Study of de-Gennes factor and effect of external magnetic field on SC and AFM in borocarbide superconductors

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ABSTRACT

We report theoretically coexistence of superconductivity (SC) and antiferomagnetism (AFM) in magnetic borocarbide superconductors RNi2B2C (R=Er, Dy, Ho, Tm). A suitable model Hamiltonian is chosen for itinerant electron system. The BCS type Cooper pairing of conduction electrons of two different Nickel sites are taken in to account. The mean field Hamiltonian is solved exactly by writing the equations of motion of single particle Greens function. Equations for appropriate single particle correlation functions are derived and the order parameters corresponding to SC and AFM are determined. The self consistent numerical calculation shows a strong interplay between SC and AFM. The plot of critical temperature (T_C) and Neel temperature (T_N) for the above compounds versus de Gennes factor shows good agreement with experiment. We also report the effect of external magnetic field on superconductivity (SC) and antiferromagnetism (AFM) in $TmNi_2B_2C$ and $HoNi_2B_2C$ at their co-existence state.

Key Words- Borocarbide Superconductors, Antiferromagnetism

I.INTRODUCTION

The RNi_2B_2C family of quaternary borocarbide superconductors discovered in 1994 has become attractive to study fundamental questions in superconductivity [1]. The interest is because the critical temperature in RNi_2B_2C is relatively high, their superconducting (SC) properties exhibit often unconventional behavior, depending on the rare earth element and coexistence of magnetism and superconductivity in these materials in a wide range of temperatures. However inspite of several publications some fundamental issues as to the nature of pairing mechanism and attractive potential are still under debate for the borocarbide superconductors.

A striking feature distinguishing the quaternary magnetic borocarbide superconductors from other superconductors is that for certain combinations of elements rare-earth and Nickel where superconductivity and antiferromagnetic order have been found to coexist in RNi_2B_2C . The values of the magnetic ordering temoerature (T_N) are comparable to the critical temperature(T_C) values i.e the magnetic energy is comparable

to the superconducting condensation energy. Therefore the investigation of these compounds is expected to result in new insight to interplay superconductivity and magnetism [2—5]. In a rare-earth antiferromagnet, two neighboring magnetic ions order spontaneously in opposite directions below the Néel temperature. Especially when it is placed in an external magnetic field, the two magnetic ions react to the field in different ways, so that they usually have different magnitudes and orientations below the magnetic transition temperature. Therefore, to describe the coexistence properties of antiferromagnetic borocarbide superconductor, the single-ion ferromagnetic-like model is inadequate. To solve this problem, a Hamiltonian of two sublattice system is considered. In the spontaneously ordered state the magnetic moments of rare-earth antiferromagnets is proposed and used in this work to investigate the interplay of SC and AFM in RNi_2B_2C.

II. MODEL AND CALCULATION

The Hamiltonian to be used is of the form

$$H = \sum_{k,\sigma} \varepsilon_0(k) (a^{\dagger}_{k,\sigma} b_{k,\sigma} + h.c) + (h/2) \sum_{k,\sigma} Z_{\sigma} (a^{\dagger}_{k,\sigma} a_{k,\sigma} - b^{\dagger}_{k,\sigma} b_{k,\sigma}) - \sum_{k,\sigma} Z_{\sigma} B (a^{\dagger}_{k,\sigma} a_{k,\sigma} + b^{\dagger}_{k,\sigma} b_{k,\sigma}) - \Delta \sum_{k} [(a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} + a_{-k\downarrow} a_{k\uparrow}) + (b^{\dagger}_{k\uparrow} b^{\dagger}_{-k\downarrow} + b_{-k\downarrow} b_{k\uparrow})] \quad (1)$$

The 1st term in Eq.(1) represents the Hamiltonian involving hopping of the quasi-particles between the neighboring sites of the two sub-lattices in Ni_2B_2C planes. Here $a^{\dagger}_{k,\sigma}(a_{k,\sigma})$ and $b^{\dagger}_{k,\sigma}(b_{k,\sigma})$are creation(annihilation) operators of the conduction electrons of Nickel ions at two sub-lattices A and B respectively with momentum k and spin σ. The hopping takes place between neighboring sites of Nickel with dispersion $\varepsilon_0(k)=-2t_0(\cos kx+\cos ky)$, where t_0 is the nearest neighbor hopping integral. The second term is due to a staggered field(h) which acts on the Ni spins and strongly reduces charge fluctuations between different cites. Zσ in the term represents +1 for up-spin and -1 for down-spin. The third term represents the Hamiltonian due to external magnetic field. It is assumed that s-wave like BCS pairing interaction mediated by some boson exchange exist within the same orbitals of a sub lattice and the same strength of the interaction is taken for the orbitals. The last term represents the super-conducting state of the system where, Δ is the superconducting gap parameter. However, we have neglected the inter-site sub lattice Cooper pairing of the conducting electrons for the simplicity of calculation.

