Functional Integral Approach to the Bound State Due to the *s-d* Exchange Interaction*)

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The Stratonovich-Hubbard transformation is applied to the partition function of the *s-d* exchange system to bring it into a functional average form over fluctuating fictitious *s-d* admixtures in order to study the singlet bound state. The static approximation is examined and effects of fluctuating components are taken into account by a perturbational method from the static approximation in the approximation of the most divergent terms. The correct binding energy is derived at 0°K. Calculations at low temperatures or at weak magnetic fields are achieved, on an assumption, to lead the normal behavior of the system. Green functions are also transformed similarly and their general property is discussed.

§1. Introduction

On the basis of the Yosida theory,[1] the ground state of a localized impurity spin in metals coupled with conduction electrons via the antiferromagnetic *s-d* exchange interaction has been worked out in the approximation of the most divergent terms by Yosida, Okiji, Ishii and Yoshimori.[2),3)] Important conclusions are: The ground state is the collective bound state with a binding energy anomalous in the interaction strength, which is a local singlet. Phase shifts of conduction electrons at the Fermi level are $\pm\pi/2$.[2)] The field dependence of magnetic properties of the bound state is shown to be normal.[3)]

In the present paper we investigate the singlet bound state in the *s-d* model, using the functional integral approach by Stratonovich and Hubbard,[4)] which has been recently applied to the Anderson model by Wang, Evenson and Schrieffer[5)] and by Hamann.[6)] Results are compared with those of the Yosida theory and a calculation of properties of the bound state at low temperatures is attempted.

The basic idea of the present approach is to bring the partition function of the system into a form of a functional average over fluctuating fictitious *s-d* mixing matrix elements by the Stratonovich-Hubbard transformation. In order to do that, we describe a localized spin in terms of an electron operator. This electron will be referred to as a *d* electron. Then we allow states of

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the d electron number n_d, 0 and 2 besides the proper states of $n_d=1$, in which the localized spin is defined. A part of the partition function from those allowed states should be separated after the functional average. The starting Hamiltonian does not connect the states of presence of a localized spin with states of no localized spin. For mathematical simplicity, appropriate potential terms are added to the Hamiltonian, which are irrelevant to the formation of the singlet bound state.

Not only the partition function but also the Green functions can be expressed in a functional average form.[7] However mainly calculation of the partition function is aimed, though a general property of Green functions is discussed. In order to perform the functional average, the fluctuating matrix elements are Fourier-transformed and a functional is expanded with respect to all the non-zero frequency components. That is, we have a perturbational expansion, of which unperturbed part contains the zero frequency component.

If one keeps only the unperturbed part (this is referred to as the static approximation) trace of the density matrix with the transformed Hamiltonian can be easily evaluated. One has an integral over amplitude of the zero frequency component left. When the extremal approximation is made for the integration, the result corresponds to the anomalous Green function method by Takano and Ogawa.[8] In the course of calculation we have the anomalous Green function similar to that by Takano and Ogawa and by Abrikosov,[9] but after the functional average this is proved to vanish completely, as it should be. This corresponds to a procedure of projecting states of presence of a localized spin by using a phase factor introduced to the anomalous average due to Nakajima.[10] However this kind of a procedure is built-in in the present formalism as a natural result due to the property of the starting Hamiltonian.

Higher order perturbational terms due to the non-zero frequency components are analyzed. After integrations over amplitudes of the non-zero frequency components, the most divergent terms, which can be identified as parquet diagrams,[15] are found. On the assumption of the weak coupling limit, only those terms are summed up to obtain an integrand in a closed form to a final integration over amplitude of zero frequency component. This integrand is correct within logarithmic accuracy. We sum the most divergent terms, referring to a series appearing in the x-ray singularity in metals with the *s-d* exchange interaction treated by Kato, Okiji and Osaka.[11] The final integration is performed in an approximation in accord with accuracy to the integrand to complete the calculation of the partition function. The regular terms with respect to the coupling constant appear in the expansion, but these are out of scope of this paper.

The antiferromagnetic isotropic exchange interaction is assumed here. Extension to the anisotropic case is not straightforward. One needs seemingly more complicated fluctuating parameters than in the present case.

This paper is organized as follows. In §2, the partition function is transformed into the functional average form. The same transformation is applied to the Green function. The static approximation is examined in §3. Higher order effects due to the finite frequency components are analyzed by the perturbation method in §4. In §5, the most divergent terms are picked up to bring into a closed form. A final integration is performed approximately in §6. Some concluding remarks are given in §7.

§2. Stratonovich-Hubbard transformation

The partition function in question for the system of conduction electrons and a localized spin $S=1/2$ is

$$Z=\mathrm{tr}\exp(-\beta H), \tag{2·1}$$

$$H=H_0+V_{sd}\,,\quad H_0=\sum_{k\sigma}\varepsilon_k c_{k\sigma}^{\dagger}c_{k\sigma}-2\mu_B H_z S_z\,, \tag{2·2}$$

$$V_{sd}=-(J/2N)\sum_{kk'}[(c_{k\uparrow}^{\dagger}c_{k'\uparrow}-c_{k\downarrow}^{\dagger}c_{k'\downarrow})S_z+c_{k\downarrow}^{\dagger}c_{k'\uparrow}S_+ +c_{k\uparrow}^{\dagger}c_{k'\downarrow}S_-], \tag{2·3}$$

where H_z is the external magnetic field acting only on a localized spin, J is negative so that the interaction is antiferromagnetic, the band energy is measured from the Fermi energy, and other notations are obvious. Instead of calculating the partition function given above, we shall calculate Z with V replaced to V_{sd}.

$$V=(J/8)\,[(\textstyle\sum_\sigma a_\sigma^{\dagger}c_\sigma+\sum_\sigma c_\sigma^{\dagger}a_\sigma)^2-(\sum_\sigma a_\sigma^{\dagger}c_\sigma-\sum_\sigma c_\sigma^{\dagger}a_\sigma)^2], \tag{2·4}$$

$$c_\sigma=N^{-1/2}\textstyle\sum_k c_{k\sigma}\,. \tag{2·5}$$

We can rewrite V as

$$V=V_{sd}-(J/4)\textstyle\sum_{\sigma\sigma'}a_\sigma^{\dagger}a_{\sigma'}c_{\sigma'}^{\dagger}c_{\sigma'}+(J/4)\sum_\sigma(a_\sigma^{\dagger}a_\sigma+c_\sigma^{\dagger}c_\sigma), \tag{2·6}$$

with

$$S_z=(1/2)(a_\uparrow^{\dagger}a_\uparrow-a_\downarrow^{\dagger}a_\downarrow),\qquad S_+=a_\uparrow^{\dagger}a_\downarrow\,, \tag{2·7}$$

where $a_\sigma^{\dagger}$ and a_σ are Fermi-operators to describe the localized d spin. In (2·1) trace is taken over states of presence of the localized spin. That is, trace is confined in states of $n_d=1$ ($n_d=a_\uparrow^{\dagger}a_\uparrow+a_\downarrow^{\dagger}a_\downarrow$). We extend trace here to states of $n_d=0$ and $n_d=2$. As we can see in (2·6), in the sub-space of $n_d=1$, V is essentially V_{sd} and in the sub-spaces of $n_d=0$ and $n_d=2$ V is merely a spin-independent potential ($V_{sd}=0$ here).

