Theoretical Investigation of the Coexistence of Superconductivity and Ferromagnetism in Bi_3Ni Superconductor

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Abstract

This research focuses on the theoretical investigation of the possible coexistence of superconductivity and Ferromagnetism in Bi_3Ni superconductor. By developing a model Hamiltonian for the system under consideration and by employing double time temperature dependent Green's function formalism and by applying a suitable decoupling approximation technique, the possible coexistence of superconductivity and ferromagnetism in Bi_3Ni 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 ferromagnetism order temperature (T_m) versus ferromagnetic order parameter (η) have been plotted. Finally, by combining the two phase diagrams, the possible coexistence of superconductivity and ferromagnetism in Bi_3Ni superconductor has been demonstrated. The finding is in agreement with the experimental observations.

Keywords: Superconductivity, ferromagnetism, Green function, Superconducting order parameter.

Resumen

Esta investigación se centra en la investigación teórica de la posible coexistencia de superconductividad y ferromagnetismo en el superconductor Bi_3Ni. Al desarrollar un modelo Hamiltoniano para el sistema en consideración y al emplear el formalismo de función de Green dependiente de la temperatura en doble tiempo y al aplicar una técnica de aproximación de desacoplamiento adecuada, se ha demostrado que la posible coexistencia de superconductividad y ferromagnetismo en el superconductor Bi_3Ni es una posibilidad muy distinta. Se han trazado los diagramas de fase del parámetro de brecha superconductora (Δ) versus temperatura (T), la temperatura de transición superconductora (T_c) y la temperatura de orden de ferromagnetismo (T_m) versus el parámetro de orden ferromagnético (η). Finalmente, al combinar los diagramas de dos fases, se ha demostrado la posible coexistencia de superconductividad y ferromagnetismo en el superconductor Bi_3Ni. El hallazgo está de acuerdo con las observaciones experimentales.

Palabras clave: Superconductividad, ferromagnetismo, función de Green, parámetro de orden superconductor.

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I. INTRODUCTION

Superconductivity which is a quantum phenomenon of zero electrical resistance and perfect diamagnetism, was discovered by Heike Kamerlingh Onnes [1]. Since then, extensive searches for novel superconductors with high critical temperature (T_C), have been performed. Condensed matter Physicists have conducted intensive researches inorder to understand the nature and properties of superconductors in general and high temperature heavy fermion superconductors in particular. Through times, many heavy fermion alloys were discovered to show superconductivity at higher transition temperatures. In materials that exhibit antiferromagnetism, the magnetic moments of atoms or molecules, 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). 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 the 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 sublattice magnetizations differing from that of the other sublattice resulting in a nonzero net magnetization. Unlike ferromagnetism, antiferromagnetic interactions can lead to multiple of 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 (*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, 5, 6], superconductivity generally occurs after suppressing the magnetic order either through doping or by 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]. 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 ordering. In spite of this, superconductivity can coexist with either remaining antiferromagnetic ordering [13] or new ferromagnetic ordering [14] and this provides an ideal platform for studying the interplay between superconductivity and magnetism.

The coexistence of 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. 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) [15]. McCallum [16] discovered the coexistence of superconductivity and long-range antiferromagnetism ordering in RMo_6S_8. Nagaraja [17] also observed the coexistence of superconductivity and long-range antiferromagnetism in rare earth transition metal borocarbide system. The discovery of the coexistence of superconductivity and antiferromagnetism in a high-TC superconductor $Gd_{1+x}Ba_{2-x}Cu_3O_{7-\delta}$ (with $x = 0.2$) has come as a big surprise [18].

The Interplay of magnetism and superconductivity in heavy fermion superconductors is a remarkable issue. This interplay has shown considerable variety by showingcompetition, coexistence, and/or coupling of the magnetic and superconducting order parameters [19].The 115 heavy-Fermion family, $CeMIn_5$,(where M= Co, Rh, Ir) has attracted interest due to the intricate relationship between antiferromagnetism and superconductivity which is found in them [20, 21].

