International Journal of Scientific Engineering and Technology
Volume No. 7, Issue No. 2, PP: 25-30

ISSN: 2277-1581
1 Feb. 2018

Study of Coexistence of Superconductivity and Antiferromagnetism in Superconducting Ce_2PdIn_8

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Abstract : Coexistence of Superconductivity and magnetism has always been the appealing area of interest for studying condensed-matter physics. Various current research efforts in strongly correlated systems focus on the interplay between magnetism and superconductivity. We report a study on the theoretical investigation of the coexistence of superconductivity and antiferromagnetism in Ce_2PdIn_8 superconductor. Hamiltonian model, double time temperature dependent Green's function formalism and a suitable decoupling approximation technique has been applying to show the coexistence of superconductivity and antiferromagnetism in Ce_2PdIn_8 superconductor. The phase diagrams of superconducting gap parameter (Δ) versus temperature (T), the superconducting transition temperature (T_C) and antiferromagnetism order temperature (T_N) versus antiferromagnetic order parameter (η) have been plotted. Finally, by combining the two phase diagrams, coexistence of superconductivity and antiferromagnetism in Ce_2PdIn_8 superconductor has been demonstrated. The model employed in this work, shows that, there is a common region where both superconductivity and antiferromagnetism can possibly coexist in superconducting Ce_2PdIn_8.

Key words: Superconductivity; Antiferromagnetism; Ce_2PdIn_8; Coexistence; Green function; Order parameter

Introduction

Superconductivity is a property whereby a material loses all resistance to the flow of electrons within it. Hence, a current, once started in a superconductor, will continue to flow indefinitely. This property was first discovered by Heike Kamerlingh Onnes in 1911 when he observed the resistance of a column of Mercury dropped to zero when cooled to about 4K [1].

In materials that exhibit antiferromagnetism, the magnetic moments of atoms or molecules, usually related to the spins of electrons, align in a regular pattern with neighboring spins (on different sublattices) 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 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 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 spins, up-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 in cuprates, 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 a 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 antiferromagnetism ordering in RMo_6S_8. Furthermore, Nagaraja [15] observed the coexistence of superconductivity and long-range antiferromagnetism in rare earth transition metal borocarbide system.

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 [16]. The 115 heavy-Fermion family $CeMIn_5$ has attracted interest due to the intricate relationship between antiferromagnetism and superconductivity that is found in them [17,18].

A new class of Ce - based heavy fermion materials with the formula $Ce_nT_mIn_{3n+2m}$ (T= transition metal; n=1, 2; m=0, 1) has recently been discovered [19]. These compounds display a variety of interesting phenomena including superconductivity (SC), antiferromagnetism (AFM), and superconductivity under pressure. The compound Ce_2PdIn_8 displays antiferromagnetic order below Neel temperature T_N= 10 K and become superconducting at T_C = 0.68 K [20].

1. Theoretical Model

To study the coexistence of antiferromagnetism and superconductivity in superconducting Ce_2PdIn_8 theoretically, systems of conduction electrons and localized electrons have been considered. The exchange interaction acts between the conduction and the localized electrons. Thus, within the frame work of the BCS model [21], we consider the Hamiltonian model as;

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_3 \qquad (1)$$

Which is written as;

$$\hat{H} = \sum_{k\sigma} E_k c^+_{k\sigma} c_{k\sigma} + \sum_{\sigma l} E_l b^+_{l\sigma} b_{l\sigma} - \sum_{kk'} V_{kk'} c^+_{k\uparrow} c^+_{-k\downarrow} c_{k'\downarrow} c_{-k'\uparrow} + \sum_{klm} \Omega^{lm}_k c^+_{k\uparrow} c^+_{-k\downarrow} b_{l\downarrow} b_{m\uparrow} + hc \qquad (2)$$

where the first and second terms of eq.(2) 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

And,

- $V_{kk'}$ defines the matrix element of the interaction potential, $c^+_{k\sigma}(c_{k\sigma})$ is the creation (annihilation) operators of an electron specified by the wave vector, k and spin, σ.
- E_k is the one electron energy measured relative to the chemical potential. $b_l^+ (b_l)$ are creation (annihilation) operators of the localized electrons of localized energy, E_l.