Now we apply the Stratonovich-Hubbard transformaion to Z,

$$\begin{aligned}Z&=\mathrm{tr}\exp[-\beta(H_0+V)]\\&=\int\delta\zeta(\tau)Z(\zeta(\tau))\exp\Big(-\int_0^1\pi|\zeta(\tau)|^2d\tau\Big),\end{aligned} \tag{2·8}$$

$$Z(\zeta(\tau))=\mathrm{tr}\,T_\tau \exp\left[-\int_0^1 \beta H_\tau(\zeta(\tau))d\tau\right], \tag{2·9}$$

$$-\beta H_\tau(\zeta(\tau))=-\beta H_{0\tau}-c\left[\zeta(\tau)\textstyle\sum_\sigma a^\dagger_{\sigma\tau}c_{\sigma\tau}+\zeta^*(\tau)\sum_\sigma c^\dagger_{\sigma\tau}a_{\sigma\tau}\right], \tag{2·10}$$

$$c=(-\pi\beta J/2)^{1/2}, \tag{2·11}$$

where $\zeta(\tau)$ is a fictitious *s-d* mixing matrix element, its real part comes from the transformation of the first term of (2·4), its imaginary part from of the second term, T_τ is the ordering operator for the imaginary time τ, and subscript τ attached for operators is the ordering label by Feynman.[12] Now the problem is to find motion of the *s-d* admixture system with a time-dependent mixing matrix element, which is a one-body problem, and then to make the functional average over all the possible time-dependent matrix elements.

If one multiplies $\zeta(\tau)$ by λ in Eq. (2·9) and differentiates both the sides of logarithm of Eq. (2·9) with respect to λ, one gets

$$(\partial/\partial\lambda)\log Z(\lambda\zeta(\tau))=-c\int_0^1 d\tau\left[\zeta(\tau)\textstyle\sum_\sigma\langle a^\dagger_{\sigma\tau}c_{\sigma\tau}\rangle+\zeta^*(\tau)\sum_\sigma\langle c^\dagger_{\sigma\tau}a_{\sigma\tau}\rangle\right], \tag{2·12}$$

where $\langle A_\tau\rangle$ is defined as

$$\langle A_\tau\rangle=Z(\lambda\zeta(\tau))^{-1}\,\mathrm{tr}\,T_\tau\left[A_\tau\exp\left(-\beta\int_0^1 H_\tau(\lambda\zeta(\tau))d\tau\right)\right], \tag{2·13}$$

and A_τ stands for any operator. If one has Green functions known,

$$g^\sigma_{ca}(\tau_1,\tau_2)=-\langle T_\tau c_{\sigma\tau_1}a^\dagger_{\sigma\tau_2}\rangle, \tag{2·14}$$

$$g^\sigma_{ac}(\tau_1,\tau_2)=-\langle T_\tau a_{\sigma\tau_1}c^\dagger_{\sigma\tau_2}\rangle, \tag{2·15}$$

the right-hand side of Eq. (2·12) can be calculated.

The Fourier transformation of g is made,

$$g^\sigma_{ca}(\tau_1,\tau_2)=\sum_{\omega_n\omega_{n'}} g^\sigma_{ca\,n,n'}\exp(-i\omega_n\tau_1+i\omega_{n'}\tau_2), \tag{2·16}$$

$$g^\sigma_{ac}(\tau_1,\tau_2)=\sum_{\omega_n\omega_{n'}} g^\sigma_{ac\,n,n'}\exp(-i\omega_n\tau_1+i\omega_{n'}\tau_2), \tag{2·17}$$

with $\omega_n=(2n+1)\pi$. If the Fourier transform of $\zeta(\tau)$ is introduced,

$$\zeta(\tau)=\sum_{\nu=-\infty}^{\infty}\zeta_\nu\exp(2\pi i\nu\tau), \tag{2·18}$$

Eq. (2·12) can be written in an integrated form as

$$Z(\zeta_\nu)=Z(0)\exp\left[-c\int_0^1 d\lambda\sum_{\sigma\nu n}(\zeta_\nu g^\sigma_{ca\,n+\nu,n}+\zeta^*_\nu g^\sigma_{ac\,n-\nu,n})\right]. \tag{2·19}$$

In the following we assume $H_z=0$ for the time being. Effects of the magnetic field will be considered in §5.

From the equation of motion,

$$(i\omega_n-\beta\varepsilon_k)g_{ka\,n,n'}=\lambda cN^{-1/2}\sum\zeta_\nu^* g_{a\,n-\nu,n'}\,, \tag{2·20}$$

$$i\omega_n g_{a\,n,n'}=\delta_{n,n'}+\lambda c\sum\zeta_\nu g_{ca\,n+\nu,n'}\,, \tag{2·21}$$

where $g_{ka\,n,n'}$ and $g_{a\,n,n'}$ are the Fourier transforms of $g_{ka}(\tau_1,\tau_2)$ and $g_a(\tau_1,\tau_2)$, respectively, defined by

$$g_{ka}(\tau_1,\tau_2)=-\langle T_\tau c_{k\sigma\tau_1}a^\dagger_{\sigma\tau_2}\rangle,$$

$$g_a(\tau_1,\tau_2)=-\langle T_\tau a_{\sigma\tau_1}a^\dagger_{\sigma\tau_2}\rangle$$

and

$$g_{ca\,n,n'}=N^{-1/2}\sum_k g_{ka\,n,n'}\,. \tag{2·22}$$

A formal solution of Eqs. (2·20) and (2·21) in a matrix notation is given by

$$g_a=(1-\lambda^2 g\eta)^{-1}g, \tag{2·23}$$

where

$$g_a=(g_{a\,n,n'}),\qquad g=(g_n\delta_{n,n'}), \tag{2·24}$$

$$g_n=(i\omega_n-\lambda^2\xi_n)^{-1},\qquad \xi_n=c^2N^{-1}|\zeta_0|^2F_n\,, \tag{2·25}$$

$$F_n=\sum_k(i\omega_n-\beta\varepsilon_k)^{-1}, \tag{2·26}$$

$$\eta=(\eta_{n,n'}), \tag{2·27}$$

$$\eta_{n,n'}=\begin{cases}c^2N^{-1}\sum\limits_\nu\zeta^*_{n-n'+\nu}\zeta_\nu F_{n+\nu} & \text{for}\quad n\neq n',\\ c^2N^{-1}\sum\limits_{\nu\neq0}|\zeta_\nu|^2F_{n+\nu} & \text{for}\quad n=n'.\end{cases} \tag{2·28}$$

An expression of g_{ca} is easily found, and a similar calculation for g_{ac} can be done to have the same contribution from the g_{ac} term in (2·19) as that from g_{ca} term. Finally, we have

$$Z(\zeta_\nu)=Z(0)\exp\Big[-\int_0^1 d\mu\, 2\,\mathrm{tr}(\xi+\eta)(1-\mu g\eta)^{-1}g\Big], \tag{2·29}$$

where $\mu=\lambda^2$ and a matrix ξ is defined by

$$\xi=(\xi_n\delta_{n,n'}). \tag{2·30}$$

The partition function is now expressed as

$$Z=\int\prod_\nu d^2\zeta_\nu Z(\zeta_\nu)\exp(-\pi\sum_\nu|\zeta_\nu|^2), \tag{2·31}$$

where integrations are over complex plane of ζ_ν.