The Hamiltonian of the system is mean field one and has been solved exactly by writing the equations of motion for the single particle Green functions by using double time electron Green function of Zubarev type[6]. The Green functions involved in the calculation are defined in our previous paper [7]. The poles of the Green functions give four quasi particle energy bands. Equations for the appropriate single particle co-relation functions are derived and the SC and AFM order parameters are determined.

$$\Delta(T) = V_0 N(0) \int_{-\omega_D}^{\omega_D} d[\varepsilon_0(k)] \times [F_1(k,T) + F_2(k,T)] \quad (2)$$

$$h(T) = -\frac{1}{2} g\mu_B N(0) \int_{-\frac{W}{2}}^{\frac{W}{2}} d[\varepsilon_0(k)] \times [F_1(k,T) - F_2(k,T)] \quad (3)$$

Where F_1 (k,T) and F_2 (k,T) are the functions of quasiparticle energy bands $\omega_{1,2} = - B \pm \sqrt{[(\frac{h}{2} - \Delta)^2 + \varepsilon_0^2(k)]}$ and $\omega_{3,4} = - B \pm \sqrt{[(\frac{h}{2} + \Delta)^2 + \varepsilon_0^2(k)]}$. We consider here the half filled band situation with the Fermi level lying at the middle of the antiferromagnetic band gap i.e the Fermi level is taken as $\varepsilon_F=0$. The different physical quantities of the atomic subsystem are made dimensionless by dividing them by the nearest neighbor hopping integral $2t_0$, with $W_b=8t_0$ being the width of the conduction band.

III. RESULT AND DISCUSSION

The SC and AFM order parameters at the coexistence state are solved self-consistently and numerically. Fig.1 shows the mean field behavior of SC and AFM for different borocarbide compounds in absence of magnetic field. The theoretically observed values of critical temperatures (Θ_C) and Neel temperatures corresponds to $TmNi_2B_2C$ is 0.00485(12.1K) and 0.00115(2.8K), $DyNi_2B_2C$ having Θ_C = 0.00263(6.57K) and Θ_N = 0.00447(11.17K), $HoNi_2B_2C$ having $\Theta_C = \Theta_N$ = 0.0034(8.5K) and $ErNi_2B_2C$ having Θ_C = 0.00441(11.025K) and Θ_N = 0.002 (5K). The theortical observed values agrees well with experimental findings of the critical and Neel temperature of the above borocarbide compounds.The detailed nature and density of states plots of these borocarbide superconductors is recently reported [8]. From the above observations we found all the three combinations i.e $\Theta_C > \Theta_N$, $\Theta_C = \Theta_N$ and $\Theta_C < \Theta_N$ which shows a strong competition between SC and AFM in RNi_2B_2C .

