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Coexistence of Magnetism and Superconductivity in $HoNi_2B_2C$

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Abstract. We have presented a microscopic theory of the effect of external magnetic field on the co-existence of superconductivity and anti-ferromagnetism in the rare earth nickel borocarbide compound, $HoNi_2B_2C$. The model proposed earlier for heavy fermion superconductors has been adopted here to take into account the effect of external magnetic field in the presence of hybridization for this rare earth compound. We have derived self-consistent equations for the superconducting and antiferromagnetic order parameter using equation of motion of Green's function in presence of external magnetic field. Also the temperature dependence of gap parameters has been studied. The calculated ratio of the effective gap and T_C has been found to be close to BCS value and also agrees quite well with the experimental results.

Keywords: Superconductivity; anti ferromagnetism; borocarbides

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1. Introduction

The quaternary rare earth transition metal borocarbides (QBC) form a class of superconductors; distinguished by relatively high T_c for intermetallic and magnetic superconductors, and possessing relatively high coexistence temperatures [1]. Some of these borocarbides exhibit magnetic ordering and superconductivity at about same temperature, offering the possibility of study of the coexistence of superconductivity and magnetism. The most spectacular case of coexistence is in the Ho-compounds, $HoNi_2B_2C$ (Tc = 8.5) [2-5].The two phenomena, superconductivity and magnetic ordering are due to the different degrees of localization of the electrons in the borocarbides. Local density approximation calculation shows that the conduction band is composed mainly of

Ni 3d electrons [6], which undergo the superconducting transition. On the other hand magnetic properties are related to the well localized electrons in the incomplete 4f-shell of Ho.

These compounds are having a layered structure in which Ni_2B_2 layers are separated by R-C planes stacked along the c-axis. Despite the layered structure, the electronic properties of borocarbides appear to be essentially three-dimensional according to electronic band structure calculations [6-7], supported by the spectroscopic studies [8]. These compounds are good metals with a large electron density of states N (E_F) at the Fermi level. The dominant contribution of N(E_F) comes from Ni 3d-states, but some contributions come from all other atoms as well [6]. Resistivity and magneto-resistance measurement on RNi_2B_2C compounds (R = Y, Lu, Er, Ho) [9] have shown similar dispersions along all directions. The band structure of borocarbides, RNi_2B_2C exhibits four bands across the Fermi level. One of these bands is a flat one, indicating that the system may be a strongly correlated one. This flat band hybridizes with the conduction band formed out of the other 3 bands. Obviously due to hybridization, the sub-lattice may partly acquire the character of the localized states of the d-band. The flat f-band of rare earth lies much below the Fermi level and hence may weakly influence the electronic structure of the system. The electronic structure calculation points towards the phonon mediated BCS mechanism for superconductivity [10] in these systems. On lowering the temperature, long range antiferromagnetic (AFM) state appears below 5.2K and superconductivity and anti-ferromagnetism truly coexist below 5.2K [5]. Neutron scattering measurement by Lynn et al.[11], on this compound gives evidence of magnetic properties of superconductivity at Tc ~ 8K. The energy gap in $HoNi_2B_2C$ studied till now gives the gap parameter as $\frac{2\Delta_0}{k_B T_C}$=3.63+0.05, close to BCS value.

2. Formalism

In the present model the anti-ferromagnetism arises due to the staggered sub-lattice magnetization from the conduction electrons which are responsible for superconductivity. In addition to that, the localized f-electrons and itinerant conduction electrons hybridize near the Fermi level. In order to simulate AFM in the system we considered two Ni sub-lattice. We have used a mean field theory for the itinerant electrons to study the effect of external magnetic field on anti-ferromagnetism in the presence of hybridization and the localized f-electron. When a magnetic field is applied, it splits the two-fold degenerate band giving

rise to quasi particle energies. We have considered the effect by replacing ϵ_k with ($\epsilon_k \pm \sigma\mu_B$B).

