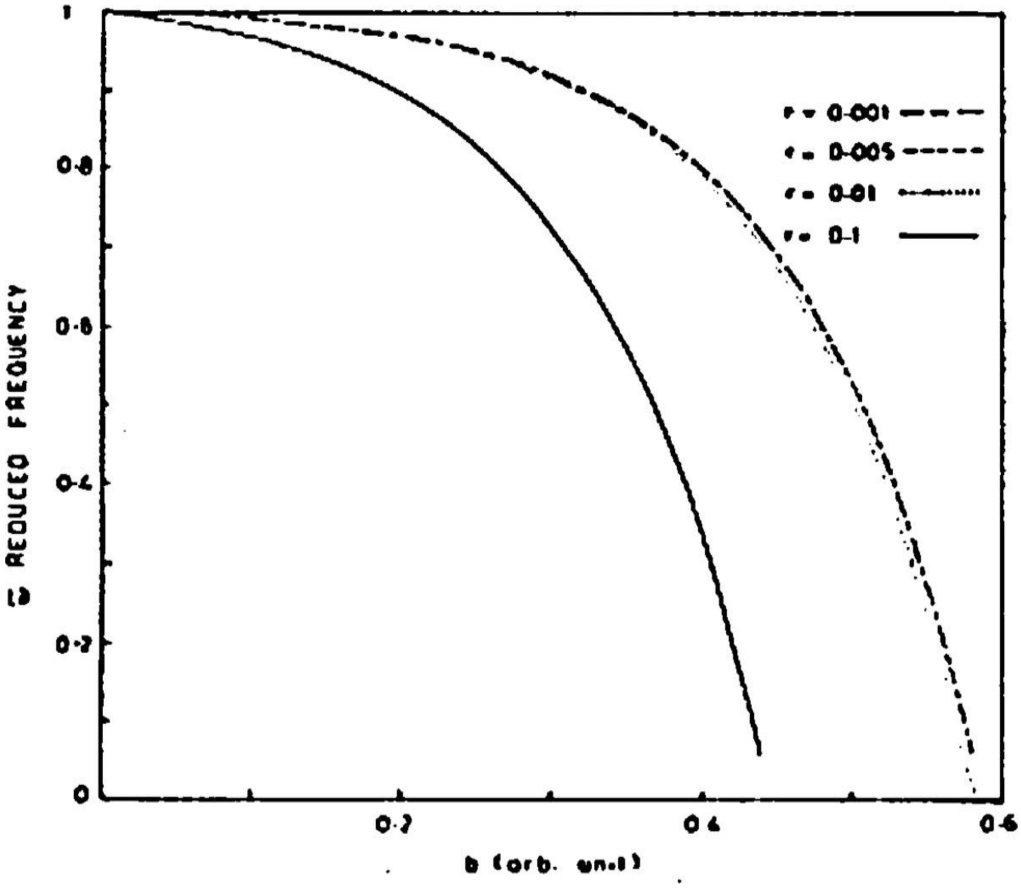


Fig .3 Plot of $\tilde{\omega}$ $(= \omega/\omega_0)$ versus temperature b for $r = 0.001, 0.005, 0.01$ and 0.1 for fixed values of $g = 0.003$ and $d = -4$.

[26]

Figure 4 illustrates the relationship between temperature and the lowered phonon frequency for various g values at r =0.01 and d = -4.0. This chart shows that the softening of the phonon frequency likewise reduces as g values are reduced from 0.05 to 0.0001. Small value of g means small value of $f_1^2(0)$ which implies that Phonons and hybridization of f and conduction electrons have a weak coupling that is insufficient to have an impact on phonons. Additionally, the variance of r in fig.3 supports this.[26]

