Two Band Models for Solids with an Ising Impurity

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Seitaro MATAYOSHI*

Summary

Using two band models for solids with an Ising impurity, we have seen the possibility of "effective" energy gap in the superconducting states. This "effective gap" appears for the existences of the both gaps; namely, the one belonging to the model of two bands and the other to the superconducting states, and, in addtion, separate into two parts; i. e. a "part" of the semiconductor-like states and a "part" of the superconducting states.

In the various "gap" in the superconducting states and in, also, the normal states, we have searched for the excited states and discussed them.

1. Introduction

Since the paper published by Abrikosov and Gorkov,[1] many works have been done experimentally and theoretically concerning the thermo-dynamic and transport properties of superconductors with small amount of paramagnetic impurities.

Recently, several authors have investigated localized low lying excited states in the energy gap of superconductors with the paramagnetic impurities.

Soda, Matsuura, and Nagaoka[2] have first found such states within the gap in the superconducting state of the s-d exchange interaction system. Their approach is a perturbational method corresponding to Yoshida' s treatment[3] in the normal s-d system. Fowler and Maki[4] have examined the states in terms of the dispersion relations, Takano and Matayoshi,[5] Zittartz and Müller-Hartmann[6] also in terms of the two-time Green's functions, respectively.

Although a satisfactory theory for the s-d system has not yet been obtained,[7] all their results have supported the existence of the localized low lying excited states in the energy gap of superconductors.

As it is well known, a paramagnetic impurity in normal and superconducting metals brings about a new kind of quantum mechanical effect, "the so-called Kondo effect",[8] but this effect makes complete solutions of the problem quite difficult.

Shiba[9] has proposed a solvable model of superconductors with a localized impurity spin which is equivalent to a local magnetic field. Using this model, he has obtained the exact solution of the Temperature Green' s function, and has discussed the excited state and others in superconductors.

Another solvable model of s-d system with an Ising spin of impurity has been suggested and investigated exactly by Yara and Matayoshi.[10]

These solvable models are almost equivalent to each other in the normal and the

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*Physics Dept., Sciences & Engineerimg Div.

superconducting states. There are, however, great differences between the two solvable models in the effects due to the existence of correlations between impurities and of an external field.

In this paper, we will show the excited states in the energy gap using one of the solvable models in a system of two bands, and will be able to see an "effective" gap in the superconducting states. This effective gap will sharply separate into" parts" of the semiconductor-like state and superconducting state.

The "part" of the semiconducting-like state has a structure sensitive on physically observable quantities, but the "part" of the superconduting state lacks not only the structure sensitive stated above but also the effect due to the gap in the two bands.

We will also see levels of localized bound state by an impurities potential especially in the "part" of the semiconductor-like, but not in the "part" of the superconducting.

In addition, we must include the explanation of the experimental fact of the "deep" bound states in the gap of the semiconductors with transition atoms as impurities in the normal state, and will give the account for the "deep" bound states in the superconducting states, too.

In calculation, the author will use the model by Yara and Matayoshi,[10] for he will study the effects of the correlations between impurities and of an external field in the future series of this paper.

In Shiba's model,[9] we cannot take into consideration the effects mentioned above, especially, the effect of an external field.

We will give the formulation of the two-time Green's functions in section 2, and in sections 3 and 4, will show various bound states in "gap" in normal and in superconducting states, respectively.

2. Formulation and Formal Solution

The Hamiltonian of our problem can be given in the following form.

$$H=\Sigma_{\ell\sigma}\ \xi_{\ell}\, C^{+}_{\ell\sigma}C_{\ell\sigma} - \Delta_{\circ}\ \Sigma_{\ell}\ (C^{+}_{\ell\uparrow}\ C^{+}_{-\ell\downarrow} + C_{-\ell\downarrow}C_{\ell\uparrow})$$

$$+\frac{V}{2N}\Sigma_{\ell\ell'\sigma}\ C^{+}_{\ell\sigma}\ C_{\ell'\sigma} - \frac{J}{2N}\Sigma_{\ell\ell'}(C^{+}_{\ell\uparrow}C_{\ell'\uparrow} - C^{+}_{\ell\downarrow}\ C_{\ell'\downarrow})\ S_z\ , \qquad (2\text{—}1)$$

where ξ_{ℓ} is the kinetic energy of an electron measured from the Fermi energy, and $C_{\ell\sigma}$ and $C^{+}_{\ell\sigma}$ are operators of the destruction and the creation of electrons with wave number ℓ and spin σ, respectively.