If a formal expansion with respect to $\mu g\eta$ for $(1-\mu g\eta)^{-1}$ and the use of relation $dg/d\mu=g\xi g$ are made, one has

$$Z(\zeta_\nu)=Z(0)\exp(A_0+A), \tag{2·32}$$

$$A_0=-2\int_0^1 d\mu\,\mathrm{tr}\,\xi g, \tag{2·33}$$

$$A=-2\sum_{p=1}^{\infty}p^{-1}\,\mathrm{tr}(g(\mu=1)\eta)^p. \tag{2·34}$$

We show here the result that the Stratonovich-Hubbard transformation is applied for Green functions and that anomalous Green functions vanish after the functional integration. A Green function can be defined by using the ordering label of Feynman as

$$G_{AB}(\tau_1,\tau_2)=-Z^{-1}\,\mathrm{tr}\,T_\tau\left[A_{\tau_1}B_{\tau_2}\exp\left(-\int_0^1 d\tau\beta H_\tau\right)\right]. \tag{2·35}$$

After a similar calculation of the exponential factor in (2·35) to that in Z, we have, for the Fourier transform of G_{AB} defined in the same way as in (2·16) and (2·17),

$$G_{AB\,n,n'}=Z^{-1}\int\prod_\nu d^2\zeta_\nu\, g_{AB\,n,n'}(\zeta_\nu)Z(\zeta_\nu)\exp(-\pi\sum|\zeta_\nu|^2), \tag{2·36}$$

where g_{AB} is a Green function similar to g_{ca} subjected to the effective Hamiltonian $H_\tau(\zeta_\nu)$ with given ζ_ν's.

Let us consider the anomalous Green function G_{ca}. The corresponding Green function g_{ca} can be found easily from Eqs. (2·20)$\sim$(2·23) as

$$g_{ca\,n,n'}=cN^{-1}F_n\sum_\nu\zeta_\nu^*\,[(1-g\eta)^{-1}]_{n-\nu,n'}g_{n'}. \tag{2·37}$$

If we expand $(1-g\eta)^{-1}$ with respect to $g\eta$, together with the expansion of (2·32), we see that each term of the expansion of $g_{ca}Z(\zeta_\nu)$ contains always at least one ζ_ν with exponent of an odd integer. Note $\eta_{n,n'}$ is a quadratic form of ζ_ν and g_n contains only the absolute square of ζ_0. As we see in the later section, the gaussian average of ζ_ν with an odd number exponent always vanishes because of the angular integration on the complex plane of ζ_ν. Therefore G_{ca} necessarily vanishes after the functional average in (2·36). We can prove this in general for the anomalous Green functions G_{AB} in which a product operator AB connects states with different values of n_a. Hence an anomalous average $\langle AB\rangle_t$ vanishes also. The average $\langle\ \rangle_t$ here denotes average with the total Hamiltonian.

§3. Static approximation

In this section we examine the static approximation. When $\zeta(\tau)$ is assumed to be τ-independent, that is, all the ζ_ν except ζ_0 are neglected, $Z(\zeta_0)$ is given by

$$Z(\zeta_0)=Z(0)\exp A_0\,, \tag{3·1}$$

from (2·32)~(2·34). The definitions (2·24), (2·25), (2·30) and (2·33) give

$$A_0=-2\int_0^1 d\mu\sum_n \xi_n(i\omega_n-\mu\xi_n)^{-1}. \tag{3·2}$$

The summation over n is converted to a contour integral around the imaginary axis as usual. One can change the contour for it along the real axis. After μ-integration one has

$$A_0=\frac{2}{\pi}\beta y\int_{-D}^{D}d\varepsilon\frac{df}{d\varepsilon}\,\mathrm{Re}\left[\log\frac{\varepsilon+iy}{D}-1+\frac{\varepsilon}{iy}\log\frac{\varepsilon+iy}{\varepsilon}\right], \tag{3·3}$$

where the constant density of states ρ is assumed for the conduction band (the band width is $2D$ and the Fermi level is at its center), $F(\varepsilon+i0^+)$ is approximated by $-i\pi\rho/\beta$ for $|\varepsilon|<D$ and by zero otherwise, and y is defined as

$$y=(\pi^2/2\beta)(-J\rho/N)|\zeta_0|^2. \tag{3·4}$$

The expression (3·3) can be evaluated with the assumption $\beta y\gg 1$ as

$$A_0=-(2/\pi)\beta y\,[\log(y/D)-1+(\pi/\beta y)\log 2-(\pi^2/6)(\beta y)^{-2}+\cdots], \tag{3·5}$$

with the use of relations, $(\beta D\gg 1)$

$$\int_0^D d\varepsilon(df/d\varepsilon)\varepsilon=-(1/\beta)\log 2,\quad \int_{-D}^{D}d\varepsilon(df/d\varepsilon)\varepsilon^2=-(\pi^2/3\beta^2).$$

Then Z in the static approximation is given by

$$Z=Z_c(2\beta/\pi)(-N/J\rho)\int_0^\infty dy\exp[(2\beta/\pi)(N/J\rho)yB_0(y)], \tag{3·6}$$

where Z_c is the partition function for the system of conduction electrons with $J=0$, the angular integration over the complex plane of ζ_0 has been made, and $B_0(y)$ is defined by

$$B_0(y)=1-(J\rho/N)\log(y/D)+(J\rho/N)+(J\rho/N)(\pi^2/6)(\beta y)^{-2}+\cdots. \tag{3·7}$$

We note a factor 4 in $Z(0)=4Z_c$, which is due to the degeneracy of d electron levels in the $J=0$ case, is canceled by the third term in the square brackets

of (3·5). This means there is no degeneracy of the ground state for any given ζ_0, as should be from the form of the effective Hamiltonian, $H(\zeta_0)$.

If one makes the extremal approximation for the integral in (3·6), that is, the integral is approximated by the maximum of the integrand, one gets

$$Z=Z_c \exp[\beta(2/\pi)\tilde{y}_0], \quad \tilde{y}_0=D\exp(N/J\rho), \tag{3·8}$$

where $\beta\to\infty$ is assumed. One can calculate easily effects of an external magnetic field and properties at finite temperatures. Results correspond to those of the anomalous Green function method by Takano-Ogawa[8] and Klein.[13] The value of the binding energy given in (3·8) is different from that by them and looks correct. However this is spurious because our starting Hamiltonian contains the potential term and it gives a spurious contribution in the static approximation to lead incidentally the correct value. This can be checked by using the anomalous Green function method for the starting Hamiltonian.

The correction terms to the extremal approximation can be calculated from (3·6) by the steepest descent method. This does not improve the results. So we must take into account the effects of the fluctuating component of $\zeta(\tau)$, which is the main subject of the remaining part of the paper.

It is noted here that the ground state in this static approximation is a local singlet. This can be seen from the value of $\langle\sigma\cdot S\rangle_1$, which should be $-3/4$ for singlet. Here, σ is the total spin of the conduction electrons and average is over only the state with the localized spin. In the static approximation one can show easily

$$\langle\sigma\cdot S\rangle=-(3/2)\textstyle\sum_k\langle c_{k\uparrow}^{\dagger}a_{\uparrow}\rangle^2=-3/8, \tag{3·9}$$

where the average is over all the states with any n_d value and under the effective Hamiltonian with any given ζ_0. Considering that the states with $n_d=0, 2$ give no contribution to this and that the absolute square of the amplitude of the ground state (for a given ζ_0) projected into the sub-space of $n_d=1$ has the weight 1/2 to the total, one may conclude $\langle\sigma\cdot S\rangle_1$ is $-3/4$. Therefore the static approximation would be a good zeroth approximation on which effects of the fluctuating components are taken into account as perturbation. We note furthermore that the anomalous Green functions like G_{ca} vanish even in the static approximation as in the general proof given in the previous section.

