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1990 J. Phys.: Condens. Matter 2 763

(http://iopscience.iop.org/0953-8984/2/3/022)

J. Phys.: Condens. Matter 2 (1990) 763–770. Printed in the UK

LETTER TO THE EDITOR

On the coherent potential approximation in the functional integral approach to itinerant electron magnetism

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Received 27 September 1989

Abstract. The so-called arbitrariness accompanying the Stratonovich–Hubbard transformation of the Hubbard model in the functional formalism is investigated in the coherent potential approximation (CPA). A dynamical theory of the CPA, which is perfectly free from the arbitrariness, and a modified static theory of the CPA, in which dynamics of the spin and charge fluctuations are taken into account partially, are proposed. In contrast with the conventional static theory of the CPA, the modified static theory of the CPA has the advantage that by means of the use of the variational principle the arbitrariness of the transformation can be removed. In the limit of a small intra-Coulomb integral, a generalised spin susceptibility is estimated and the result of the Hartree–Fock approximation is reproduced in both the dynamical and modified static theories of the CPA.

Functional integral formalism based on the Stratonovich–Hubbard transformation has been extensively used in the study of itinerant electron magnetism. In particular, the coherent potential approximation (CPA) developed by Soven (1967) so as to investigate the electronic structure of the alloying system has been successfully applied to the Hubbard model in the functional integral scheme (for example Hubbard 1979, Hasegawa 1980, Morkowski and Wosicki 1989). As is well known, there is an arbitrariness in the Stratonovich–Hubbard transformation and it does not give a unique result in the approximate theory of which we are eventually forced to make use. Therefore, the results do not always reduce to that of the Hartree–Fock approximation in the limit of small intra-Coulomb integral U. In our previous work (Hirooka and Shimizu 1988, hereafter referred to as I) we have discussed this subject in the Gaussian approximation and shown that the results of the Hartree–Fock approximation are reproduced by including dynamics of the fluctuations and that the arbitrariness is removed by means of the variational principle. In this letter we discuss the same subject in the CPA. The static approximation has been exclusively adopted in the treatment of random fields in the conventional theories of the CPA. It is shown that the difficulties in these theories are removed by taking into account dynamics of the fluctuating fields. We investigate the applicability of the variational principle in approximate methods involving the CPA and the nature of the methods in the limit of small U.

We adopt a single-band Hubbard model and the Hamiltonian is given by

$$H = \sum_{i,j,\sigma} t_{ij} a_{i\sigma}^{+} a_{j\sigma} + U \sum_{i} n_{i+} n_{i-}. \tag{1}$$

Here $a_{i\sigma}$ ($a_{i\sigma}^{+}$) is the annihilation (creation) operator for an electron with spin σ at the

0953-8984/90/030763 + 08 $03.50

Wannier site i, $n_{i\sigma} = a_{i\sigma}^{+} a_{i\sigma}$, and t_{ij} are the transfer integrals. The interaction term in equation (1) may be rewritten as follows:

$$U \sum_i n_{i^+} n_{i^-} = - \sum_i (\tfrac{1}{4} J \sigma_i^2 + \tfrac{1}{4} K n_i^2 - W n_i) \tag{2}$$

with $K = 3J - 2U$ and $W = (3J - U)/2$, where J is an arbitrary parameter. Through the Stratonovich–Hubbard transformation the partition function of the system is expressed in the form of a functional integral of fluctuating fields $\xi_i(u)$ and $\kappa_i(u)$, which are conjugate to the spin and charge operators $\sigma_i(u)$ and $n_i(u)$, respectively, as follows:

$$Z = \mathrm{e}^{-\beta\Omega} = \mathrm{Tr}(\mathrm{e}^{-\beta(H - \zeta N)}) = N \int \mathrm{D}\xi \, \mathrm{D}\kappa \, \mathrm{e}^{-\beta \Psi(\xi, \kappa)} \tag{3a}$$

