Journal of Multidisciplinary Engineering Science and Technology (JMEST)
ISSN: 2458-9403
Vol. 12 Issue 2, February - 2025

Crystal Structure And Mechanism Of Superconductivity In Cerium Based Heavy Fermions

[1]Horace Kibe, [2]Michael Nakitare Waswa, [3]Godwin Wabuyi

[1]Department of Physical and Biological Sciences (Bomet University College)

[2] Department of Science Technology and Engineering (Kibabii University)

[3] Department of Science Technology and Engineering (Kibabii University)

***Abstract*—Superconductivity in certain inter-metallic rare-earth compounds takes place amongst it's electron-hole elementary excitations referred to as excitons. No theoretical study has been performed taking account of these excitons. In the present attempt it has been done.**

Formation of Cooper pair in heavy electrons due to electron-hole interaction has been shown in our study. This knowledge is consistently used in the present investigation of bulk superconductivity in Ce-based silicons.

Singlet superconducting electron-hole pairing of excitonic-type in heavy fermion system has been used to explain superconductivity, quite unlike earlier studies where conduction and f-electrons and their hybridization were considered independently. It turns out that one can explain $T_c = 0.6$ K in $CeCu_2Si_2$ and other Ce-based silicons with tetragonal crystal structure.

In these materials magnetism and superconductivity do not coexist and has non-Fermi Liquid (NFL) behaviour with critical temperature $T_c \approx 0.7K$. The superconducting cooper pairs are particle having large effective masses. The tetragonal crystal $CeCu_2Si_2$ has the layers of $CeSi_2$ separated by layers of $CuSi_2$.

Electron – hole coupling has extensively been studied in Graphene bilayer and very little on heavy fermion systems. Graphene which is one atomic layer separated from graphite crystal. The pairing of electrons and holes due to their coulomb attraction in two parallel independently gated layers separated by a barrier which is a dielectric material shows the existence of the BCS-like pair – condensed state at weak coupling.

The total energy increases with increase in temperature since a sigmoid- like curve was observed. The specific heat capacity data revealed the fact that at the transition temperature, an energy gap is created at the Fermi energy level and hence there is a sudden change in the value of specific heat capacity of these heavy fermion system. The Gaussian – like curve obtained skewed to the left suggests that superconductivity is a bulk phenomenon in these compounds. At the peak, the Cv was observed to be 0.4560 eV/K. The transition temperature obtained was 0.59K.

***Keywords*—Cooper pair, superconductivity, transition temperature, excitons**

INTRODUCTION

Electron – hole coupling has extensively been studied in Graphene bilayer and very little on heavy fermion systems. Graphene which is one atomic layer separated from graphite crystal [7]. It has its band structure consisting in linear dispersion of electron energy near two inequivalent points of the Brillouin zone. An electron wave function close to these points is well described by the 2-Dimensional Dirac equation for massless particles. The pairing of electrons and holes due to their coulomb attraction in two parallel independently gated layers separated by a barrier which is a dielectric material shows the existence of the BCS-like pair – condensed state at weak coupling [5]. The localized electron – hole pairs are absent in Graphene hence this makes the behaviour of the system versus the coupling strength to be cardinally different from the BCS-BEC crossover [2].

Further, the interlayer pairing of electron – hole system is unstable with respect to the BCS type. The problem of pairing of identical fermions is well examined in the BCS but the problem of pairing of a bound state between an electron and a hole has not been discussed for a long period in condensed matter physics [1]. Such a bound electron-hole pair is known as exciton. According to [4], the cooper pairs carry a magnetic moment. Magnetism in the 5f electrons is of itinerant nature which allows for superconductivity and ferromagnetism to be carried by the same electrons.