We have taken our model Hamiltonian as,

$$H = H_C + H_h + H_v + H_S + H_f + H_B \quad (1)$$

Where H_C describes the conduction which represents the hopping of the quasi particles between the neighboring sites of the two sub-lattices.

$$H_c = \sum_{k\sigma} \epsilon_0(k)\left(a^\dagger_{k\sigma} b_{k\sigma} + h.c\right) \quad (2)$$

$a^\dagger_{k\sigma}(a_{k\sigma})\ and\ b^\dagger_{k\sigma}(b_{k\sigma})$ are the creation (annihilation) operators of electrons at site 1 and 2 of Ni respectively with momentum k and σ.

Hopping takes place between nearest neighbor sites of Ni with dispersion,

$$\epsilon_0(k) = -2t_0\left(cos\ k_x + cos\ k_y\right) \quad (3)$$

Where t_0 is the nearest neighbor hopping integral.

A staggered magnetic field of strength h stimulates a strongly AFM correlation of conduction Ni d-electrons and its contribution to the Hamiltonian is given as,

$$H_h = (h/2) \sum_{k\sigma} \sigma (a^\dagger_{k\sigma} a_{k\sigma} - b^\dagger_{k\sigma} b_{k\sigma}) \quad (4)$$

The staggered field is defined by,

$$h = \frac{-1}{2} g\mu_B \sum_{k\sigma} < a^\dagger_{k\sigma} a_{k\sigma} > - < b^\dagger_{k\sigma} b_{k\sigma} > \quad (5)$$

Effective hybridization between the f-electrons of the rare earth atom and the conduction electrons of Ni atom also contributes to the Hamiltonian, represented as H_V has been given by

$$H_v = V \sum_{k\sigma}\left(a^\dagger_{k\sigma} f_{1,k\sigma} + b^\dagger_{k\sigma} f_{2,k\sigma} + h.c\right) \quad (6)$$

Where $f^\dagger_{ik\sigma}(f_{ik\sigma})$ is the creation (annihilation) operator of the f-electrons and V is the strength of hybridization. Only on-site hybridization is included here.

The attractive part of intra-band interaction term leads to superconductivity. The mean field BCS Hamiltonian describing phonon mediated superconductivity is given by,

$$H_s = -\Delta \sum_k \left[\left(a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} + h.c\right) + \left(b^\dagger_{k\uparrow} b^\dagger_{-k\downarrow} + h.c\right)\right] \quad (7)$$

Here BCS type of phonon mediated cooper pairing of conduction electrons of different Ni sites is taken into account. The inter sub-lattice pairing may be significant here but has not been taken into consideration for simplicity of numerical calculation. The superconducting order parameter Δ, is given as

$$\Delta = -\sum_K \tilde{V}_k \left(< a^\dagger_{k\uparrow}\, a^\dagger_{-k\downarrow} > + < b^\dagger_{k\uparrow}\, b^\dagger_{-k\downarrow} >\right) \quad (8)$$

$V_k$is the strength of the attractive interaction between two electrons mediated by the phonons.

The intra f-electron Hamiltonian in the presence of external magnetic field B is described by

$$H_f=\left(\in_f+\frac{1}{2}g\mu_B B\right)\sum_{i,ki=1,2} f^{\dagger}_{ik\uparrow} f_{ik\uparrow} + \left(\in_f-\frac{1}{2}g\mu_B B\right)\sum_{i,ki=1,2} f^{\dagger}_{ik\downarrow} f_{ik\downarrow} \quad (9)$$

g and μ_B are Lande g-factor and Bohr magnetron respectively.