with

$$\Psi(\xi, \kappa) = \sum_{i,u} (\xi_i(u)^2 + \kappa_i(u)^2) + \Omega_0(\xi, \kappa) \tag{3b}$$

$$\Omega_0(\xi, \kappa) = - \frac{1}{\beta} \log[\mathrm{Tr}(\mathrm{e}^{-\beta(H_0 - \zeta N)} T(S))] \tag{3c}$$

$$S = \exp\left(\beta \sum_{i,u} (\sqrt{J} \xi_i(u) \sigma_i(u) + \sqrt{K} \kappa_i(u) n_i(u) - W n_i(u))\right) \tag{3d}$$

where $\beta = 1/k_{\mathrm{B}} T$, ζ is the chemical potential, N is the normalisation constant, T is Wick's time ordering operator, H_0 is the non-interacting part of equation (1) and

$$\sum_{i,u} = (1/\beta) \int_0^\beta \mathrm{d}u \sum_i .$$

Now, equation (3a) is rewritten as follows:

$$Z = N_0 \int \prod_i \mathrm{D}\xi_i \, \mathrm{D}\kappa_i \, \mathrm{e}^{-\beta \varphi_0(\xi, \kappa)} \langle\!\langle \mathrm{e}^{-\beta \Omega_0(\xi, \kappa)} \rangle\!\rangle \tag{4a}$$

where

$$\langle\!\langle A(\xi, \kappa) \rangle\!\rangle = \int \prod_{l \neq 0} \mathrm{D}\xi_i[\omega_l] \, \mathrm{D}\kappa_i[\omega_l] \, \mathrm{e}^{-\beta \varphi'(\xi, \kappa)} \, A(\xi, \kappa) \times \left(\int \prod_{l \neq 0} \mathrm{D}\xi_i[\omega_l] \, \mathrm{D}\kappa_i[\omega_l] \, \mathrm{e}^{-\beta \varphi'(\xi, \kappa)} \right)^{-1} \tag{4b}$$

$$\varphi_0(\xi, \kappa) = \sum_i (\xi_i^2 + \kappa_i^2) \tag{4c}$$

$$\varphi'(\xi, \kappa) = \sum_{i, l \neq 0} (|\xi_i[\omega_l]|^2 + |\kappa_i[\omega_l]|^2) \tag{4d}$$

with $\xi_i = \xi_i[\omega_0]$ and $\kappa_i = \kappa_i[\omega_0]$ and the Fourier transformations for $\xi_i(u)$ and $\kappa_i(u)$ are defined as

$$\eta_i[\omega_l] = \frac{1}{\beta} \int_0^\beta \eta_i(u) \exp(\mathrm{i}\omega_l u) \, \mathrm{d}u$$

with $\eta_i(u) = \xi_i(u)$ or $\kappa_i(u)$ and $\omega_l = 2l\pi/\beta$ (l: integer). Generally we have the inequality $\langle \mathrm{e}^{-f(\xi, \kappa)} \rangle > \mathrm{e}^{-\langle f(\xi, \kappa) \rangle}$, where $\langle A \rangle$ means A averaged over an arbitrary probability distribution. Therefore, we find from equation (4a) that

$$\Omega < \Omega_{\mathrm{m}} = - \frac{1}{\beta} \log\left(N_0 \int \mathrm{D}\xi \, \mathrm{D}\kappa \, \mathrm{e}^{-\beta \Psi_{\mathrm{m}}(\xi, \kappa)}\right) \tag{5a}$$

with $\Psi_{\mathrm{m}}(\xi, \kappa) = \varphi_0(\xi, \kappa) + \Omega_{0\mathrm{m}}(\xi, \kappa)$ and

$$\Omega_{0\mathrm{m}}(\xi, \kappa) = \langle\!\langle \Omega_0(\xi, \kappa) \rangle\!\rangle \tag{5b}$$

where Ω is an exact thermodynamic potential and $\Omega_{0\mathrm{m}}(\xi, \kappa)$ is a functional of only ξ_i

