CHAPTER, IV

PROXIMITY EFFECT SANDWICHES

CONTAINING

NONMAGNETIC LOCALIZED STATES

In this chapter, we present the extension of McMillan's calculation to the case when the normal side contains nonmagnetic localized states. The Hamiltonian of the total system therefore is identical to that of McMillan except for the inclusion of resonance scattering and Coulomb correlation terms describing the effects of the nonmagnetic impurities in the normal film. As in McMillan's theory, the transfer Hamiltonian is treated self-consistently up to second order in perturbation theory.

4.1 Gap Equations

The physical system we are interested in is similar to that of McMillan (7) (see Fig. 3.1) except that the normal layer contains randomly distribution of nonmagnetic localized states. Both N and S films are assumed to be clean ($\ell \sim d$) and the coherence length ξ be much larger than d. The purpose of this section is to derive self-consistent equations for the renormalized superconductivity energy-gap functions in each film. The gap functions determine the nature of the one-electron excitation spectrum in the superconducting state.

The Hamiltonian for such a sandwich in the McMillan tunneling model (7) is given by

$$H = H_{S} + H_{N} + H_{T}$$
(4.1)

(a) H_{S} is the total Hamiltonian of film S and is given by

$$H_{S} = H_{OS} + H_{SS}^{BCS}$$
(4.2)

 H_{OS} is the noninteracting Hamiltonian for the superconducting film and H_{SS}^{BCS} is the BCS interaction between superconducting pairs with coupling constant λ_{c} .

(b) ${\rm H}_{\rm N}$ is the total Hamiltonian for the nonmagnetic alloy film and is written

$$H_{N} = H_{ON} + H_{res} + H_{corr}$$
(4.3)

H is the noninteracting Hamiltonian for the alloy. The resonance scattering are described by

$$H_{res} = \sum_{i} \sum_{k'js} (V_{kj'}c_{js}^{\dagger}b_{k's}^{+}V_{k'j}b_{k's}^{\dagger}c_{js})$$
(4.4)

where $b_{k's}^{\dagger}$ and $b_{k's}^{\dagger}$ are creation and destruction operators for an s-electron state with spin s in the alloy film, and similarly c_{js}^{\dagger} and c_{js}^{\dagger} for a d-electron state and spin s. $\sum_{i}^{}$ is the sum over impurity sites. It is assumed that there is no significant interaction between different impurity sites.

The effect on the pairing of the d-d Coulomb repulsion U is given by

$$H_{corr} = -\sum_{i} \sum_{j} \Delta_{a} (c_{j\dagger}^{\dagger} c_{j\downarrow}^{\dagger} + c_{j\downarrow} c_{j\downarrow})$$
(4.5)

where



(c) The electrical contact between these films is described by the transfer Hamiltonian ${\rm H}_{\rm T}$ given by

$$H_{T} = T_{m} \sum_{kk'} (a_{k}^{\dagger} b_{k'} + b_{-k'}^{\dagger} a_{-k'}) + H.c. \qquad (4.7)$$

 T_m is the transfer matrix element assumed independent of k and k'.

 $\Delta_{d} = - U \langle c_{d} c_{d} \rangle$

The Hamiltonian H in Eq. (4.1) is treated self-consistently to second order in both T and V in the Nambu-Schrieffer formalism for superconductivity (60). The equations for the 2 x 2 matrix self-energies are presented in diagrammatic form in Fig. 4.1. $\Sigma_{s}(\omega)$ and $\Sigma_{n}(\omega)$ are the self-energies of superconducting electrons in the superconducting and normal films. $\Sigma_{d}(\omega)$ is the self-energy of d electrons in the normal film. The double lines represent the full matrix propagators $G_{s}(\omega)$, $G_{n}(\omega)$ and $G_{d}(\omega)$ for electrons in the superconducting and normal films.