§4. Higher order perturbation

We consider here effects of the fluctuating components ζ_ν $(\nu\neq0)$. That is, the term A (2·34) neglected by the static approximation is now taken into account. Let us introduce an average which represents the integral over ζ_ν $(\nu\neq0)$ for given ζ_0 by

$$\langle\cdots\rangle_{\zeta_0}=\int\prod_{\nu\neq 0}d^2\zeta_\nu\exp(-\pi\sum_{\nu\neq 0}|\zeta_\nu|^2)\cdots. \tag{4·1}$$

Then the partition function Z is expressed as

$$Z=Z(0)\int d^2\zeta_0\exp(-\pi|\zeta_0|^2)\exp A_0\,\langle\exp A\rangle_{\zeta_0}. \tag{4·2}$$

The last factor which results from fluctuations of the mixing is rewritten in terms of cumulant averages, $\langle\cdots\rangle^c_{\zeta_0}$,[14] as

$$\langle\exp A\rangle_{\zeta_0}=\exp\{\langle\exp A\rangle^c_{\zeta_0}-1\}=\exp\left\{\sum_{m=1}^{\infty}\frac{\langle A^m\rangle^c_{\zeta_0}}{m!}\right\}. \tag{4·3}$$

We are going to calculate the averages $\langle A^m\rangle^c_{\zeta_0}$ or $\langle A^m\rangle_{\zeta_0}$ perturbationally with the aid of a diagrammatic representation. Rules for the correspondence of a term in the formula to a diagram element are summarized in Table I. Then, for instance, the p-th term in the expansion of A (2·34),

Table I.

term in the formula	element in the diagram
g_n	n (spin line)
F_n	n (electron line)
$c/\sqrt{N}\,\zeta^*_\nu$	ν (mixing line)
$c/\sqrt{N}\,\zeta_\nu$	ν (mixing line)

$$-\frac{1}{p}\mathrm{tr}(g\eta)^p=-\frac{1}{p}\left(\frac{c^2}{N}\right)^p\sum_{1\sim p}{\sum_{\nu_1\sim\nu_p}}'\prod_{i=1}^{p}\zeta^*_{\nu_i}\zeta_{i-(i-1)+\nu_{i-1}}F_i\,g_{i-\nu_i}, \tag{4·4}$$

is represented by Fig. 1. In (4·4), $(i-1)=p$ for $i=1$ and a dash attached to the summation means that each ν_i should not satisfy $\nu_i=\nu_{i-1}+i-(i-1)=0$, because of the definition of η, (2·27), (2·28). In the diagram, frequencies associated with g, F and ζ are conserved at any vertex point. When we average (4·4) over the frequencies, there remain only terms with same number of ζ_ν and ζ^*_ν for each frequency ν because of

$$\langle\zeta^{*m}_\nu\zeta^n_\nu\rangle_{\zeta_0}=\delta_{n,m}\frac{n!}{\pi^n}.$$

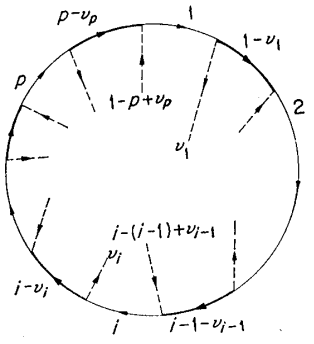

Fig. 1. The p-th term in the expansion of A.

In the diagram, after the averaging procedure, we connect dotted arrows with

same frequencies together. There are several possibilities to do so and to give non-vanishing elements in the result. Here we write down the first few terms of the resulting averaged expansion of $\langle A\rangle^c_{\zeta_0}$, some of which are shown by the diagrams in Fig. 2;

$$\langle A\rangle^c_{\zeta_0}=\langle A\rangle_{\zeta_0}=-2\{U\sum_1\sum_\nu{}' F_1 g_{1-\nu} \tag{4·5-1}$$

$$+(1/2)U^2\{\pi|\zeta_0|^2 2\sum_1\sum_\nu{}' F_1^2 g_1 g_{1-\nu} \tag{4·5-2a}$$

$$+\sum_1\sum_{\nu\nu'}{}' F_1^2 g_{1-\nu}g_{1-\nu'} \tag{4·5-2b}$$

$$+\sum_{12}{}'\sum_\nu{}' F_1 F_2 g_{1-\nu}^2 \tag{4·5-2c}$$

$$+2\sum_1\sum_\nu{}' F_1^2 g_{1-\nu}^2\} \tag{4·5-2d)*}$$

$$+(1/3)U^3\{\pi|\zeta_0|^2 3\sum_{123}{}' F_1F_2F_3 g_1 g_2 g_{1+2-3} \tag{4·5-3a}$$

$$+\sum_{123}{}'\sum_\nu{}' F_1F_2F_3 g_{1-\nu}g_{2-\nu}g_{1+2-3-\nu} \tag{4·5-3b}$$

$$+3\sum_{12}{}'\sum_{\nu_1\nu_2}{}' F_1^2F_2 g_{1-\nu_1}^2 g_{1-\nu_2} \tag{4·5-3c}$$

$$+\pi|\zeta_0|^2 6\sum_{13}{}' F_1^2F_3 g_1^2 g_{1+1-3}\} \tag{4·5-3d)**}$$

$$+[\text{other terms of } O(J^3)]$$

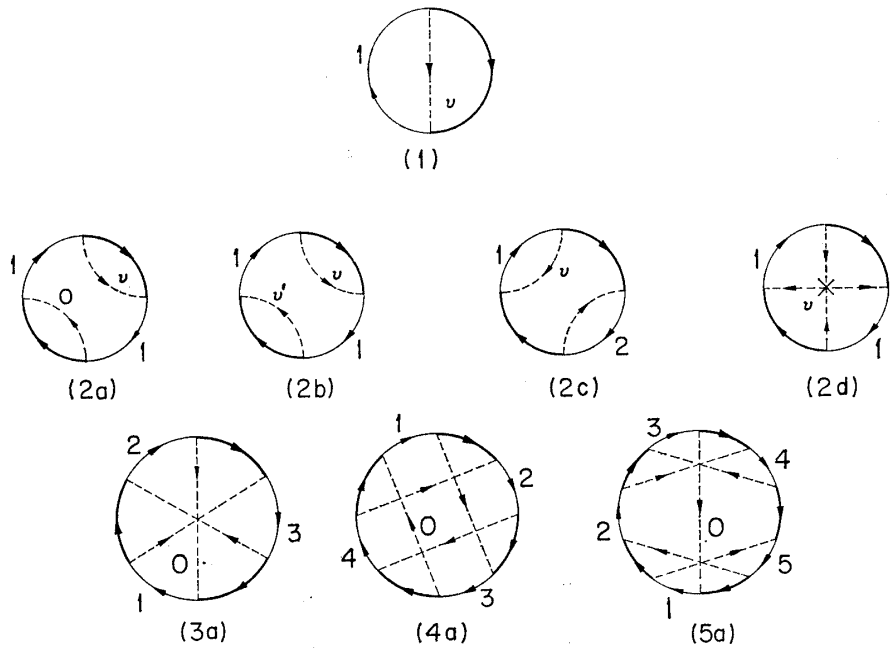

Fig. 2. Diagrammatic representation of $\langle A\rangle^c_{\zeta_0}$, (4·5).

*) (2d) should not be included if the restrictions $1\neq 2$ in (2c) and $\nu\neq\nu'$ in (2b) are omitted.