and κ_i, which are the zero-frequency components of $\xi_i(u)$ and $\kappa_i(u)$. The inequality (5*a*) shows that the variational principle is applicable to Ω_m. In the so-called static approximation, the thermodynamic potential Ω_s is given as

$$\Omega_s = -\frac{1}{\beta}\log\left(N_0\int \mathrm{D}\xi\,\mathrm{D}\kappa\,\mathrm{e}^{-\beta(\varphi_0(\xi,\kappa)+\Omega_{0s}(\xi,\kappa))}\right) \tag{6}$$

where $\Omega_{0s}(\xi, \kappa)$ is given by putting $\xi_i[\omega_l] = 0$ and $\kappa_i[\omega_l] = 0$ for $l \neq 0$ or $\xi_i(u) = \xi_i$ and $\kappa_i(u) = \kappa_i$ in $\Omega_0(\xi, \kappa)$ of equation (3*c*). If $\Omega_0(\xi, \kappa)$ has a maximum value at $\xi_i[\omega_l] = 0$ and $\kappa_i[\omega_l] = 0$ for $l \neq 0$, we have $\Omega_{0m}(\xi, \kappa) = \langle\langle\Omega_0(\xi, \kappa)\rangle\rangle < \Omega_{0s}(\xi, \kappa)$ and so $\Omega < \Omega_m < \Omega_s$. However, we cannot prove the inequality $\Omega < \Omega_m < \Omega_s$ or $\Omega < \Omega_s$ for arbitrary values of J in equation (2). It is rather probable that the inequality $\Omega < \Omega_s$ is broken for some values of the parameter J. This fact should be kept in mind when we apply the variational principle to Ω_s in equation (6). This subject will be referred to later in the case of small U. From now on we describe the approximation used when deriving Ω_m in equation (5) as the modified static approximation.

As discussed in I, the approximate thermodynamic potential Ω_m or Ω_s is dependent on the arbitrary parameter J, unlike the exact Ω. For Ω_m, because of the inequality (5*a*), the variational principle can be applied to determine the optimum value of J. Then, the relation $\partial\Omega_m/\partial J = 0$ gives

$$\tfrac{1}{3}\langle\langle\bar{\sigma}_i^2\rangle\rangle - \langle\langle\bar{\sigma}_i\rangle\rangle^2\rangle + \langle\langle\bar{n}_i^2\rangle\rangle - \langle\langle\bar{n}_i\rangle\rangle^2\rangle = 0 \tag{7}$$

where

$$\bar{A} = \frac{1}{\beta}\int_0^\beta [A(u)]\,\mathrm{d}u \qquad [A(u)] = \mathrm{Tr}\{\mathrm{e}^{-\beta(H_0-\zeta N)}T[A(u)S]\}/Z_0$$

with

$$Z_0 = \mathrm{Tr}\{\exp[-\beta(H_0 - \zeta N)]T[S]\}$$

and $\langle\ldots\rangle$ means averaging over the distribution $\exp(-\beta\Psi_m(\xi, \kappa))$. Equation (7) gives for $U/t \ll 1$

$$J \simeq U/2 \tag{8}$$

which agrees with the result obtained in I in the Gaussian approximation. Moreover, we can derive the results of the Hartree–Fock approximation, regardless of the value of J, by the use of Ω_m in equation (5*a*) in contrast to the case for the static approximation.