Δ_0 is the order parameter or the gap energy of the superconducting states defined by

$$\Delta_{\circ}=g\Sigma_{\ell}< C^{+}_{\ell\uparrow}\ C^{+}_{-\ell\downarrow} > =g\Sigma_{\ell}<C_{-\ell\downarrow}C_{\ell\uparrow}> \qquad (2\text{—}2)$$

g being the coupling constant in the B. C. S. Hamiltonian[11) 12)] and $\langle A\rangle$ denoting the statistical average of an operator A. N is the number of atoms in the system, V is the strength of a scattering potential impurity, and J is the coupling constant of the exchange interaction between electrons and an Ising impurity of operator Sz which is located at the origin of the system.

The Green's functions in Nanbu space[11] to be calculated in the following are

$$\hat{G}_{kk'}(\omega)=\begin{pmatrix} \langle\langle C_{k\uparrow} \mid C^{+}_{k'\uparrow}\rangle\rangle_{\omega} & \langle\langle C_{k\uparrow} \mid C^{-}_{k'\downarrow}\rangle\rangle_{\omega} \\ \langle\langle C^{+}_{-k\downarrow} \mid C^{+}_{k'\uparrow}\rangle\rangle_{\omega} & \langle\langle C^{+}_{-k\downarrow} \mid C_{-k'\downarrow}\rangle\rangle_{\omega} \end{pmatrix}, \tag{2—3}$$

and

$$\hat{\Gamma}_{kk'}(\omega)=\begin{pmatrix} \langle\langle C_{k\uparrow}S_Z \mid C^{+}_{k'\uparrow}\rangle\rangle_{\omega} & \langle\langle C_{k\uparrow}S_Z \mid C_{k'\downarrow}\rangle\rangle_{\omega} \\ \langle\langle C^{+}_{-k\downarrow}S_Z \mid C^{+}_{k'\uparrow}\rangle\rangle_{\omega} & \langle\langle C^{+}_{-k\downarrow}S_Z \mid C_{-k'\downarrow}\rangle\rangle_{\omega} \end{pmatrix}, \tag{2—4}$$

where $\langle\langle A \mid B\rangle\rangle_{\omega}$ denotes the Fourier transform of the Green's function of two operators A and B.

There are various kinds of the Green's functions, i. e. the retarded or advanced two-time Green's function, the temperature Green's function, and so on.

The only differences are the definition of the frequencies and the relation between the Green's function $\langle\langle A \mid B\rangle\rangle_{\omega}$ and the average $\langle BA\rangle$.

The former Green's function has simpler analytical properties, while the latter is convenient for perturbational calculations. Though the two-time Green's functions will be used in the following, it can be easily rewritten by means of the temperature Green's function which will also be utilized in the forthcoming series.

Equations for $\hat{G}_{kk'}(\omega)$ and $\hat{\Gamma}_{kk'}(\omega)$ are derived in the usual way. We have the following,

$$\hat{\Omega}_{k}(\omega)\hat{G}_{kk'}(\omega)-\frac{V}{2N}\Sigma_{l}\hat{G}_{lk'}(\omega)+\frac{J}{2N}\Sigma_{l}\hat{\Gamma}_{lk'}(\omega)=\delta_{kk'}, \tag{2—5}$$

$$\hat{\Omega}_{k}(\omega)\hat{\Gamma}_{kk'}(\omega)-\frac{V}{2N}\Sigma_{l}\hat{\Gamma}_{lk'}(\omega)+\frac{J}{8N}\Sigma_{l}\hat{G}_{lk'}(\omega)=0, \tag{2—6}$$