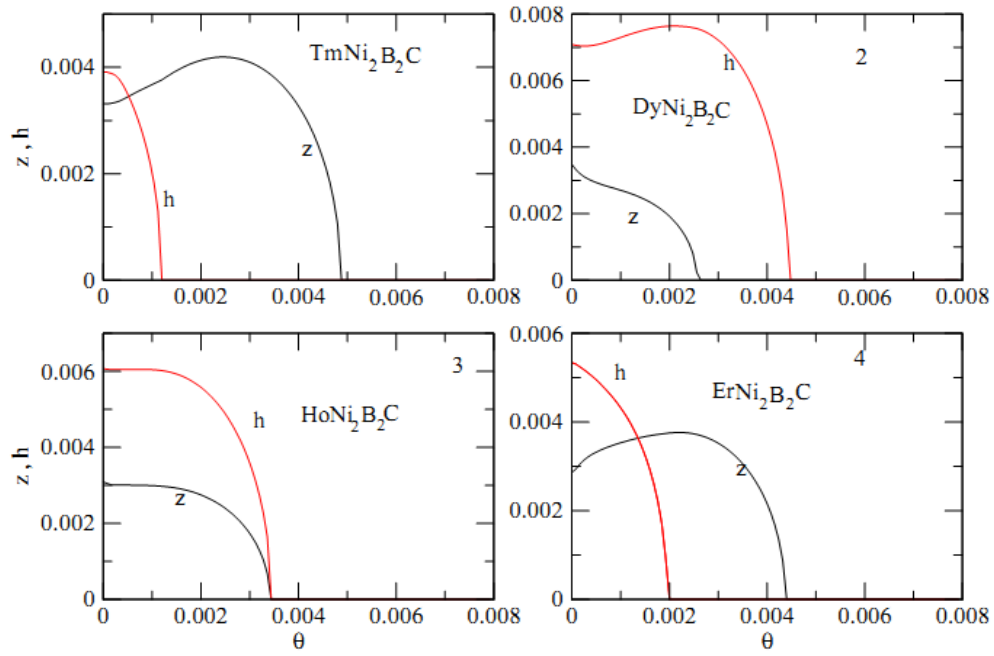

Fig.1 shows the plot of dimensionless SC gap (z) and AFM gap (h) vs. temperature parameter (Θ) for magnetic borocarbide superconductors RNi_2B_2C(R=Tm,Dy,Ho,Er).

Fig. 2 represents the critical temperature and Neel temperature versus de Gennes factor. The de-Gennes factor is expressed as $dG = (g-1)^2 J(J+1)$ where j is the lande factor and J is the total angular momentum of the R^{3+} Hunds rule ground state [9]. By substituting the proper value of total angular momentum (J), lande factor (g), the de Gennes factor for $TmNi_2B_2C$ is 1.167, for $ErNi_2B_2C$ is 2.55, for $HoNi_2B_2C$ is 4.5 and for $DyNi_2B_2C$ is 7.083. Here we plot a graph between critical temperature and Neel temperature (values taken from Fig.1) vs. de Gennes factor. The phase diagram shows in Fig.2 is almost linear. Our theoretical study agrees well with similar type of de Gennes scaling which was reported earlier by Machida et al.[10]. Here, the enhancement of antiferromagnetism and the supression of superconductivity are governed by exchange interaction of conduction electrons and rare earth f- electrons.

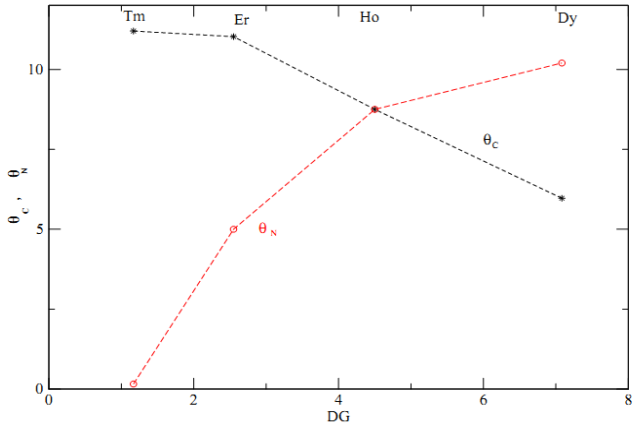

Fig.2 shows critical temperature ($Θ_C$) and Neel Temperature ($Θ_N$) versus de-Gennes factor (DG) of RNi_2B_2C (R=Tm, Er, Ho, Dy).

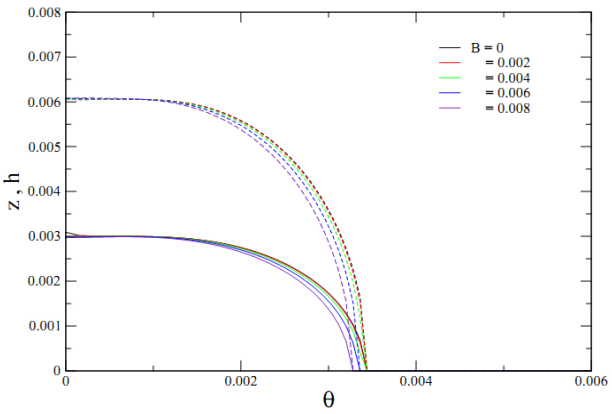

Fig.3 Self-consistent plot of SC and AFM long range orders for the external magnetic field b=0(0 Tesla), 0.0002(0.86 Tesla), 0.0004(1.72 Tesla), 0.0006(2.58T) and 0.0008(3.44 T) for the compound HoNi2B2C.