On the other hand, the optimum condition $\partial\Omega_s/\partial J = 0$ in the static approximation gives

$$\tfrac{1}{3}\langle[\overline{\sigma_i(u)^2}]\rangle + \langle[\overline{n_i(u)^2}]\rangle - 2\langle[\overline{n_i(u)}]\rangle = 0 \tag{9}$$

where

$$\bar{A} = \frac{1}{\beta}\int_0^\beta A(u)\,\mathrm{d}u.$$

The corresponding equation in the exact theory is given by $\bar{B} = 0$ with $B(u) = \tfrac{1}{3}\langle[\sigma_i(u)^2]\rangle + \langle[n_i(u)^2]\rangle - 2\langle[n_i(u)]\rangle$. Then the identity $B(u) = 0$ holds regardless of the values of J and U because of the nature of the Fermi operator. However, equation (9) is not satisfied even when $U = 0$ and $J = 0$; but it gives $J \neq 0$ in the limit of $U = 0$. On the other hand, we have $\Omega_s(U = 0, J = 0) = \Omega(U = 0)$ from equations (3*a*) and (6). Considering the function $f(J) = \Omega_s(U = 0, J) - \Omega\,(U = 0)$, we have $f(0) = 0$ and

$f'(0) \neq 0$, where $f'(J) = \mathrm{d}f(J)/\mathrm{d}J$. This means that a value of J that satisfies $f(J) < 0$ exists in the small region around $J = 0$. Assuming that $\Omega_s(U, J)$ is a continuous function of the variables U and J, it is concluded that values of U and J that satisfy the inequality $\Omega_s(U, J) < \Omega(U)$ exist, at least in the small region around $U = 0$ and $J = 0$.

From equations (3*c*) and (3*d*) we obtain $\Delta\Omega_0(\xi, \kappa) = -(1/\beta)\,\mathrm{Tr}(\log(1 - gV))$ in the matrix representation, where

$$\Delta\Omega_0(\xi, \kappa) = \Omega_0(\xi, \kappa) - \Omega_0$$
$$\Omega_0 = -(1/\beta)\log(\mathrm{Tr}(\mathrm{e}^{-\beta(H_0 - \zeta N)}))$$
$$V_{ij}(u, u') = -(\sqrt{J}\xi_i(u)\sigma + \sqrt{K}\kappa_i(u) - W)\delta(u - u')\delta_{ij}$$

in the spinor representation, σ is the Pauli spin matrix and g is a Green function of a free electron. In order to apply the CPA to our system, we rewrite $\Delta\Omega_0(\xi, \kappa)$ as follows,

$$\Delta\Omega_0(\xi, \kappa) = \mathrm{Tr}(\log(1 - g\Sigma)) - \mathrm{Tr}(\log(1 - F(V - \Sigma)) - \mathrm{Tr}(\log(1 - Dt))] \tag{10}$$

where the self-energy function Σ and renormalised Green function G are defined by

$$G = (g^{-1} - \Sigma)^{-1} = \langle (g^{-1} - V)^{-1} \rangle. \tag{11}$$

$F = G_{ij}\delta_{ij}$ and $D = (1 - \delta_{ij})G_{ij}$ are the diagonal and off-diagonal parts of G, respectively, and $t = (V - \Sigma)(1 - F(V - \Sigma))^{-1}$ is a t-matrix. Here, $\langle \ldots \rangle$ in equation (11) means averaging over the appropriate distribution of the random fields ξ and κ. Following the argumentation used when deriving the inequality (5*a*), we find from equations (3*a*) and (3*b*) that

$$\Delta\Omega < \Delta\Omega_{\mathrm{d}}^{\mathrm{CPA}} = -\frac{1}{\beta}\mathrm{Tr}(\log(1 - g\Sigma)) - \frac{1}{\beta}\log\left(N_0 \int \mathrm{D}\xi\, \mathrm{D}\kappa\, \mathrm{e}^{-\beta\Psi_{\mathrm{dc}}(\xi, \kappa)}\right)$$
$$-\frac{1}{\beta}\langle \mathrm{Tr}(\log(1 - Dt)) \rangle \tag{12a}$$

with

$$\Psi_{\mathrm{dc}}(\xi, \kappa) = \sum (\xi_i(u)^2 + \kappa_i^2(u)) - \frac{1}{\beta}\mathrm{Tr}[\log(1 - F(V - \Sigma))] \tag{12b}$$