This therefore implies that magnetism and superconductivity occupy the same volume and coexists on a microscopic scale. Further, magnetism and superconductivity are two states that are mutually exclusive and antagonistic which do not occur or coexist at the same temperature and place in a sample [3]. Critically, the findings above have not exhausted the field of superconductivity in heavy fermions based on electron- hole coupling of excitonic type. Low temperature superconductors have wide applications ranging from the magnetic resonance imaging, the nuclear magnetic resonance, high speed computing, marine propulsion motors, MAGLEV trains, (SQUIDS) and in making conductors for large scale high current transmissions cables. Adequate low temperature superconductors once are in place for use, they will save our environment that many countries in the world are facing due to large emissions of carbon dioxide gases by local and international airlines and vehicles since the consumption rate of petrol energy is high. [3] looks at coexistence of AFM and superconductivity only as a thermal property of $CePtIn_{11}$ by deriving a Hamiltonian that takes into account of localized electrons and conduction electrons yet the compound is ceramic, not putting the holes interaction into consideration. [7] also looks at the coherent Kondo effect by considering localized and conduction electrons in the partially filled f- shell in heavy fermions, leaving out the hole interaction. This research looked at the thermodynamic phase transition of singlet superconducting electron – hole coupling in $CeCu_2Si_2$ and other Ce-based silicons heavy fermions where the hybrid Hamiltonian was developed and diagonalized by the BVT technique.

In these materials magnetism and superconductivity do not coexist and has non-Fermi Liquid (NFL) behaviour with critical temperature (Tc) ≈0.7K [3]. The superconducting cooper pairs are particle having large effective masses. The tetragonal crystal $CeCuSi_2$ has the layers of $CeSi_2$ separated by layers of $CuSi_2$.Tetragonal $CeRh_2Si_2$ show antiferromagnetism at T_N≈36K.Below T_N=25 K, the antiferromagnetism is replaced by superconducting state at critical pressure ≈ 9kbar, superconductivity appears at critical temperature (Tc) ≈0.4K.

The Cerium based silicon compounds have a tetragonal crystal structure. In $CePd_2Si_2$ antiferromagnetism is replaced by superconductivity at quantum critical point under applied pressure [4].

The heavy fermion superconductors that exhibit anti- ferromagnetism has their magnetic moments of atoms or molecules usually related to the spins of electrons aligned in a regular pattern with neighbouring spins on different lattices pointing in opposite directions [8]. The antiferromagnetic interaction can lead to multiple optimal states that is ground states of minimal energy. Further, magnetism and superconductivity are two states that are mutually exclusive and antagonistic which do not occur or coexist at the same temperature and place in a sample [3]. Researchers have been seen to cleave on a single property of a material to classify it as a heavy fermion, yet several properties are supposed to be unravelled to fully enable description of these heavy fermion materials which are currently inadequate.

A remarkable feature in Ce-based superconductors is the strong correlation between crystal structure and superconductivity. The fact that superconductivity can also be induced by the application of pressure indicates that crystal structure can be a key factor for the appearance of superconductivity [6].

Cerium based heavy fermion superconductors with Tc and crystal structure are given in table I

Table 1: Cerium based heavy fermion superconductors with T_C and crystal structure

Materials	$T_C(K)$	Crystal Structure
$CeCu_2Si_2$	0.6	bc tetragonal
$CePd_2Si_2$	0.43	bc tetragonal
$CeRh_2Si_2$	0.3	bc tetragonal
$CePt_3Si_2$	0.75	tetragonal

Heavy fermion superconductors with their thermodynamic property values adapted from Shailaj Kumar Shrivastava (2020) [4].

This research looked at the thermodynamic phase transition of singlet superconducting electron – hole coupling in heavy fermions where the hybrid Hamiltonian was developed and diagonalized by the BVT technique.

THEORETICAL FORMULATION

In this model, we consider a system that describes singlet superconducting electron-hole pairing of excitonic type that induces effective f-d hybridization. The total Hamiltonian will be expressed as.

$$H_T = \sum k,\sigma\{ \varepsilon_f(k)(f^+{}_{k\sigma} f_{k\sigma}) + \varepsilon_d(k)(d^+{}_{k\sigma} d_{k\sigma}) + V(f^+{}_{k\sigma} d_{k\sigma} + h.c) \} \quad (1)$$

$$H_T = \sum_{k\sigma}\left\{\varepsilon_f(k)(f^+_{k\sigma} f_{k\sigma} + f^+_{-k\sigma} f_{-k\sigma}) + \varepsilon_d(d)(d^+_{k\sigma} d_{k\sigma} + d^+_{-k\sigma} d_{-k\sigma}) + \sum_{k,\sigma}\{V(f_{k\sigma} b_{-k\sigma} - f_{-k\sigma} b_{k\sigma} + f^+_{-k\sigma} b^+_{k\sigma} - f^+_{k\sigma} b^+_{-k\sigma})\}\right\} \quad (2)$$

