CHAPTER VII

CONCLUSION

From chapter VI we have the response kernel

$$Q(k') = \frac{\pi T}{2} \sum_{\omega} \frac{\Delta'^2}{(\omega^2 + \Delta'^2 + C^2)^{3/2}}$$

$$= \frac{\pi T N^2 V^4 \Delta_g^2}{2(2\pi)^2} \sum_{\omega} \frac{1}{(\omega^2+B^2+\Delta_g^2)^2 (\omega^2+\Delta'^2+C^2)^{3/2}} \qquad (7.1)$$

where

$$C^2 = \left(\frac{N^2 V^4 \omega^2}{4\pi^2 (\omega^2+B^2+\Delta_g^2)^2} - \frac{N V^2 \omega^2}{\pi (\omega^2+B^2+\Delta_g^2)} \right) \qquad (7.2)$$

Since $\Delta_g(T) \longrightarrow 0$ at T_c, we expect that near T_c it is small compare to ω. Therefore we can neglect Δ_g^2 appearing in the denominator when the temperature is close to T_c.

$$Q(k') = \frac{\pi T}{2} \cdot \frac{N^2 V^4 \Delta_g^2}{(2\pi)^2} \sum_{\omega} \frac{1}{(\omega^2+B^2)^2 (B^2+C^2)^{3/2}} \qquad (7.3)$$

and

$$C^2 = \frac{N^2 V^4 \omega^2}{4\pi^2 (\omega^2+B^2)^2} - \frac{N V^2 \omega^2}{\pi (\omega^2+B^2)} \qquad (7.4)$$

$$\omega^2 + C^2 = \omega^2 \left[1 + \frac{N V^2}{\pi(\omega^2+B^2)} \left(\frac{N V^2}{4\pi (\omega^2+B^2)} - 1 \right) \right] \qquad (7.5)$$

$$B = E + U\langle n \rangle + \frac{2 m P_0 V^2}{(2\pi)^3} \ln \frac{\omega - \omega_D}{\omega + \omega_D} \qquad (7.6)$$

For weak-coupling limit[1] V is small compare to E and U, so we can neglect the last term in B.

Now let us consider the function

$$\frac{NV^2}{\pi(\omega^2+B^2)}\left(\frac{NV^2}{4\pi(\omega^2+B^2)}-1\right) . \qquad (7.7)$$

By setting

$$\frac{NV^2}{\pi(\omega^2+B^2)} = \frac{1}{X}$$

the function (7.7) can be written as

$$Y = \frac{1}{X}\left(\frac{1}{4X}-1\right) ;$$

Looking at Fig. 10, we see that this function is small compare to one if $X \gg 1$.

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[1]For transition metals $U \sim$ 2-5 eV ; $E \sim -\frac{U}{2}$; $N\langle\omega\rangle V^2 \sim 1$ eV ; $T_c \sim$ 1-10 °K , 9.5 °K for Nb and 4.5°K for Ta.

From Mamada, H., and F. Takano, " Self- Consistent Treatment of Anderson Model and Magnetic Susceptibility ", Prog. Theor Phys. , 43 , 1458 (1970). and Parks, R.D., Superconductivity, Vol. II, Marcel Dekker, Inc; New York 1969.

