CHAPTER V

ANDERSON MODEL FOR

TRANSITION METAL SUPERCONDUCTORS

V.1 Anderson Model

There are two or more groups of electrons (`i.e., s , d and f electrons) present in the transition metals. One of these groups, the s - electrons, behave like free electrons while the others are localized about the nuclei located at the lattice sites[1]. In 1961 Anderson[2] introduced a model Hamiltonian, which takes into account the presence of both free electron states and localized states. Included in his Hamiltonian are terms for the hybridyzation of the conduction electrons with localized d- electrons and for the Coulomb interaction between electrons of opposite spins occupying the localized orbital state. While this model was intended for the study of the occurrence of a localized magnetic moments on iron-group atoms, which are dissolved as dilute impurities in nonmagnetic

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[1] Friedel, J., " Transition Metals : Electronic Structure of the d-Band. Its Role in the Crystalline and Magnetic " The Physics of Metals 1. Electron. Edited by J.M. Ziman, Cambridge 1969, p. 340

[2] Anderson, P.W., "Localized Magnetic States in Metals " Phys. Rev. , 124 , 41 (1961)

metals, it contains the essential features of the narrow d-band transition metals.

In its simplest form, the Anderson model is described by the Hamiltonian

$$H = \sum_{k\sigma} \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{j\sigma} E_j d^{\dagger}_{j\sigma} d_{j\sigma} + \sum_{j,k,\sigma} V_{kj} c^{\dagger}_{k\sigma} d_{j\sigma} + \sum_{j,k,\sigma} V^{*}_{jk} d^{\dagger}_{j\sigma} c_{k\sigma} + \frac{1}{2} U \sum_{j\sigma} d^{\dagger}_{j\sigma} d_{j\sigma} d^{\dagger}_{j-\sigma} d_{j-\sigma} , \qquad (5.1)$$

where σ labels the spin orientation ; $c^{\dagger}_{k\sigma}$ and $c_{k\sigma}$ are the creation and destruction operators for a s-electron of momentum k, respectively, and ϵ_k is its energy; $d^{\dagger}_{j\sigma}$ and $d_{j\sigma}$ are the creation and destruction operators for a d- orbital electron or Wannier function, respectively, and E_j is its energy. U is Coulomb repulsion between d- electrons, and V_{kj} is the matrix element that connects the localized states at position j and the conduction state with the momentum k .

If we now carry out the Hartree Fock approximation[3] ; we get

$$H = \sum_{k,\sigma} \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{j\sigma} (E_j + U\langle n_{\sigma}\rangle) d^{\dagger}_{j\sigma} d_{j\sigma} + \sum_{j,k,\sigma} (V_{kj} c^{\dagger}_{k\sigma} d_{j\sigma} + V^{*}_{jk} d^{\dagger}_{j\sigma} c_{k\sigma}) - \frac{1}{2} \Delta_d \sum_{j\sigma} d^{\dagger}_{j\sigma} d_{j-\sigma} - \frac{1}{2} \Delta^{*}_d \sum_{j\sigma} d_{j-\sigma} d_{j\sigma} \qquad (5.2)$$

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[3] Shiba, H., " A Hartree-Fock Theory of Transition Metal Impurities in a Superconductor" , Prog. Theor. Phys., 50 , 50 (1973) See also Appendix B.

where $$n_\sigma = d^+_{j\sigma} d_{j\sigma} \qquad (5.3)$$

and $$\Delta_d = -U\langle d_{j-\sigma} d_{j\sigma}\rangle \qquad (5.4)$$

V.2 Hamiltonian for Superconducting Transition Metals

We have mentioned the BCS theory for superconductivity which have been remarkably successful in accounting for the superconducting properties of simple metals. For transition metal superconductors many experimental results do not egree with the predictions of the BCS theory[4] such as the isotope effect, the critical temperature and the pressure effect. Many theories have been proposed to describe the transition metal superconductors. The SMW two-band model which have mentioned in section IV.2 is the one of these theories. In this theory electrons in both s- band and d- band form Cooper pairs. It can describe some experimental results from very pure transition metal superconductors especially in the existent of two energy gaps (see sect. IV.2).

However, most of the recent theories of superconductivity in the transition metals[5] suggested that the d-d pairing interaction

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[4]Gladstone, G., et al , "Superconductivity in the Transition Metals : Theory and Experiment " Superconductivity, Vol II,Edited by R.D. Parks, Marcel Dekker, Inc., New York, 1969.

[5]Appel, J., and W. Kohn, "Transition Temperature of Transition Metal Superconductors " ; Bennermann, K.H. and J.W. Garland " Theory for Superconductivity in d- Band Metals " , AIP Conf. Proc. No. 4 Superconductivity in d- and f- Band Metals. Edited by David H., Douglass American Institute of Physics, New York 1972.

is usually more important than the s-s or s-d interaction, because of a large d- electron density of states at the Fermi surface. Appel and Kohn [5] have shown that the vertex function constructed with Wannier function representation of the d- orbital electrons exhibit the singularities which indicate an instability against the formation of Cooper pairs. They have also calculated T_c and discussed the isotope effect which exhibit a behavior in agreement with experiments. Bennermann and Garland[5] have shown that the electron-phonon matrix element between localized d- orbitals leads to an expression for the critical temperature which allows for the variation in T_c seen in three transition metal series. They have also shown that the McMillan equation[6], which is based on the virtual exchange of the phonons between the d- electrons, can explain the pressure dependence of the transition temperatures seen in the transition metal superconductors.

From the ideas just have mentioned we add to the Anderson Hamiltonian, the term

$$-\tfrac{1}{2} g \sum_{j,m,\sigma} d^{+}_{j\sigma} d^{+}_{j-\sigma} d_{m-\sigma} d_{m\sigma} \qquad (5.5)$$

where g is the strength of the electron-phonon interaction between d- orbitals located on the j^{th} and m^{th} site and is taken to be the electron-phonon coupling constant in McMillan's work. It is similar to the attractive interaction term in the BCS

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[6] McMillan, W.L., " Transition Temperature of Strong-Coupled Superconductors ", Phys. Rev., 167, 331 (1968)

theory which leads to the formation of Cooper pairs in simple metal superconductors .

Applying the Hartree - Fock approximation to (5.5) ; we obtain the following Hamiltonian

$$H = \sum_{k,\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma} + \sum_{j,\sigma} (E_j + U\langle n_\sigma \rangle) d^+_{j\sigma} d_{j\sigma}$$
$$+ \sum_{j,k,\sigma} (V_{kj} c^+_{k\sigma} d_{j\sigma} + V^*_{jk} d^+_{j\sigma} c_{k\sigma})$$
$$- \frac{1}{2} \sum_{j,\sigma} (\Delta^*_g d_{j-\sigma} d_{j\sigma} + \Delta_g d^+_{j\sigma} d^+_{j-\sigma}) \quad , \qquad (5.6)$$

where

$$\Delta_g = g \sum_{j,\sigma} \langle d_{j-\sigma} d_{j\sigma} \rangle + \Delta_d \qquad (5.7)$$

is the gap parameter similar to that in the BCS theory.

For the reasons we have mentioned previously, the Hamiltonian (5.6) should be a fairly good description of the superconducting phase of the transition metals.