Applying BVT technique equation (2) yields

$$H_T = \sum_{k\sigma}\{2\varepsilon_f v_k^2 + (u_k^2 - v_k^2)(m_k + m_{-k}) + 2u_k v_k(\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k}\gamma_k)\} + \sum_{k\sigma} \varepsilon_d \left[2v_k^2 + (u_k^2 - v_k^2)\left((n_k + n_{-k}) + 2u_k v_k(b_k^+ b_{-k}^+ + b_{-k} b_k)\right)\right] + \sum_{k\sigma} V_{k\sigma}(2v_k^2 - 2u_k^2)(\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k}\gamma_k) + 4V u_k v_k(m_k + m_{-k} - 1). \quad (3)$$

The values of u_k and v_k that diagonalize the Hamiltonian in (3) are found to be $u_k = 0.46$ and $v_k = 1.10$.

Hence

$$E_o = 0.42\, \varepsilon_f + 0.42\varepsilon_d - 2.02V_{k\sigma} \quad (4)$$

If the d- bands are too narrow, then for the cerium –based silicon heavy Fermion compounds have: □□ = □□ = 1 □□□ and the f-d hybridization V = -4 □□□ [14]. From which we estimate $E_o = 0.0089eV$. The total energy of the system is obtained by introducing the thermal activation factor thus.

$$E_T = 8.943 \times 10^{-3} e^{-\frac{1.036}{T}} \quad (5)$$

Energy of the system

The total energy of a system results from the coupling between the electrons and holes of system. The energy due to this coupling increases as the temperature increases. The results obtained are shown in Figure **1.0**

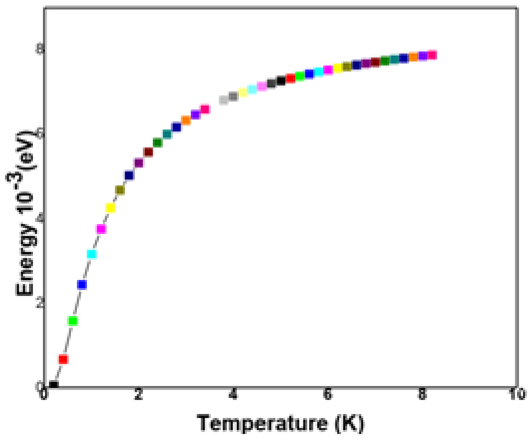


Figure **1.0:** Energy versus temperature

In Figure **1.0**, it is observed that at T= 0, E = 0 and this is consistent with the nature of the super-fluid system. In Figure **1.0**, it is observed that at T= 0, E = 0 and this is consistent with the nature of the super-fluid system. As the temperature increases, the magnitude of the superconducting gap decreases slowly at low temperatures but decreases rapidly near T_c. The temperature-dependent feature in both the gaps was qualitatively described by a two-band BCS model with interband interactions. The gap energy disappears when the temperature rises above the critical temperature and the superconductor changes into an ordinary material.

Thus, at finite temperatures, thermal conductivity for the superconductor is very small (see Fig. 1.0), since only the excited quasiparticles of the electron-hole pairs can contribute to thermal conductivity. The low thermal conductivity of superconductors for $T < Tc$, can be utilized in a low temperature heat switch.

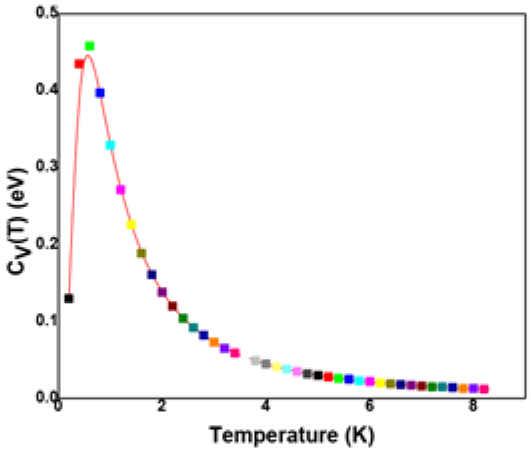
Specific heat capacity of the system

$$\mathrm{C_V} = \frac{\mathrm{dE_T}}{\mathrm{dT}} = \frac{(\mathrm{E_o})^2}{\mathrm{K_B T^2}} \mathrm{e}^{-\frac{\mathrm{E_o}}{\mathrm{K_B T}}} = \frac{0.927}{\mathrm{T^2}} \mathrm{e}^{-\frac{(1.036)}{\mathrm{T}}}$$