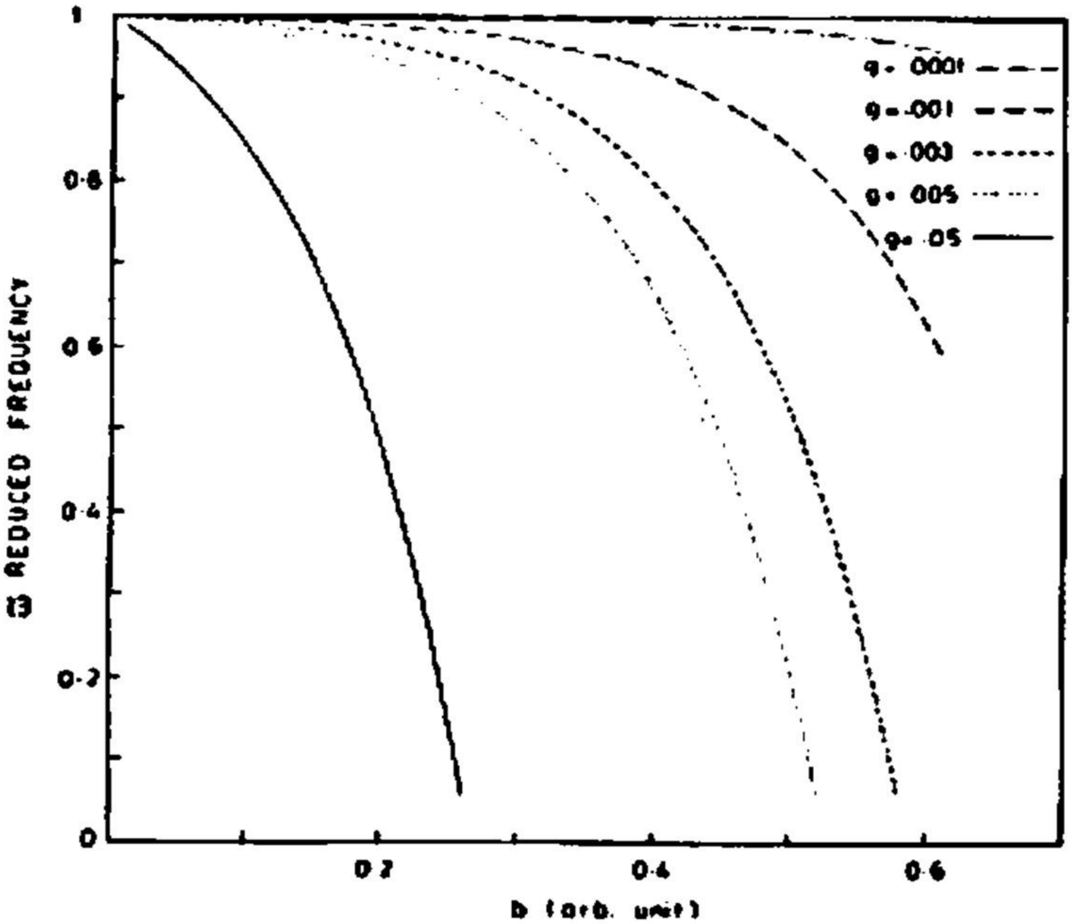


Fig .4 . Plot of $\bar{\omega}\ (= \omega/\omega_0)$ versus temperature b for $g = 0.0001$, 0.001, 0.003, 0.005 and 0.05 for fixed values of $r = 0.01$ and $d = -4$.[26]

In Fig. 5, the f level's position is adjustable, but the other two parameters are set to r=0.01 and g=0.003. The phonon softening is demonstrably significant for negative values of d, namely -6, -4, and -2. As the f-level decreases from 6 to 2 or gets closer to the conduction band, the phonon softening becomes less severe. For positive values of d, the phonon softening is barely noticeable.

Since b is an inverse function of temperature in all of these plots, an increase in b implies a drop in temperature. Figure 5 shows that the phonon softening reduces for the given values of r, g, and d as the value of d is raised.[26]

Figure 6 shows the effect of correlation U on phonon softening. The variation in phonon energy with temperature is examined to illustrate this impact by maintaining the starting values of the parameters r, g, and d while accounting for a range of U′ values, including U′ = 0. As the value of U′ increases, the softening decreases.

Thus, an increase in correlation causes phonons to harden. It is evident from the analysis that the correlation causes the f level's position to change. The value of parameter d becomes less negative when the value of U increases from U=0 to some positive values, causing the f level to approach the fermi level.[26]

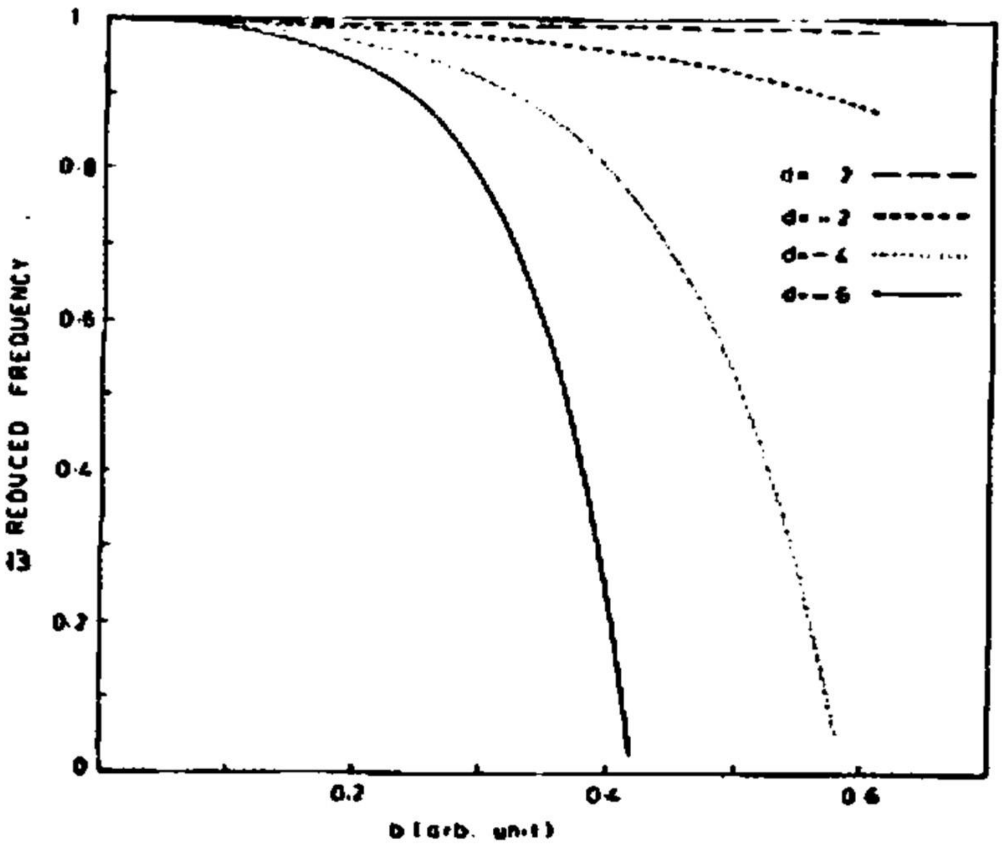


Fig .5 Plot of $\tilde{\omega}$ $(= \omega/\omega_0)$ versus temperature b for $d = -6, -4, -2$, and 2 for fixed values of $r = 0.01$ and $g = 0.003$. [26]

