Coexistence of Superconductivity and Anti-ferromagnetism in Heavy FermionCe_3PtIn_{11}Superconductor

Tamiru Negussie

Department of Physics, College of Natural & Computational Science, Debre Markos University, Ethiopia.

email: abeneyb@gmail.com

This work focuses on the theoretical investigation of the possible coexistence of superconductivity and anti-ferromagnetism in Ce_3PtIn_{11} superconductor. By developing a model Hamiltonian for the system under consideration, by employing double time temperature dependent Green's function formalism and by applying a suitable decoupling approximation technique, the possible coexistence of superconductivity and anti-ferromagnetism in Ce_3PtIn_{11} superconductor has been shown to be a very distinct possibility. The phase diagrams of superconducting gap parameter (Δ) versus temperature (T), the superconducting transition temperature T_C and anti-ferromagnetism order temperature T_N versus antiferromagnetic order parameter η are plotted. Finally, by combining the two phase-diagrams, the possible coexistence of superconductivity and anti-ferromagnetismin Ce_3PtIn_{11} superconductor is demonstrated. Our finding is in agreement with the experimental observations.

1. Introduction

Superconductivity was first observed by H. K. Onnes [1] and after the discovery of superconductivity, many other materials were subsequently observed in the superconducting state. Many investigations were made to understand how superconductors behave. Through times, many alloys were also found to show superconductivity at higher transition temperatures. The transition of a normal metal into the superconducting state was revealed by the total disappearance of the electrical resistance at low temperature, which subsequently results in the continuous flow of electric currents for a long period of time without decay.

In materials that exhibit anti-ferromagnetism, the magnetic moments of atoms or molecules, usually related to the spins of electrons, align in a regular pattern with neighboring spins (on different sub-lattices) pointing in opposite directions. Generally, antiferromagnetic orders may exist at sufficiently low temperatures, vanishing at and above a certain temperature known as the Neel temperature (T_N). Above the Neel temperature, the material is typically in a paramagnetic state. When no external field is applied, the antiferromagnetic structure corresponds to a vanishing of total magnetization.

In an external magnetic field, a kind of ferromagnetic behavior may be displayed in the antiferromagnetic phase, with the absolute value of one of the sub-lattice magnetizations differing from that of the other sub-lattice resulting in a nonzero net magnetization. Unlike ferromagnetism, antiferromagnetic interactions can lead to multiple optimal states (ground states of minimal energy).

In one dimension, the antiferromagnetic ground state is an alternating series of spin up and down. Since the discovery of superconductivity (SC) the effects of magnetic impurities and the possibility of magnetic ordering in superconductors have been a central topic of condensed matter physics. Due to strong spin scattering, it has generally been believed that, the conduction electrons cannot be both magnetically ordered and superconducting [2, 3]. Even though it is thought that Cooper pairs incuprate, heavy fermions, and iron-based superconductors are mediated by spin fluctuations [4- 6], superconductivity generally occurs after suppressing the magnetic order either through doping or the application of hydrostatic pressure [7, 8]. However, there is a growing evidence for the coexistence of superconductivity with either ferromagnetic (FM) [9, 10] or antiferromagnetic (AFM) order [11, 12].

The coexistence of superconductivity and magnetism has recently re-emerged as the central topic in condensed matter physics due to the competition between magnetic ordering and superconductivity, in some compounds. In general, these two states are mutually exclusive and antagonistic which do not coexist at the same temperature and place in a sample. The coexistence of superconductivity and magnetism was shown in the ternary rare earth compounds such as RMo_6X_8 type (where X = S, Se) [13]. McCallum [14] discovered the coexistence of superconductivity and long-range anti-ferromagnetism ordering in RMo_6S_8. Furthermore, Nagaraja [15] observed the coexistence of superconductivity and long-range anti-ferromagnetism in rare earth transition metal borocarbide system. The discovery of the coexistence of superconductivity and anti-ferromagnetism in a high-T_C (92K) superconductor $Gd_{1+x}Ba_{2-x}Cu_3O_{7-\delta}$ (with x = 0.2) for the first time has come as a big surprise [16].