which are exact equations and make use of the usual relation $\langle S_Z\rangle=0$ obtained from the axial symmetry of the sytem. The inverse matrix of $\hat{\Omega}_{k}(\omega)$ in eqs. (2—5) and (2—6) is the free Green's function of a pure superconductor and is given by

$$\hat{\Omega}_{k}^{-1}(\omega)=\frac{1}{\omega^{2}-\xi_{k}^{2}-\Delta_{\circ}^{2}}\begin{pmatrix} \omega+\xi_{k} & -\Delta_{\circ} \\ -\Delta_{\circ} & \omega-\xi_{k} \end{pmatrix}, \tag{2—7}$$

These coupled Equations (2—5) and (2—6) can be solved easily to give the solution in the following simple forms:

$$\hat{G}_{kk'}(\omega)=\delta_{kk'}\hat{\Omega}_{k}^{-1}(\omega)+\hat{\Omega}_{k}^{-1}(\omega)\,\hat{t}_{1}(\omega)\,\hat{\Omega}_{k'}^{-1}(\omega), \tag{2—8}$$

$$\hat{\Gamma}_{kk'}(\omega)=\hat{\Omega}_{k}^{-1}(\omega)\,\hat{t}_{2}(\omega)\,\hat{\Omega}_{k'}^{-1}(\omega), \tag{2—9}$$

$$\hat{t}_1(\omega)=\left(\frac{V}{4N}\hat{\tau}_3-\frac{J}{8N}\right)\left[1-\frac{V}{2}\hat{F}(\omega)\hat{\tau}_3+\frac{J}{4}\hat{F}(\omega)\right]^{-1}$$

$$+\left(\frac{V}{4N}\hat{\tau}_3+\frac{J}{8N}\right)\left[1-\frac{V}{2}\hat{F}(\omega)\hat{\tau}_3-\frac{J}{4}\hat{F}(\omega)\right]^{-1}, \qquad (2\text{—}10)$$

$$\hat{t}_2(\omega)=\frac{1}{2}\left(\frac{V}{4N}\hat{\tau}_3-\frac{J}{8N}\right)\left[1-\frac{V}{2}\hat{F}(\omega)\hat{\tau}_3+\frac{J}{4}\hat{F}(\omega)\right]^{-1}$$

$$-\frac{1}{2}\left(\frac{V}{4N}\hat{\tau}_3+\frac{J}{8N}\right)\left[1-\frac{V}{2}\hat{F}(\omega)\hat{\tau}_3-\frac{J}{4}\hat{F}(\omega)\right]^{-1}, \qquad (2\text{—}11)$$

$$\hat{\tau}_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \qquad (2\text{—}11')$$

and

$$\hat{F}(\omega)=\frac{1}{N}\Sigma_l\,\hat{\Omega}_l^{-1}(\omega) \qquad (2\text{—}12)$$

These solutions coincide with eqs. (2—8) in the reference (10) , if we put the strength V of a impurity potential equal to zero. Using these solutions, we can investigate various physical quantities. In the next section, discussions of excited states in the energy gap of normal state will be given.

3. Normal State

To calculate the function $F(\omega)$ specifically, we must assume a form of the state density $\rho(\xi_k)$ as shown in Fig. I for simplicity.

Both the upper and lower energy bands are supposed to have the same band width $D-\Delta$ and the same uniform state density ρ, It is further assumed that the total number of electrons in the system just equals the total number of one-electron states in the lower band.

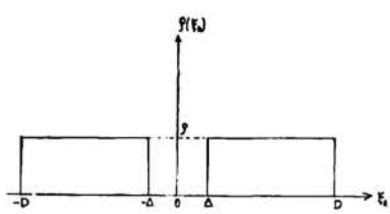


Fig. I . State density of the two band models.

Consequently, the lower energy band is fully occupied by electrons, while the upper band is completely empty in the ground state of the system without an interaction between electrons and impurities. This state density will be used in this section and thereafter.