where $\Delta\Omega = \Omega - \Omega_0$ and $\langle \ldots \rangle$ denotes averaging over the distribution $\mathrm{e}^{-\beta\Psi_{\mathrm{dc}}(\xi, \kappa)}$. The inequality (12*a*) shows again that the variational method is applicable to $\Delta\Omega_{\mathrm{d}}^{\mathrm{CPA}}$. The variational function is a self-energy function Σ. Thus we have the thermodynamic potential in the dynamical CPA, which is given by omitting the third term in equation (12*a*) (Ducastelle and Gautier 1976, Paquet and Leroux-Hugon 1983). Then, the self-energy function Σ is determined by the so-called Soven equation as $\langle t \rangle = 0$ or

$$\Sigma = \langle V(1 - F(V - \Sigma))^{-1} \rangle \tag{13}$$

where a single-site approximation is adopted:

$$\Sigma = \Sigma_i \delta_{ij}.$$

The static approximation is obtained by putting $\xi_i(u) = \xi_i$ and $\kappa_i(u) = \kappa_i$ in equation (12*b*), which defines $\Psi_{\mathrm{sc}}(\xi, \kappa)$ in place of $\Psi_{\mathrm{dc}}(\xi, \kappa)$. On the other hand, we get a thermodynamic potential $\Delta\Omega_{\mathrm{m}}^{\mathrm{CPA}}$ in the modified static CPA by using $\Psi_{\mathrm{mc}}(\xi, \kappa)$ in place of $\Psi_{\mathrm{dc}}(\xi, \kappa)$ in equation (12*a*):

$$\Psi_{\mathrm{mc}}(\xi, \kappa) = \varphi_0(\xi, \kappa) - (1/\beta)\langle\langle \mathrm{Tr}[\log(1 - F(V - \Sigma))] \rangle\rangle \tag{14}$$

where $\varphi_0(\xi, \kappa)$ and the definition of $\langle\langle \ldots \rangle\rangle$ is given in equations (4*c*) and (4*b*). The Soven

equation is given by $\langle\langle\langle t\rangle\rangle\rangle = 0$ or $\Sigma = \langle\langle\langle V(1 - F(V - \Sigma))^{-1}\rangle\rangle\rangle$, where $\langle \ldots \rangle$ means averaging over the distribution $e^{-\beta\Psi_{mc}(\xi,\kappa)}$. Then, we have inequalities

$$\Delta\Omega < \Delta\Omega_m < \Delta\Omega_m^{CPA} \tag{15a}$$

and

$$\Delta\Omega < \Delta\Omega_d^{CPA} < \Delta\Omega_m^{CPA} \tag{15b}$$

where $\Delta\Omega_m = \Omega - \Omega_0$ is a thermodynamic potential in the modified static approximation and $\Delta\Omega_m^{CPA}$ is that in the modified static CPA. It is worth noting that the thermodynamical potential $\Delta\Omega_d^{CPA}$ in the dynamical CPA, like the exact potential $\Delta\Omega$, is independent of J. In fact, we can verify the identity $\partial\Delta\Omega_d^{CPA}/\partial J = 0$ by direct calculation, but this will be left to forthcoming work because it involves a somewhat lengthy manipulation. On the other hand, $\Delta\Omega_m^{CPA}$ is dependent on J and so the optimum value of J is determined by the relation $\partial\Delta\Omega_m^{CPA}/\partial J = 0$ and the variational principle, as in the case of $\Delta\Omega_m$, because of the inequality (15*a*). In the static CPA, although we have the relation $\Delta\Omega_s < \Delta\Omega_s^{CPA}$, the inequality $\Delta\Omega < \Delta\Omega_s^{CPA}$ is not always guaranteed for all values of J, where $\Delta\Omega_s = \Omega_s - \Omega_0$. Therefore, we do not have the best choice for the value of J in the static theory of the CPA.