Interplay of magnetism and superconductivity in heavy fermion materials is a remarkable issue. This interplay has shown considerable variety by showing competition, coexistence, and/or coupling of the magnetic and superconducting order parameters [17]. The 115 heavy-Fermion family, $CeMIn_5$,(where M= Co, Rh, Ir) has attracted interest due to the intricate relationship between anti-ferromagnetism and superconductivity that is found in them [18, 19]. The discovery of superconductivity in iron-based superconductors has sparked enormous interest in the scientific community. Although iron is the most known ferromagnet, iron-based superconductors exhibit antiferromagnetic ordering though superconductivity, which is induced after suppressing the anti-ferromagntic ordering. Despite this, superconductivity can coexist with either remaining antiferromagnetic ordering [20] or new ferromagnetic ordering [21] and this provides an ideal platform for studying the interplay between superconductivity and magnetism.

2. Model System Hamiltonian

The system under consideration consists of conduction electrons and localized electrons, between which exchange interaction exists. Thus, the Hamiltonian of the system can be written as

$$\hat{H} = \sum_{k\sigma} E_k a^+_{k\sigma} a_{k\sigma} + \sum_{\sigma l} E_l b^+_{l\sigma} b_{l\sigma} - \sum_{kk'} V_{kk'} a^+_{k\uparrow} a^+_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow} + \sum_{klm} \Omega^{lm}_k a^+_{k\uparrow} a^+_{-k\downarrow} b_{l\downarrow} b_{m\uparrow} + hc \quad (1)$$

Where, the first and second terms are the energy of conduction electrons and localized electrons respectively, the third term is the interaction (electron-electron) BCS type electron-electron pairing via bosonic exchange, and the last term represents the interaction term between conduction electrons and localized electrons with a coupling constant Ω^{lm}_k. $V_{k,k'}$ defines the matrix element of the interaction potential, $a^+_{k\sigma}(a_{k\sigma})$ are the creation (annihilation) operators of an electron specified by the wave vector, k and spin, σ. E_k is the one electron energy and measured relative to the chemical potential, where μ. $b^+_l(b_l)$ represents creation (annihilation) operators of the localized electrons of localized energy E_l.

3. Conduction Electrons

In order to obtain the self-consistent expression for the superconducting order parameter (Δ) and superconducting transition temperature (T_C), we derived the equation of motion using the Hamiltonian given in Eqn. (1) and the Green's function formalism [22] and obtained,

$$(\omega - E_k)\langle\langle a_{k\uparrow}, a^+_{\downarrow}\rangle\rangle = 1 - (\Delta - \eta)\langle\langle a^+_{-k\downarrow}, a^+_{k\uparrow}\rangle\rangle, \quad (2)$$

The equation of motion for the higher order Green's function correlation can be also derived and obtained to be,

$$\omega\langle\langle a^+_{-k\downarrow}, a^+_{k\uparrow}\rangle\rangle = -E_{-k}\langle\langle a^+_{-k\uparrow}, a^+_{k\downarrow}\rangle\rangle - \sum_p V\langle a^+_{p\downarrow}, a^+_{-p\uparrow}\rangle\langle\langle a_{k\downarrow}, a^+_{k\uparrow}\rangle\rangle + \sum_{klm}\Omega^{lm}_k\langle b^+_{l\downarrow} b^+_{m\uparrow}\rangle\langle\langle a_{k\downarrow}, a^+_{k\uparrow}\rangle\rangle \quad (3)$$

For $E_k = E_{-k}$, $\Delta = \Delta^*$, *and* $\eta = \eta^*$ (assuming that the order parameters are real), we get,

$$(\omega + E_k)\langle\langle a^+_{-k\downarrow}, a^+_{k\uparrow}\rangle\rangle = -(\Delta - \eta)\langle\langle a_{k\downarrow}, a^+_{k\uparrow}\rangle\rangle \tag{4}$$