The external magnetic field B contributes to the Hamiltonian $H_{B,}$written as,

$$H_B = \frac{1}{2}g\mu_B B\sum_{k\sigma}\left(a^{\dagger}_{k\sigma}a_{k\sigma}+b^{\dagger}_{k\sigma}b_{k\sigma}\right) \quad (10)$$

We have calculated the one electron Green's function using the Model Hamiltonian [eqn.(1)] for the superconducting and anti-ferromagnetic state of borocarbide system. The double time electron Green's function of Zubarev type has also been calculated by the equation of motion method. The poles of the Green's function give four quasi particle energy bands. By using equation for appropriate single particle correlation functions in presence of external magnetic field and hybridization we have derived SC and AFM order parameters. By solving them we have obtained the quasi particle energies as,

$$\omega'_{1,2}=\sqrt{\frac{1}{2}}\left(E^2_{1k}+\sqrt{E^4_{1k}-4V^4}\right) \quad (11)$$

and

$$\omega'_{3,4}=\sqrt{\frac{1}{2}}\left(E^2_{2k}+\sqrt{E^4_{2k}-4V^4}\right) \quad (12)$$

where

$$E^2_{1,2} = \in^2_0(\mathrm{k}) + (\Delta \pm \frac{h}{2})^2 + 2V^2 \quad (13)$$

We have made all the parameters (used in the above equations) dimensionless by dividing them by 2t.

3. Results and Discussion

We have solved the two order parameters self consistently and their temperature dependencies are shown in figure (1) and (2).The graphs show the superconductivity and anti-ferromagnetic order parameters for different hybridizations and for different external magnetic fields respectively . On

increasing the magnetic field, superconducting critical temperature decreases from 8.66 to 7.5 and $2\frac{\Delta_0}{k_B T_C}$ increases from 2.59 to 4.03. Similarly anti-ferromagnetic order parameter also decreases with increase in external magnetic field. But with increasing hybridization both the order parameters decrease. By increasing hybridization of localized level with conduction band, hybridization gap increases in the quasi particles spectrum which results in the decrease of density of states at Fermi level. Consequently the transition temperature decreases.

Our model shows coexistence of SC & AFM and the obtained result agrees well with experimental value.

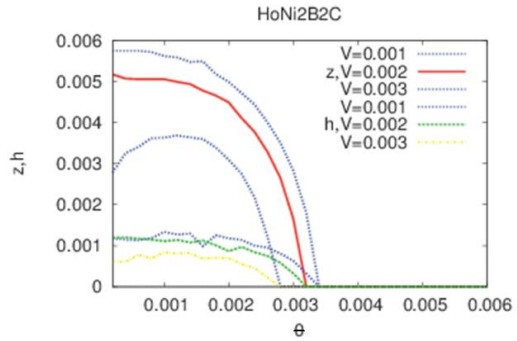

Fig.1: Sc gap (z) and AFM gap (h) Vs. temperature for various hybridization parameters (0.001 to 0.003) for a constant magnetic field parameter (0.001)

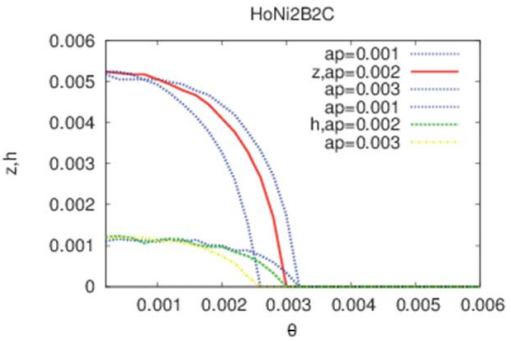

Fig.2: Sc gap (z) and AFM gap (h) Vs. temperature for various magnetic field parameters (0.001 to 0.003) at a constant hybridization parameter (0.002)

4. Conclusion

In this paper we have studied the effect of external magnetic field in the coexisting state of SC and AFM. In the present model, the study of external magnetic field in both SC and AFM long-range order, obtained for $HoNi_2B_2C$ compound, produces the experimentally observed values of T_C and T_N. The graph presented in this paper shows the co-existence of superconductivity and long range anti-ferromagnetic order in the $HoNi_2B_2C$ below T_N. With the increase of hybridization strength, the order parameters are suppressed which is verified experimentally.

In the BCS theory of superconductivity, the conduction electrons in a metal cannot be both superconducting and antiferromagnetic. But the situation has

changed in case of $HoNi_2B_2C$. Here, antiferromagnetic transition takes place well below the superconducting state and truly, the superconductivity and long-range antiferromagnetic order coexist below T_N.

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