**) The factor 6 in (3d) changes to 3 if the restriction $1\neq 2$ of the sum in (3a) is omitted.

$$+(1/4)U^4\pi|\zeta_0|^2 4\sum_{1\sim4}{}' F_1F_2F_3F_4 g_1 g_{1+2-4} g_{2+3-4} g_3 \qquad (4\cdot5\text{–}4a)$$

$$+[\text{other terms of } O(J^4)]$$

$$+(1/5)U^5\pi|\zeta_0|^2 5\sum_{1\sim5}{}' F_1F_2F_3F_4F_5 g_1 g_2 g_3 g_{1+2-5} g_{2+3-4} \qquad (4\cdot5\text{–}5a)$$

$$+[\text{other terms of } O(J^5)]+\cdots\}, \qquad (4\cdot5)$$

where $U\equiv c^2/(\pi N)\propto J$. The dash attached to the summation designates that all the frequencies are to be summed with special attentions not to equate a dotted line frequency to another independent one or to zero if there is no indication. On the other hand a small cross at the center in the diagram (2d) represents that all the dotted lines connected to it have the same frequencies. In a similar way we obtain the following expansion for $\langle A^2\rangle^c_{\zeta_0}$, which corresponds to Fig. 3;

$$\langle A^2\rangle^c_{\zeta_0}=\langle A^2\rangle_{\zeta_0}-\langle A\rangle^2_{\zeta_0}$$

$$=4\{U^2\sum_{12}\sum_{\nu}{}' F_1F_2 g_{1-\nu} g_{2-\nu} \qquad (4\cdot6\text{–}2a)$$

$$+U^3\{\pi|\zeta_0|^2 2\sum_{12}\sum_{\nu}{}' F_1^2F_2 g_1 g_{1-\nu} g_{2-\nu} \qquad (4\cdot6\text{–}3a)$$

$$+2\sum_{12}\sum_{\nu\nu'}{}' F_1^2F_2 g_{1-\nu} g_{1-\nu'} g_{2-\nu'} \qquad (4\cdot6\text{–}3b)$$

$$+2\sum_{123}{}'\sum_{\nu}{}' F_1F_2F_3 g_{1-\nu}^2 g_{1-2+3-\nu} \qquad (4\cdot6\text{–}3c)$$

$$+4\sum_{12}\sum_{\nu}{}' F_1^2F_2 g_{1-\nu}^2 g_{2-\nu}\} \qquad (4\cdot6\text{–}3d)$$

$$+U^4\pi|\zeta_0|^2 2\{\sum_{1234}{}' F_1F_2F_3F_4 g_1 g_2 g_{1+2-3} g_{2+4-3} \qquad (4\cdot6\text{–}4a)$$

$$+\sum_{1234}{}' F_1F_2F_3F_4 g_1 g_2 g_{1+2-3} g_{1+4-3} \qquad (4\cdot6\text{–}4b)$$

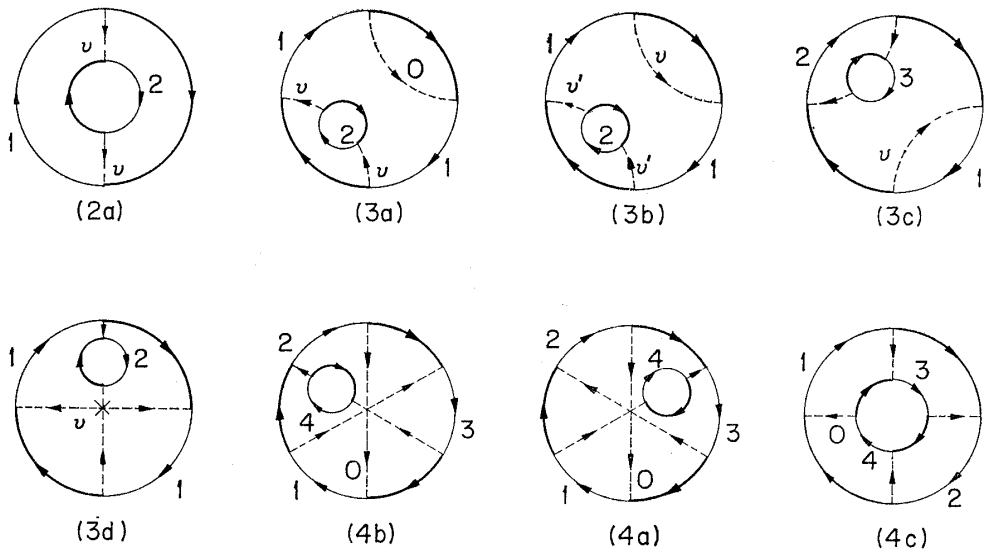

Fig. 3. Diagrammatic representation of $\langle A^2\rangle^c_{\zeta_0}$, (4·6).

$$+\sum_{1234}{}' F_1F_2F_3F_4g_1g_4g_{1+4-2}g_{1+4-3}\} \qquad (4\cdot6\text{–}4c)$$

$$+[\text{other terms of order } O(J^4)]+\cdots\}. \qquad (4\cdot6)$$

The higher order cumulants are obtainable by using formulae,

$$\langle A^3\rangle^c_{\zeta_0}=\langle A^3\rangle_{\zeta_0}-3\langle A\rangle_{\zeta_0}\cdot\langle A^2\rangle_{\zeta_0}+2\langle A\rangle^3_{\zeta_0}, \quad \text{etc.}$$

In these expansions, terms which are factorizable into more than two independently averaged traces and so correspond to disconnected graphs have disappeared from the result, according to a general property of the cumulant.[14] Each term of $\langle A^n\rangle^c_{\zeta_0}$, being an averaged product of n traces, has n circles made of g- and F-lines in the diagram representation. $\langle A^n\rangle^c_{\zeta_0}$ forms a series beginning with $O(J^n)$ terms.

§5. Most divergent terms

By examining each term of the cumulant expansions discussed above we can find they contain divergent terms like $(J\rho/N)^m(\log\{y/D\})^n$, among which the most divergent ones (with $n=m$) are chosen to sum.

At first, a series with the coefficient $\pi|\zeta_0|^2$ is discussed. An only one candidate of second order, (4·5–2a), is not divergent. Among the third order terms, (4·5–3a) can be evaluated by contour integrals in the logarithmic accuracy as

$$\begin{aligned}
&-2\pi|\zeta_0|^2U^3\sum_{12}g_1g_2F_1F_2\frac{-\beta}{2\pi i}\int_c dzf(z)\frac{F(-\beta z)}{\beta z+i\omega_1+i\omega_2-\xi(\beta z+i\omega_1+i\omega_2)}\\
&\simeq 2\pi|\zeta_0|^2(U\rho/\beta)^3\,\mathrm{Re}\iint_{-D}^{D}d\varepsilon d\varepsilon' f(\varepsilon)f(\varepsilon')\frac{\log\{(\varepsilon+\varepsilon'+iy)/D\}}{(\varepsilon+iy)(\varepsilon'+iy)}\\
&\simeq-\pi|\zeta_0|^2\frac{1}{12}(J\rho/N)^3\{\log^3(y/D)+3\log^2(y/D)(\pi^2/6)(\beta y)^{-2}\}, \qquad (5\cdot1)
\end{aligned}$$

where the integral path is shown in Fig. 4, and the result is expanded up to $(\beta y)^{-2}$. Although the temperature dependent term itself seems to be next divergent in comparison with the independent ones, we retain it because it is the highest in temperature dependent terms. Other third order terms like (4·5–3d) are not most divergent. The fourth order most divergent contributions come from $\langle A^2\rangle^c_{\zeta_0}$, namely terms (4·6–4a), (4·6–4b) and (4·6–4c). The former two give the argument of the exponential (4·3) the value

$$\begin{aligned}
&-\pi|\zeta_0|^2 2(U\rho/\beta)^4\,\mathrm{Re}\int_{-D}^{D}d\varepsilon_1 f(\varepsilon_1)\int_{-D}^{D}d\varepsilon_2 f(\varepsilon_2)\\
&\qquad\times\int_{-D}^{0}d\varepsilon_3\frac{\log\{(\varepsilon_2+\varepsilon_3+iy)/D\}}{(\varepsilon_1+iy)(\varepsilon_2+iy)(\varepsilon_1+\varepsilon_2+\varepsilon_3+iy)}\\
&\simeq-\pi|\zeta_0|^2\frac{1}{6\cdot2^4}\left(-\frac{J\rho}{N}\right)^4[\log^4(y/D)+4\log^3(y/D)\cdot(\pi^2/6)(\beta y)^{-2}],
\end{aligned} \qquad (5\cdot2)$$

where we have used

$$\sum_4 F_4 g_{2+4-3} \simeq (\rho/\beta) \log\{[i\omega_2 - i\omega_3 - \xi(i\omega_2 - i\omega_3)]/(-\beta D)\},$$

$$\sum_3 F_3 g_{1+2-3} \sum_4 F_4 g_{2+4-3} \simeq -(\rho/\beta)^2 \int_{-D}^{0} d\varepsilon \frac{\log\{[\beta\varepsilon + i\omega_2 - \xi(i\omega_2)]/(-\beta D)\}}{\varepsilon + (i\omega_1 + i\omega_2)/\beta - \xi(i\omega_1 + i\omega_2)/\beta}.$$