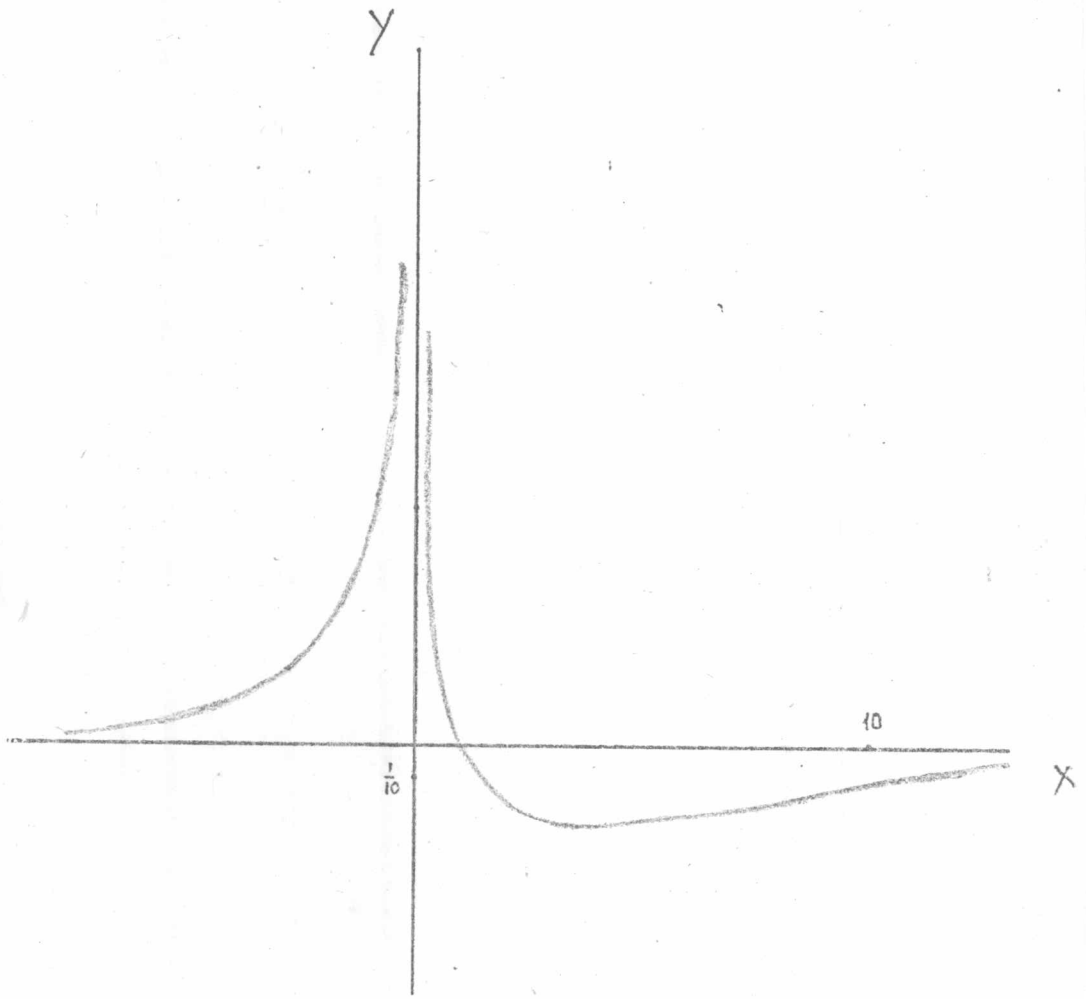

Fig. 10 $y = \frac{1}{x}\left(\frac{1}{4x} - 1\right)$

This happens when

$$\omega^2 + B^2 \gg \frac{NV^2}{\pi} \qquad (7.8)$$

The summation over ω is carried out by setting

$$\omega = (2n+1)\pi T \quad ; \quad n = 0, 1, 2, 3 \ldots$$

$$Q(k') = \frac{\pi}{2}\frac{N^2V^4\Delta_g^2 T}{(2\pi)^2}\sum_n \frac{1}{[(2n+1)^2\pi^2T^2 + B^2]^2[(2n+1)^2\pi^2T^2 + C^2\cdot]^{3/2}} \qquad (7.9)$$

If we now assume that $B^2 \gg \frac{NV^2}{\pi}$ we can neglect the C^2 term appearing in the denominator of (7.9) since C^2 is nothing but the function y shown in Fig. 10 and goes to zero when inequality (7.8) is satisfied.

Therefore, close to T_c, the response kernel is

$$Q(k') = \frac{\pi}{2}\frac{N^2V^4\Delta_g^2 T}{(2\pi)^2}\sum \frac{1}{[(2n+1)^2\pi^2T^2 + B^2]^2[(2n+1)\pi T]^3}$$

If we assume that B^2 is very small, the summation gives

$$Q(k') = \frac{1}{2\pi^6(2\pi)^2}\left(\frac{NV^2}{T^2}\right)^2\left(\frac{\Delta_g}{T}\right)^2\left(1 - 2^{-7}\right)\zeta(7)$$

$$= \frac{1}{(2\pi)^2}\frac{127}{128}\cdot\frac{1}{2\pi^6}\left(\frac{NV^2}{T^2}\right)^2\left(\frac{\Delta_g}{T}\right)^2\zeta(7) \qquad (7.10)$$

where $\zeta(\cdot\cdot)$ is the Riemann Zeta function. However, if we assume that B^2 is large, the summation gives

$$Q(k') = \frac{1}{(2\pi)^2}\cdot\frac{1}{2\pi^2}\left(\frac{NV^2}{B^2}\right)^2\left(\frac{\Delta_g}{T}\right)^2\left(1 - 2^{-3}\right)\zeta(3)$$

$$= \frac{1}{(2\pi)^2}\cdot\frac{7}{16\pi^2}\left(\frac{NV^2}{B^2}\right)^2\left(\frac{\Delta_g}{T}\right)^2\zeta(3) \qquad (7.11)$$