To compute the equation of motion for mobile electrons, we use the double-time temperature dependent Green's function [22], which is defined by:

$$G_r(t-t') \equiv \langle\langle \hat{A}(t); \hat{B}(t') \rangle\rangle \qquad (3)$$

Or $G_r(t,t') = -i\theta(t-t')\langle[\hat{A}(t), \hat{B}(t)]\rangle$

And we use $\omega G_r(\omega) = \langle[\hat{A}(t), \hat{B}(t')]\rangle_\omega + \langle\langle[\hat{A}(t), \hat{H}], \hat{B}(t')]\rangle\rangle_\omega$ (4)

2. 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 eq.(2) and the Green's function formalism[22] we have:

$$\omega\langle\langle \hat{c}_{k\uparrow}, \hat{c}^{\uparrow}_{k'\downarrow} \rangle\rangle_\omega = \delta_{kk'} + \langle\langle[\hat{c}_{k\uparrow}, \hat{H}_{BCS}]; \hat{c}^{\uparrow}_{k\uparrow} \rangle\rangle_\omega \qquad (5)$$

Applying elementary Commutation relation, computing the following:

$$[\hat{c}_{k\uparrow}, \hat{H}] = [\hat{c}_{k\uparrow}, \hat{H}_1] + [\hat{c}_{k\uparrow}, \hat{H}_2] + [\hat{c}_{k\uparrow}, \hat{H}_3] \qquad (6)$$

And the result is substituted in the equation of motion eq.(5) we get:

$$\omega \ll \hat{c}_{k\uparrow}, \hat{c}^+_{k\uparrow} \gg = 1 + \epsilon_k \ll \hat{c}_{k\uparrow}, \hat{c}^+_{k\uparrow} \gg - \sum_p V_{pk'} \ll \hat{c}^+_{-k\uparrow}\, \hat{c}_{-p\uparrow} \hat{c}_{p\uparrow} \hat{c}^+_{k\uparrow} \gg + \sum_{l,m} \alpha_{l,m} \ll \hat{c}^+_{-k\uparrow} \hat{b}_{l\uparrow} \hat{b}_{m\uparrow}, \hat{c}^+_{k\uparrow} \gg \qquad (7)$$

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

$$\omega\langle\langle c^+_{-k\downarrow}, c^+_{k\uparrow}\rangle\rangle = -\varepsilon_{-k}\langle\langle c^+_{-k\uparrow}, c^+_{k\downarrow}\rangle\rangle - \sum_p v\langle c^+_{p\downarrow}, c^+_{-p\uparrow}\rangle\langle\langle c_{k\downarrow}, c^+_{k\uparrow}\rangle\rangle + \sum_{klm}\Omega^{lm}_k\langle b^+_{l\downarrow} b^+_{m\uparrow}\rangle\langle\langle c_{k\downarrow}, c^+_{k\uparrow}\rangle\rangle$$

(8)

The higher order Green's function is written into lower order Green's function by using Wick's theorem. Thus, we have,

$$(\omega - \varepsilon_k)\langle\langle c_{k\uparrow}, c^+_{\downarrow}\rangle\rangle = 1 - (\Delta - \eta)\langle\langle c^+_{-k\downarrow}, c^+_{k\uparrow}\rangle\rangle \quad (9)$$

For real order parameters: $\varepsilon_k = \varepsilon_{-k}$, $\Delta = \Delta^*$, and $\eta = \eta^*$, we get,

$$(\omega + \varepsilon_k)\langle\langle c^+_{-k\downarrow}, c^+_{k\uparrow}\rangle\rangle = -(\Delta - \eta)\langle\langle c_{k\downarrow}, c^+_{k\uparrow}\rangle\rangle \quad (10)$$

Where $\Delta = v\sum_{k'}\langle c_{-k'\downarrow}, c_{k'\uparrow}\rangle$ and $\eta = \sum_{klm}\Omega^{lm}_k\langle b_{l\downarrow}, b_{m\uparrow}\rangle$