Where, $\Delta = V\sum_{k'}\langle a_{-k'\downarrow}, a_{k'\uparrow}\rangle$ and $\eta = \sum_{klm}\Omega_k^{lm}\langle b_{l\downarrow}, b_{m\uparrow}\rangle$

Now using Eqns. (2) and (4), we get,

$$\langle\langle a_{k\uparrow}, a^+_{k\uparrow}\rangle\rangle = \frac{(\omega + E_k)}{\left(\omega^2 - E_k^2 - (\Delta - \eta)^2\right)} \tag{5}$$

$$\langle\langle a^+_{-k\downarrow}, a^+_{k\uparrow}\rangle\rangle = \frac{-(\Delta - \eta)}{\left(\omega^2 - E_k^2 - (\Delta - \eta)^2\right)} \tag{6}$$

Now, using the relation, $\Delta = \frac{V}{\beta}\sum_k \langle\langle a^+_{-k\downarrow}, a^+_{k\uparrow}\rangle\rangle$, the summation with respect to k extends over all allowed pair states, where, $\beta = \frac{1}{k_B T}$.

Thus we get,

$$\Delta = -\frac{1}{\beta}\sum_n \int_{-\varepsilon_F}^{\infty} dE\, N(0)V\left[\frac{\Delta - \eta}{\omega^2 - E_k^2 - (\Delta - \eta)^2}\right]$$

Attractive interaction is effective for the region $-\hbar\omega_b \langle E \langle \hbar\omega_b$ and assuming the density of states does not vary over this integral, we get,

$$\Delta = -\frac{2}{\beta}N(0)V\sum_k \int_0^{\hbar\omega_b} dE\left[\frac{\Delta - \eta}{\omega^2 - E_k^2 - (\Delta - \eta)^2}\right]. \tag{7}$$

For $N(0)V = \lambda$, Eqn. (7) becomes,

$$(\Delta - \eta) = 2\hbar\omega_b \exp\left[-\frac{1}{\lambda(1 - \frac{\eta}{\Delta})}\right] \tag{8}$$

For $\eta = 0$, Eqn. (8) reduces to the well known BCS model.

If we use the value of $\Delta(0)$ at T = 0, we get,

$$2\Delta(0) = 3.5 k_B T_C. \tag{9}$$

For Ce_3PtIn_{11}, $T_C = 0.32$K, [23],

Thus, we obtain, $\Delta(0) = 7.7X10^{-24}$.

Furthermore, using Eqns. (8) and (9), we get

$$\eta \approx 1.75 k_B T_C - 2\hbar\omega_b \exp\left[-\frac{1}{\lambda(1 - \frac{\eta}{1.75 k_B T_c})}\right]. \tag{10}$$

4. Localized Electrons

Now, using double time temperature dependent Green's functions formalism, we can derive the equation of motion for the localized electrons and obtained,

$$\omega\langle\langle b_{l\uparrow}, b^+_{l\uparrow}\rangle\rangle = 1 + E_l\langle\langle b_{l\uparrow}, b^+_{l\uparrow}\rangle\rangle + \sum_{klm}\Omega_k^{lm}\langle a_{-k\uparrow}a_{k\uparrow}\rangle\langle\langle b^+_{m\downarrow}, b^+_{l\uparrow}\rangle\rangle$$

$$\Rightarrow (\omega - E_l)\langle\langle b_{l\uparrow}, b^+_{l\uparrow}\rangle\rangle = 1 + \Delta_l\langle\langle b^+_{m\downarrow}, b^+_{l\uparrow}\rangle\rangle$$

From which we get,

$$\langle\langle b_{l\uparrow}, b^+_{l\uparrow}\rangle\rangle = \frac{1}{(\omega - E_l)} + \frac{\Delta_l}{(\omega - E_l)}\langle\langle b^+_{m\downarrow}, b^+_{l\uparrow}\rangle\rangle, \tag{11}$$

Where, $\Delta_l = \sum_{klm}\Omega_k^{lm}\langle a_{-k\uparrow}a_{k\uparrow}\rangle$.