On the other hand the latter (4·6–4c) is evaluated as

$$\pi|\zeta_0|^2 (U\rho/\beta)^4 \mathrm{Re} \int d\varepsilon f(\varepsilon) \int d\varepsilon' f(\varepsilon') \frac{\log^2\{(\varepsilon + \varepsilon' + iy)/D\}}{(\varepsilon + iy)\cdot(\varepsilon' + iy)}$$
$$\simeq -1 \times (5\cdot 2). \qquad (5\cdot 3)$$

That is, these three terms of fourth order cancel one another giving no most divergent contribution.

We notice here that each most divergent term in the series has one to one correspondence to the Abrikosov's parquet diagram[15] describing the vertex part if one has integrated the vertexes multiplied by external lines with respect to external frequencies of electrons, too. For instance, (4·5–3a) can be represented by Fig. 5 (3a), while (4·6–4a), (4·6–4b) and (4·6–4c) by Fig. 5 (4a), (4b) and (4c) respectively.

The fifth order terms can be also evaluated in a similar way, where the terms represented by Fig. 6 are found to be most divergent. In Fig. 6 the corresponding parquet diagrams are also illustrated. The sum of them amounts to

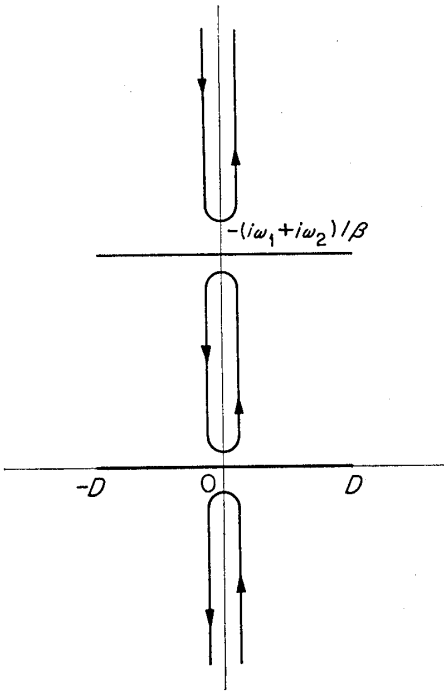

Fig. 4. The integral path used in (5·1). The cuts are due to F or ξ. For the most divergent terms, only F's cuts are important.

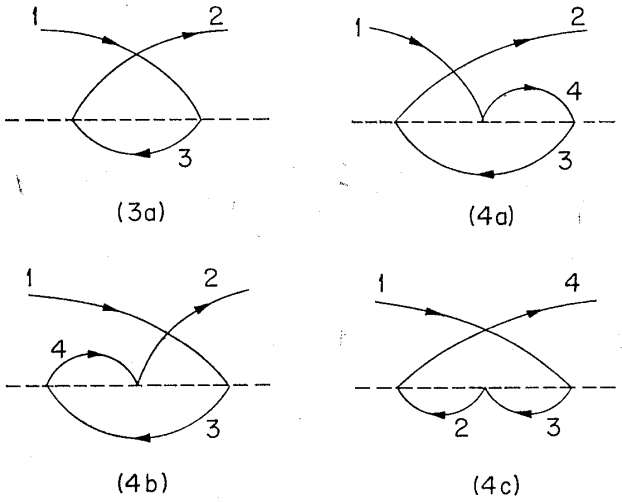

Fig. 5. Parquet diagrams corresponding to most divergent terms in (4·5) and (4·6).

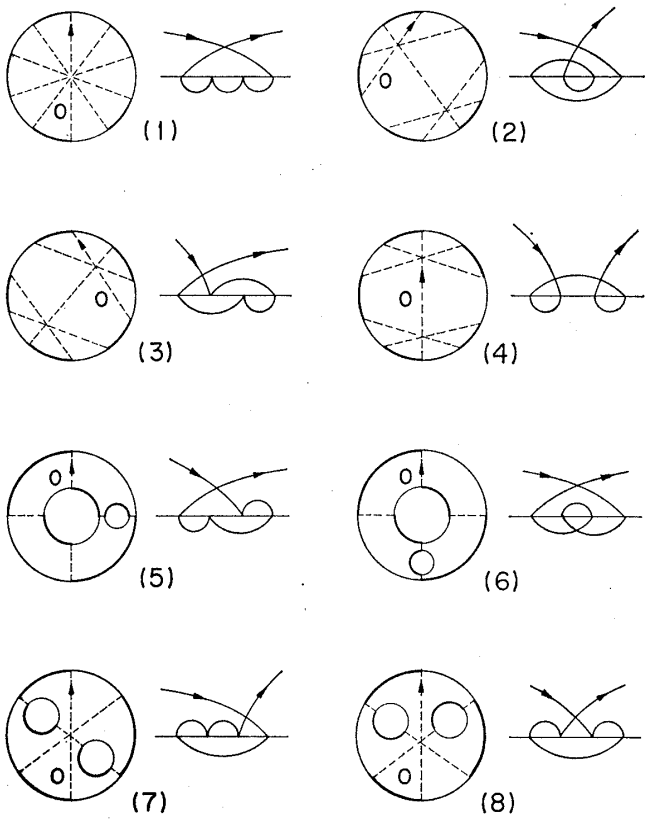

Fig. 6. Diagrams describing the fifth order most divergent terms.

$$\pi|\zeta_0|^2\frac{7}{480}\left(\frac{J\rho}{N}\right)^5\left[\log^5(y/D)+5\log^4(y/D)\frac{\pi^2}{6(\beta y)^2}\right]. \qquad (5\cdot4)$$

If the effects of fluctuations up to fifth order in J are added to the static contribution in (3·6), we obtain, for the argument of the exponential (4·3),

$$-\pi|\zeta_0|^2[g(X,\beta)+(J\rho/N)(\pi^2/3)/(\beta y)^2+(J\rho/N)], \qquad (5\cdot5)$$

where

$$g(X,\beta)=g(X)+y(dg(X)/dy)(\pi^2/6)(\beta y)^{-2}, \qquad (5\cdot6)$$

$$g(X)\equiv1-X+(1/12)X^3-(7/480)X^5+\cdots, \qquad (5\cdot7)$$

$$X\equiv(J\rho/N)\log(y/D).$$

Relating to the series $g(X)$, (5·7), we note here the following fact: When we consider a system of conduction electrons coupled with an impurity by both the exchange and potential interactions, $V_{sd}+(J/4)\sum_\sigma c_\sigma^\dagger c_\sigma$, an amplitude of the wave function of the singlet ground state, $\Gamma(\varepsilon)$, satisfies the following integral equation in the most divergent approximation, of which integration kernel is given by Kato, Okiji and Osaka[11] for the problem of singularities in the x-ray absorption,

$$\Gamma(\varepsilon)(\varepsilon-\widetilde{E})+(J\rho/N)\int_0^D d\varepsilon'\Gamma(\varepsilon')+\int_0^D d\varepsilon'\Gamma(\varepsilon')K(\varepsilon,\varepsilon')=0, \tag{5·8}$$

$$K(\varepsilon,\varepsilon')=-(1/16)(J\rho/N)^2\log[(\varepsilon+\varepsilon'-\widetilde{E})/D]$$
$$+(3/16)(J\rho/N)^2\log[(\varepsilon+\varepsilon'-\widetilde{E})/D]\,[1-(J\rho/N)\log((\varepsilon+\varepsilon'-\widetilde{E})/D)]^{-1}$$
$$+(3/8)(J\rho/N)\log[1-(J\rho/N)\log((\varepsilon+\varepsilon'-\widetilde{E})/D)]. \tag{5·9}$$

