Improved Analysis of Rare Earth Magnetic Superconductors

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Abstract

We present an improved analysis of the phase transitions in rare earth superconductor within Ginzburg-Landau theory. Our work is based on the systematic study of critical field and superconducting order parameters in the presence of localized magnet due to rare earth atom. We present the different phases that can occur and analyze the conditions of phase transition from the normal phase to the coexistence phase of anti-ferromagnetism and superconductivity. We calculate the critical field and Ginzburg-Landau parameters to show the coexistence property. We compare our theoretical results with existing experimental results.

Keywords  Superconductor · Phase transition · Magnetic properties

1 Introduction

The magnetic and superconducting order parameters of rare earth compounds \((RNi_2B_2C)\) are in the same range [1, 2] and thus attract the attention of researchers all around the globe. Antiferromagnetic and superconducting properties exhibited by these compounds contradict each other. The superconducting behavior is observed for both types of compounds, i.e., having nonmagnetic rare earth elements (Y, Lu) [1, 3] and elements (Tm, Er, Ho, and Dy) with high magnetic moments [2, 4]. Several compounds of the “\(RNi_2B_2C\)” group exhibit superconductivity, magnetism, and coexisting properties of both [5–10] for different R (rare earth). The coexisting property in these compounds is due to the localized rare earth 4\(f\) magnetic moments coupling with the conduction electrons \(Ni(3d)\) via exchange interaction. The band structure calculation shows that the Fermi energy bands consist of \(Ni(3d)\) orbital along with B and C 2p orbitals, and the dominant contribution is from Ni orbitals [10–12]. Superconducting condensation is associated with itinerant conduction electrons [10], and anisotropic magnetic properties are related to localized 4\(f\) electrons [13, 14]. These compounds exhibit various commensurate and incommensurate magnetic structures. The experimental tunneling data shows that \(RNi_2B_2C\) superconductors are weak-coupling BCS type. They are type II superconductors with a small coherence length of 50–100 Å. The different theoretical models and experimental observations have been proposed to study various features, precisely the upper critical field, specific heat, using neutron diffraction, magnetization measurements, and resistive transition curves [14–23]. The upper critical field provides knowledge of coupling strength, exchange interaction, the electronic structure, and anisotropy of the order parameter.

The purpose of this present work is to have an exhaustive understanding of the phase transition from the normal state to the coexistence state, and the thermodynamic properties of these rare earth compounds theoretically. The Ginzburg-Landau approach [22–26] helps to study the coexistence of magnetism and superconductivity in the multi-band picture. These theories explain magnetic fluctuations and anomalous behavior of the upper critical field \(H_{c2}\) [12, 23, 24]. We have done a systematic study of critical field and other Ginzburg-Landau parameters within a single phenomenological model, including magnetism and superconductivity. We construct our phenomenological model of two order parameters [24] corresponding to the two dominant correlations based on the experimental information. The next section discusses the
The Ginzburg-Landau theory simply postulates the existence of a magnetic field with a superconducting order parameter. The differential equation which couples the spatial variation of the magnetic field with the superconducting order parameter is a phenomenological approach to describe phase transition using a unified theoretical framework. It can explain a variety of phenomena without going into the technical process. The Ginzburg-Landau theory is nonlinear second order differential equation which couples the spatial variation of a magnetic field with a superconducting order parameter. The Ginzburg-Landau theory simply postulates the existence of macroscopic quantum wave function \( \psi(\mathbf{r}) \), which is equivalent to an order parameter. The transition from superconducting to the normal state is assumed to take place at the thermodynamic critical field. So the difference in free energy between the normal and superconducting state is given by the magnetic field energy between the normal and superconducting state. The anti-ferromagnetic order of rare earth magnetic superconductor can be described by \( M_a \) and \( M_b \). Here \( M_a \) and \( M_b \) are the magnetic order of two identical inter penetrating lattices labeled by “a” and “b.” Furthermore, we assume \( M_a = -M_b \). For the superconducting order parameter, we define \( \psi_a(\mathbf{r}) \) and \( \psi_b(\mathbf{r}) \) as two superconducting order parameters in the lattices “a” and “b” respectively.