Similarly, the equation of motion for the higher order Green's function is obtained as

$$\omega\langle\langle b^+_{m\downarrow}, b^+_{l\uparrow}\rangle\rangle = -E_l \langle\langle b^+_{m\downarrow}, b^+_{l\uparrow}\rangle\rangle + \sum_{klm}\Omega_k^{lm}\langle a^+_{k\uparrow}a^+_{-k\uparrow}\rangle\langle\langle b_{l\uparrow}, b^+_{l\uparrow}$$

$$\Rightarrow \langle\langle b^+_{m\downarrow}, b^+_{l\uparrow}\rangle\rangle = \frac{\Delta_l}{(\omega + E_l)}\langle\langle b_{l\uparrow}, b^+_{l\uparrow}\rangle\rangle \tag{12}$$

where $\Delta_l^* = \sum_{klm}\Omega_k^{lm}\langle a^+_{k\uparrow}a^+_{-k\downarrow}\rangle$.

Now combining Eqns. (11) and (12), we get,

$$\langle\langle b^+_{m\downarrow}, b^+_{l\uparrow}\rangle\rangle = \frac{\Delta_l}{\omega^2 - E_l^2 - \Delta_l^2}, \tag{13}$$

and

$$\langle\langle b_{l\uparrow}, b_{l\uparrow}^{+}\rangle\rangle = \frac{(\omega + E_l)}{\omega^2 - E_l^2 - \Delta_l^2} \quad . \tag{14}$$

5. Equation of Motion demonstrates the Correlation between Conduction and Localized electrons

The equation of motion which shows the correlation between the conduction and localized electrons can be demonstrated by using a similar definition as above.The relation for the magnetic order parameter(η) is given by,

$$\eta = \frac{\Omega}{\beta}\sum_{lm}\langle\langle b_{l\uparrow}^{+}, b_{m\downarrow}^{+}\rangle\rangle \tag{15}$$

Now using Eqn. (12) in Eqn. (14) we get,

$$\eta = \frac{\Omega}{\beta}\sum_{l}\frac{\Delta_l}{\omega^2 - E_l^2 - \Delta_l^2} \tag{16}$$

The summation in Eqn. (16) may be changed into an integral by introducing the density of states at the fermilevel, N(0)and obtain,

$$\eta = -\frac{\Omega}{\beta}\sum_{l}\int_{-\varepsilon_F}^{\infty} dEN(0)\left[\frac{\Delta_l}{\omega^2 - E_l^2 - \Delta_l^2}\right] \tag{17}$$

For effective attractive interaction region and assuming the density of state is constant, eq. (17) becomes,

$$\eta = -\frac{2}{\beta}N(0)\Omega\sum_{l}\int_{0}^{\hbar\omega_b} dE\left[\frac{\Delta_l}{\omega^2 - E_l^2 - \Delta_l^2}\right]. \tag{18}$$

Let $N(0)\Omega = \lambda_l$,

Hence, we get,

$$\eta = \lambda_l\int_{0}^{\hbar\omega_b} dE\,\frac{|\Delta_l|}{\sqrt{E_l^2 + \Delta_l^2}}\tanh\left(\frac{\beta(E_l^2 + \Delta_l^2)^{\frac{1}{2}}}{2}\right). \tag{19}$$

Since Δ_l is very small, Eqn. (19) becomes,

$$\eta = -\lambda_l\Delta_l \ln 1.14\frac{\hbar\omega_b}{k_B T_N},$$

Thus, the antiferr magnetic order temperature (T_N) is given by,

$$T_N = \frac{1.14}{k_B}\hbar\omega_b \exp\left(\frac{\eta}{\lambda_l\Delta_l}\right). \tag{20}$$