Now using eq, (2) and (10), we get,

$$\langle\langle c_{k\uparrow}, c^+_{k\uparrow}\rangle\rangle = \frac{(\omega + \varepsilon_k)}{(\omega^2 - \varepsilon_k^2 - (\Delta - \eta)^2)} \quad (11)$$

and

$$\langle\langle c^+_{-k\uparrow}, c^+_{k\uparrow}\rangle\rangle = \frac{-(\Delta - \eta)}{(\omega^2 - \varepsilon_k^2 - (\Delta - \eta)^2)} \quad (12)$$

Now, using the relation, $\Delta = \frac{v}{\beta}\sum_k\langle\langle c^+_{-k\uparrow}, c^+_{k\uparrow}\rangle\rangle$ the summation with respect to k extends over all allowed pair states. Thus we get,

$$\Delta = -\frac{1}{\beta}\sum_n\int_{-\varepsilon_F}^{\infty} d\varepsilon\, N(0)v\left[\frac{\Delta - \eta}{\omega^2 - \varepsilon_k^2 - (\Delta - \eta)^2}\right] \quad (13)$$

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

$$\Delta = -\frac{2}{\beta}N(0)v\sum_k\int_0^{\hbar\omega_b} d\varepsilon\left[\frac{\Delta - \eta}{\omega^2 - \varepsilon_k^2 - (\Delta - \eta)^2}\right]. \quad (14)$$

For $N(0)v = \lambda$, eq. (14) becomes,

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

(15)

For $\eta = 0$, eq. (15) reduces to the well-known BCS model.

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

$$2\Delta(0) = 3.5k_BT_C . \quad (16)$$

For Ce_2PdIn_8 experimentally, $T_C = 0.68K$ [20],

Thus, we obtain, $\Delta(0) = 1.64\times10^{-23}$.

Furthermore, for T = 0K, eq. (15) can be expressed as,

$$\eta \approx 1.75k_BT_C - 2\hbar\omega_b \exp\left[-\frac{1}{\lambda(1 - \frac{\eta}{1.75k_BT_c})}\right] \quad (17)$$

3. Localized Electrons

The equation of motion for the localized electrons can be obtained using double time temperature dependent Green's functions technique as,

$$\omega\langle\langle b_{l\uparrow}, b^+_{l\uparrow}\rangle\rangle = 1 + \varepsilon_l\langle\langle b_{l\uparrow}, b^+_{l\uparrow}\rangle\rangle + \sum_{klm}\Omega^{lm}_k\langle c_{-k\uparrow}c_{k\uparrow}\rangle\langle\langle b^+_{m\uparrow}, b^+_{l\uparrow}\rangle\rangle$$

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

$$\langle\langle b_{l\uparrow}, b^+_{l\uparrow}\rangle\rangle = \frac{1}{(\omega - \varepsilon_l)} + \frac{\Delta_l}{(\omega - \varepsilon_l)}\langle\langle b^+_{m\uparrow}, b^+_{l\uparrow}\rangle\rangle, \quad (18)$$

Where, $\Delta_l = \sum_{klm}\Omega^{lm}_k\langle c_{-k\uparrow}c_{k\uparrow}\rangle$.

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

$$\omega\langle\langle b^+_{m\uparrow}, b^+_{l\uparrow}\rangle\rangle = 1 + \varepsilon_m\langle\langle b^+_{m\uparrow}, b^+_{l\uparrow}\rangle\rangle + \sum_{klm}\Omega^{lm}_k\langle c^+_{k\uparrow}c^+_{-k\uparrow}\rangle\langle\langle b_{l\uparrow}, b^+_{l\uparrow}\rangle\rangle \quad (19)$$

Assuming, $\varepsilon_l = \varepsilon_m$ we have;

 ISSN: 2277-1581
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$$\Rightarrow \langle\langle b_{m\uparrow}^{+}, b_{l\uparrow}^{+}\rangle\rangle = \frac{\Delta_l}{(\omega+\varepsilon_l)}\langle\langle b_{l\uparrow}, b_{l\uparrow}^{+}\rangle\rangle \quad (20)$$

Where $\Delta_l^{*} = \sum_{l,m}\Omega_k^{lm}\langle c_{k\uparrow}^{+}c_{-k\uparrow}^{+}\rangle$.