In both cases, the response kernel is independent of $\vec{k}'$. Therefore if we take the Fourier inverse of

$$\vec{j}(k') \sim Q(k') A(k') \qquad (7.12)$$

with the relations

$$\vec{j}(\vec{r}) = \frac{1}{(2\pi)^3} \int j(k') e^{i\vec{k}'\cdot\vec{r}} d\vec{k}'$$

$$A(\vec{r}) = \frac{1}{(2\pi)^3} \int A(\vec{k}') e^{i\vec{k}'\cdot\vec{r}} d\vec{k}'$$

we get

$$\vec{j}(\vec{r}) \sim \text{constant } \vec{A}(\vec{r}) \qquad (7.13)$$

where the constant is (7.10) if B^2 is small and is (7.11) if B^2 is large.

From Eq. (7.13) and London Theory of superconductivity (see Sect. III.2 and III.2.2), we conclude that near T_c, the s- electrons also goes into superconducting phase.

Therefore the transport properties of transition metal which are mostly due to the s- electrons in normal state should not change abruptly when changing from normal to superconducting state at T_c. This behavior has been found experimentally in several researches. For example we show the result from the experiment of Connolly and Mendelssohn[2] in Fig. 11. In this experiment,

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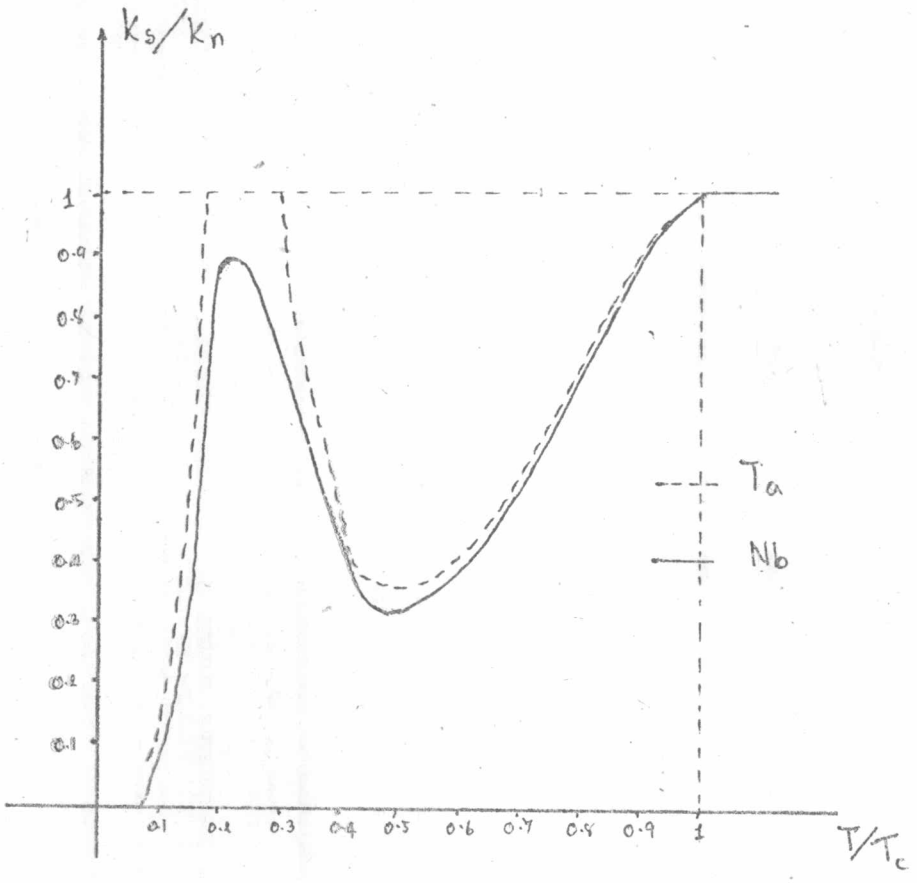
[2] Connolly, A. and K. Mendelssohn, " Thermal Conductivity of Tantalum and Niobium Below 1 °K " Proc. Roy. Soc. Lon., A 266, 429 (1962)



K_s = Thermal conductivity in superconducting state

K_n = Thermal conductivity in normal state

Fig.11 Thermal Conductivity of Ta and Nb .

measurement of thermal conductivity of tantalum and niobium have been done for both the normal and superconducting phases. The result shows continuous change at T_c.