The secular equation for it is

$$0=1+(J\rho/N)\left\{\int_0^D\frac{d\varepsilon}{\varepsilon-\widetilde{E}}-\iint_0^D d\varepsilon d\varepsilon'\frac{K(\varepsilon,\varepsilon')}{(\varepsilon-\widetilde{E})(\varepsilon'-\widetilde{E})}\right.$$
$$\left.+\iiint_0^D d\varepsilon d\varepsilon' d\varepsilon''\frac{K(\varepsilon,\varepsilon')K(\varepsilon',\varepsilon'')}{(\varepsilon-\widetilde{E})(\varepsilon'-\widetilde{E})(\varepsilon''-\widetilde{E})}+\cdots\right\}$$
$$=1-x+(1/12)x^3-(7/480)x^5+\cdots \tag{5·10}$$

in an expanded form, or

$$0=\left\{1+\int_0^x du(1-u)^{-3/2}\exp(u/2)\right\}^{-1} \tag{5·11}$$

in a closed form which can be derived by the differential equation method[16] and gives a root of $x=1$. We put here $x=(J\rho/N)\log(-\widetilde{E}/D)$. Since the series for the secular equation (5·10) is the same in the result and in the structure*) as $g(X)$ we are summing up, we identify $g(X)$ with the right-hand side of (5·10) and put

$$g(X)=\left\{1+\int_0^X du(1-u)^{-3/2}\exp(u/2)\right\}^{-1} \tag{5·12}$$

in the closed form.

The other possibility giving most divergent terms is there in the terms with no ζ_0 component from η. For instance let us consider a series of terms corresponding diagrams obtainable by changing a $\nu=0$ dotted line to $\nu\neq0$ in the most divergent diagrams above discussed. (4·5–3b) corresponding to (4·5–3a) is one of them. Now the sum over ν is restricted by $\nu\neq0$, then all the frequencies ($\nu\neq0$) are averaged at once. If the sum is rearranged as

$$\sum_{\nu\neq0}=\sum_{\nu}-\sum_{\nu=0}$$

after averaging, the first term of the right hand gives the result which can be interpreted as the regular part of the energy shift, which is out of scope of this paper and will not be discussed further. The second term becomes most

*) For instance, the fifth order term of Fig. 6 (4) corresponds to one of the terms in the third integral (5·10) with double $K(\varepsilon,\varepsilon')$ integrand, while our other terms appearing so far correspond to ones in the first and the second integral.

divergent and this kind of terms form a series which can be summed up as $g(X)-1$ with inclusion of the term (4·5–1).

We can also gather p products of terms each diagram of which is obtained by replacement of a $\nu=0$ dotted line by a $\nu\neq 0$ line in a most divergent graph. Two examples of these terms with $p=2$ are shown in Fig. 7(a) and (b). In these cases the most divergent terms are extracted as follows:

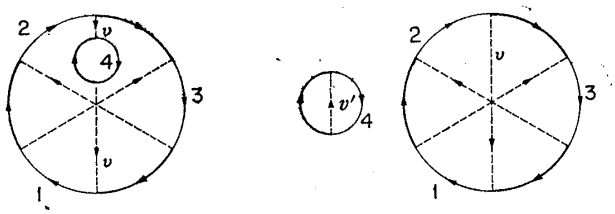

Fig. 7. All the frequencies of the mixing lines are confined to be different from each other and not to be zero.

term (a)

$$3\cdot 2!\,U^4\sum_{\nu}'\sum_{1\,2\,3}'F_1F_2F_3\,g_{1-\nu}g_{2-\nu}g_{1+2-3-\nu}\sum_{4}F_4\,g_{4-\nu}$$
$$=3\cdot 2!\,U^4\Big(\sum_{\nu}-\sum_{\nu=0}\Big)\to -2(-X)(X^3/12).$$

term (b)

$$U^4\sum_{\nu\neq\nu'}'\sum_{1\sim 3}'F_1F_2F_3\,g_{1-\nu}g_{2-\nu}g_{1+2-3-\nu}\sum_{4}'F_4\,g_{4-\nu'}$$
$$=U^4\Big(\sum_{1\,2\,3\,\nu}'\cdots\Big)\Big(\sum_{4\,\nu'}'\cdots\Big)-3U^4\sum_{\nu=\nu'}'\Big(\sum_{1\,2\,3}'\cdots\Big)\Big(\sum_{4}\cdots\Big)$$
$$\to(\text{disconnected part})+(-X)(X^3/12).$$

Sum of them contributes to the exponential argument as

$$-(2/2)(-X)(X^3/12).$$

In this way, such terms as them with $p=2$ can be brought to

$$-(1/2)\,[g(X)-1]^2,$$

and, in general,

$$-(-1)^p/p\cdot\,[g(X)-1]^p \qquad (5\cdot 13)$$

can be found in connection with the series for p products. Therefore, the most divergent terms without $\pi|\zeta_0|^2$ coefficients become collected as

$$\log[g(y,\beta)] \qquad (5\cdot 14)$$

in all together at finite temperatures. Hereafter the variable in the function g will be described by using y rather than X.

Combining (3·6), (4·2), (5·5) and (5·14) we finally obtain the expression for the partition function in an integral form,

$$Z=Z_c(2\beta/\pi)(-N/J\rho)\int dy g(y,\beta)\exp[(2\beta/\pi)(N/J\rho)yB'(y)], \quad (5\cdot15)$$

$$B'(y)=g(y,\beta)+(J\rho/N)(\pi^2/3)(\beta y)^{-2}+(J\rho/N)$$

in the most divergent approximation omitting the regular terms. Comparing this with (3·6), we see a great difference. We note furthermore that the expression of the integrand is an expansion of $(\beta y)^{-1}$, $(\beta y \gg 1)$, in the exponent, where the first three terms are given, and, in each coefficient the most divergent terms are summed up into the closed form.

At the end of this section we consider the effect of the magnetic field H_z acting on the localized spin. A magnetic field acting on the conduction electrons gives merely the Pauli paramagnetic term in addition to the result obtained here.[17] When we have the Zeeman term in H_0 given by (2·2), the Green function g_n^σ given by (2·25) turns out to be

$$g_n^\sigma=(i\omega_n+\sigma\mu_B H_z-\lambda^2\xi_n)^{-1}, \quad (5\cdot16)$$

where $\sigma=+1$ for the up spin d-electron and -1 for the down spin. The other part of the calculation of the Green functions is the same as in the case of $H_z=0$. Through §§4 and 5 the calculation is also the same. Only care to be made is to discriminate between $g_n^\uparrow$ and $g_n^\downarrow$. We confine ourselves in the case of the weak magnetic field at the absolute zero of temperature. The calculation up to H_z^2 is straightforward in parallel with that of $H_z=0$. Omitting details, we show here the expression corresponding to (5·15),

$$Z=Z_c(2\beta/\pi)(-N/J\rho)\int dy g(y,H_z)\exp[(2\beta/\pi)(N/J\rho)yB''(y)], \quad (5\cdot17)$$

$$B''(y)=g(y,H_z)+(J\rho/N)(\mu_B H_z/y)^2+(J\rho/N),$$

$$g(y,H_z)=g(X)+y[dg(X)/dy](1/2)(\mu_B H_z/y)^2, \quad (5\cdot18)$$

where $g(X)$ is defined by (5·7).