Now, we can obtain the concrete results of $F(\omega)$ in the following.

$$F^{\pm}(\omega)=F\ (\omega\pm i\,\delta)=\frac{1}{N}\Sigma_{\ell}\frac{1}{\omega-\xi_{\ell}\ \pm i\,\delta}$$

$$\begin{cases} \dfrac{\rho}{N}\ln\left|\dfrac{\omega-\Delta}{\omega+\Delta}\right| \mp i\pi\dfrac{\rho}{N} & \text{for } |\omega|>\Delta \quad (3\text{—}1) \\ \dfrac{\rho}{N}\ \ln\left|\dfrac{\omega-\Delta}{\omega+\Delta}\right|, & \text{for } |\omega|<\Delta \quad (3\text{—}2) \end{cases}$$

which are approximately calculated using an assumption, i. e. $D\gg |\omega|,\ \Delta$.

The low lying excited levels are obtained by seeking singular points of the normal Green's function $G_{kk'}(\omega)$ or $t_l(\omega)$ matrix without spin flip : namely by the zero points in the following equations

$$1-\frac{V}{2}F^{\pm}(\omega)\ \pm\frac{J}{4}F^{\pm}(\omega)\ =0, \qquad (3\text{—}3)$$

To find bound states in the gap Δ, it is convenient to divide the discussions into two cases and consider them separately.

CaseA

$$\gamma_1\equiv\frac{\rho V}{2N}\neq 0\ \text{ and }\quad \gamma_2\equiv\frac{\rho J}{4N}=0, \qquad (3\text{—}4)$$

For this case we have, from eqs. (3—3) ,

$$1-\gamma_1\ \ell n\left|\frac{\omega-\Delta}{\omega+\Delta}\right|=0$$

and obtain the excited state, i. e.

$$\omega=-\Delta\,\mathrm{th}\ \frac{1}{2\gamma_1} \qquad (3\text{—}5)$$

The $\omega-\gamma_1$ curve is shown in Fig. Ⅰ.

Case B.

$$\gamma_1\neq 0\ \text{ and }\ \gamma_2\neq 0.$$

For this case we can achieve the following as the final results,

$$\omega=-\Delta\,\mathrm{th}\frac{1}{2(\gamma_1\pm\gamma_2)} \qquad (3\text{—}6)$$

in the same way as in the Case A.

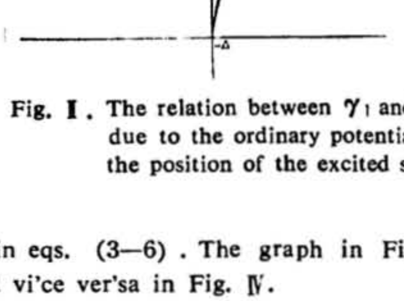


Fig. Ⅰ. The relation between γ_1 and ω, due to the ordinary potential, i. e., the position of the excited states.

We can easily depict the curve of ω by γ in eqs. (3—6) . The graph in Fig. Ⅲ give the $\omega-\gamma_1$ curve for a constant γ_2 and vi'ce ver'sa in Fig. Ⅳ.

The low excited energy ω in the eq. (3—5) is the single-valued function of γ_1 , but the ω in the eq. (3—6) are two-valued. We can graphically see the connection between eq 's (3—5) and (3—6) in the Fig. Ⅱ and Fig. Ⅲ, when γ_2 approaches zero.

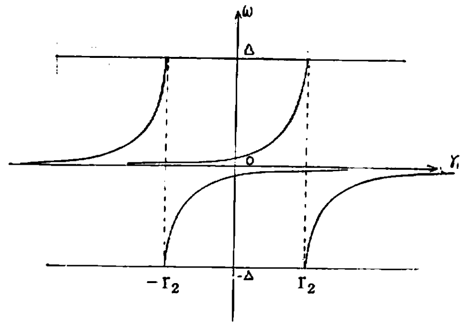


Fig. Ⅲ. $\omega - \gamma_1$ curve for a constant γ_2 in the normal states.