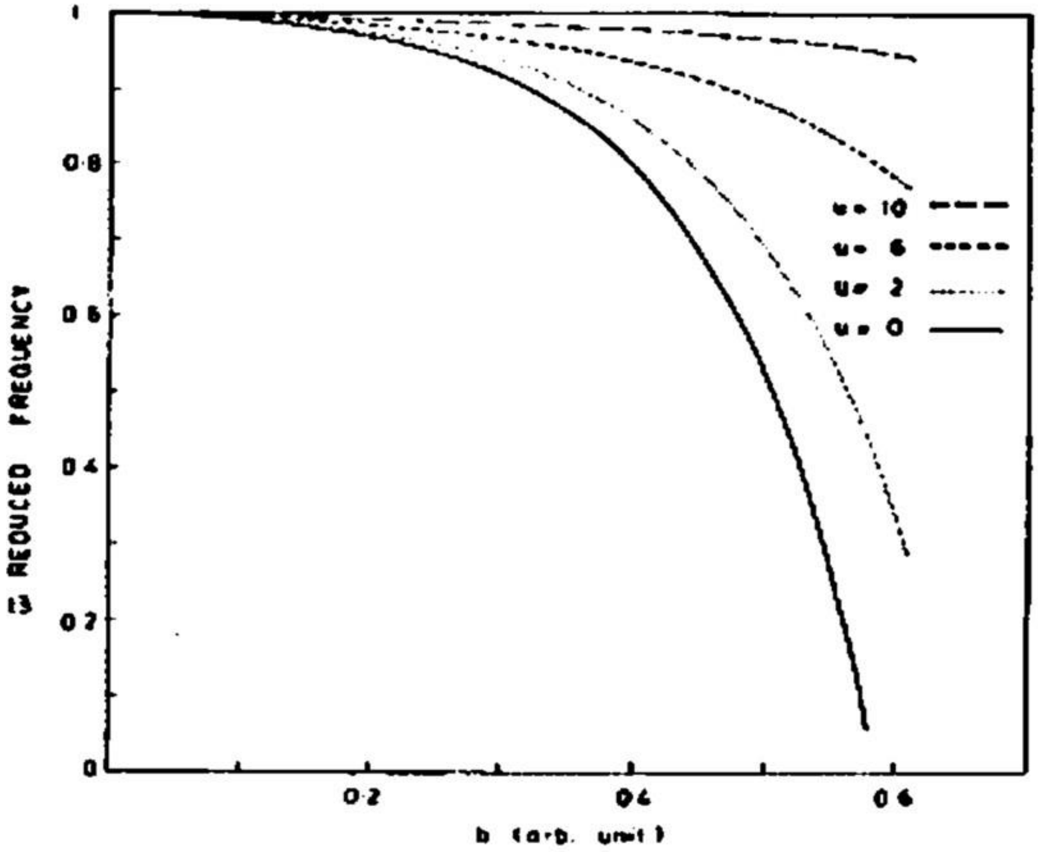


Fig .6 , Plot of $\tilde{\omega}$ $(= \omega/\omega_0)$ versus temperature b for $U' = 0, 2, 6$ and 10 for fixed values of $r = 0.01$, $g = 0.003$ and $d = -4$. [26]

2.2 INFLUENCE OF ELECTRON-PHONON INTERACTION ON EFFECTIVE MASS

The electron-phonon interaction raises the quasi particle mass for ordinary metals, which is a well-known fact. In contrast, Fulde et al. [27] recently discovered that it decreases for some heavy Fermion systems

Here, we will examine the impact of the electron-phonon interaction on effective mass via the self energy, which has the following relationships with effective mass:

$$m^*/m = \tilde{m} = 1/\left[1+\partial\Sigma(k,\omega)/\partial\varepsilon_k\right].$$

All of these systems' anomalous characteristics can be explained by the high hybridization of their correlated γ- electrons with those in the conduction band close to the Fermi level. Furthermore, it has been demonstrated that phonon coupling to the hybridised f- and conduction band electrons is stronger than phonon coupling to the f- band electrons alone.

The phonons are primarily affected by the variables d, g, and r. Renormalized phonon energy, which again affects the effective mass, has been researched in order to understand how these parameters behave in heavy fermion systems. The results of the numerical calculations are shown in two pictures that illustrate how the effective mass $\tilde{m}$ changes with the effective coupling strength g keeping other parameters constant.[28]

In Figure 7, the variation of $\tilde{m}$ is made with g keeping other parameters at fixed values as r =0 .1, z = 2.5, a_0 = 0.1, X_f =0, b= 0.2 and d = -2,

Where z=w_0/γ_0, $x_f = \frac{\varepsilon_f}{\gamma_0}$, $\langle a_0 \rangle = \langle b_q + b^{+}_{-q} \rangle_{q=0}$

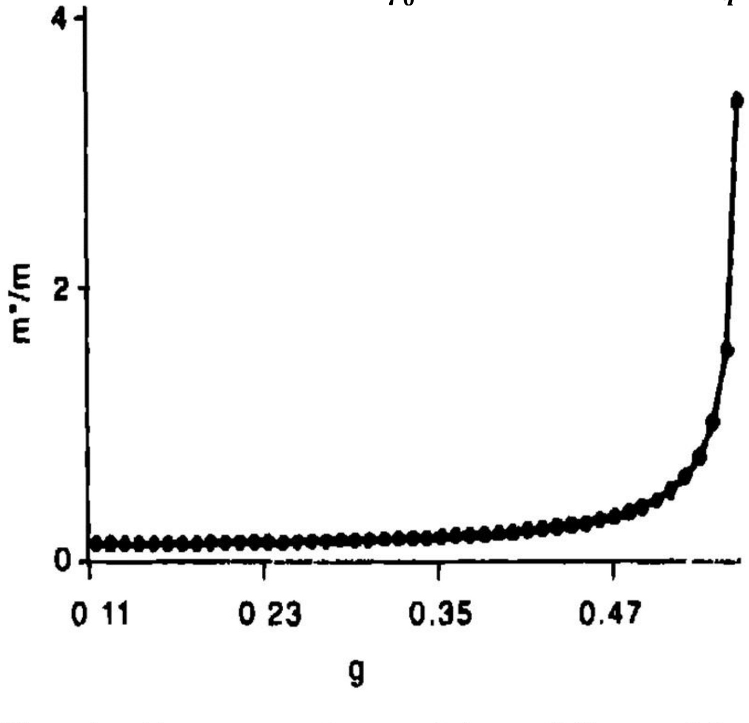


Fig .7 1. Plot of m^*/m versus g for $r = 0.1$, $z = 2.5$, $x_m = 0.1$, $a_0 = 0.1$, $x_f = 0$, $b = 0.2$ and $d = -2$ [28]

The same figure is shown in Figure 8 for a different value of d (= - 1), with the values of the other parameters remaining the same as they did in the first instance.

