Research Article *http://dx.doi.org/10.4314/mejs.v16i2.1* ***Open Access***

Theoretical Investigation of the Coexistence between Superconductivity and Antiferromagnetism in Heavy Fermion $CeCu_2Si_2$ Superconductor

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ABSTRACT

The current research work has theoretically investigated the possible coexistence between superconductivity and antiferromagnetism in heavy fermion CeCu2Si2 superconductors. By developing a model Hamiltonian for the system under consideration, and by employing the double time-temperature dependent Green's function formalism, mathematical computations have been conducted, and phase diagrams of superconducting gap parameter (Δ) versus temperature (T), superconducting transition temperature (T_C) and antiferromagnetism order temperature (T_N) versus antiferromagnetic order parameter (η) have been plotted separately by using MATLAB script. Finally, the possible coexistence between superconductivity and antiferromagnetism in heavy fermion CeCu2Si2 superconductor has been demonstrated by combining the two-phase diagrams. The model we employed in this research shows a common region where superconductivity and antiferromagnetism can coexist in superconducting $CeCu_2Si_2$. The results we obtained in this work are compatible with previous findings.

Keywords: Superconductivity, Antiferromagnetism, Coexistence, Green function, $CeCu_2Si_2$, Superconducting order parameter.

1. INTRODUCTION

Heike Kamerlingh Onnes discovered superconductivity by measuring the electrical conductivity of metals and observed the abrupt disappearance of the resistance of solid mercury (Onnes, 1911). Subsequently, several superconductors have been discovered with increasing transition temperatures (T_C) and it is believed that room-temperature superconductors could be ultimately discovered. Prior to the discovery of unconventional superconductors such as $CeCu_2Si_2$ (Steglich et al., 1979) the properties of superconductors were treated within the context of the BCS theory (Bardeen et al., 1957). However, the discovery of superconductivity in $CeCu_2Si_2$ had brought a paradigm shift since the superconducting pairing mechanism of electrons is not related to the conventional phonon mediated type of pairing of electrons. Recently, a few Ce-based heavy fermion compounds have been discovered demonstrating the coexistence between superconductivity and antiferromagnetism.

Submitted: 30th September 2020 Accepted: 30th January 2024 Published: 14th September 2024

It is a well-known fact that superconductivity and magnetism are mutually exclusive due to their essentially different order states (Sinha and Kakani, 1989). Even though the superconducting transition temperatures of UGe_2 (Saxena et al., 2001), $ZrZn_2$ (Pfleiderer et al., 2001), URhGe (Aoki et al., 2001), UIr (Akazawa et al., 2004) and UCoGe (Huy et al., 2007) are very low, the discovery of superconductivity in a single crystal of these materials invigorated the interest in the coexistence between superconductivity and magnetism in the same homogenous system. The fascinating relationship between superconductivity and magnetic ordering has been a central issue in condensed matter physics for several decades. It has been generally believed that, within the context of the BCS theory, the conduction electrons cannot be both magnetic and superconducting simultaneously as they are two antagonistic entities. Even though the superconducting pairing in cuprates, heavy fermions, and iron-based superconductors is believed to be mediated by antiferromagnetic spin fluctuations (Maple, 1976; Ginzburg, 1957), superconductivity can be generally induced by suppressing the magnetic order with chemical doping or pressure (Mathur et al., 1998; Onufrieva and Pfeuty, 2012).