The term (a) in Fig 4.1 represents the BCS pairing correlation in film S. It is given by

$$\Sigma_{s}^{BCS} = \Delta_{s} \gamma_{1} \qquad (4.8)$$

where Δ is the usual BCS order parameter.

Term (c) and (e) describe the resonance scattering of s electrons with d electrons in film N. These terms are obtained by using the standard technique developed by Edwards (60) and by Abrikosov and Gor'kov (61) and are given by

$$\sum_{n}^{\text{res}} = |v_{kj}|^2 \sum_{j} \zeta_{3} G_{dj} (\omega) \zeta_{3}$$
(4.9)

and

$$\Sigma_{d}^{\text{res}} = | v_{kj} | \sum_{k'} \chi_{3} G_{Nk'}(\omega) \chi_{3} \qquad (4.10)$$

Term (b) and (d) represent the penetration of electrons through the barrior. These self-energy terms are

$$\Sigma_{s} = T_{m}^{2} \sum_{k'} \chi_{3} G_{Nk}, (\omega) \chi_{3}$$
(4.11)

and

$$\Sigma_{N}^{\text{tunneling}} = T_{m}^{2} \sum_{k} \zeta_{3} G_{Sk}^{} (\omega) \zeta_{3}^{} (4.12)$$

Term (f)arises from the Coulomb repulsion of opposite spin d electrons and is given by

$$\Sigma_{d}^{\text{corr}} = \Delta_{d} \chi_{1}$$
 (4.13)

In the usual way, we write

$$G_{sk}(\omega) = \left[z_{s}(\omega) \omega \mathbf{1} - \mathcal{E}_{k} \tau_{3} - \phi_{s}(\omega) \tau_{1} \right]^{1} \quad (4.14a)$$

$$G_{Nk}(\omega) = \left[Z_{N}(\omega) \omega \mathbf{1} - \varepsilon_{k}, \ \tau_{3} - \phi_{N}(\omega) \ \tau_{1} \right]^{-1}$$
(4.14b)

$$G_{dj}(\omega) = \left[z_{d}(\omega)\omega \mathbf{1} - \varepsilon_{j} z_{3} - \phi_{d}(\omega) z_{1} \right]^{-1}$$
(4.14c)

where **1** is the 2 x 2 unit matrix, γ_1 and γ_3 are Pauli matrices. Substitution of Eq. (4.8) into equations represented by the diagrams of Fiq. 4.1 gives the following self-consistent equations (at temperature T) :

$$z_{s}(\omega) = \frac{1+}{\left[\phi_{N}^{2}(\omega) + z_{N}^{2}(\omega)\omega^{2}\right]^{\frac{1}{2}}}$$
(4.15a)

$$\varphi_{\rm S}(\omega) = \Delta_{\rm S}^{\rm ph} + \frac{\Gamma_{\rm S} Z_{\rm N}(\omega)}{\left[\phi_{\rm N}^{2}(\omega) + Z_{\rm N}^{2}(\omega) \omega^{2}\right]^{\frac{1}{2}}}$$
(4.15b)

$$Z_{N}(\omega) = 1 + \left[\frac{\phi_{S}^{2}(\omega) + Z_{S}^{2}(\omega) - \omega^{2}}{\left[\phi_{S}^{2}(\omega) + Z_{S}^{2}(\omega) - \omega^{2}\right]}\right]^{\frac{1}{2}}$$

+
$$\frac{n_{\mathrm{I}} \Gamma_{\mathrm{d}}}{\Re N_{\mathrm{N}}^{(0)}} \frac{Z_{\mathrm{d}}^{(\omega)}}{\phi_{\mathrm{d}}^{2}(\omega) + Z_{\mathrm{d}}^{2}(\omega) \omega^{2} + E_{\mathrm{d}}^{2}}$$
 (4.16a)