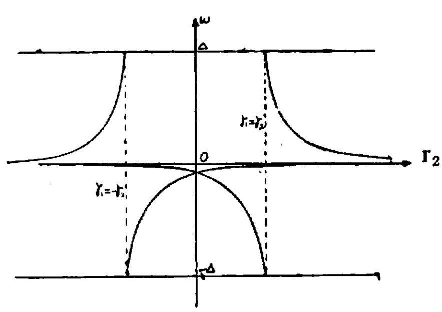


Fig. Ⅳ. The bound state position as a function of γ_2 for a positive constant γ_1 in the normal states.

It will be convenient for discussions on the superconducting states in the next section to have the Fig. Ⅳ.

4 Superconducting State

The treatments are quite the same as in the normal state in the section 3. To begin with, we must caluculate the function $\hat{F}(\omega)$ in this section, too. The final result of this function is given in the following,

$$\hat{F}(Z) = \begin{pmatrix} Z & -\Delta_0 \\ -\Delta_0 & Z \end{pmatrix} I(Z), \qquad (4\text{—}1)$$

and

$$I(Z) = \frac{1}{N} \Sigma_l \frac{1}{Z^2 - \xi_l^2 - \Delta_0^2}, \qquad (4\text{—}1')$$

where Z is the complex number, and the function I is shown to be easily obtained on the real axis in the complex plane; namely,

$$I^{\pm}(\omega) = I(\omega \pm i\delta) = \frac{\rho}{N} \frac{1}{\sqrt{\omega^2 - \Delta_0^2}} \; ln \left| \frac{\sqrt{\omega^2 - \Delta_0^2} - \Delta}{\sqrt{\omega^2 - \Delta_0^2} \pm \Delta} \right|$$

$$+ \begin{cases} \mp \dfrac{i\pi\rho}{N} \dfrac{}{\sqrt{\omega^2 - \Delta_0^2}}, & \text{for } \omega > \sqrt{\Delta^2 + \Delta_0^2} \\ \pm \dfrac{i\pi\rho}{N} \dfrac{1}{\sqrt{\omega^2 - \Delta_0^2}}, & \text{for } \omega < -\sqrt{\Delta^2 + \Delta_0^2} \end{cases} \qquad (4\text{—}2)$$

$$I^{\pm}(\omega)=\frac{\rho}{N}\frac{1}{\sqrt{\omega^2-\Delta_o^2}}\quad \ln\left|\frac{\sqrt{\omega^2-\Delta_o^2}-\Delta}{\sqrt{\omega^2-\Delta_o^2}+\Delta}\right|,\ \text{for}\ \Delta_o<|\omega|<\sqrt{\Delta_o^2+\Delta^2} \tag{4—3}$$

and

$$I^{\pm}(\omega)=-\frac{\pi\rho}{N}\ \frac{1}{\sqrt{\Delta_o^2-\omega^2}}\ , \qquad \text{for}\quad |\omega|<\Delta_o \tag{4—4}$$

which coicide with eqs. (3—1) and (3—2) at the normal limit of $\Delta_o=0$, and with that of the superconducting metals at the limit of $\Delta=0$, respectively.

The equations of the position of the bound state in the energy gap are given by

$$\det\left|1-\frac{V}{2}\hat{F}^{\pm}(\omega)\,\hat{\tau}_3\pm\frac{J}{4}\hat{F}^{\pm}(\omega)\right|=0 \tag{4—5}$$

or

$$\left[1\pm\frac{J}{4}\omega I^{\pm}(\omega)\right]^2-\left[\frac{V}{2}\omega I^{\pm}(\omega)\right]^2+\left(\frac{V^2}{4}-\frac{J^2}{16}\right)\Delta_o^2 I^{\pm 2}(\omega)=0. \tag{4—6}$$

The solutions of this equations are grouped into several cases for the sake of discussions.

Case A $\gamma_1\neq 0$ and $\gamma_2=0$ for $|\omega|<\Delta_o$.

We have no solution of the ω.

Case A' $\gamma_1\neq 0$ and $\gamma_2=0$ for $\Delta_o<|\omega|<\sqrt{\Delta_o^2+\Delta^2}$.