6. Pure Superconducting System

For pure superconducting system, i.e., for $\eta = 0$, Eqn. (10) gives an expression similar to the BCS model given by, $\frac{1}{\lambda} = \ln 1.14\frac{\hbar\omega_b}{k_B T_c}$,

From which we get,

$$k_B T_c = 1.14\hbar\omega_b \exp\left(-\frac{1}{\lambda}\right). \tag{21}$$

But from the BCS model, at $T = T_c$,

$\frac{1}{\lambda} = 1.14\frac{\hbar\omega_D}{k_B T_c}$ and assuming $\omega_b = \omega_D$, we get,

$$\Delta(T) = 3.06k_B T_c\left(1 - \frac{T}{T_c}\right)^{\frac{1}{2}}. \tag{22}$$

7. Results and Discussion

Using the model Hamiltonian we developed and the double time temperature dependent Green's function formalism, we obtain expressions for superconducting order parameter Δ, antiferromagnetic order parameter η , superconducting transition temperature T_C and anti-ferromagnetic order temperature T_N. The expression we obtained for pure superconductor when magnetic effect is zero η = 0), is in agreement with the BCS model. Now using Eqn. (22), the experimental value, T_C = 0.32K,for Ce_3PtIn_{11}[23]and considering some plausible approximations, we plotted the phase diagram of Δ versus T_C as shown in figure 1. It can be easily seen that the superconducting order parameter decreases with increasing temperature until it vanishes at the superconducting transition temperature T_C.

Similarly, by employing Eqn. (10), the phase diagram of T_C versus η is plotted as depicted in Fig. 2. Furthermore, the Phase diagram of T_N versus η is plotted by using Eqn. (20) as shown in figure3. Now by merging figures 2& 3, the possible coexistence of superconductivity and anti-ferromagnetism in $Ce_3PtIn_{11}$is demonstrated as shown in Fig. 4.

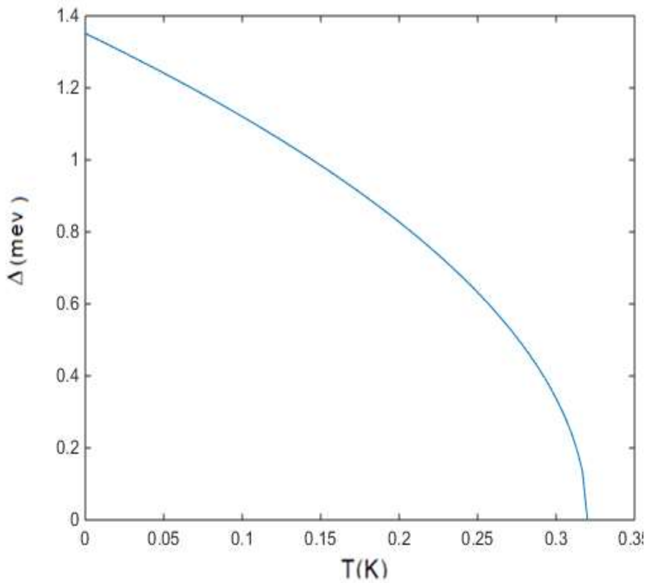

Fig. 1. Superconducting order parameter Δ versus temperature for the Ce_3PtIn_{11}Superconductor

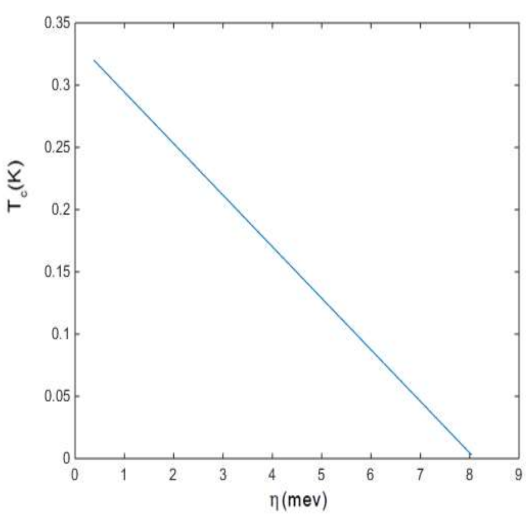

Fig. 2. Superconducting transition temperature (T_c) versus magnetic order parameter (η) for the Ce_3PtIn_{11} superconductor

