CHAPTER II

ANTIFERROMAGNETIC SUPERCONDUCTORS

Introduction to Antiferromagnetic Superconductor (AFS)

The study on the interplay of superconductivity and magnetism was started more than three and half decades ago. The first theoretical study on the interplay of superconductivity and ferromagnetism was published by Ginzburg (Ginzburg,1957) in 1957. He showed that superconductivity is almost impossible to coexist with ferromagnetic order. Baltensperger and Strassler(Baltensperger and Strassler,1963) first pointed out the possibility of the coexistence of superconductivity and antiferromagnetic order. The experimental attempts on the coexistence were initiated by Matthias ,Suhl and Corenzwit (Matthias ,Suhl and Corenzwit ,1959). They studied the mutual interaction between superconductivity and magnetism by introducing magnetic impurities into usual superconductors. However, with this method, the coexistence of superconductivity and long range magnetic order could not be obtained.

In 1977, Matthias' group (Fertig et al.,1977) and Fischer's group (Ishikawa and Fischer,1977) discovered the coexistence of superconductivity and long range magnetic order in the ternary rare earth (RE) compounds $RERh_4B_4$ and $REMo_6S_8$ (the Chevrel compounds) . Of these compounds $ErRh_4B_4$ and $HoMo_6S_8$ are ferromagnetic superconductor. Over a narrow temperature range above the ferromagnetic transition temperature, the superconducting state coexists with magnetic order. The compounds

$REMo_6S_8$ with RE=Gd,Tb,Dy,Er and $RERh_4B_4$ with RE=Nd,Sm,Tm are antiferromagnetic superconductors. These compounds become superconductor at $T=T_c$ and with the temperature being lowered further suffer a phase transition to an antiferromagnetic state at $T_N<T_c$ (T_N is Neel temperature) . At temperature below T_N the superconducting and antiferromagnetic orderings coexists. This kind of coexistence has also been found in $Tb_2Mo_3Si_4$, a heavy fermion superconductor (Broholm et al.,1987) and high-T_c superconductor $REBa_2Cu_3O_{7-x}$ (RE=Gd,Er,Dy) (Willis et al.,1987)..For instance, the value of $T_c$and T_N respectively, have been about 1.4 K and 0.8 K for $GdMo_6S_8$, 1.8 K and 1.0 K for $TbMo_6S_8$, and 2.0 K and 0.4 K for $DyMo_6S_8$ (Ishikawa and Fischer,1977;Hamaker et al.,1979).

For definiteness we will focus on Chevrel compounds and ternary rare-earth borides, in these materials the antiferromagnetism is associated with the f electron of the rare-earth atoms and the superconductivity is due to the d conduction electrons of Mo or Rh. Below T_N, the interaction between the magnetic and the conduction electrons is replaced by a staggered molecular field (H_Q) which acts on the conduction electrons. This field is detrimental to BCS pairing because it acts in opposite ways on the spins of the electrons making the Cooper pair.

Neutron Scattering Studies of AFS

While neutrons unfortunately cannot couple directly to the superconducting order parameter, they are an ideal probe for studying the magnetic order parameter at microscopic level. We cosider neutron diffraction experiments carried out on the antiferromagnetic superconductors. These are summarized in table 2.1 . For all of these materials, below T_N, superconductivity and antiferromagnetic long-range order coexist all the down to the lowest temperature. Hamaker et al.(Hamaker et al.,1983) have studied, by powder diffraction, the compound $Ho(Rh_{0.3}Ir_{0.7})_4B_4$, where a continuous transition occurs to an antiferromagnetic state at 2.7 K from a normal paramagnetic state. Superconductity then sets in at a lower temperature of T_c=1.34 K and coexists

Table 2.1

Magnetic structures of antiferromagnetic superconductors as determined by neutron diffraction (Matsubara and Kotani,1984).

Compound	T_c	T_N	Direction of q	Moment Direction
$GdMo_6Se_8$	5.6 K	0.75 K	[100]	-
$DyMo_6S_8$	2.05 K	0.4 K	[100]	[111]
$TbMo_6S_8$	2.05 K	1.0 K	[100]	[111]
$TmRh_4Bh_4$	9.8 K	0.7 K	[101]	[010]

with the magnetic long-range order for lower temperatures. The onset of superconductivity has no discernible effect on the magnetic ordering which is estimated to be long range. Another way to understand this is that the antiferromagnetic interaction has a wave vector which much shorter than either the London penetration depth or coherence length of the superconductor and hence is not strongly affected by either the supercurrent screening effects or the singlet pairing effects.