Experiments on ultrasonic attenuation also show this continuity. Fig. 12 shows result from the work of Levy[3].

If the attenuations were discontinuous at T_c the slope at that point should be infinity.

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[3]Levy, M. and I. Rudnick, " Ultrasonic Determination of the Superconducting Energy Gap in Tantalum " Phys. Rev., 132, 1073(1963)

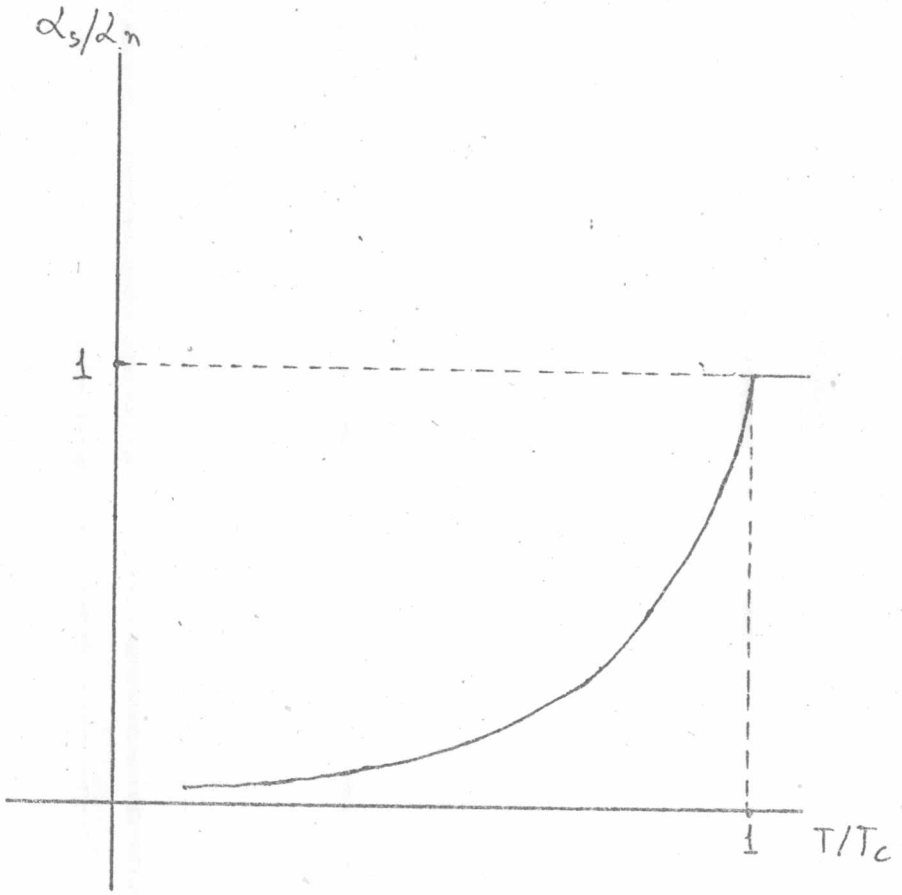

Fig. 12 Ultrasonic Attenuation Ratio α_s/α_n VS T/T_c on Ta

APPENDIX A

GREEN'S FUNCTIONS

The retarded double - time temperature dependent Green's function is defined as [1]

$$\ll A(t);\ B(t')\gg \;=\; -i\,\Theta(t-t')\,\langle\{A(t),\ B(t')\}\rangle \qquad (A.1)$$

where

1. $\langle \cdots \rangle$ denotes a grand canonical ensemble average

$$\langle A\rangle = \frac{\sum \langle n|A|n\rangle\, e^{-\beta E_n}}{\sum e^{-\beta E_n}}$$

2. $\Theta(t-t')$ is the Heaviside step function

$$\Theta(x) = \begin{cases} 1, & x>0 \\ 0, & x<0 \end{cases}$$

3. $\{\cdots\}$ denotes an anti-commutation relation.