Now, we add an external field V_e to our system in order to estimate the magnetic or the electric susceptibility. Then, equation (12*a*) becomes

$$\Delta\Omega_d^{GPA} = -\frac{1}{\beta}\mathrm{Tr}[\log(1 - g(V_e + \Sigma))] - \frac{1}{\beta}\log\left(N_0 \int \mathrm{D}\xi\, \mathrm{D}\kappa\, e^{-\beta\Psi_{dc}(\xi,\kappa)}\right) \tag{16}$$

and also we have the Soven equation (13) with a renormalised single-particle Green function $G = (g^{-1} - V_e - \Sigma)^{-1}$. From equation (16) the generalised susceptibility can be derived by using the functional derivative method by Baym (1962) and Baym and Kadanoff (1961) as was done in I. We put $V_e = -h_i(1, 1')\delta_{ij}$, where the argument 1 or 1′ represents the imaginary time and the spin state. A generalised susceptibility is defined as follows:

$$L_{ij}(12, 1'2') = -\partial G_{ii}(1,1')/\partial h_j(2',2) \tag{17}$$

and it satisfies the following integral equation:

$$L_{ij}(12,1'2') = L_{ij}^0(12,1'2') - \sum_l L_{il}^0(1\underline{2},1'\underline{2'})\Xi(\underline{2'1'},\underline{21})L_{lj}(\underline{1}2,\underline{1'}2'), \tag{18}$$

where $L_{ij}^0(12,1'2') = -G_{ij}(1,2')G_{ji}(2,1')$ and $\Xi(12,1'2') = \partial\Sigma(1,1')/\partial F(2',2)$ is the effective interaction. The underlining of $\underline{1}$ and $\underline{2}$ denotes taking the summation with respect to the argument 1 or 2. Equation (13) defines the self-energy function Σ as a functional of a single-particle Green function G, from which the integral equation for the effective interaction Ξ is derived as

$$\Xi(12,1'2') = \Xi_0(12,1'2') - \sum \Xi_0(1\underline{2},1'\underline{2'})F(\underline{2'},1)F(\underline{1'},2)\Xi(\underline{1}2,\underline{1'}2') \tag{19a}$$

with

$$\Xi_0(12,1'2') = \langle t(1,2')t(2,1')\rangle - \langle t(1,1')t(r,r')\rangle \tag{19b}$$

in the case of the dynamical or the static CPA and

$$\Xi_0(12,1'2') = \langle\langle\langle t(1,2')t(2,1')\rangle\rangle\rangle - \langle\langle\langle t(1,1')\rangle\rangle\rangle\langle\langle\langle t(2,2')\rangle\rangle\rangle \tag{19c}$$

in the case of the modified static CPA, where the meaning of $\langle\langle\langle \ldots \rangle\rangle\rangle$ is given by equation

(4*b*) and $\langle \ldots \rangle$ means averaging over the distribution $e^{-\beta\Psi_{dc}(\xi,\kappa)}$, $e^{-\beta\Psi_{sc}(\xi,\kappa)}$ or $e^{-\beta\Psi_{dc}(\xi,l)}$.

As an example of the solution of equations (18) and (19*a*) we will derive the transverse spin susceptibility below in the limit of small U. Then we make the approximation $t \simeq V$ in equations (19*b*) and (19*c*). We need $\Xi_0^{-+-+}(u_1, u_2; u_1', u_2')$ and its Fourier transformation is given by, in the lowest order of U and J,

$$\Xi_0^{-+-+}(\omega,\omega',\omega'') \simeq -U/\beta \tag{20a}$$

in the dynamical CPA,

$$\Xi_0^{-+-+}(\omega,\omega',\omega'') \simeq (K-J)/2\beta - (J/\beta)\delta(\omega) \tag{20b}$$

in the modified static CPA and

$$\Xi_0^{-+-+}(\omega,\omega',\omega'') \simeq [(K-J)/2\beta]\delta(\omega+\omega'-\omega'') - (J/\beta)\delta(\omega) \tag{20c}$$