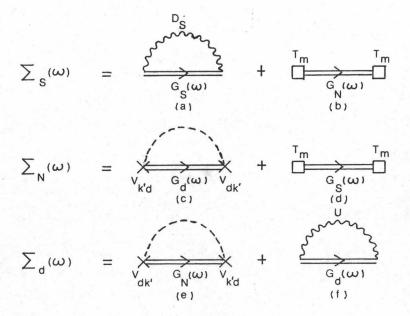


Fig. 4.1. Self-energy equations in diagrammatic form in film S and N. $G_S(\omega)$ is the full electron propagator in film S. $G_N(\omega)$ and $G_d(\omega)$ are the full s- and d-electron propagators in film N. T_m is the tunneling matrix element. D_S is the BCS electronphonon interaction in film S, U the Coulomb repulsion of opposite spin d electrons; the crosses represent resonance scattering at an impurity site, with matrix elements V_{kd} .

$$\phi_{N}(\omega) = \frac{\Gamma_{N} \phi_{S}(\omega)}{\left[\phi_{S}^{2}(\omega) + z_{S}^{2}(\omega)\omega^{2}\right]^{\frac{1}{2}}} + \frac{n_{\perp} \Gamma_{d}}{\pi_{N_{N}}(o)} \frac{\phi_{d}}{\phi_{d}^{2}(\omega) + z_{d}^{2}(\omega)\omega^{2} + E_{d}^{2}}$$
(4.16b)

$$Z_{d}(\omega) = \Delta_{d} + \frac{\int_{d}^{Z} Z_{N}(\omega)}{\left[\phi_{N}^{2}(\omega) + Z_{N}^{2}(\omega) \omega^{2}\right]^{\frac{1}{2}}}$$
(4.17a)

$$\phi_{d}(\omega) = \frac{\int_{d} \phi_{N}(\omega)}{\left[\phi_{N}^{2}(\omega) + z_{N}^{2}(\omega) \omega^{2}\right]^{\frac{1}{2}}}$$
(4.17b)

where $\omega = (2n + 1) \, \, {}^{\Lambda}k_{\rm B}{}^{\rm T}$, n is an integer. $\Gamma_{\rm S}$ and $\Gamma_{\rm N}$ are the McMillan tunneling parameters, defined as in Eq. (3.8). $\Gamma_{\rm d}$ is the half-width of the d resonance and ${}^{\rm E}_{\rm d}$ is the displacement of its centre from the Fermi level. $\Gamma_{\rm d}$ is given by

$$\Gamma_{d} = N_{N}(0)\pi |V_{k'j}|^{2}$$
(4.18)

 $\mathbf{n}_{_{\mathrm{T}}}$ is the impurity concentration in atomic fraction.

At temperature T, the self-consistent potential $\Delta_S^{\ \rm ph}$ is given by

$$\Delta_{s}^{ph} = 2 \lambda_{s} N_{s}(0) \pi k_{B}^{T} \sum_{(|\omega| < \omega_{D})} \frac{\phi_{s}(\omega)}{\left[\phi_{s}^{2}(\omega) + z_{s}^{2}(\omega) \omega^{2}\right]^{\frac{1}{2}}}$$
(4.19)

Eqns. (4.9), (4.10), (4.11) and (4.13) can be simplified by introducing

$$u_{\rm S} = \frac{Z_{\rm S} \omega}{\phi_{\rm S}}, \ u_{\rm N} = \frac{Z_{\rm N} \omega}{\phi_{\rm N}} \text{ and } u_{\rm d} = \frac{Z_{\rm d} \omega}{\phi_{\rm d}}$$
 (4.20)

so that

$$u_{s} \Delta_{s}^{ph} = \omega + \frac{\int_{s}^{(u_{N} - u_{s})}}{(1 + u_{N}^{2})}$$
(4.21)

$$\frac{\Gamma_{N}(u_{N}-u_{S})}{(1+u_{S}^{2})^{\frac{n}{2}}} = \omega + \frac{n_{I}\Gamma_{d}}{\pi_{N_{N}}(0)}$$