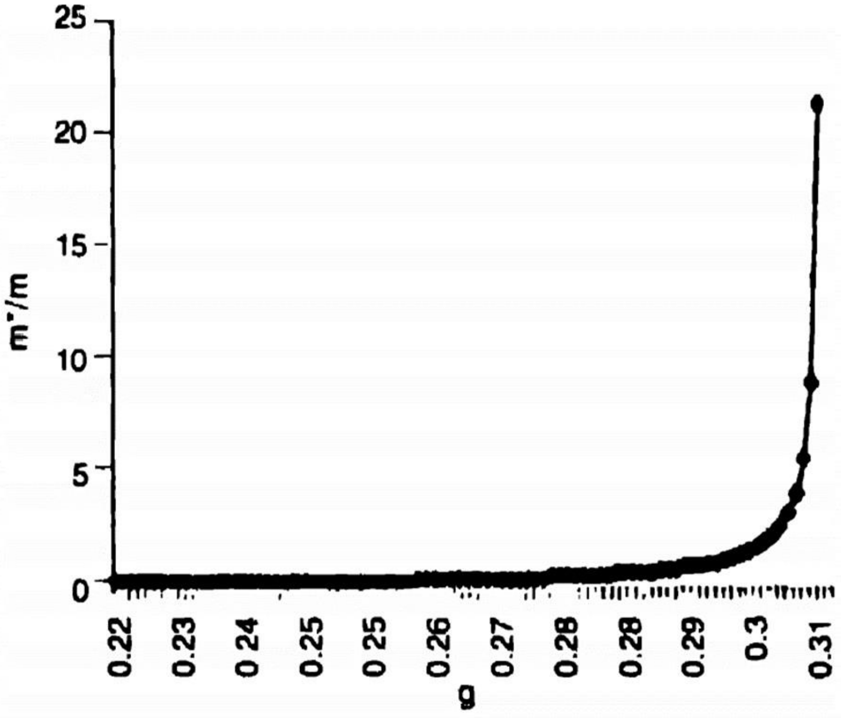


Fig.8 Plot of m^*/m *versus* g for $r = 0.1$, $z = 2 5$, $x_m = 0 1$, $a_0 = 0.1$, x_f =0, $b = 0.2$ and $d = -1$. [28]

It can be seen in both figures that the effective mass grows and lowers depending on the values of g and d. In other words, the effective mass has a value greater than one for some ranges of g values and less than one for others.

Additionally, the value of the location of the f-level has a significant impact on the g value range. In the first scenario, the effective mass is less than one and the range of g values ranges from 0 to 0.53. However, as the g values exceed this threshold, i.e., 0.53, the effective mass quickly rises and approaches 4.0 for g = 0.56 [28]

If g is raised much further, the system becomes unstable and the effective mass produces unphysical outcomes. The effective mass is smaller than one for the second curve when d shifts from -2 to -1 for the range of g values from 0 to 0.294. The effective mass is more than one when the value of $\tilde{m}$ exceeds 0.294, and the value of $\tilde{m}$ increases to $\tilde{m}$ =21 at g=0.301.

Therefore, it can be inferred from these two figures that the placement of the f-level has a significant impact on the range of g values. It is obvious that the value of effective mass increases with the distance between the f-level and the fermi level. It is clear that the electron density rises when the f-level approaches fermi level. The value of effective mass increases since it is directly proportional to this amount. Additionally, as anticipated by Fulde et al., the present study also explains the drop in effective mass for some Heavy Fermion systems.[28]

CHAPTER-3

SUPERCONDUCTIVITY IN HEAVY FERMION MATERIALS

The enormous specific heat and large effective masses of the heavy fermion materials are reflected in their lower superconducting transition temperature and large specific heat. At low temperatures, these materials' superconductivity coexists with ferromagnetic or antiferromagnetic order. It displays features such unconventional superconductivity, non-fermi liquid, quantum critical points, and magnetic instabilities. The fundamental physics underlying the pairing mechanism can be visualised by comparing the superconducting characteristics, phase diagram, and impact of magnetic field and pressure on heavy fermions based on uranium, cerium, and praseodymium.[29]

These materials' critical temperature is below 2.0 K. They exhibit magnetic field penetration depths λ of over a few thousand and coherence lengths ξ are 100-200 Å .

It was discovered that rather of being caused by lattice vibrations, the cooper-pairing in these materials results from the magnetic interactions of the electron spins. Superconductivity and ferromagnetic or antiferromagnetic order coexist in uranium-based heavy fermions that have a periodic array of uranium ions. The magnetic ordering of atoms is broken by a little change in pressure at the quantum critical point (QCP). Superconductivity can exist in the environment created by the quantum critical point. Phase variations with the material extend in both space and time close to quantum critical regions, aiding in the production of cooper pairs. The significant value of specific heat (Cp/T) at the transition temperature (Tc) suggests that large mass quasi-particles are crucial to the superconducting pairing.

3.1 URANIUM BASED HEAVY FERMION SUPERCONDUCTORS

The coexistence of superconductors with a magnetic long-range order is visible in the uranium-based superconducting materials.

In UPt_3, UBe_{13}, URu_2Si_2, UPd_2Al_3, UNi_2Al_3 a transition from to an antiferromagnetic state to a superconducting state takes place.

In UGe_2, URhGe and UCoGe, because of the coexistence of superconductivity and ferromagnetism, Cooper pairs are in the spin-triplet state.[30]

In URhGe and UCoGe following changes occurs

when magnetic field is applied

- T_curie is overpowered.
- Ferromagnetic fluctuations are enhanced.
- Superconductivity behaviour is enhanced.