We have the following,

$$1-\gamma_1^2\ \ln^2\left|\frac{\sqrt{\omega^2-\Delta_o^2}-\Delta}{\sqrt{\omega^2-\Delta_o^2}+\Delta}\right|=0\ , \tag{4—7}$$

from eqs. (4—3) and (4—6) and take

$$\omega=\pm\sqrt{\Delta_o^2+\Delta^2\ \mathrm{th}^2\ \frac{1}{2\gamma_1}}\ , \tag{4—8}$$

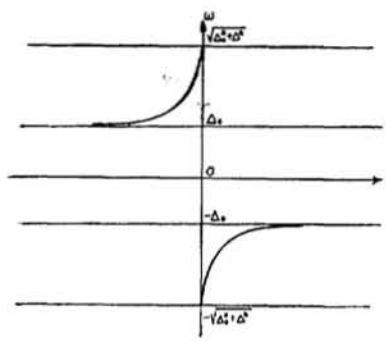


Fig. V. Impurity levels for the case of the ordinary potential only in the "part" of the semiconductor-like states. Such levels have not appeared in the single band model.

as the solutins of eqs. (4—7) . We must select the signs of eqs. (4—8) approaching eq. (3—5) at the limit $\Delta_o=0$.

Therefore we obtain the final results as follows:

$$\omega=-\sqrt{\Delta_o^2+\Delta^2\ \mathrm{th}^2\ \frac{1}{2\gamma_1}}\ . \qquad \text{for}\ \gamma_1>0$$

and (4—9)

$$\omega = \sqrt{\Delta_o^2 + \Delta^2 \, \mathrm{th}^2 \frac{1}{2\gamma_1}} \quad . \text{ for } \gamma_1 < 0$$

or

$$\omega = -(\mathrm{sgn}\, \gamma_1) \quad \sqrt{\Delta_o^2 + \Delta^2 \, \mathrm{th}^2 \frac{1}{2\gamma_1}} . \qquad (4-9').$$

Case B. $\gamma_1 \neq 0$ and $\gamma_2 \neq 0$ for $|\omega| < \Delta_o$.

The bound states are given by

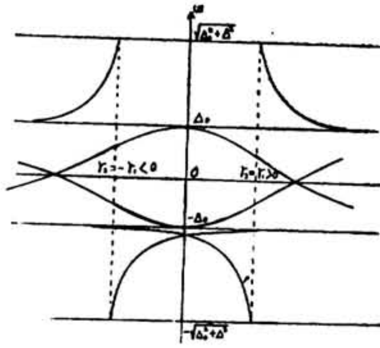
$$\omega = \pm \frac{1+\pi^2 \gamma_1^2 - \pi^2 \gamma_2^2}{\sqrt{(1+\pi^2 \gamma_1^2 - \pi^2 \gamma_2^2)^2 + 4\pi^2 \gamma_2^2}} \Delta_o , \qquad (4-10)$$

as the final solution of eqs. (4—6) .

Case B′ $\gamma_1 \neq 0$ and $\gamma_2 \neq 0$ for $\Delta_o < |\omega| < \sqrt{\Delta_o^2 + \Delta^2}$.

We cannot obtain the explicit form of the ω in term of either γ_1 or γ_2 , but can give an outline of the curve of the ω in terms of γ^1 for a constant γ_2 and vi'ce ver'sa, for we can use the results and the figures obtained previously.

The figures of the Case A with A′ are given in Fig. V and the Case B with B′, in Fig. VI.



Fgi. VI. The excited state position as a function of γ_2 for a positive constant γ_1 in the "part" of semiconductor-like states and in the "part" of the superconducting states. Attention should be paid to the "part" of the superconducting states of $|\omega| < \Delta_o$. The bound states in this "part" are completely equivalent to that of the gap of superconductors in the single band model.

5. Results and Discussions

Using the two-band model for solids with an Ising impurity, we have investigated the various kinds of the excited states within the "gap" in the normal states and the superconducting states.