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

$$\langle\langle b_{m\uparrow}^{+}, b_{l\uparrow}^{+}\rangle\rangle = \frac{\Delta_l}{\omega^2-\varepsilon_l^2-\Delta_l^2}, \quad (21)$$

And

$$\langle\langle b_{l\uparrow}, b_{l\uparrow}^{+}\rangle\rangle = \frac{(\omega+E_l)}{\omega^2-\varepsilon_l^2-\Delta_l^2} \quad (22)$$

4. Correlation between Conduction and Localized electrons

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

$$\eta = \frac{\Omega}{\beta}\sum_{lm}\langle\langle b_{l\uparrow}^{+}, b_{m\uparrow}^{+}\rangle\rangle \quad (23)$$

Now using eq. (18) in eq. (22) we get,

$$\eta = \frac{\Omega}{\beta}\sum_{l}\frac{\Delta_l}{\omega^2-\varepsilon_l^2-\Delta_l^2} \quad (24)$$

The summation in eq. (24) may be changed into an integral by introducing the density of states at the fermi level and obtain,

$$\eta = \frac{\Omega}{\beta}\sum_{l}\int_{-\varepsilon_F}^{\infty} d\varepsilon N(0)\left[\frac{\Delta_l}{\omega^2-\varepsilon_l^2-\Delta_l^2}\right] \quad (25)$$

For effective attractive interaction region and assuming the density of state is constant, the expression becomes,

$$\eta = \frac{2}{\beta}N(0)\Omega\sum_{l}\int_{0}^{\omega_b} d\varepsilon\left[\frac{\Delta_l}{\omega^2-\varepsilon_l^2-\Delta_l^2}\right]. \quad (26)$$

Let $N(0)\Omega = \chi_l$, we get,

$$\eta = \chi_l\int_0^{\hbar\omega_b} dE\frac{|\Delta_l|}{\sqrt{E_l^2+\Delta_l^2}}\tanh\left(\frac{\beta\sqrt{E_l^2+\Delta_l^2}}{2}\right). \quad (27)$$

Since Δ_l is very small, eq. (27) becomes,

$$\eta = -\chi_l\Delta_l \ln 1.14\frac{\hbar\omega_b}{k_B T_N}, \quad (28)$$

Thus, the magnetic order temperature is given by,

$$T_N = \frac{1.14}{k_B}\hbar\omega_b \exp\left(\frac{\eta}{\chi_l\Delta_l}\right). \quad (29)$$

5. *The Superconducting State*

For $\eta = 0$ (pure superconducting system), the previous calculation gives an expression similar to the BCS model.

That is, $\frac{1}{\lambda} = \ln 1.14\frac{\hbar\omega_b}{k_B T_C}$, From which we get,

$$k_B T_c = 1.14\hbar\omega_b \exp\left(-\frac{1}{\lambda}\right). \quad (30)$$

But from the BCS model, at $T = T_C$, $\frac{1}{\lambda} = \ln 1.14\frac{\hbar\omega_b}{k_B T_C}$ and assuming $\omega_b = \omega_D$, we get,

$$\Delta(T) = 3.06k_B T_c\left(1-\frac{T}{T_c}\right)^{\frac{1}{2}}. \quad (31)$$

6. Results and Discussion

Using the model Hamiltonian and the double time temperature dependent Green's function formalism, the researcher develop expressions for superconducting order parameter(Δ), antiferromagnetic order parameter(η), superconducting transition temperature(T_C) and antiferromagnetic order temperature (T_N). The expression here obtained for pure superconductor is that, when magnetic effect is zero($\eta = 0$), it is in agreement with the BCS model. Using eq. (31) and the experimental value, T_C =0.68K for Ce_2PdIn_8, the researcher plotted the phase diagram of the superconducting order parameter(Δ) versus Temperature (T) as shown in figure 1. It

ISSN: 2277-1581
1 Feb. 2018

can be easily seen that the superconducting order parameter, which is a measure of pairing energy decreases with increasing temperature until it vanishes at the superconducting transition temperature (T_C).