Condensed matter Physicists have conducted extensive research to understand the nature and properties of superconductors in general and high temperature heavy fermion superconductors in particular. Thus, through times, many heavy fermion alloys were discovered to manifest superconductivity at higher transition temperatures. In materials that exhibit antiferromagnetism, the magnetic moments of atoms or molecules are usually related to the spins of electrons and align in a regular pattern with neighboring spins pointing in opposite directions. Generally, antiferromagnetic orders may exist at sufficiently low temperatures, vanishing at and above the Neel temperature (T_N). When no external field is applied, the antiferromagnetic structure corresponds to a vanishing of the total magnetization. In an external magnetic field, a kind of ferrimagnetic behavior may be displayed in the antiferromagnetic phase with the absolute value of one of the sublattice magnetizations differing from that of the other sublattice resulting in a non-zero net magnetization. Unlike ferromagnetism, antiferromagnetic interactions can lead to multiple optimal states or ground states of minimal energy. In one dimension, the antiferromagnetic ground state is an alternating series of up and down spins. Since the discovery of superconductivity, 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 scatterings, it has generally been believed that the conduction electrons could not be both magnetically ordered and superconducting (Maple, 1976; Ginzburg, 1957). However, there is growing evidence for the coexistence between superconductivity with either ferromagnetic (Ishikawa and Fischer, 1977) or antiferromagnetic ordering (Maple and Fischer, 1982; Kenzelmann et al., 2008). Furthermore, the discovery of superconductivity in iron-based superconductors has sparked enormous interests in the scientific community. Although iron is the most well-known ferromagnet, iron-based superconductors exhibit antiferromagnetic ordering though superconductivity is induced after suppressing the antiferromagntic order. Despite this, superconductivity can coexist with either remaining antiferromagnetic order (Mathias et al., 1977) or new ferromagnetic order (Fertig et al., 1977) and this provides an ideal platform for studying the interplay between superconductivity and magnetism.

The coexistence between superconductivity and magnetism has recently reemerged as a central topic in condensed matter physics due to the competition between magnetic ordering and superconductivity in some compounds such as RMo_6X_8 type (where R = rare earth elements and X = S, Se). McCallum as cited in (Gebregziabher and Singh, 2016) discovered the coexistence between superconductivity and long-range antiferromagnetism ordering in RMo_6S_8. Moreover, the interplay between superconductivity and long-range antiferromagnetism in heavy fermion systems was observed by muon spin relaxation studies (Heffner, 1994). The discovery of the coexistence between superconductivity and antiferromagnetism in a high T_C superconductor $Gd_{1+x}Ba_{2-x}Cu_3O_{7-\delta}$ (with x = 0.2) was seen as a big surprise by condensed matter researchers (Thompson and Fisk, 2012).

The interplay between superconductivity and magnetism in heavy fermion superconductors has been considered as a remarkable phenomenon. This phenomenon has demonstrated considerable varieties by showing competition, coexistence, and/or coupling of the magnetic and superconducting order parameters (Bauer et al., 2010). The 115 heavy-Fermion family, $CeMIn_5$ (where M= Co, Rh, Ir) has attracted interest due to the intricate relationship that exists between antiferromagnetism and superconductivity (Steglich et al., 1979; Steglich et al., 1996). Theoretical investigations on the coexistence between superconductivity and magnetism has been shown in various heavy fermion superconductors (Tamiru and Gebregziabher, 2017; Tamiru and Gebregziabher, 2018; Tamiru, 2019). Since, the discovery of superconductivity in

$CeCu_2Si_2$ (Assmus et al., 1984), antiferromagnetic spin excitations have been proposed as a viable mechanism for superconductivity (Rauchschwalbe et al., 1982; Sarrao and Thompson, 2007; Ren et al., 2009).

Finally, as was stated above, the current work focuses on the theoretical investigation of the coexistence between superconductivity and antiferromagnetism in Ce-based heavy fermion $CeCu_2Si_2$ superconductors. The coexistence has been demonstrated by developing a model Hamiltonian for the systems and using double time temperature dependent Green's function formalism. Then by plotting phase diagrams, we demonstrated the required coexistence between superconductivity and antiferromagnetism in heavy fermion $CeCu_2Si_2$ superconductor.