- Superconductivity in UGe_2 was observed on the border of ferromagnetism[32] . Fig. 1 shows variation of P as a function of T for UGe_2 in which the superconducting dome is completely inside the ferromagnetic phase. Here superconductivity coexists with strong ferromagnetism. It is an orthorhombic crystal having critical temperature Tc≈0.8K at 12kbar. When pressure is applied the ferromagnetism is overpowered at Tcurie.

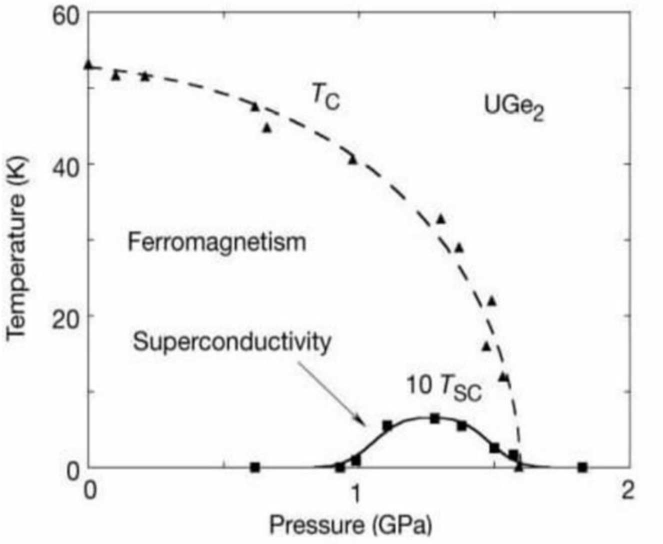


Fig. 9 : P-T phase diagram of UGe_2[33]

- In hexagonal UPt_3, superconductivity is achieved around Tc≈0.53K, and below Tc, many superconducting phases can be observed. UPt_3 is antiferromagnetic below Neel temperature (TN) = 5K and has a magnetic moment of around (μ= 0.02μB) . At the same pressure, the two superconducting transitions combine into one and antiferromagnetism is destroyed. It displays a spin triplet pairing condition that is consistent with the spin fluctuation process.
- The superconducting transition temperature (Tc) of UBe_{13}, a non-fermi liquid (NFL) superconductor with a cubic crystal structure, is (≈0.93K). The high effective mass (m*/m≈260) and high specific heat (1100 m J/mol-K^2) demonstrate the role of quasi-particles with huge masses in superconductivity.
- The body centered tetragonal crystal URu_2Si_2[31] has transition temperature (Tc) ≈ 1.5K. It is a multiband superconductor . The hidden order transition takes place at 17.5K.

- With a Tcurie ≈ 9.5K , URhGe exhibits ferromagnetism at atmospheric pressure and superconductivity at 0.3K in fields less intense than 2T. The coexistence of ferromagnetic and superconducting behaviour at the microscopic level is demonstrated by the presence of the same 5f electrons in these materials.
- UTe_2 has superconducting transition temperature Tc≈1.6K at ambient pressure and zero magnetic fields .[34] The upper critical field Hc2 (0) ≈ 40 tesla is very large. It has body centered orthorhombic structure with lattice constants a=4.165Å, b=6.139Å and c=13.979Å.

- UPd_2Al_3 has transition temperature Tc≈2.0 K and having Neel temperature T_N≈ 14.5 K. When pressure is increased up to 6.5GPa the Neel temperature T_N deceases while the onset of superconductivity remains unchanged but above 6.5GPa the critical temperature starts decreasing. Here pairing is mediated by spin fluctuation.

- Hexagonal UNi_2Al_3 has transition temperature Tc≈1.6 K. At 4.5K, the co-existence of a small magnetic moment with disproportionate spin density wave recommend spin triplet state.

Theoretically, $Hc1 \propto 1/\lambda^2$, which may leads to anomalously small value of Hc1 and $Hc2 \propto 1/\xi^2$ which may lead to large value of Hc2 in heavy fermion superconductors.

MATERIAL	T_C (K)	STRUCTURE	MAGNETISM	COMMENT
UPt_3	0.53	Hexagonal	Paramagnetic	several distinct superconducting phases
UBe_{13}	0.93	Cubic	Paramagnetic	p-wave superconductor
URu_2Si_2	1.53	bc tetragonal	Antiferromagnetic ($T_N = 17.5K$)	mysterious hidden-order phase below 17K
URhGe	0.25	Orthorhombic	Ferromagnetic ($T_{curie} = 9.5K$)	ferromagnetic and superconducting behaviour coexists on the microscopic scale
UPd_2Al_3	2.0	Hexagonal	Antiferromagnetic ($T_N = 14.5K$)	pairing is mediated by spin fluctuation
UNi_2Al_3	1.6	Hexagonal	Antiferromagnetic ($T_N = 4.6K$)	at 4.5K the co-existence of a small magnetic movement with disproportionate spin density wave recommend spin triplet state
UGe_2	0.8	Orthorhombic	Ferromagnetic ($T_{curie} = 30K$)	superconductivity coexist with strong ferromagnetism
UTe_2	1.6	Orthorhombic	Nearly Ferromagnetic	Spin triplet pairing

(Table 2 : list of uranium based heavy fermion superconductors)[38]

Table 3 : **Superconducting parameters of uranium based superconductors**

Materials	λ (Å)	ξ (Å)	$H_{c1}(0)$ mT	$H_{c2}(0)$ T
UPt_3	~7000	100-120	3.0	2.8
UBe_{13}	~8000	100	4.6	10.1
UNi_2Al_3	~3000	240	1.5	1.5
UPd_2Al_3	~5000	85	1.0	3.6
URu_2Si_2	~15000	100-150	1.4	3.0

3.2 CERIUM BASED HEAVY FERMION SUPERCONDUCTORS

- Magnetism and superconductivity cannot coexist in $CeCu_2Si_2$, which exhibits non-Fermi liquid behaviour at a critical temperature of (Tc) ≈0.6K.[32] The superconducting cooper pairs are extremely massive particles .
- The layers of $CeIn_3$ are separated by layers of $RhIn_2$ in the tetragonal crystal $CeRhIn_5$. With a Neel temperature of $T_N \approx 3.8K$ at ambient pressure, it exhibits antiferromagnetism. A superconducting state with a transition temperature (Tc) ≈2.2 K replaces this antiferromagnetic state at pressures of about 2.3 to 2.5 GPa. The superconducting and antiferromagnetic phases of $CeRhIn_5$ coexist at 2.4GPa, as seen in Fig. 2's T-P phase diagram.