Nass-Levin-Grest Theory

We consider the theory introduced by Nass, Levin, and Grest(Nass, Levin ,and Grest,1981,1982). Nass, Levin, and Grest have applied a mean field theory to AFS . They considered that in the rare earth borides there are two groups of electrons of interest. The first, the 4f electrons on the rare earth atoms, form localized moments. The second group are the d-band conductions electrons which undergo the superconducting pairing. With this fact, the Hamiltonian contains the d-electron kinetic energy, the d-f electron exchange interaction, and d-d interaction arising from the phonon, they have for the Hamiltonian

$$H = \sum_{k\sigma} \varepsilon_k C^{+}_{k\sigma} C_{k\sigma} - \sum_{kk'q\sigma\sigma'} V_{kk'q} C^{+}_{k+q\,\sigma} C^{+}_{k'-q\,\sigma'} C_{k'\sigma'} C_{k\sigma} - (I/2N) \sum_{kk'\sigma\sigma'} \vec{S}_i \cdot \vec{S}\, C_{k\sigma} C_{k'\sigma'} \exp[i(\vec{k}-\vec{k}')\cdot\vec{R}_i] \qquad (2.1)$$

where $\vec{S}$ ($\vec{S}_i$) is the spin angular momentum operator of the 4f electrons (on site i). Below T_N, a staggered temperature independent molecular field $H_Q = I\langle S_Q\rangle/2N$ is non-zero. Here $\vec{S}_Q$ is the Fourier transform of $\vec{S}_i$ and $\vec{Q}$, the wave vector of the antiferromagnetic state. Finally $\langle S_Q\rangle$ is the magnetic order parameter of the localized spins. $V_{kk'q}$ is the usual BCS pairing potential. I is the d-f electron exchange interaction. Since $Q \neq 0$, they have allowed for $q \neq 0$ contributions in the second term of Eq.(2.1). The mean field decoupling of the Hamiltonian yields

$$H = \sum_{k\sigma} \varepsilon_k C^{+}_{k\sigma} C_{k\sigma} - \sum_{k\sigma} H_{Q\sigma} (C^{+}_{k\sigma} C_{k+Q\sigma} + h.c.) - \sum_{k} \Delta_0(k) (C^{+}_{k\uparrow} C^{+}_{-k\downarrow} + h.c.)$$

$$- \sum_{k} \Delta_Q(k) (C^{+}_{k+Q\uparrow} C^{+}_{-k\downarrow} + h.c.) - \sum_{k} \Delta_{-Q}(k) (C^{+}_{k\uparrow} C^{+}_{-k-Q\downarrow} + h.c.) \qquad (2.2)$$

Here, the parameters $\Delta_0(k)$ and $\Delta_{\pm Q}(k)$ are determined by the self-consistent equations

$$\Delta_0(k) = \sum_{k'} \langle C_{-k'\downarrow} C_{k'\uparrow} \rangle V_{kk'0} \qquad (2.3.1)$$

$$\Delta_Q(k) = 2 \sum_{k'} \langle C_{-k'\downarrow} C_{k'+Q\uparrow} \rangle V_{kk'Q} \qquad (2.3.2)$$

$$\Delta_{-Q}(k) = 2 \sum_{k'} \langle C_{-k'-Q\downarrow} C_{k'\uparrow} \rangle V_{kk'-Q} \qquad (2.3.3)$$

The prime on the summation in Eqs.(2.2) and (2.3) indicates that the summation is restricted to regions of the Fermi surface in which both $\varepsilon_{k'}$ and $\varepsilon_{k'+Q}$ are within ω_D of Fermi energy. In this formalism there are three self-consistent gap equations to solve, Eq.(2.3) must be solved numerically. However, one special case leads to an analytical solution, that is when the system is one dimensional so that $\varepsilon_k = -\varepsilon_{k+Q}$ for $|k| \approx k_F$, $Q \approx 2k_F$ and $\Delta_Q = -\Delta_{-Q}$. A general detailed numerical study suggests that the case $\Delta_0 \neq 0$ with $\Delta_Q = -\Delta_{-Q} = 0$, $Q \neq 0$, is the only allowed nontrivial solution of Eq.(2.2), so that in one dimension the usual BCS pairing is preferred. Physically, this is a consequence of the fact that $Q \approx 2k_F$ is large compared to the inverse coherence length ξ^{-1}, so that Cooper pairing of this large momentum Q is highly favorable.