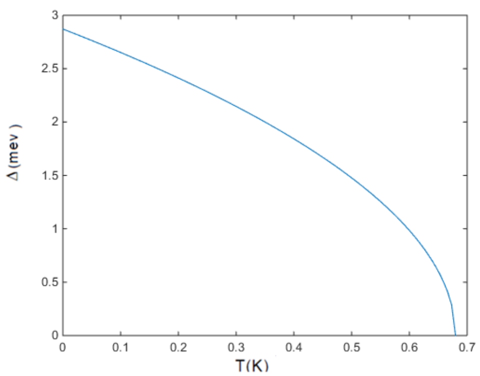

Figure.1: Superconducting order parameter ($\triangle$) versus temperature for the superconductor Ce_2PdIn_8.

Similarly, using eq. (17) the phase diagram of T_C versus η is plotted as depicted in figure 2.

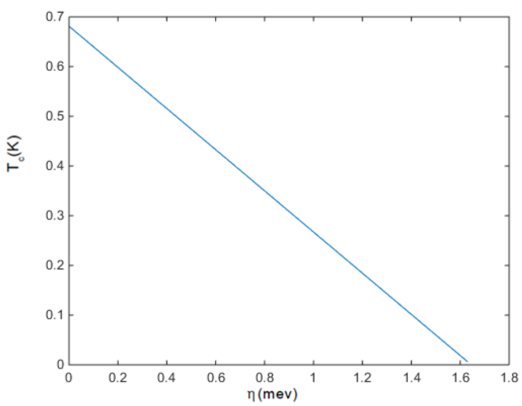

Figure 2: Superconducting transition temperature (T_C) versus magnetic order parameter (η) for the superconductor Ce_2PdIn_8.

Furthermore, the Phase diagram of T_N versus η is plotted by using eq. (29) as shown in figure.3.

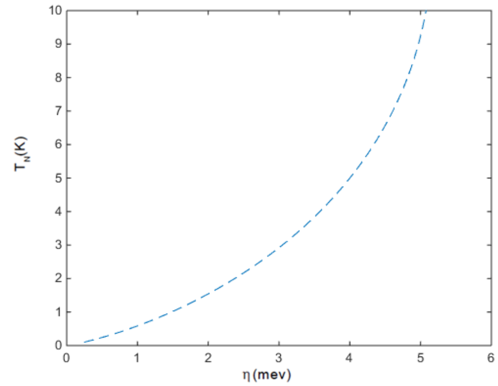

Figure 3: Magnetic ordering temperature (T_N) versus magnetic order parameter (η) for the superconductor Ce_2PdIn_8.

Now by merging figures 2 & 3, the possible coexistence of superconductivity and antiferromagnetism in Ce_2PdIn_8 is demonstrated as shown in figure 4.

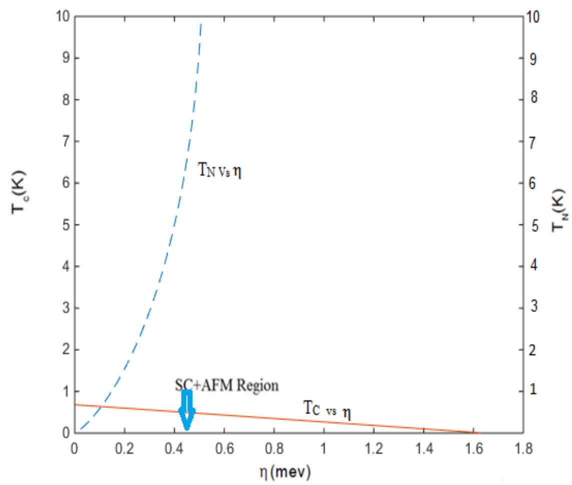

Figure 4: Coexistence of Superconductivity and antiferromagnetism in Ce_2PdIn_8.

From figure 4, it can be seen that, T_C decreases with increasing η, whereas T_N increases with increasing η and there a common region where both superconductivity and antiferromagnetism can coexist in superconducting Ce_2PdIn_8. The current finding is in agreement with experimental finding [20].

7. Conclusion

In this work, we have studied the possible co-existence of Antiferromagnetism and superconductivity in Ce_2PdIn_8. Using 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 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 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 developed. As is well known, superconductivity and antiferromagnetism are two cooperative phenomena which are mutually incompatible 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 antiferromagnetism can possibly coexist in superconducting Ce_2PdIn_8. Our findings are in broad agreement with experimental results [20].

Acknowledgements

We gratefully acknowledge Tamiru Negussie for useful discussions and valuable suggestion to complete the work.

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