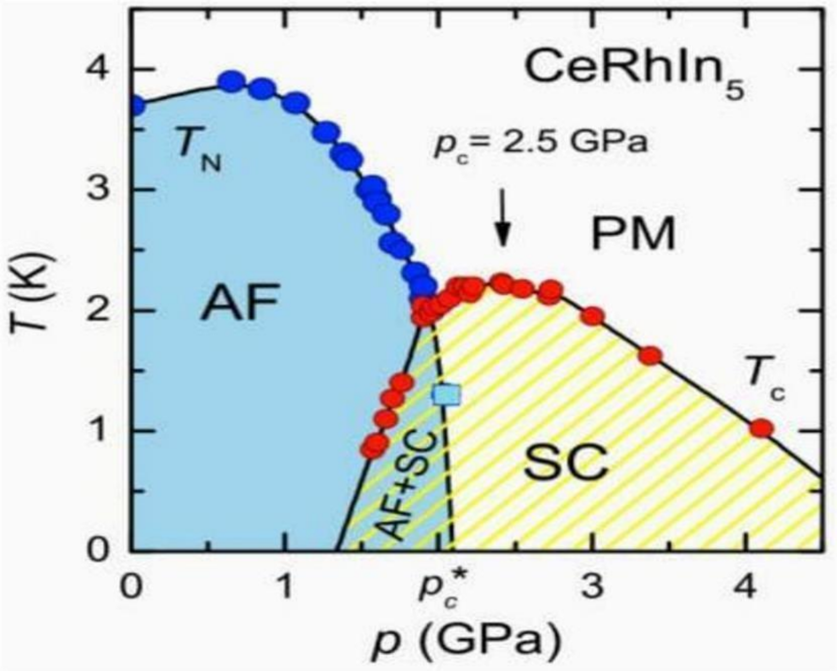


Fig.10 **T-P phase diagram of CeRhIn5** [35]

- The quasi-2D structure of the tetragonal $CeCoIn_5$ has lattice constants of a=b=4.612Å and c=7.551Å. The critical temperature for it is Tc = 2.3K. At critical temperature (Tc), a specific heat jump of 290 mJ/mol-K2 has been recorded. The layers of $CeIn_3$ in $CeCoIn_5$ are separated by layers of $CoIn_2$. Magnetic interactions in it cause superconductivity. Under pressure, the nonfermi liquid state's fermi liquid behaviour is broken, and $CeCoIn_5$ exhibits superconductivity.
- At T_N≈36K, tetragonal $CeRh_2Si_2$ exhibit antiferromagnetism. At a critical pressure ≈ 9 kbar and a critical temperature(Tc) ≈0.3K. superconductivity replaces antiferromagnetism below T_N=25 K.

- $CeIn_3$ demonstrate antiferromagnetism at atmospheric pressure with T_N=10.2 K. At a critical pressure of around 26 kbar when pressure is applied at around 0.19 K, T_N vanishes, and below this temperature antiferromagnetism is replaced by a superconducting state. Its pressure-temperature phase diagram leads to the conclusion that superconductivity is mediated by magnetism.
- Tetragonal $CePt_3Si$ (36), when subjected to ambient pressure, exhibits a magnetic transition at T_N=2.2 K and a superconducting transition atTc≈0.75 K. The absence of a centre of inversion symmetry in this substance indicates that superconductivity may not be possible. A spin triplet pairing state may be possible if Hc2 (0) ≈5T has a higher value.

MATERIAL	**T_C (K)**	**STRUCTURE**	**COMMENT**
$CeCu_2Si_2$	0.6	bc tetragonal	1st unconventional superconductor
$CeRhIn_5$	2.2	tetragonal	Antiferromagnetic and superconducting phase coexists at 2.4 GPa
$CeCoIn_5$	2.3	tetragonal	Highest T_C of all Ce based heavy fermions
$CeIn_3$	0.19	cubic	Superconducting only at high pressure
$CePd_2 Si_2$	0.43	bc tetragonal	Superconductivity is magnetically mediated
$CeRh_2Si_2$	0.3	bc tetragonal	Below T_N=25K antiferromagnetism is replaced by superconducting state at critical pressure =9kbar
$CePt_3Si$	0.75	tetragonal	1st heavy fermion superconductor with non-centrosymmetric crystal structure

(Table 4 : list of cerium based heavy fermion superconductors)[38]

3.3 PRASEODYMIUM BASED HEAVY FERMION SUPERCONDUCTORS

Materials	T_c(K)	Crystal Structure
$PrOs_4Sb_{12}$	1.85	Skutterudite
PrV_2Al_{20}	0.05	Cubic
$PrTi_2Al_{20}$	0.2	Cubic