$$X = \frac{(u_{d} - u_{N})(1 + u_{N}^{2})^{\frac{2}{2}}}{\left[\alpha \Delta_{s}^{ph}(1 + u_{N}^{2})^{\frac{1}{2}} + \Gamma_{d}\right](1 + u_{d}^{2})}$$
(4.22)

$$\alpha u_{d} \Delta_{S}^{ph} = \omega + \frac{\Gamma_{d}^{(u_{N} - u_{d})}}{(1 + u_{N}^{2})^{\frac{1}{2}}}$$
 (4.23)

and

$$\Delta_{\rm S}^{\rm ph} = \lambda_{\rm S}^{\rm N}{}_{\rm S}^{\rm (0)} \cdot 2\pi \, {\rm k}_{\rm B}^{\rm T} \sum_{(|\omega| < \omega_{\rm D})} \frac{1}{(1 - {\rm u}_{\rm S}^{\rm 2})^{\frac{1}{2}}}$$
(4.24)

where, as in Tang and Roongkeadsakoon theory (5), $\alpha = \Delta_d / \Delta_S^{ph} = constant.$

4.2 Transition Temperature

The equation of the critical temperature T_c for the NS sandwich is obtained by linearizing Eqs. (4.15) to (4.18) by the expansion method of Shiba (60), by substituting into them the expansion of u_s , u_N , u_d in power of Δ_s^{ph}

$$u_{s} = a_{l} \Delta_{s} \frac{ph}{s} + a_{-l} \Delta_{s}^{ph}$$
(4.25a)

$$u_{N} = b_{1} \Delta_{S}^{ph} + b_{-1} / \Delta_{S}^{ph}$$
 (4.25b)

$$u_{d} = c_{l} \Delta_{s}^{ph} + c_{-l} \Delta_{s}^{ph}$$
(4.25c))

Equating the coefficients of Δ_S^{ph} and 1/ Δ_S^{ph} of the resulting equations, we have (See Appendix A)

$$a_{-1} = \frac{(\omega + \Gamma_{s})b_{-1}}{(b_{-1} + \Gamma_{s})}$$
(4.26)

$$b_{-1} = \frac{\omega + \frac{\Gamma_{N}\omega}{(\omega + \Gamma_{n})} + \frac{n_{I}\Gamma_{d}}{\pi N_{N}(0)} \frac{\omega}{(\omega + \Gamma_{d})^{2}}}{\frac{\Gamma_{N}}{\omega + \Gamma_{s}} + \frac{n_{I}\Gamma_{d}}{\pi N_{N}(0)} \frac{\omega}{(\omega + \Gamma_{d})^{2}}}$$
(4.27)

$$c_{-1} = \frac{(\omega + \Gamma_{d})b_{-1}}{(\alpha b_{-1} + \Gamma_{d})}$$
(4.28)

$$a_{1} = \frac{\Gamma_{S}}{b_{-1} + \Gamma_{S}} \left[\frac{a_{-1}b_{1}}{a_{-1}} - \frac{(b_{-1} - a_{-1})}{2b_{-1}} \right]$$
(4.29)

and

$$b_{1} = \left[\frac{n_{1} \Gamma_{d}}{\pi_{N_{N}}(0)} \frac{(c_{-1} - b_{-1})(\Gamma_{d}c_{-1} - \Gamma_{d}b_{-1} - \alpha b_{-1}^{2})}{c_{-1}^{4}(\alpha b_{-1} + \Gamma_{d})^{2}} + \frac{\Gamma_{N}(a_{-1} - b_{-1})(\Gamma_{S}a_{-1} - \Gamma_{S}b_{-1} - b_{-1}^{2})}{2a_{-1}^{3}b_{-1}(b_{-1} + \Gamma_{S})} \right] / \left[\frac{\Gamma_{N}b_{-1}}{a_{-1}(b_{-1} + \Gamma_{S})} \right]$$

$$+ \frac{n_{I} \left[\frac{d^{b} - 1}{d^{b} - 1} \right]}{\pi N_{N}(0) c_{-1}^{2} (b_{-1} + \Gamma_{d})}$$
(4.30)

$$c_{\perp} = \frac{\int_{a} \left[\frac{c_{-\perp}b_{\perp}}{b_{-\perp}} - \frac{b_{-\perp}-a_{-\perp}}{2b_{-\perp}} \right]}{\alpha b_{-\perp} + \int_{a} \left[\frac{c_{-\perp}b_{\perp}}{b_{-\perp}} - \frac{b_{-\perp}-a_{-\perp}}{2b_{-\perp}} \right]}$$
(4.31)