Fig.3 shows the self consistent plot of SC gap(z) and AFM gap(h) vs. temperature parameter (Θ) of $HoNi_2B_2C$ for different external magnetic field parameter(b)=0 ,0.0002, 0.00004,0.0006,0.0008. When magnetic field w.r.t some quantized axis is applied, the SC gap and AFM gap remains unaffected. But the critical temperature and Neel temperature get reduced due to the application of magnetic field.

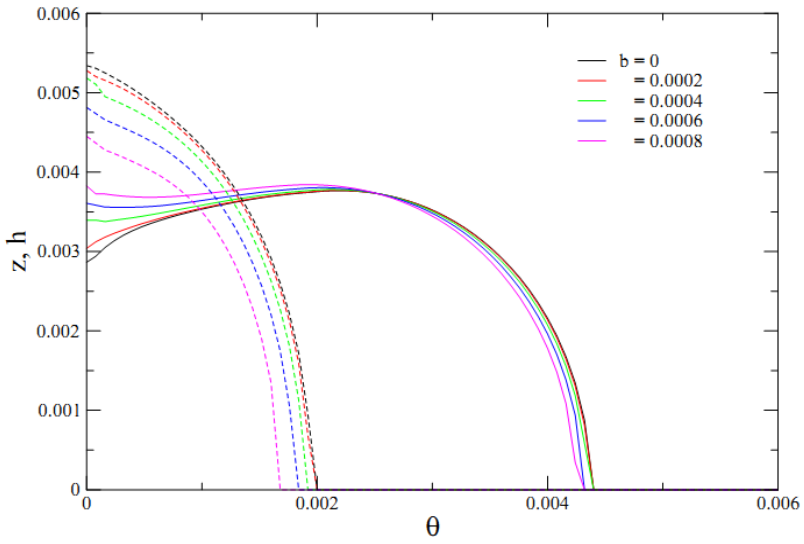

Fig4. Self consistent plot of SC gap(z) and AFM gap(h) vs. temperature parameter (Θ) of $TmNi_2B_2C$ for different external magnetic field parameter(b)=0,0.0002, 0.00004,0.0006,0.0008.

Fig. 4 depicts the self-consistent plot of SC and AFM long range orders for the same external magnetic fields b=0(0 Tesla), 0.0002(0.86 Tesla), 0.0004(1.72 Tesla), 0.0006(2.58T) and 0.0008(3.44 T) for the compound $ErNi_2B_2C$. When magnetic field is applied, the SC gap is suppressed in the pure SC phase due to the Cooper pairing as expected from metallic superconductors. On the contrary, SC gap is enhanced in the co-existence phase on application of external magnetic field. It is observed that AFM gap value is suppressed throughout the temperature range with the application of the magnetic field. In our earlier communication, the critical temperature shows both increasing and decreasing tendency in he pure SC state only [11]. In normal state, the antiferromagnetism (both Neel temperature and AFM order parameter) shows both increasing and decreasing trend on the application of external magnetic field which is also reported [12]. But here, i.e on the coexistence state of SC and AFM, the antiferromagnetism (both Neel temperature and AFM order parameter) only reduces due to the application of external magnetic fields. This interesting result for the compound $ErNi_2B_2C$ may be due to the breaking of spin symmetry and formation of Cooper pairs. Here, we have not mentioned the effect of external magnetic field for other two compounds in this series $TmNi_2B_2C$ and $DyNi_2B_2C$. For these two compounds, the effect of external magnetic field on SC and AFM is robust and our model could not solve SC and AFM self-consistently.

IV.CONCLUSION

A mean field Hamiltonian model is proposed to study the critical temperature and Neel temperature of magnetic borocarbide superconductors. Out of several rare-earth compounds, we only study the magnetic borocarbide superconductors RNi_2B_2C (R=Tm, Dy, Ho, Er). The phase diagram shows the critical temperature decreases and the Neel temperature increases with de-Genns factor which indicates the competition of SC and AFM. The effect of external magnetic field is studied for $HoNi_2B_2C$ and $ErNi_2B_2C$. This model is further improved to study the effective de Gennes factor and effect of dopant concentration on SC and AFM borocarbide superconductors.

V. ACKNOWLEDGMENT

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