According to Nass-Levin-Grest theory, they found that in the one-dimensional system the Hamiltonian of the AFS system is

$$H = \sum_{k\alpha} \varepsilon_k C^{+}_{k\alpha} C_{k\alpha} - \Delta \sum_{k} (C^{+}_{k\uparrow} C^{+}_{-k\downarrow} + \text{h.c.}) - H_Q \sum_{k\alpha\beta} (\sigma_Z)_{\alpha\beta} (C^{+}_{k\alpha} C_{k+Q\,\beta} + \text{h.c.}) \qquad (2.4)$$

where ε_k is the band energy of the conduction electron measured from the Fermi energy. $C^{+}_{k,\alpha}$ ($C_{k,\alpha}$) is the creation (annihilation) operator for electron with momentum k and spin α, σ_z is the Pauli matrix, Δ is the superconducting order parameter, H_Q is the staggered molecular field which is taken to be temperature independent. The superconducting order parameter is given by

$$\Delta = g \sum_{k} \langle C^{+}_{k\uparrow} \; C^{+}_{-k\downarrow} \rangle = g \sum_{k} \langle C_{-k\downarrow} \; C_{k\uparrow} \rangle \qquad (2.5)$$

where g is the BCS coupling constant and the bracket $\langle\,\rangle$ denotes the thermal average.

The Hamiltonian given by Eq.(2.4) is the same as that given by Machida, Nokura, and Matsubara (Machida, Nokura, and Matsubara ,1980) and Nass, Levin, and Grest (Nass,Levin,and Grest,1981). When H_Q=0, it corresponds to the ones studied by Sarma (Sarma,1963) and Maki and Tsuneto (Maki and Tsuneto,1964). It also agrees with the model given by Suzumura and Nagi (Suzumura and Nagi,1981) who studied the effect of a homogenous magnetic field on AFS.

Assuming a one-dimensional-like half-filled band which safisfies the condition $\varepsilon_k=-\varepsilon_{k+Q}$, Suzumura and Nagi obtain the finite-temperature Green's function as

$$G^{-1}(k,\omega_n) \;=\; i\,\omega_n - \varepsilon_k\,\rho_3\sigma_3 + \Delta\,\sigma_1 + H_Q\,\rho_1 \tag{2.6}$$

where $\omega_n = \pi T(2n+1)$, T is temperature, n is an integer, and σ_i and ρ_i (i=1,2,3) are the Pauli matrices operating on the spin and electron-hole states respectively.

The critical temperature T_c of AFS as obtained by Suzumura and Nagi (Suzumura and Nagi , 1981) is related to the critical temperature of pure BCS superconductor T_{c0} as follows :

$$\ln(T_c/T_{c0}) = -\sum_{n=0}^{\infty}\{(n+1/2)^{-1} + [(n+1/2)^2+(H_Q/2\pi T_c)^2]^{-1/2} + (H_Q/2\pi T_c)^2\,[(n+1/2)^2+(H_Q/2\pi T_c)^2]^{-3/2}\} \tag{2.7}$$

here T_{c0} is the critical temperarture of pure superconductor. The behavior of T_c/T_{c0} as a function of H_Q/Δ_0 ($\Delta_0$is the BCS order parameter) is shown in Fig. 2.1 .