Theoretical investigations on the coexistence of superconductivity and magnetism has been shown in various heavy fermion superconductors [22, 23, 24]. The coexistence of superconductivity and ferromagnetism in Bi_3Ni is observed, with superconductivity emerging in the ferromagnetically ordered phase [25].

II. 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 measured relative to the chemical potential, μ . $b^+_l(b_l)$ are creation (annihilation) operators of the localized electrons oflocalized energy (E_l).

III. 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.(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,

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

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

Now using Eqs, (2) and (4), we get,

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

and

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

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

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

For $\eta = 0$, eq. (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 Bi_3Ni, $T_C =$ 4.1K, [26]. Thus, we obtain, $\Delta(0) = 9.9X10^{-23} J$. Furthermore, using Eqs. (8) and (9), we get

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

IV. 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 to be,

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

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

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

Now combining Eqs. (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

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

V. EQUATION OF MOTION WHICH 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 Eq. (12) in Eq. (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 Eq.(16) may be changed into an integral by introducing the density of states at the fermilevel, $N(0)$and obtain,

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

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

$$\eta = -\frac{2}{\beta} N(0)\Omega \sum_l \int_0^{\hbar\omega_b} dE \left[\frac{\Delta_l}{\omega^2 - E_l^2 - \Delta_l^2} \right]. \quad (18)$$

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

Hence, we get,

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

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

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

Thus, the ferromagnetic order temperature (T_m) is given by,

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

VI. PURE SUPERCONDUCTING SYSTEM

For pure superconducting system, i.e., for $\eta = 0$, Eq. (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,

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

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,

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

VII. RESULTS AND DISCUSSION

Using the model Hamiltonian we developed and the double time temperature dependent Green's function formalism, we obtained expressions for superconducting order parameter (Δ), ferromagnetic order parameter (η), superconducting transition temperature(T_c) and ferromagnetic order temperature (T_m). The expression we obtained for pure superconductor when magnetic effect is zero (η = 0), is in agreement with the BCS model. Now using Eq. (22), the experimental value, T_c = 4.1K, for Bi_3Ni [26] 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 Eq. (10), the phase diagram of T_c versus η is plotted as depicted in figure 2. Furthermore, the Phase diagram of T_m versus η is plotted by using Eq. (20) as shown in figure 3. Now by merging figures 2 & 3, the possible coexistence of superconductivity and ferromagnetism in Bi_3Ni is demonstrated as shown in figure 4.

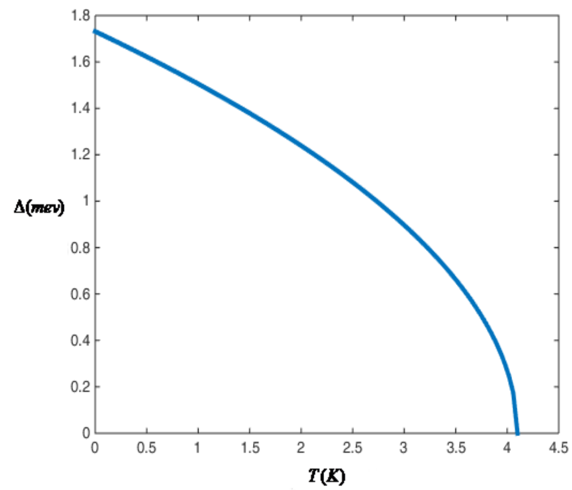

FIGURE 1. Superconducting order parameter(Δ) versus temperature for the Bi_3Ni Superconductor.