The temperature T_C can be interpreted as the temperature of dissociation of electron-hole pairs.

The temperature dependence of the specific heat of these compounds well below T_C is an indication of the unconventional superconductivity.

The specific heat increases with an increase in temperature up to a point when $T = Tc = 0.59K$ which is a point observed to give a sharp turning point of the curve.There is a maximum in Cv at $Tc = 0.59K$, suggesting a phase transition.This is a point where the system is very unstable and the 2nd order phase transition from the normal metal to a superconducting state is much like the superfluid state. Further, it is at this point ($Tc = 0.59K$) when more electron – hole pairs are formed thus causing a phase transition.



Assmus *et al.,* (1984) while investigating superconductivity in CeCu2Si_2 single crystals obtained heat capacity as $0.9\mathrm{J/mol.K}$ at $T_C = 0.6K$. The results are in good agreement with results obtained by other researchers [9].

CONCLUSION

The tetragonal crystal structure favors the electron -hole pairing mechanism as explained in this study. The silicon compounds transition temperature was determined, and the results agree with the experimental results obtained for tetragonal crystal structures as seen in table 1. The unusual magnetic and the gap structure were not considered.

The complicated crystal structures, unusual magnetic and superconducting transition, co-existence of superconductivity and antiferromagnetism, appearance of superconductivity at quantum critical point and the gap structure indicate that pairing mechanism is still a difficult problem in heavy fermion superconductors.

ACKNOWLEDGEMENTS

The authors would like to express their gratitude to Bomet University College and Kibabii University for the opportunity and enabling environment to conduct this research.

REFERENCES

1.Fil, D. V., & Shevchenko, S. I. (2018). Electron-hole superconductivity. *Low Temperature Physics, 44*(9), 867-909.

2. Fujimori, S. I. (2016). Band structures of 4f and 5f materials studied by angle-resolved photoelectron spectroscopy Journal of Physics: Condensed Matter. *Journal of Physics: Condensed Matter, 28*(15), 153002.

3. Negussie, T. (2019). Coexistence of Superconductivity and Anti-ferromagnetism in Heavy

Fermion ceptin11 superconductor. *The African Review of Physics*, 14.

4. Shrivastava, S. K. (2017). Search for higher critical temperature (Tc) in superconducting materials. *Journal Home page: http://www. ijmra. us, 5*(8).

5. Beille, J., Maple, M. B., Wittig, J., Fisk, Z., & DeLong, L. E. (1983). Suppression of the energy gap in Sm B 6 under pressure. *Physical Review B,,28*(12), 7397.

6. Lozovik, Y. E., & Yudson, V. I. (1976). A new mechanism for superconductivity: pairing between spatially separated electrons and holes. *Zh. Eksp. iTeor. Fiz, 71*, 738-753.

7. Dolgov, O. V., Fetisov, E. P., Khomskii, D. I., & Svozil, K. (1987). Model of interband pairing in mixed valence and heavy fermion systems. *Zeitschrift für Physik B Condensed Matter, 67*(1), 63-68.

8. Falkowski, M., & Strydom, A. M. (2017). A new ternary magnetically ordered heavy fermion compound Pr2Rh3Ge: magnetic, electronic and thermodynamic properties. *Journal of Physics: Condensed Matter, 29*(39), 395601.

9. Kibe, H. E., Sakwa, T. W., & Khanna, K. M. (2017). Thermodynamics Of S-Wave Pairing in Uranium and Cerium Based Heavy Fermion Compounds. *journal of multidisciplinary engineering science and technology (JMEST), 4*(8), 7950-7955.