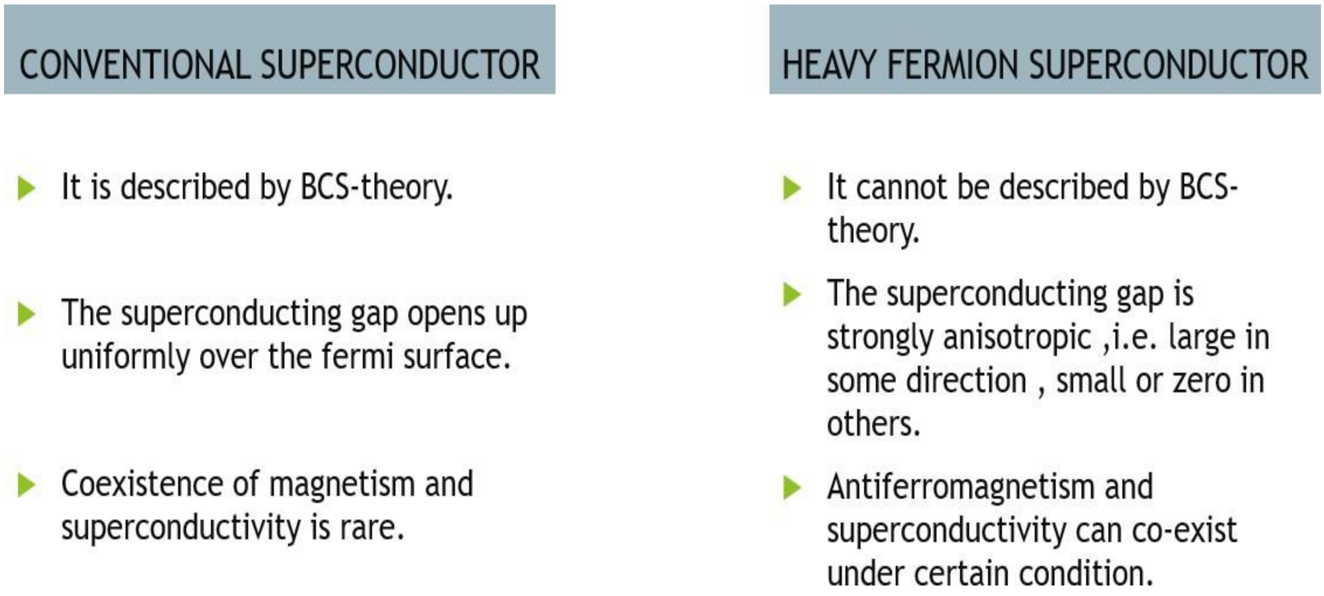
(Table 5 : list of praseodymium based heavy fermion superconductors)

- With a broken time reversal symmetry and a superconducting critical temperature Tc ≈1.85K , $PrOs_4Sb_{12}$ is a filled skutterudites heavy fermion complex [37]. There are multiple superconducting phases in it. Just above the upper critical field, there is a field-induced antiferroquadrupolar order phase, which suggests that electric quadrupole fluctuations are crucial to the superconducting mechanism.

- The nonmagnetic cubic Γ_3 doublet ground state is found in PrV_2Al_{20}. When the transition temperature Tc≈50mK and ambient pressure is present, it displays superconductivity. The function of orbital fluctuation of the f electrons at ambient pressure is indicated by the large $\gamma \approx 300$ m J. $mol^{-1}.K^{-2}$ and related large m*/m ≈140. Cubic temperature dependence of specific heat capacity shows the gapless mode associated with quadrupolar ordering.

- The quadrupolar ordered state of cubic $PrTi_2Al_{20}$ is present, and the 4f and outer shell electrons interact strongly. The transition temperature for the non-magnetic ferro-quadrupolar state is Tc = 200 mK..

3.4 COMPARISON BETWEEN CONVENTIONAL SUPERCONDUCTOR AND HEAVY FERMION SUPERCONDUCTOR



CONVENTIONAL SUPERCONDUCTOR	HEAVY FERMION SUPERCONDUCTOR
▶ It is described by BCS-theory.	▶ It cannot be described by BCS-theory.
▶ The superconducting gap opens up uniformly over the fermi surface.	▶ The superconducting gap is strongly anisotropic ,i.e. large in some direction , small or zero in others.
▶ Coexistence of magnetism and superconductivity is rare.	▶ Antiferromagnetism and superconductivity can co-exist under certain condition.

CONCLUSION

Heavy fermions have been studied for some of their interesting characteristics, such as their huge effective mass, high specific heat, and strong electron-phonon interaction, etc.

The correlation effect on the electron-phonon interactions in HF systems, which indirectly affects the many physical parameters exhibiting phonon anomalies, has been attempted to be explained. Calculating the renormalized phonon frequencies is necessary in order to examine the various phonon anomalies displayed by these systems. Correlation has the effect of moving the f-level closer to the Fermi level, which lessens the phonon softening.

It is discussed how the effect of electron-phonon interaction, which directly affects the effective mass, works in the heavy fermion systems. In heavy fermion compounds, the actual interaction between localised magnetic moments and conduction electrons is still not well understood.

Based on research into the superconducting properties of several heavy fermion compounds, a comparison between heavy fermion superconductors and ordinary superconductors was conducted. Pairing mechanism in heavy fermion superconductors is still a challenging problem, as evidenced by the complex crystal structures, unusual magnetic and superconducting transitions, coexistence of antiferromagnetism and superconductivity, multiple superconducting phases, appearance of superconductivity at quantum critical point, and the gap structure.

REFERENCES

[1] P. Coleman (2007). "Heavy Fermions: Electrons at the Edge of Magnetism. Handbook of Magnetism and Advanced Magnetic Materials". In Helmut Kronmuller; Stuart Parkin (eds.). Handbook of Magnetism and Advanced Magnetic Materials. 1. pp. 95–148. arXiv:condmat/0612006 (https://arxiv.org/abs/cond-mat/0612006).

[2] P.Fulde, J. Phys. F: Met. Phys. 18, 601 (1988).

[3] K.Andres, J. Graebner, H. R. Ott, Phys. Rev. Lett. 35, 1779 (1975).

[4] . K. Andres; J.E. Graebner; H.R. Ott (1975). "4f-Virtual-Bound-State Formation in CeAl3 at Low Temperatures". Physical Review Letters. 35 (26): 1779–1782.Bibcode:1975PhRvL..35.1779A (https://ui.adsabs.harvard.edu/abs/1975PhRvL..35.1779A). doi:10.1103/PhysRevLett.35.1779

(https://doi.org/10.1103%2FPhysRevLett.35.1779).