4. $A(t)$, $B(t')$ are general products of particle creation and annihilation operators in the Heisenberg representation. The time dependence arises from

$$A(t) = e^{iH't}\, A\, e^{-iH't} \qquad ;\ \hbar = 1$$

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[1] Matsubara, T., " A New Approach to Quantum Statistical Mechanics " Prog. Theor. Phys., 14 , 351 (1955) and Abrikosov, A.A. et al , Quantum Field Theoretical Methods In Statistical Physics, 2nd Ed., Pergamon Press, Oxford (1965) Chapter 7.

where $H' = H - \mu N$; N is the total number of particles opertor and μ is the chemical potential (for temperature near o° K $\mu = E_F$)

$$i\frac{d}{dt}\langle\langle A(t); B(t')\rangle\rangle = \frac{d}{dt}\theta(t-t')\langle\{A(t), B(t')\}\rangle - i\theta(t-t')\langle\{i\frac{d}{dt}A(t), B(t')\}\rangle \quad \text{A.2)}$$

and

$$\frac{d}{dt}\theta(t-t') = \delta(t-t') \quad \text{(A.3)}$$

$$i\frac{dA(t)}{dt} = i(iH'e^{iH't}Ae^{-iH't} + e^{iH't}A(-iH')e^{-iH't})$$

$$= [A(t), H'] \quad \text{(A.4)}$$

$[\cdots]$ = commutation relation,

substituting (A.3) and (A.4) into (A.2) yields

$$i\frac{d}{dt}\langle\langle A(t); B(t')\rangle\rangle = \delta(t-t')\langle\{A(t), B(t')\}\rangle - i\theta(t-t')\langle\{[A(t), H'], B(t')\}\rangle$$

$$= \delta(t-t')\langle\{A(t), B(t')\}\rangle + \langle\langle[A(t), H']; B(t')\rangle\rangle \quad \text{(A.5)}$$

This equation is called the " Green's differential equation ". If we now introduce the Fourier transform of the Green's function

$$\langle\langle A; B\rangle\rangle_\omega = \frac{1}{2\pi}\int_{-\infty}^{\infty}\langle\langle A(t); B(t')\rangle\rangle e^{i\omega(t-t')}\,d(t-t') \quad \text{(A.6)}$$

and substitute it into Green's differential equation, we obtain the algebraic equation

$$\omega\langle\langle A; B\rangle\rangle_\omega = \frac{1}{2\pi}\langle\{A, B\}\rangle + \langle\langle[A, H']; B\rangle\rangle_\omega \quad \text{(A.7)}$$

The special case of $A = c_k$ and $B = c_{k'}^+$ gives the so called one particle Green's function $\langle\langle c_k; c_{k'}^+\rangle\rangle_\omega$. The equation (A.7)

gives a prescription for calculating these one particle Green's functions. In the case that c_k , c_k^+ are fermion operators, we find

$$\omega \ll c_k, c_{k'}^+ \gg_\omega = \frac{1}{2\pi} \langle \{ c_k, c_{k'}^+ \} \rangle + \ll [c_k, H'] ; c_{k'}^+ \gg_\omega ,$$

$$\omega \ll [c_k, H'] ; c_{k'}^+ \gg_\omega = \frac{1}{2\pi} \langle \{ [c_k, H'], c_{k'}^+ \} \rangle + \ll [[c_k, H'], H'] ; c_{k'}^+ \gg_\omega ,$$

etc

The Green's functions satisfy a set of coupled equation. The function $\ll [A, H'] ; B \gg_\omega$ contains higher order Green's function than $\ll A, B \gg_\omega$. This hierarchy of coupled equation connecting the Green's functions of higher orders is exact ; but ; in general, does not terminate in a finite set which would allow an exact solution. One usually introduces some approximation in order to decouple this hierarchy of equations to obtain a finite set.

APPENDIX B

THE HARTREE FOCK APPROXIMATION

The Hartree Fock approximation can be written in the form[1]

$$ABCD = \langle AB\rangle CD + \langle CD\rangle AB - \langle AC\rangle BD - \langle BD\rangle AC \quad (B.1)$$