Equations (4.18) and (4.19a) give the equation for T_{c}

$$\ln \frac{T_{c}}{T_{c}^{B}} = 2 \mathcal{T} k_{B} T_{c} \sum_{\omega} \left(\frac{1}{a_{-1}} - \frac{1}{\omega} \right)$$
(4.32)

where T^B_{c} is the transition temperature of the Bulk material of film c.

Eq. (4.26) have been solved by computer using a trial-error procedure (see Appendix C). We have plotted the resulting values of T_c as a function of impurity concentration n_I in Fig. 4.2.

4.3 Jump of the Specific Heat at the Transition temperature

The jump of the specific heat $\triangle C$ is easily evaluated by employing the equation for the order parameter near T_{c} . In fact. after substituting Eq. (4.19a) into Eq. (4.18), we have

$$\ln \frac{T_{c}^{B}}{T} = B_{O}(n_{I}, T) + \frac{1}{2} B_{I}(n_{I}, T) \left(\frac{\Delta s^{ph}}{2\pi k_{B}^{T}}\right)^{2} + \dots \qquad (4.33)$$

where

$$B_{0}(n_{1},T) = 2 \pi k_{B}T \qquad \sum_{n=0}^{\infty} (\frac{1}{\omega} - \frac{1}{a_{-1}})$$
 (4.34)

and

$$B_{1}(n_{1},T) = (2\pi k_{B}T)^{3} \sum_{n=0}^{\infty} (2a_{1} + \frac{1}{a_{-1}}) (\frac{1}{a_{-1}})^{2}$$
(4.35)

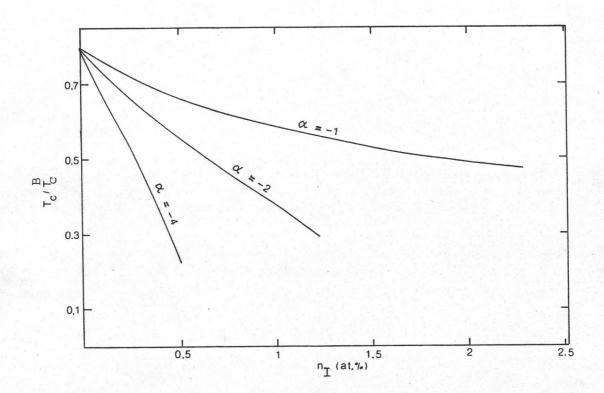


Fig. 4.2. Reduced transition temperature T_c/T_c_0 vs. impurity concentration n_I for $\Gamma_d = 0.75$ eV, $E_d = 0$, $\Gamma_S = 0.2 \Delta_B$, $\Gamma_N = 0.8 \Delta_B$ (Δ_B is the order parameter of the bulk superconductor).

 a_{-1} and a_{1} are determined from Eqns. (4.20) and (4.23). The difference between the values of the thermodynamic potential for the superconducting and normal states of the S layer is expressed as (see Appendix B)

$$\Omega_{s} - \Omega_{n} = \int_{0}^{\Delta_{s} \text{ph}} d\Delta_{s}^{\text{ph}} (\Delta_{s}^{\text{ph}})^{2} \frac{d(1/\lambda_{s})}{d\Delta_{s}^{\text{ph}}}$$
(4.36)