Now the free energy density of rare earth magnetic superconductor should be expressed in terms of an expansion of \( \psi_a, \psi_b, M_a, \) and \( M_b \):

\[
F = \int d^3r \left[ F_n + a_1 |\psi_a|^4 + a_2 |\psi_b|^4 + \frac{1}{2} b_1 |\psi_a|^4 + \frac{1}{2} b_2 |\psi_b|^4 + \alpha (M_a^2 + M_b^2) + \frac{1}{2} \beta (M_a^4 + M_b^4) + 2\delta M_a M_b + \gamma_1 |\psi_a|^2 (M_a^2 + M_b^2) + \gamma_2 |\psi_b|^2 (M_a^2 + M_b^2) + 2\eta_1 \psi_a^2 \Psi_b^2 - \kappa_1 \psi_a \psi_b + \frac{1}{2m_a} \left| -i\hbar \nabla - \frac{2eA}{c} \right| \psi_a^2 + \frac{1}{2m_b} \left| -i\hbar \nabla - \frac{2eA}{c} \right| \psi_b^2 \right. \\
+ \kappa_2 \left( i\hbar \nabla - \frac{2eA}{c} \right) \psi_a \left( -i\hbar \nabla - \frac{2eA}{c} \right) \psi_b + \frac{H^2}{8\pi} \right] \tag{2.1}
\]

where \( F_n \) is the free energy density of the normal phase. \( a_1, a_2, b_1, b_2, \alpha, \delta, \) and \( \beta \) are material parameters. \( \gamma_1, \gamma_2, \eta, \kappa_1, \) and \( \kappa_2 \) are the coupling constants. \( \gamma_1 \) and \( \gamma_2 \) are assumed to be positive for the stability of the superconducting state. \( e, m_a, \) and \( m_b \) are the elementary electron charge and mass, respectively. Here \( \delta > 0, \beta > 0, \) and \( b > 0 \). The parameter \( a_1 \) is proportional to \( (T - T_C1) \), \( a_2 \) is proportional to \( (T - T_{C2}) \), and \( \alpha \) is proportional to \( (T - T_a) \). Thus, \( a_1 = a_{01} (T - T_C1), a_2 = a_{02} (T - T_{C2}), \) and \( \alpha = \alpha_0 (T - T_a) \). \( a_{01}, a_0, \) and \( \alpha_0 \) are positive constants. The \( \psi_a \) and \( \psi_b \) are the superconducting order parameters associated with Ni(3d).

First, we consider the uniform system in zero field \( H = 0 \). After the minimization of Eq. (2.1) with respect to \( \psi_a, \psi_b, M_a, \) and \( M_b \), we get the following four stable phases:

I. Normal phase (N): \( |\psi_a| = 0, |\psi_b| = 0, M_a = 0, M_b = 0 \). This phase exists for \( a_1 > 0, a_2 > 0, \) and \( \alpha > 0 \).

II. Anti-ferromagnetic phase (AFM): \( |\psi_a| = 0, |\psi_b| = 0, M_a \neq 0, M_b \neq 0 \). This phase exists for \( a_1 > 0, a_2 > 0, \) and \( \alpha < 0 \).

III. Superconducting phase (SC): \( |\psi_a| \neq 0, |\psi_b| \neq 0, M_a = 0, M_b = 0 \). This phase exists for \( a_1 < 0, a_2 < 0, \) and \( \alpha > 0 \).

IV. Coexistence of superconductivity and antiferromagnetism phase (AFS): \( |\psi_a| \neq 0, |\psi_b| \neq 0, M_a \neq 0, M_b \neq 0 \). This phase exists for \( a_1 < 0, a_2 < 0, \) and \( \alpha < 0 \).

From these solutions, it is clear that six types of phase transition are possible: N-SC, N-AFM, N-AFS, SC-AFM, AFM-AFS, SC-AFS. The N-SC, N-AFM, and SC-AFM transitions are second order. We will now discuss the N-AFS phase transition. The spontaneous magnetization in the AFS phase \( (M_a = -M_b) \) is given by:

\[
M_{sa}^2 = M_{sb}^2 = \frac{(\delta - \alpha - \gamma_1 |\psi_a|^2 - \gamma_2 |\psi_b|^2)}{\beta} \tag{2.2}
\]

Now the substitution of Eq. (2.2) into Eq. (2.1), we get:

\[
F = \int d^3r \left[ F_n^* + a_1^* |\psi_a|^4 + a_2^* |\psi_b|^4 + \frac{1}{2} b_1^* |\psi_a|^4 + \frac{1}{2} b_2^* |\psi_b|^4 + \frac{1}{2m_a} \left| -i\hbar \nabla - \frac{2eA}{c} \right| \psi_a^2 + \frac{1}{2m_b} \left| -i\hbar \nabla - \frac{2eA}{c} \right| \psi_b^2 \right.
\\
+ \kappa_2 \left( i\hbar \nabla - \frac{2eA}{c} \right) \psi_a \left( -i\hbar \nabla - \frac{2eA}{c} \right) \psi_b + \frac{H^2}{8\pi} \left. \right] \tag{2.3}
\]