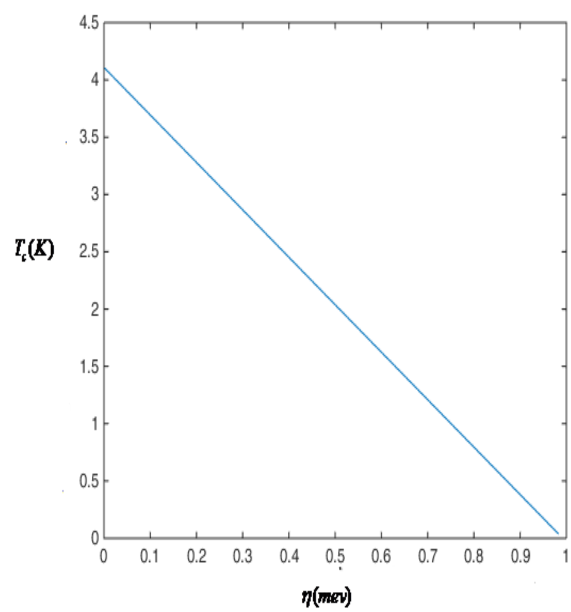

FIGURE 2. Superconducting transition temperature (T_c) versus magnetic order parameter (η) for the Bi_3Ni superconductor.

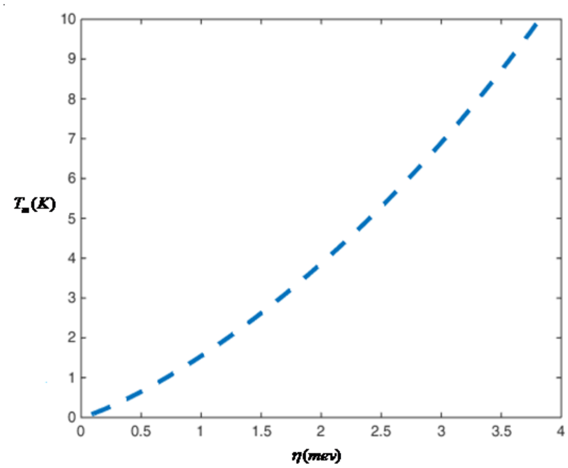

FIGURE 3. Ferromagnetic order temperature (T_m) versus magnetic order parameter (η) for the Bi_3Ni superconductor.

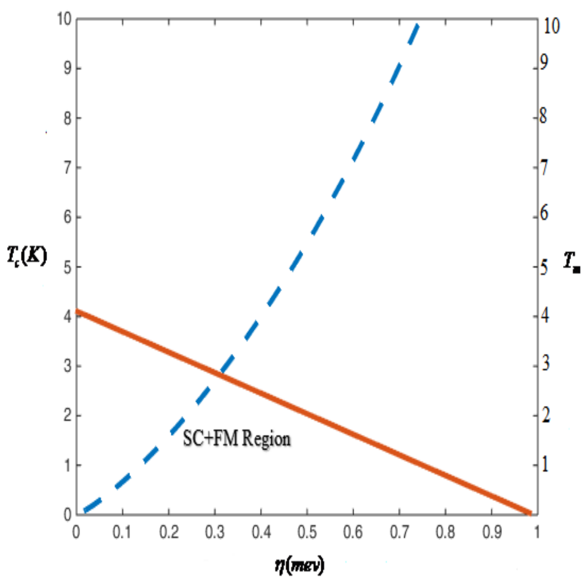

FIGURE 4. Coexistence of Superconductivity and ferromagnetism in Bi_3Ni Superconductor.

From Fig. 4, it can be seen that, T_c decreases with increasing η, whereas T_m increases with increasing η and there is a common region where both superconductivity and ferromagnetism coexist in Bi_3Ni.

VIII. CONCLUSION

In the present work, we have demonstrated the basic concepts of superconductivity with special emphasis on the interplay between superconductivity and ferromagnetism which are closely connected to the superconducting Bi_3Ni. 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 and carried out various correlations by using suitable decoupling procedures and obtained expressions for superconducting order parameter, ferromagnetic order parameter, superconducting transition temperature and ferromagnetic order temperature. By using appropriate experimental values and considering suitable approximations, we plotted phase diagrams using the equations developed. As is well known, superconductivity and 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 ferromagnetism can possibly coexist in superconducting Bi_3Ni. as demonstrated in Fig. 4. Our finding is in agreement with experimental results [25].

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