which reduces to

$$\Omega_{\rm s} - \Omega_{\rm n} = -\frac{1}{4} N_{\rm s}^{(0)} B_{\rm l}^{(n_{\rm l}, T)} \frac{(\Delta_{\rm s}^{\rm ph})^4}{(2 \pi k_{\rm B}^{\rm T} c)^2}$$
(4.37)

near T. Here use has been made of the relation

$$\delta \left(\frac{1}{\lambda_{s}} \right) = -N_{s}(0)B_{1}(n_{I},T) \frac{\Delta_{s}^{ph} \delta \Delta_{s}^{ph}}{\left(2\pi k_{B}T_{c}\right)^{2}}$$
(4.38)

which is derivable from Eq. (4.27) for $T \leq T_c$. For temperature closed to T_c , Δ_s^{ph} can be determined by expanding both sides of Eq. (4.27) about T_c to give

$$(\Delta_{\rm S}^{\rm ph})^2 = \frac{2(2\pi k_{\rm B}T_{\rm c})^2}{B_{\rm l}(n_{\rm l},T_{\rm c})} \left(1 + T_{\rm c}\frac{\partial B_{\rm O}(N_{\rm l},T_{\rm c})}{\partial T_{\rm c}}\right)$$
$$\times \left(1 - \frac{T}{T_{\rm c}}\right) \qquad (4.39)$$

The jump in the specific heat at T of the S layer can be obtained from the thermodynamic relation

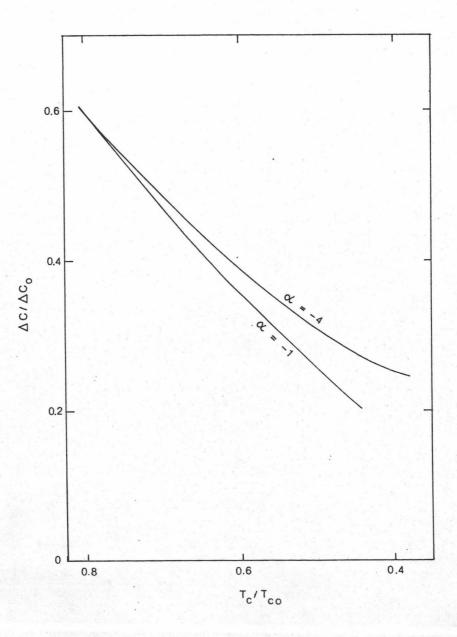


Fig. 4.3. Reduced specific heat jump $\Delta C/\Delta C_0$ at T_c vs. reduced transition temperature T_c/T_c for $\Gamma_d = 0.75$ eV, $E_d = 0$, $\Gamma_S = 0.2 \Delta_B$, $\Gamma_N = 0.8 \Delta_B$.

$$\Delta C = -T_{C} \frac{\partial^{2} (\Omega_{s} - \Omega_{n})}{\partial T^{2}} \Big|_{T=T_{C}}$$

$$= \frac{2(2\pi k_{B})^{2} T_{C} N_{S}(0)}{B_{L} (n_{I}, T_{C})} (1 + T_{C} \frac{\partial B_{O} (n_{I}, T_{C})}{\partial T_{C}})^{2} (4.40)$$

which finally gives

$$\frac{\Delta C}{\Delta C_{O}} = \frac{T_{C}}{T_{CO}} \frac{B_{1}^{(0,T_{O})}}{B_{1}^{(n_{I},T_{O})}} \left(1 + T_{C} \frac{\partial B_{O}^{(n_{I},T_{O})}}{\partial T_{O}}\right)^{2}$$
(4.41)

where $\triangle C_0$ is the jump in the specific heat at T of the pure proximity effect sandwich.

Shown in Fig. 4.3 is a plot of the specific heat jump $\Delta C/\Delta c_0$ vs. reduced transition temperature T_c/T_{c0} . The numerical values of $\Delta C/\Delta C_0$ are computed from Eq. (4.35) by substituting into it the values of n_I and the corresponding T_c as obtained from Eq. (4.26) (see Appendix C).