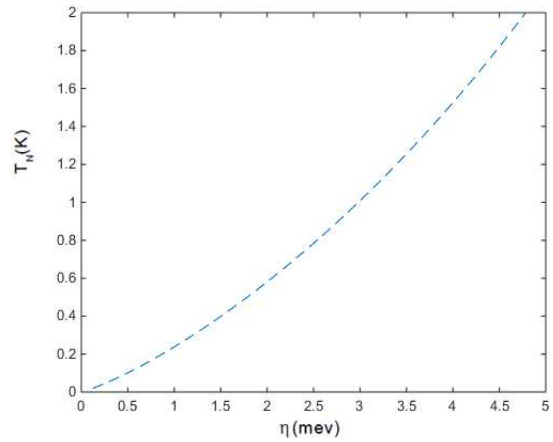

Fig.3. Antiferromagnetic order temperature T_N versus magnetic order parameter η for the Ce_3PtIn_{11} superconductor

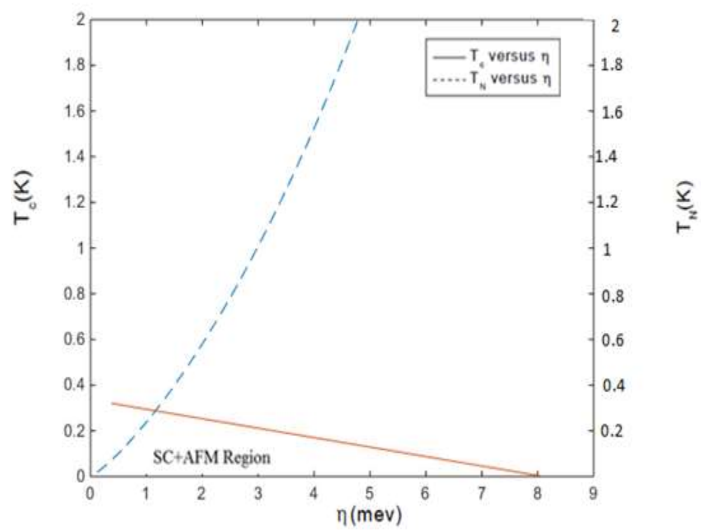

Fig.4. Coexistence of Superconductivity and Antiferromagnetism in Ce_3PtIn_{11} Superconductor

From fig. 4, it can be seen that, T_C decreases with increasing η, whereas T_N increases with increasing η and there is a common region where both superconductivity and anti-ferromagnetism co-exist in Ce_3PtIn_{11}.

8. Conclusion

In the present work, we have demonstrated the basic concepts of superconductivity with special emphasis on the interplay between superconductivity and anti-ferromagnetism closely connected to the superconducting Ce_3PtIn_{11}. Employing the double time temperature dependent Green's functions formalism, we developed the Model Hamiltonian for the system and derived equations of motion for conduction electrons, localized electrons and for pure superconducting system.

We carried out various correlations by using suitable decoupling procedures. In developing the Model Hamiltonian, we considered spin triplet pairing mechanism and obtained expressions for superconducting order parameter, antiferromagnetic order parameter, superconducting transition temperature and anti-ferrmagnetic order temperature. By using appropriate experimental values and considering suitable approximations, we plotted figures using the equations developed.