2. MODEL SYSTEM HAMILTONIAN

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

$$\widehat{H}=\sum_{k\sigma}E_k a_{k\sigma}^{+}a_{k\sigma}+\sum_{\sigma l}E_\ell b_{\ell\sigma}^{+}b_{\ell\sigma}-\sum_{kk'}V_{kk'}a_{k\uparrow}^{+}a_{-k\downarrow}^{+}a_{k'\downarrow}a_{-k'\uparrow}+\sum_{k\ell m}\Omega_k^{\ell m}a_{k\uparrow}^{+}a_{-k\downarrow}^{+}b_{\ell\downarrow}b_{m\uparrow}+hc \tag{1}$$

Where, the first and second terms are the energy of conduction and localized electrons respectively, the third term is the BCS type electron-electron pairing via bosonic exchange and the last term represents the interaction term between conduction and localized electrons with a coupling constant $\Omega_k^{\ell m}$, $V_{kk'}$ denotes 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 kinetic energy measured relative to the chemical potential, μ . $b_\ell^{+}(b_\ell)$ are creation (annihilation) operators of the localized electrons of localized energy, E_ℓ , hc is to mean Hermitian conjugate of all the 4 terms used to define the Hamiltonian in equation (1) and its significance is seen in the sense that adding its own conjugate to an operator guarantees that the combination is Hermitian.

3. CONDUCTION ELECTRONS

In order to obtain a 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 equation (1) and the Green's function formalism (Zubarev, 1960) and obtained,

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

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

$$\omega\langle\langle a_{-k\downarrow}^{+}, a_{k\uparrow}^{+}\rangle\rangle = -E_{-k}\langle\langle a_{-k\uparrow}^{+}, a_{k\downarrow}^{+}\rangle\rangle - \sum_{p} V\langle a_{p\downarrow}^{+}, a_{-p\uparrow}^{+}\rangle\langle\langle a_{k\downarrow}, a_{k\uparrow}^{+}\rangle\rangle$$
$$+ \sum_{k\ell m}\Omega_{k}^{\ell m}\langle b_{\ell\downarrow}^{+} b_{m\uparrow}^{+}\rangle\langle\langle a_{k\downarrow}, a_{k\uparrow}^{+}\rangle\rangle \tag{3}$$

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 $\eta = \sum_{k\ell m}\Omega_{k}^{\ell m}\langle b_{\ell\downarrow}, b_{m\uparrow}\rangle$

From equations (2) and (4), we obtained,

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

and

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

Hence, using the relation, $\Delta^{*} = \frac{V}{\beta}\sum_{k}\langle\langle a_{-k\downarrow}^{+}, a_{k\uparrow}^{+}\rangle\rangle$, we got,

$$\Delta = -\frac{1}{\beta}\sum\int_{-\varepsilon_F}^{\infty} dE\, N(0)V\left[\frac{\Delta - \eta}{\omega^2 - E_k^2 - (\Delta - \eta)^2}\right], \text{ where, } \beta = 1/k_B T.$$

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

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

For $N(0)V = \lambda$, equation (7) becomes, $(\Delta - \eta) = 2\hbar\omega_b \exp\left[-\frac{1}{\lambda(1 - \frac{\eta}{\Delta})}\right]$ (8)

For $\eta = 0$, equation (8) reduces to the well known BCS model (Bardeen et al., 1957).

Now, if we use the value of $\Delta(0)$ at T = 0, we got, $\Delta(0) = 1.76\, k_B T_C$ (9)

For $CeCu_2Si_2$, $T_C =$ 0.6 K (Stockert et al., 2011). Thus, we get, $\Delta(0) = 1.45 * 10^{-23} J$.

Furthermore, using equations (8) and (9), we obtained,

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

4. LOCALIZED ELECTRONS

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

$$\omega\langle\langle b_{\ell\uparrow}, b^+_{\ell\uparrow}\rangle\rangle = 1 + E_\ell \langle\langle b_{\ell\uparrow}, b^+_{\ell\uparrow}\rangle\rangle + \sum_{k\ell m} \Omega_k^{\ell m} \langle a_{-k\uparrow} a_{k\uparrow}\rangle \langle\langle b^+_{m\downarrow}, b^+_{\ell\uparrow}\rangle\rangle$$