In the normal states, the gap in this system is only the gap Δ owing to the model of two bands. We have given the excited state, namely $\omega - \gamma_1$ curve in the Fig. II, corresponding to the usual results due to the existence of impurity potentials. However, the absolute values of γ_1 seeming to be very small, we cannot in fact obtain the "deep" excited levels as they have been shown in many experimental data.

We also know the experimental facts concerning the "deep" levels in a system with the transition atoms as impurities. In the Fig. III or the Fig. IV, the graphs of $\omega - \gamma_s$ curves are shown for the case when an impurity spin exists. These graphs give the reason for the appearance of the "deep" levels, if the property of the structure sensitive is taken into consideration.

The occurence of the structure sensitive is due to the existence of the small gap owing to the two-band system and the existence of impurities.

In the superconducting states, we have had the "effective gap" consisting of the gaps owing to Δ in the two-band model and Δ_0 in the superconductors. This effective gap has sharply separated into two parts: i. e., the "parts" of the semiconductor-like and the superconducting. The "part" of the semiconductor-like has a structure sensitive property for physical quantities, but the "part" of the superconducting does not. In the appearance of the superconducting state at very low impurity concentration, any systems are necessary to have energy gap owing to the formation of many Cooper pairs.

In addition, the energy gap owing to many Cooper pairs is the universal function independent of a form of electron state density and dependent only on a value of the density in the neighborhood of the Fermi surface. Therefore, the "part" of the superconducting states in this two-band model is completely equivalent to the gap of the superconducting states in a single band model, or in a metal. Consequently, the graphs in the "part" of the superconducting states in Fig. VI correspond to the ones in Fig. I in Ref. (10). Contrary to the superconducting case, the "part" of the semiconductor-like is due to the gap in the two-band system and has effect for the sake of the superconducting states. This effect is largest at $|\omega| = \Delta_0$, decreasing as $|\omega|$ approaches the gap edge $\sqrt{\Delta_0^2 + \Delta^2}$, and is smallest at the edge $\sqrt{\Delta_0^2 + \Delta}$; so, the "part" of the semiconductor-like becomes the part of the superconductor-like in the neighborhood of the edge $|\omega| = \Delta_0$, and becomes also the part of the normal semiconductor-like in the neighborhood of the edge $|\omega| = \sqrt{\Delta_0^2 + \Delta^2}$. We know the relation of correspondence between Fig. II and VI, or Fig. IV and VI, respeotively.

As it is seen in Fig. V, we can obtain the excited states for the ordinary potential in the "part" of the semiconductor-like states. The excited states for the potential have not been obtained in the normal states and in the superconducting states for the single band model.

It is interesting to discuss the case of a solid with a finite concentration of Ising impurity spins. Using the discussion of equivalence between the "part" of the superconducting state in the two-band model and the gap of the supercoductors in a single band model, and also using the results in Ref. (9) and (10), we can presume that at extremely low concentration, the growth of impurity band begins with the localized levels near the edge $|\omega| = \Delta_0$, and at higher concentration, the growth of band begins also with the edge Δ_0 and with levels near $\omega = 0$.

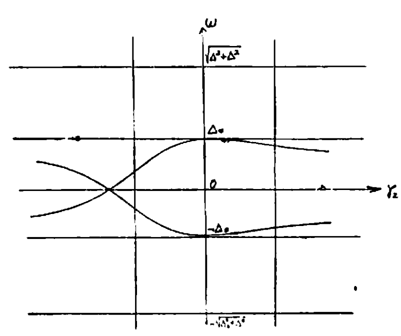


Fig. VII. The positions of the impurity levels taking the "Kondo effect" into consideration in the "part" of the superconducting states.

Next, we must refer to the "Kondo effect". It is very difficult to take the Kondo effect problem into consideration, but we will be able to infer it as shown in Fig. VII, if we utilize the equivalent property mentioned above and the result in Ref. (6) .

On both the finite concentration problem and the Kondo effect problem, we have given some suggestions in the "part" of the superconducting state, but not in the "part" of the semiconductor-like state. As it seems to be very interesting, we will investigate the problems in our future work.

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