§6. Final integration for the partition function

First we consider the case at the absolute zero and $H_z=0$. For the expression (5·15) at the absolute zero,

$$Z=Z_c(2\beta/\pi)(-N/J\rho)\int dy g(X)\exp[(2\beta/\pi)y((N/J\rho)g(X)+1)], \quad (6\cdot1)$$

the extremal approximation being made, we get for $\beta\to\infty$

$$Z=Z_c\exp[(2\beta/\pi)\tilde{y}], \quad (6\cdot2)$$

where $\tilde{y}$ is determined by maximizing the exponent in the approximation of the most divergent terms,

$$g(X)=0, \quad \tilde{y}=D\exp(N/J\rho). \tag{6·3}$$

We note here the condition (6·3) is the eigenvalue equation (5·11) for the singlet bound state. The ground state energy $-(2/\pi)\tilde{y}$ obtained in (6·2) is the correct one.

The fact mentioned above indicates convincingly that the extremal approximation is a good one for deriving the ground state energy and that the integrand in the approximation of the most divergent terms is sufficiently accurate for it. However, before we proceed to the case at low temperatures or at weak magnetic fields, it should be noted that the function $g(X)$ becomes complex for $X>1$ ($y<\tilde{y}$) as one can see from (5·12). Then, a contribution from the integral over $0<y<\tilde{y}$ in (6·1) becomes also complex. This is of course unreasonable and due to the approximation of the most divergent terms. In the following we assume simply this part of the integral for $X>1$ can be neglected in our approximation in order to carry out the integration over y.*) By doing so we show first the result due to the extremal approximation can be reproduced correctly and then we proceed to the cases at low temperatures or at weak fields.

We put $g(X)=1+g_1(X)$, then integration by parts for (6·1) gives in the approximation of the most divergent terms

$$\begin{aligned} Z/Z_c=&-\exp[(2\beta/\pi)(N/J\rho)y]\exp[(2\beta/\pi)(N/J\rho)yB_1(y)]\,g(X)\,|_{\tilde{y}}^{\infty} \\ &+(2\beta/\pi)(N/J\rho)\int_{\tilde{y}}^{\infty}dy\exp[(2\beta/\pi)(N/J\rho)y] \\ &\times\exp[(2\beta/\pi)(N/J\rho)yB_1(y)]\,g(X)g_1(X), \\ B_1(y)=&\,g_1(X)+(J\rho/N). \end{aligned} \tag{6·4}$$

Applying the similar integration by parts repeatedly, we obtain

$$Z=Z_c\exp[(2\beta/\pi)y((N/J\rho)g(X)+1)]\,g(X)(1+g_1(X))^{-1}|_{y=\tilde{y}}. \tag{6·5}$$

This gives the result (6·2) with the use of the condition (6·3), namely $g(X)|_{y=\tilde{y}}=0$. We note the factor $g(X)$ in the front of the exponential in (6·1) is important to have vanishing zero point entropy as seen in (6·5).

In the cases at low temperatures or at weak fields given by (5·15) or (5·17) one has

$$g(y,\beta)=g(X'), \quad g(y,H_z)=g(X''), \tag{6·6}$$

from (5·6) or (5·18) in the lowest order of $(\beta y)^{-2}$ or $(\mu_B H_z/y)^2$ for $\beta y\gg 1$ and $\mu_B H_z/y\ll 1$, respectively, where X' and X'' are defined by

*) An alternative assumption may be to put $g(X)=0$ in the exponent for this interval. However this does not change our conclusion at 0°K.

$$X'=(J\rho/N)\log[y(1+(\pi^2/6)(\beta y)^{-2})/D], \tag{6·7}$$

$$X''=(J\rho/N)\log[y(1+(1/2)(\mu_B H_z/y)^2)/D]. \tag{6·8}$$

Then neglecting parts of the integrals for X', $X''>1$, that is, putting $\tilde{y}'$ or $\tilde{y}''$ into the lower limit of the integrals in (5·15) or (5·17) respectively, $(X'|_{y=\tilde{y}'}=1, X''|_{y=\tilde{y}''}=1)$

$$\tilde{y}'=\tilde{y}[1-(\pi^2/6)(\beta\tilde{y})^{-2}], \quad \tilde{y}''=\tilde{y}[1-(1/2)(\mu_B H_z/\tilde{y})^2], \tag{6·9}$$

we can perform the integrations by the method similar to (6·4) and (6·5). In these cases, however, the calculation must be done correctly in the approximation of the most divergent terms for each term up to $(\beta y)^{-2}$ or $(\mu_B H_z/y)^2$. The results are given by

$$Z=Z_c\exp[(2\beta/\pi)y((N/J\rho)g(X')+1+(\pi^2/3)(\beta y)^{-2})]|_{y=\tilde{y}'}, \tag{6·10}$$

$$Z=Z_c\exp[(2\beta/\pi)y((N/J\rho)g(X'')+1+(\mu_B H_z/y)^2)]|_{y=\tilde{y}''}. \tag{6·11}$$

Note that $g(X')$ and $g(X'')$ are valid in the lowest order of $(\beta y)^{-2}$ and $(\mu_B H_z/y)^2$. Since $g(X')|_{y=\tilde{y}'}=0$ and $g(X'')|_{y=\tilde{y}''}=0$, we get

$$Z=Z_c\exp[(2\beta/\pi)\tilde{y}(1+(\pi^2/6)(\beta\tilde{y})^{-2})], \tag{6·12}$$

$$Z=Z_c\exp[(2\beta/\pi)\tilde{y}(1+(1/2)(\mu_B H_z/\tilde{y})^2)], \tag{6·13}$$

from (6·10) and (6·11) with (6·9) up to $(\beta\tilde{y})^{-2}$ and $(\mu_B H_z/\tilde{y})^2$. These results give immediately the specific heat at low temperatures and the susceptibility at 0°K,

$$C_v=k_B^2(\pi/3)T/\tilde{y}, \qquad \chi=2\mu_B^2/\pi\tilde{y}.$$

The expression of the susceptibility is in accordance with the result by Ishii and Yosida.[17] These expressions have the same form as those calculated by the anomalous Green function theory due to Takano and Ogawa.[8] However, the binding energy $\tilde{y}$ appearing in them is replaced by the correct one. The obtained normal behavior at low temperatures are in agreement with the expectation by Ishii[3] and by Anderson, Yuval and Hamann[18] and also with recent experimental observations.[19]

§7. Concluding remarks

The calculation of the partition function for the *s-d* exchange system has been made in the approximation of the most divergent terms by using the functional integral method due to the Stratonovich-Hubbard transformation. The correct binding energy has been obtained. In order to derive the expression at low temperatures we made an assumption that a part of the integrand for the final integration for the partition function, which cannot be obtained

in the approximation of the most divergent terms, can be neglected. The behavior of the free energy is concluded to be normal.

At the absolute zero the ground state projected into the subspace of $n_d=1$ for any value of ζ_0 in the static approximation is shown to be a singlet. The perturbation series $g(X)$ coincides with that appearing in the eigenvalue equation for the singlet bound state, and further, in the extremal approximation, the binding energy is determined by the very eigenvalue equation. These facts suggest that the final ground state in the present calculation is the singlet bound state.

We are unable to derive the contribution from the states in the subspaces of $n_d=0, 2$ to the partition function, though physically uninteresting. This will be done by having the expression of the integrand neglected in the final integration. In other words, we expect that this part of the integrand will be primarily related to this irrelevant contribution. However, it is necessary to have a complete expression of the integrand beyond the most divergent terms to derive the behavior of the bound state at all temperatures and magnetic fields. For this purpose the time dependent approach[6),7)] may be promising.

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