From which we got, $(\omega - E_\ell)\langle\langle b_{\ell\uparrow}, b^+_{\ell\uparrow}\rangle\rangle = 1 + \Delta_\ell \langle\langle b^+_{m\downarrow}, b^+_{\ell\uparrow}\rangle\rangle$

Thus, we have, $\langle\langle b_{\ell\uparrow}, b^+_{\ell\uparrow}\rangle\rangle = \frac{1}{(\omega - E_\ell)} + \frac{\Delta_\ell}{(\omega - E_\ell)} \langle\langle b^+_{m\downarrow}, b^+_{\ell\uparrow}\rangle\rangle,$ (11)

Where, $\Delta_\ell = \sum_{km} \Omega_k^{\ell m} \langle a_{-k\uparrow} a_{k\uparrow}\rangle$.

Similarly, by decoupling the higher order Green's function to lower order, we obtained the equation of motion to be,

$$\omega\langle\langle b^+_{m\downarrow}, b^+_{\ell\uparrow}\rangle\rangle = -E_\ell << b^+_{m\downarrow}, b^+_{\ell\uparrow}\rangle\rangle + \sum_{k\ell m} \Omega_k^{\ell m} \langle a^+_{k\uparrow} a^+_{-k\uparrow}\rangle \langle\langle b_{\ell\uparrow}, b^+_{\ell\uparrow}\rangle\rangle$$

From which we got $\langle\langle b^+_{m\downarrow}, b^+_{\ell\uparrow}\rangle\rangle = \frac{\Delta_\ell}{(\omega + E_\ell)} \langle\langle b_{\ell\uparrow}, b^+_{\ell\uparrow}\rangle\rangle$ (12)

Where, $\Delta^*_\ell = \sum_{km} \Omega_k^{\ell m} \langle a^+_{k\uparrow} a^+_{-k\downarrow}\rangle$. Now, using equations (11) and (12), we obtained,

$$\langle\langle b^+_{m\downarrow}, b^+_{\ell\uparrow}\rangle\rangle = \frac{\Delta_\ell}{\omega^2 - E_\ell^2 - \Delta_\ell^2} \quad (13)$$

and

$$\langle\langle b_{\ell\uparrow}, b^+_{\ell\uparrow}\rangle\rangle = \frac{(\omega + E_\ell)}{\omega^2 - E_\ell^2 - \Delta_\ell^2} \quad . \quad (14)$$

5. EQUATION OF MOTION WHICH DEPICTS 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 procedure as above.Thus, the expression for the magnetic order parameter (η) is given by,

$$\eta = \frac{\Omega}{\beta}\sum_{\ell m}\langle\langle b^{+}_{\ell\uparrow}, b^{+}_{m\downarrow}\rangle\rangle \tag{15}$$

Using eqution (13) in equation (15) we got,

$$\eta = \frac{\Omega}{\beta}\sum_{\ell}\frac{\Delta_{\ell}}{\omega^2 - E_{\ell}^2 - \Delta_{\ell}^2} \tag{16}$$

The summation in equation (16) may be changed into an integration by introducing the density of state at the fermi level, N(0) and obtained,

$$\eta = -\frac{\Omega}{\beta}\sum_{\ell}\int_{-\varepsilon_F}^{\infty} dE N(0)\left[\frac{\Delta_{\ell}}{\omega^2 - E_{\ell}^2 - \Delta_{\ell}^2}\right] \tag{17}$$

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

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

Let $N(0)\Omega = \lambda_{\ell}$. Hence, we got,

$$\eta = \lambda_l \int_0^{\hbar\omega_b} dE\left[\frac{|\Delta_l|}{\sqrt{E_l^2 + \Delta_l^2}}\tanh\left(\frac{\beta\left(E_l^2 + \Delta_l^2\right)^{\frac{1}{2}}}{2}\right)\right] \tag{19}$$

Since, Δ_{ℓ} is very small, equation (19) becomes, $\eta = -\lambda_{\ell}\Delta_{\ell}\ln 1.14\frac{\hbar\omega_b}{k_B T_N}$.