[5] Steglich, F.; Aarts, J.; Bredl, C. D.; Lieke, W.; Meschede, D.; Franz, W.; Schäfer, H. (1979-12-17)."Superconductivity in the Presence of Strong Pauli Paramagnetism : CeCu2Si2". Physical Review Letters. 43 (25): 1892–1896. Bibcode:1979PhRvL..43.1892S

(https://ui.adsabs.harvard.edu/abs/1979PhRvL..43.1892S).doi:10.1103/PhysRevLett.43.1892(https://doi.org/10.1103%2FPhysRevLett.43.1892).hdl:1887/81461(https://hdl.handle.net/1887%2F81461).

[6] https://en.wikipedia.org/wiki/Heavy_fermion_material

[7] H.R. Ott, H. Rudigier, Z. Fisk, and J.L. Smith, in W.J.L. Buyers (ed.): Proceedings of the NATO Advanced Study Institute on Moment Formation in Solids, Vancouver Island, August 1983, Valence Fluctuations in Solids (Plenum, 1985), p. 309.

[8] J. Kondo, Prog. Theo. Phys. 28, 772 (1962).

[9] J. Kondo, Prog. Theo. Phys. 32, 37 (1964).

[10]Hewson, Alex C ; Jun Kondo(2009)."Kondo effect"

(https://doi.org/10.4249%2Fscholarpedia.7529).Scholarpedia.4(3):7529.Bibcode:2009SchpJ. 4.7529H(https://ui.adsabs.harvard.edu/aExamplesReferencesbs/2009SchpJ. 4.7529H).doi:10.4249/scholarpedia.7529)

(https://doi.org/10.4249%2Fscholarpedia.7529).

[11] W. Meissner and B. Voigt, Ann. Phys. 7, 761, 892 (1930).

[12] Kondo ,Jun(1964)."Resistance Minimum in Dilute Magnetic Alloys" (https://doi.org/10.1143%2FPTP.32.37). Progress of Theoretical Physics. 32 (1): 37–49.
Bibcode:1964PThPh..32.. 37K(https://ui.adsabs.harvard.edu/abs/1964PThPh..32...37K).doi:10.1143/PTP.32.37

(https://doi.org/10.1143%2FPTP.32.37).

[13] https://en.wikipedia.org/wiki/Kondo_effect

[14] J. Kondo. , Prog. Theor. Phys. 32: 37-69, (1964).

[15] G R Stewart, Rev. Mod. Phys. 56, 755 (1984)

[16] P Thalmeir and B Luthi, in Handbook on the physics and chemistry of rare earth edited by K A Schneider Jr and L Eyring (North Holland, Amsterdam, 1991) vol. 1, p. 226

[17] F Steglich, Theory of heavy fermion and valence fluctuation edited by T Kasuya and T Saso in Springer Series in Solid State Sciences (Springer, Berlin, 1985) vol. 62

[18] Luthi and Yoshizawa, (1987)

[19] P W Anderson, Phys. Rev. 124, 41 (1961)

[20] J D Lee, K Kong and B I Min, Phys. Rev. B51, 3850 (1995)

[21] K Miyake, T Matsuura, H Jichu and Y Nagaoka, Prog. Theor. Phys. 72, 1063 (1984)

[22] J E Hirsch, Phys. Rev. Lett. 54, 1317 (1985)

[23] B I Min, J D Lee and K Kang, Physica 206 & 207, 736 (1995)

[24] P Fulde, J Keller and G Zwicknagle, Solid State Physics 41, 1 (1988)

[25] D N Zubarev, Sov. Phys. Usp. 3, 320 (1960)

[26] P Nayak B Ojha S N Behera Pramana - J Phys 54 305 (2000)

[27] P Fulde. P Horsch and A Ramsack Z Phys B 90 125 (I993)

[28] P Nayak B Ojha S N Behera Indian J . Phys .76A(l), 35-38 (2002)

[29] Superconductivity in heavy fermion materials Shailaj Kumar Shrivastava International Journal of Engineering and Advanced Technology (IJEAT)ISSN: 2249 – 8958, Volume-9 Issue-3, February, 2020

[30] D.Aoki, K.William, I.Sheikin. "Heavy fermions in high magnetic fields". Comptes rendus-physique", 14, 1, 53-77, 2013

[31] N.Shah, P. Chandra, P. Coleman and J.A. Mydosh" Hidden order inURu_2Si_2" Phys. Rev. B,61(564),2000

[32] B.D.White, J.D. Thompson, M.B. Maple. "Unconventional superconductivity in heavy-fermion compounds".Physica C: superconductivity and its applications.514, 246-278, 2015

[33] S.S. Saxena, P. Agarwal, K. Ahilan et al., "Superconductivity on the border of itinerant-electron ferromagnetism in UGe2" . Nature, 406(6796), 587-92, 2000

[34] Sheng Ran, Chris Eckberg, Quing-ping-Ding, Yuji Furukawa et al."Nearly ferromagnetic spin-triplet superconductivity". Science,365(6454) 684, 2019

[35] G.Knebel, D.Aoki and J. Flouquet. "Antiferromagnetism and superconductivity in cerium based heavy fermion compounds", Comptes Rendus Physique, 12(5-6), 542-566, 2011

[36] K.V. Samokhin, E.S. Zijlstra, S.K. Bose. "CePt3Si: an unconventional superconductor without inversion centre". Phys. Rev.B , 69, 094514 , 2004.

[37] M.B. Maple, N.A. Frederick P.-C. Ho, W.M. Yuhasz, T. Yanagisawa.“Unconventional superconductivity and heavy fermion behaviour inPrOs4Sb12”. J. Supercond. And Novel Magnetism19, 3-5,299-315,2006

[38] https://en.wikipedia.org/wiki/Heavy_fermion_superconductor