As is well known, superconductivity and anti-ferromagnetism are two cooperative phenomena, which are mutually antagonistic since superconductivity is associated with the pairing of electron states related to time reversal while in the magnetic states the time reversal symmetry is lost. Because of this, there is strong competition between the two phases. This competition between superconductivity and magnetism made coexistence unlikely to occur. However, the model we employed in this work, shows that, there is a common region where both superconductivity and anti-ferromagnetism can possibly coexist in superconducting Ce_3PtIn_{11}.The result we obtained in our current research work is in agreement with experimental findings [23].

References

[1] Onnes, K. H., Akad. Weten Schappen (Amsterdam) **14**, 113, 1911

[2] Maple M. B., Superconductivity-a probe of the magnetic state of local moments in metals, Appl. Phys. (Berl) **9(3)**:179-204,1976

[3] Ginzburg V. L., Ferromagnetic superconductors, Sov. Phys. JETP **4**:153-161, 1957

[4] Mathur N. D., et al., Magnetically mediated superconductivity in heavy fermion compounds, Nature **394(6688)**:39-43, 1998

[5] Onufrieva F. and Pfeuty P., Low-doping anomalies in high-Tc cuprate superconductors as evidence of a spin-fluctuation-mediated superconducting state, Phys. Rev. Lett **109 (25)**:257001, 2012

[6] Chubukov A., Pairing mechanism in Fe-based superconductors, Annual Rev. Cond Matt Phys. **3**:57-92, 2012

[7] Heffner S et al. Two gaps make a high temperature superconductor, Rep Prog. Phys. **71(6)**, 062501, 2008

[8] Kamihara Y. et al, Iron-based layered superconductor LaO1−xFxFeAs (x = 0.05 -0.12) with Tc = 26 K, J Am Chem. Soc. **130(11)**: 3296-3297, 2008

[9] Fertig W. A., et al. Destruction of superconductivity at the onset of long-range magnetic order in the compound ErRh4B4, Phys. Rev. Lett **38(17)**:987-990, 1977

[10] Ishikawa M, Fischer, Destruction of superconductivity by magnetic ordering in $Ho_{1.2}Mo_6S_8$, Solid State Comm. **23(1)**:37-39, 1977

[11] Maple MB, Fischer, Magnetic superconductors. Superconductivity in Ternary Compounds II: Topics in Current Physics, eds. Maple M. B., Fischer (Springer, Berlin), **34**, pp 1-10, 1982

[12] Kenzelmann M. et al., Coupled superconducting and magnetic order in CeCoIn5, Science **321(5896)**:1652-1654, 2008

[13] Mathias, B.T., et al., Proc. Natl. Acad. Sci. **74**, 1334, 1977

[14] McCallum, R.W. et al., Phys. Rev. Lett. **38**, 987,1977

[15] Nagaraja, R., et al., Phys. Rev. Lett. **72**, 274, 1994

[16] Gebregziabher, K. and Singh, P, J Supercond. Nov. Magn. **29** (8), 2031–2034, 2016

[17] R. H. Heffner, J. Alloys and Compounds, **213-214**, 232, 1994

[18] J. D. Thompson and Z. Fisk, J. Phys. Soc. Jpn.**81**, 011002, 2012

[19] E. D. Bauer et al., Phys. Rev. B **81**, 180507, 2010

[20] J. L. Sarrao and J. D. Thompson, J. Phys. Soc. Jpn.**76**, 051013, 2007

[21] Ren Z, et al. Superconductivity induced by phosphorus doping and its coexistence with

ferromagnetism in $EuFe_2(As0.7P0.3)_2$, Phys. Rev. Lett **102 (13)** :137002,2009
[22] Zubarev, D. N, Double-time Green Functions in Statistical Physics, *Sov. Phys. Usp.* **3**, 320, 1960
[23] J. Prokleska, et al., Magnetism, superconductivity, and quantum criticality in the multisite cerium heavy-fermion compound Ce_3PtIn_{11}, Phys. Rev. B **92**, 161114(R), 2015

Received: 19 September, 2018

Accepted: 10 September, 2019