Thus, the antiferrmagnetic order temperature (T_N) becomes, $T_N = \frac{1.14}{k_B}\hbar\omega_b\exp(\frac{\eta}{\lambda_{\ell}\Delta_{\ell}})$ (20)

6. PURE SUPERCONDUCTING SYSTEM

For pure superconducting system, that is, for $\eta = 0$, equation (10) gives an expression similar to the BCS model which is given by, $\frac{1}{\lambda} = \ln 1.14\frac{\hbar\omega_b}{k_B T_C}$. From which we obtained

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

Assuming $\omega_b = \omega_D$, obtained, $\frac{1}{\lambda} = 1.14(\frac{\hbar\omega_D}{k_B T_C})$.

Finally, we hav $\Delta(T) = 3.06 k_B T_C (1-\frac{T}{T_C})^{1/2}$ (22)

7. RESULTS AND DISCUSSION

Using the model Hamiltonian, we developed and the double time temperature dependent Green's function technique, we obtained expressions for superconducting order parameter (Δ) , antiferromagnetic order parameter (η), superconducting transition temperature (T_C) and antiferromagnetic order temperature (T_N). The expression we obtained for pure superconductor that is, when magnetic effect is zero ($\eta = 0$), is in good agreement with the BCS model (Bardeen et al., 1957). Now, using equation (22), the experimental value, T_C =0.6 K, for $CeCu_2Si_2$ (Stockert et al., 2011) and considering some plausible approximations, we plotted the phase diagram of Δ versus T as shown in figure 1A.

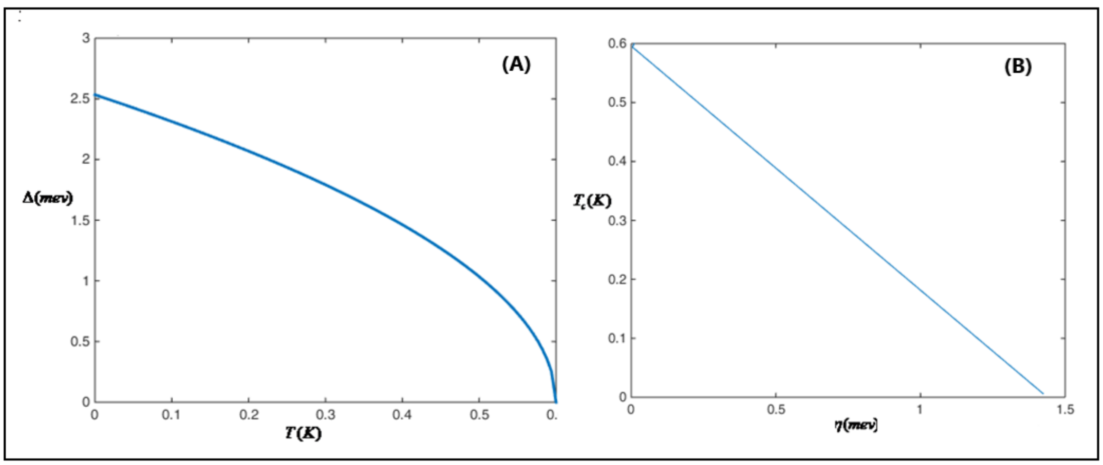

Figure 1. (A) Superconducting order parameter (Δ) versus temperature for $CeCu_2Si_2$ superconductor; (B) Superconducting transition temperature (T_C) versus magnetic order parameter (η) for the $CeCu_2Si_2$ superconductor.

It can be easily seen from the figure that, the superconducting order parameter decreases as temperature increases and vanishes at the transition temperature (T_C) of $CeCu_2Si_2$ as Cooper pairs break there and a change from a superconducting state to a normal state occurs (Stockert et al., 2011). Similarly, by employing equation (10), the phase diagram of T_C versus η is plotted as depicted in figure 1B. From the figure, it can be observed that, magnetism has a suppression effect on superconductivity.