From Eq. (B.1) the Hartree Fock approximation for Coulomb repulsion term can be written as

$$\begin{aligned} U d^{\dagger}_{j\sigma} d_{j\sigma} d^{\dagger}_{j-\sigma} d_{j-\sigma} &= U\langle d^{\dagger}_{j\sigma} d_{j\sigma}\rangle d^{\dagger}_{j-\sigma} d_{j-\sigma} + U\langle d^{\dagger}_{j-\sigma} d_{j-\sigma}\rangle d^{\dagger}_{j\sigma} d_{j\sigma} \\ &\quad - U\langle d^{\dagger}_{j\sigma} d^{\dagger}_{j-\sigma}\rangle d_{j\sigma} d_{j-\sigma} - U\langle d_{j\sigma} d_{j-\sigma}\rangle d^{\dagger}_{j\sigma} d^{\dagger}_{j-\sigma} \\ &= U\langle d^{\dagger}_{j\sigma} d_{j\sigma}\rangle d^{\dagger}_{j-\sigma} d_{j-\sigma} + U\langle d^{\dagger}_{j-\sigma} d_{j-\sigma}\rangle d^{\dagger}_{j\sigma} d_{j\sigma} \\ &\quad + U\langle d^{\dagger}_{j\sigma} d^{\dagger}_{j-\sigma}\rangle d_{j-\sigma} d_{j\sigma} + U\langle d_{j-\sigma} d_{j\sigma}\rangle d^{\dagger}_{j\sigma} d^{\dagger}_{j-\sigma} \\ &= U\langle n_{j\sigma}\rangle n_{j-\sigma} + U\langle n_{j-\sigma}\rangle n_{j\sigma} - \Delta^{*}_{d} d_{j-\sigma} d_{j\sigma} - \Delta_{d} d^{\dagger}_{j\sigma} d^{\dagger}_{j-\sigma} \end{aligned}$$

where

$$\Delta_{d} = -U\langle d_{j-\sigma} d_{j\sigma}\rangle \quad .$$

In equilibrium $\langle n_{j\sigma}\rangle = \langle n_{j-\sigma}\rangle$, thus the Anderson

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[1] Shiba, H., " A Hartree-Fock Theory of Transition Metal Impurities in a Superconductor " , Prog. Theor. Phys., 50, 50 (1973) Abrikosov, A.A., L.R. Gorkov and I.Y. Dzyaloshinskii, Quantum Field Theoretical Methods In Statistical Physics, 2nd Ed., Pergamon Press, Oxford (1965) Chapter 7 .

Hamiltonian (5.1), in the Hartree Fock approximation, becomes

$$H = \sum_{k,\sigma} \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{j,\sigma} (E_j + U\langle n_\sigma \rangle) d^{\dagger}_{j\sigma} d_{j\sigma}$$
$$+ \sum_{j,k,\sigma} (V_{kj} c^{\dagger}_{k\sigma} d_{j\sigma} + V^{*}_{jk} d^{\dagger}_{j\sigma} c_{k\sigma})$$
$$- \tfrac{1}{2} \Delta_d \sum_{j,\sigma} d^{\dagger}_{j\sigma} d^{\dagger}_{j-\sigma} - \tfrac{1}{2} \Delta^{*}_d \sum_{j,\sigma} d_{j-\sigma} d_{j\sigma} \qquad (B.2)$$

Similarly the BCS coupling term,

$$- \tfrac{1}{2} g \sum_{j,m,\sigma} d^{\dagger}_{j\sigma} d^{\dagger}_{j-\sigma} d_{m-\sigma} d_{m\sigma} \quad ,$$

can be written in the Hartree Fock approximation as

$$- \tfrac{1}{2} \Delta^{*}_o \sum_{j,\sigma} d_{j-\sigma} d_{j\sigma} - \tfrac{1}{2} \Delta_o \sum_{j,\sigma} d^{\dagger}_{j\sigma} d^{\dagger}_{j-\sigma} \quad , \qquad (B.3)$$

where $\Delta_o = g \sum_j d_{j-\sigma} d_{j\sigma}$; and we change m to j in the last step.

To get the Hamiltonian for superconducting transition metals in the Hartree Fock approximation we add (B.3) into Eq. (B.2). The result is

$$H = \sum_{k,\sigma} \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{j,\sigma} (E_j + U\langle n_\sigma \rangle) d^{\dagger}_{j\sigma} d_{j\sigma}$$
$$+ \sum_{j,k,\sigma} (V_{kj} c^{\dagger}_{k\sigma} d_{j\sigma} + V^{*}_{jk} d^{\dagger}_{j\sigma} c_{k\sigma})$$
$$- \tfrac{1}{2} \sum_{j,\sigma} \Delta_g d^{\dagger}_{j\sigma} d^{\dagger}_{j-\sigma} - \tfrac{1}{2} \sum_{j,\sigma} \Delta^{*}_g d_{j-\sigma} d_{j\sigma} \quad ,$$

where

$$\Delta_g = \Delta_o + \Delta_d \quad .$$