where:

\[
f_n^* = F_n - \frac{a_2^*}{\beta} - \frac{\delta^2}{\beta} + \frac{\delta \alpha}{\beta},
\]

\[
a_1^* = a_1 + \frac{2\delta \gamma_1}{\beta} - \frac{2\gamma_1 \alpha}{\beta},
\]

\[
a_2^* = a_2 + \frac{2\delta \gamma_2}{\beta} - \frac{2\gamma_2 \alpha}{\beta},
\]

\[
b_1^* = b_1 - \frac{2\gamma_1^2}{\beta},
\]

\[
b_2^* = b_2 - \frac{2\gamma_2^2}{\beta},
\]

\[
\eta^* = \eta - \frac{\gamma_1 \gamma_2}{\beta}.
\]
Minimization of Eq. (2.3) with respect to $\psi_a$ and $\psi_b$ (for uniform system and $\kappa_1 = 0$) yields:

$$|\psi_a|^2 = \frac{a_1^* b_2^* - 2\eta^* a_2^*}{4\eta^* - b_2^* b_2^*}$$  \hspace{1cm} (2.4)

$$|\psi_b|^2 = \frac{a_2^* b_1^* - 2\eta^* a_1^*}{4\eta^* - b_1^* b_1^*}$$  \hspace{1cm} (2.5)

Substitution Eqs. (2.4) and (2.5) into Eq. (2.2), we get:

$$M_a^2 = M_b^2 = \frac{(\delta - \alpha)(4\eta^* - b_1^* b_2^*) - \gamma_1 (a_1^* b_2^* - 2\eta^* a_2^*) - \gamma_2 (a_2^* b_1^* - 2\eta^* a_1^*)}{\beta(4\eta^* - b_1^* b_2^*)}$$  \hspace{1cm} (2.6)

Equations (2.4), (2.5), and (2.6) are the values of superconducting order parameters and spontaneous magnetization in the AFS phase.

$T_{C1} > T < T_{af}$ and $T_{C2} > T < T_{af}$ are the conditions for the existence of the AFS phase. Then $a_1$, $a_2$, and $\alpha$ are negative. For the AFS phase, both Eqs. (2.4), (2.5), and (2.6) must be positive. Thus, the necessary conditions for the existence of the AFS phase are:

1. $a_1^* b_2^* > 2\eta^* a_2^*$,
2. $a_2^* b_1^* > 2\eta^* a_1^*$,
3. $4\eta^* - b_1^* b_2^*$
4. $(\delta - \alpha)(4\eta^* - b_1^* b_2^*) > \gamma_1 (a_1^* b_2^* - 2\eta^* a_2^*) + \gamma_2 (a_2^* b_1^* - 2\eta^* a_1^*)$.

The above four conditions should hold simultaneously for the existence of the AFS phase. In this case, the free energy will be in the lowest energy state. So the N-AFS phase transition occurs. The superconductor has three characteristic parameters associated with them: the Ginzburg-Landau coherence length ($\xi$), the penetration depth ($\lambda$), and the Ginzburg-Landau parameter ($\kappa$).

The correlation length, penetration depth, and critical magnetic field can be calculated for the AFS phase by the same method as adapted for the normal superconductor which are given by:

$$\xi_{GLa}(T) = \xi_{GLa}(0)(T_{C1}^*-T)^{-1/2}$$  \hspace{1cm} (2.7)

$$\xi_{GLb}(T) = \xi_{GLb}(0)(T_{C2}^*-T)^{-1/2}$$  \hspace{1cm} (2.8)

$$\lambda_{GLa}(T) = \lambda_{GLa}(0)(T_{C1}^*-T)^{-1/2}$$  \hspace{1cm} (2.9)

$$\lambda_{GLb}(T) = \lambda_{GLb}(0)(T_{C2}^*-T)^{-1/2}$$  \hspace{1cm} (2.10)

$$H_{Ca} = \frac{2m_a a_0^1 c}{\hbar e}(T_{C1}^*-T)$$  \hspace{1cm} (2.11)

$$H_{Cb} = \frac{2m_a a_0^2 c}{\hbar e}(T_{C2}^*-T)$$  \hspace{1cm} (2.12)

where:

$$\xi_{GLa}(0) = \frac{h}{\sqrt{2m_a a_0^1}},$$

$$\xi_{GLb}(0) = \frac{h}{\sqrt{2m_a a_0^2}},$$

$$\lambda_{GLa}(0) = \frac{m_a e^2 b_1^*}{8\pi e^2 a_0^1},$$

$$\lambda_{GLb}(0) = \frac{m_a e^2 b_2^*}{8\pi e^2 a_0^2},$$

$$a_0^1 = a_0^1 - \frac{2\eta a_0^1}{b_2^*} + \frac{2\gamma_1 a_0^1}{b_2^*} + \frac{4\eta a_0^2}{b_2^*},$$

$$a_0^2 = a_0^2 - \frac{2\eta a_0^1}{b_1^*} + \frac{2\gamma_2 a_0^1}{b_1^*} + \frac{4\eta a_0^2}{b_1^*},$$

$$T_{C1}^* = a_0^1 T_{C1} - 2\eta a_0^1 T_{C1} + 2\gamma_1 a_0^1 T_{C1} - 2\gamma_2 a_0^1 T_{C1} - 2\eta a_0^2 T_{C1} - 2\gamma_2 a_0^1 T_{C1} - 2\gamma_2 a_0^2 T_{C1},$$

$$T_{C2}^* = a_0^2 T_{C2} - 2\eta a_0^1 T_{C2} + 2\gamma_1 a_0^1 T_{C2} - 2\gamma_2 a_0^1 T_{C2} - 2\eta a_0^2 T_{C2} - 2\gamma_2 a_0^1 T_{C2} - 2\gamma_2 a_0^2 T_{C2},$$

$$b_2^* = b_2^* - \frac{4\eta^2}{b_2^*},$$

$$b_1^* = b_1^* - \frac{4\eta^2}{b_1^*}.$$

### 3 Results and Discussion

We have determined the value of the upper critical magnetic field for various rare earth compounds, specifically $HoNi_2B_2C$, $ErNi_2B_2C$, $TmNi_2B_2C$, and $DyNi_2B_2C$ using Eqs. (2.11 and 2.12) from the previous section. The curves for both the equations are more or less identical. The corresponding graphs are plotted along with experimental results in Figs. 1, 2, 3, and 4. The numerical results are given in Table 1.

![Fig. 1 Variation of upper critical magnetic field $H_{C2}$ with the temperature for $HoNi_2B_2C$](image)
Fig. 2 The upper critical field $H_{c2}$ as a function of temperature for $DyNi_2B_2C$ along with experimental results [21]. Inset shows Ginzburg-Landau parameters (coherence length and penetration depth) with temperature. The calculated $\zeta(0)$ 285.6 Å while the experimental one is given by 220 Å.

It is observed that the critical field plot for all the compounds shows similar trends as that of the experimental one. The theoretical value of $H_{c2}(0)$ for $HoNi_2B_2C$ is 5.9 T, which is larger than the experimental value of 0.84 T. Similarly, for $TmNi_2B_2C$ $H_{c2}(0)$ is 3.9 while the experimental value is 2.0. However, for $DyNi_2B_2C$ and $ErNi_2B_2C$, the theoretical values of $H_{c2}(0)$ are 0.21 T and 0.78 T, respectively which matches their experimental ones, i.e., 0.7 T and 0.112–0.113 T. The coherence length and penetration depth plotted using the above equations for all the compounds increases with temperature and diverge as $T$ tends to $T_c$.

4 Conclusion

Ginzburg’s theory is valid in the superconducting phase boundary. Our multi-band model describes the behavior and mutual influence of two magnetic and two superconducting order parameters. We have studied the coexistence of superconducting and anti-ferromagnetism for rare earth superconductors using Ginzburg-Landau theory. We have calculated the effect of coherence length, penetration depth, and critical field with temperature using the above model. Our theoretical results agree with the experimental observations. Our model describes some of the physical properties of the system in the coexisting state. We do not find any anomalous behavior in the measurements of the upper critical field.

| Compounds  | $T_C$ in K | $T_N$ in K | $H_{c2}(0)$ in T | $\zeta_{GL}(0)$ in Å | $\lambda_{GL}(0)$ in Å |
|------------|------------|------------|------------------|----------------------|----------------------|
| $HoNi_2B_2C$ | 8.5 | 5.2 | 5.9 | 104.9 | 293.5 |
| $DyNi_2B_2C$ | 6.5 | 10.5 | 0.807 | 285.6 | 1102.5 |
| $ErNi_2B_2C$ | 11.5 | 6 | 1.9 | 186.9 | 877 |
| $TmNi_2B_2C$ | 11 | 1.5 | 3.99 | 128.5 | 535.4 |
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