Furthermore, the Phase diagram of T_N versus η is plotted by using equation (20) as shown in figure 2A. The figure shows that the magnetic ordering parameter supports the Neel temperature. Now, by merging figures 1B and 2A, the coexistence between superconductivity and antiferromagnetism in $CeCu_2Si_2$ has been demonstrated in figure 2B.

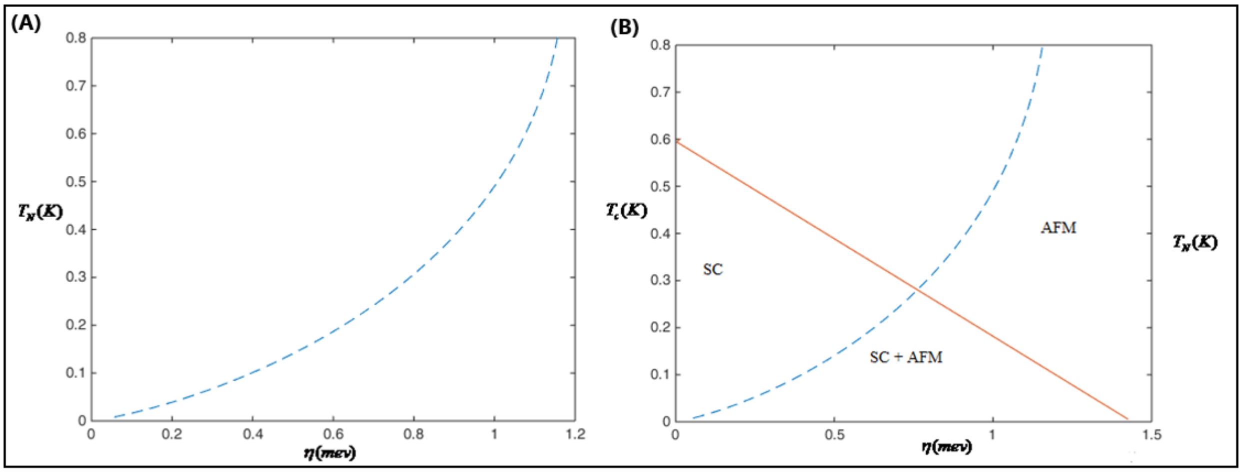

Figure 2. (A) Antiferromagnetic order temperature (T_N) versus magnetic order parameter (η) for the CeCu2Si$_2$ superconductor; (B) Coexistence between superconductivity and antiferromagnetism in $CeCu_2Si_2$ superconductor.

From figure 2B, it can be observed that, T_C decreases with increasing the magnetic order parameter (η), whereas T_N increases with increasing η and there is a common region where both superconductivity and antiferromagnetism coexist in $CeCu_2Si_2$ superconductor.

8. CONCLUSION

In the present work, we have demonstrated the basic concepts of superconductivity with special emphasis on the coexistence between superconductivity and antiferromagnetism which are closely connected to the heavy fermion $CeCu_2Si_2$ superconductor. Employing the double time temperature dependent Green's functions formalism, we developed a model Hamiltonian for the system and derived equations of motion for conduction electrons, localized electrons and for pure superconducting system and carried out various correlations by using suitable decoupling procedures. In developing the model Hamiltonian, we considered spin triplet pairing mechanism and obtained expressions for the superconducting order parameter, antiferromagnetic order parameter, superconducting transition temperature and antiferromagnetic order temperature. By using appropriate experimental values and considering suitable approximations, we plotted figures using the equations we developed.

As is well known, superconductivity and antiferromagnetism 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, demonstrates that, there is a common region where both superconductivity and antiferromagnetism can possibly coexist in superconducting $CeCu_2Si_2$. The results we obtained in this research work agree with the experimental findings of Stockert et al. (2011).

9. ACKNOWLEDGEMENTS

The authors would like to express their gratitude to the Department of Physics of Bahir Dar University for the material support it provided for the research work.

10. CONFLICT OF INTERESTS

No conflict of interest.

11. REFERENCE

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