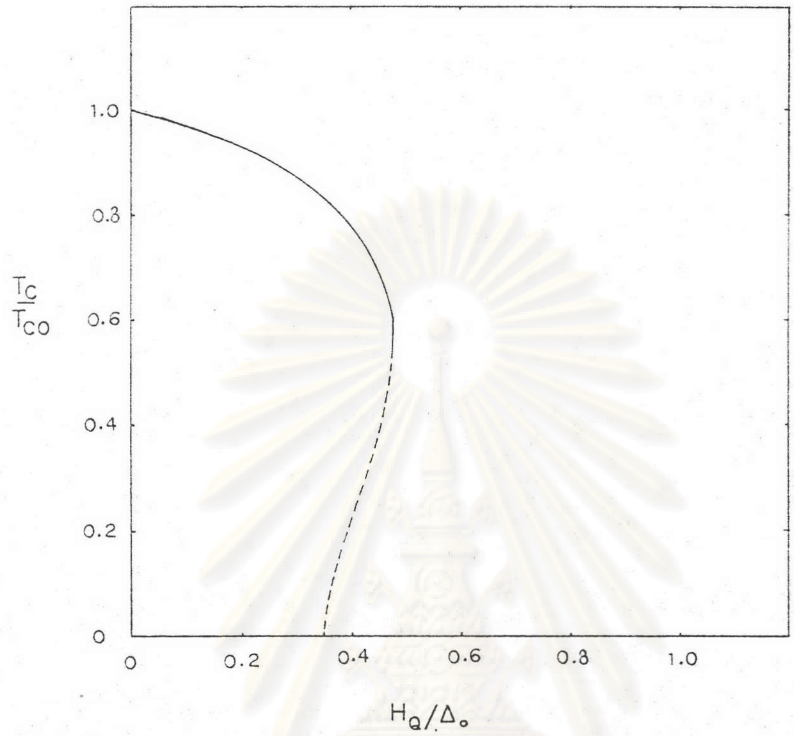

Fig. 2.1 T_c/T_{c0} as a function of H_Q/Δ_0 (Suzumura and Nagi , 1981)

Replacing $(2n+1)\pi T$ by ω_n in Eq.(2.7), we have

$$\ln(T_c/T_{c0}) \;=\; 2\pi T_c \sum_{n\geq 0}^{\omega_D/2\pi T_c} \{\, \omega_n^2\,[\omega_n^2+H_Q^2]^{-3/2} - 1/\omega_n \,\} \qquad (2.8)$$

Suzumura and Nagi found that Eqs.(2.7) and (2.8) agrees with T_c formula of Machida ,Nokura ,and Matsubara (Machida,Nokura,and Matsubara,1980) and when the stable T_c exists, T_c decreases monotonously as H_Q/Δ_0 is increased.

Finally,we will describe briefly the attempts by many researchers to explain and study the problem of coexistence between superconductivity and antiferromagnetism.

Machida, Nokura, and Matsubara (Machida,Nokura,and Matsubara,1980) have demonstrated that AFS can be well described by a model in which a spin-density wave ordering with a wave vector $\vec{Q}$ coexists with superconductivity , they predicted the existence of a new pairing state in these superconductors. Nass ,Levin ,and Grest (Nass, Levin,and Grest,1981) have applied a mean field theory to AFS and found that the usual BCS pairing state is more stable than the new pairing state in the presence of H_Q.Suzumura and Nagi (Suzumura and Nagi,1982) have studied the effect of a homogeneous magnetic field (H_0) on one-dimensional AFS.The effect of impurities on AFS has also been studied by Nass, Levin ,and Grest (Nass,Levin,and Grest,1982). They have found that nonmagnetic impurities can make AFS gapless at moderate concentrations.Ishino and Suzumura (Ishino and Suzumura,1982) have studied the effect of a sinusoidal magnetic field, homogeneous magnetic field, and staggered molecular field on superconductivity and the magnetic susceptibility of AFS. They have found that H_0 has an additive effect of destroying the superconducting state in the presence of H_Q . Okabe and Nagi (Okabe and Nagi,1983) have studied the effect of nonmagnetic impurities on AFS and found the condition for the appearance of the gapless superconductor. The temperature dependence of the upper critical field in AFS has been computed by Ro and Levin (Ro and Levin,1984). Prohammer and Schachinger (Prohammer and Schachinger,1986) have applied mean field model of Nass-Levin-Grest to strong coupling system of AFS. In this system the critical value of H_Q is largely affected by the strong coupling corrections. Chi and Nagi (Chi and Nagi,1987,1988, 1990,1992) have applied a mean field theory given by Nass,Levin, and Grest to investigate the following properties of the AFS (I) the critical curve of a transition of the second kind in AFS with nonmagnetic impurities.(II) the order parameter and the maximum Josephson current for AFS. (III) the effect of all types of impurities (nonmagnetic, magnetic,and spin-orbit) on AFS by studying the transition temperature and the specific heat jump.(IV) the superconducting density of states and the tunneling differential conductivity for AFS in both paramagnetic and antiferromagnetic phases. (V) the transport properties of AFS with $T_N<T_c$.

To the best of our knowledge, the study of the bilayered AFS system has never been investigated. This motivated us to address ourselves to question of calculating the T_c of a bilayered AFS sandwich. In the next chapter, we will describe the theory of a superconducting sandwich and use it to obtain the T_c formula of a bilayered AFS sandwich.