in the static CPA, respectively. Here, the Fourier transformation is defined as

$$f(u_1, u_2; u_1', u_2') = \sum f(\omega,\omega',\omega'') \exp\{i[\omega(u_1-u_2) + \omega'(u_1-u_1') + \omega''(u_2-u_2')]$$

and $\omega = 2\pi n/\beta$ (n: integer) etc and it is noted that $(K-J)/2 - J = -U$. The transverse spin susceptibility is defined as

$$\chi_{-+}(\omega, \boldsymbol{q}) = (1/\beta)\sum_{\underline{\omega}} L_{-+-+}(\omega, \underline{\omega}; \boldsymbol{q})$$

with

$$L_{-+-+}(\omega,\omega';\boldsymbol{q}) = (1/N)\sum L_{ij}^{-+-+}(u_1,u_2,u_1',u_2') \times \exp\{-i[\omega(u_1-u_2)+\omega'(u_1-u_1')]\} \exp(i\boldsymbol{q}\cdot\boldsymbol{R}_{ij}).$$

Finally, we have, in the lowest order of U,

$$\chi_{-+}(\boldsymbol{q}, \omega) = \chi_{0-+}(\boldsymbol{q}, \omega)/(1 - U_{\text{eff}}(\omega)\chi_{0-+}(\boldsymbol{q}, \omega)) \tag{21a}$$

in the dynamical CPA, where

$$\chi_{0-+}(\boldsymbol{q}, \omega) = (1/\beta)\sum_{\underline{\omega}} L^{0}_{-+-+}(\omega, \underline{\omega}; \boldsymbol{q})$$

and

$$U_{\text{eff}}(\omega) = U/(1 + U\Gamma(\omega)) \tag{21b}$$

where

$$\Gamma(\omega) = -(1/\beta)\sum_{\underline{\omega}} F_-(\omega+\underline{\omega})F_+(\underline{\omega}).$$

In the modified CPA, the static susceptibility is obtained as $\chi_{m-+}^{CPA}(\boldsymbol{q}) = \chi_{-+}(\boldsymbol{q}, 0)$ in equation (21*a*). Then, Σ is given as $\Sigma_\sigma(\omega) \simeq Un_{-\sigma}$ in the limit of small U both in the dynamical and in the modified static CPA, where

$$n_\sigma = (1/\beta)\sum_{\underline{\omega}} F_\sigma(\underline{\omega}).$$

Equation (21*b*) shows the reduction of an effective interaction by the local spin fluctuations. Moreover, we have $\chi_{s-+}^{CPA}(q) = \Pi_1(q)/(1 - J_{\text{eff}}\Pi_2(\boldsymbol{q}))$ in the static CPA, where

$J_{\text{eff}} = J/(1 + J\Gamma(0))$ and $\Pi_1(q) \simeq \Pi_2(q) \simeq \chi_{0-+}(q, 0)$ in the limit of $J, K = 0$, and $\Sigma_\sigma(\omega) \simeq -\frac{1}{2}(K-J)n_{-\sigma} - \frac{1}{2}(K+J)n_\sigma + JF_{-\sigma}(\omega)/\beta + \frac{1}{2}(K+J)F_\sigma(\omega)/\beta$. Thus, the results in the dynamical and the modified static CPA reduce to that in the Hartree–Fock theory, regardless of the value of J, in the limit of small U, in contrast with the case for the static CPA.

Unfortunately, we cannot solve analytically equations (18) and (19*a*) with the full expression of the t-matrix in (19*b*). In particular, it is very difficult to solve equation (13) even numerically in the dynamical CPA, because we are forced to carry out the functional integration along the path of the imaginary time. Equation (13) may be simplified by adopting the decoupling approximation introduced by Hasegawa (1980), which seems to be useful in the dynamical CPA and the modified static CPA, too. However, Hasegawa's decoupling method has been criticised by Paquet and Leroux-Hugon (1983) as it yields unphysical results at high temperature. These authors have investigated the nature of the static CPA in detail by solving equation (13) directly. Calculation such as that carried out by them seems to be possible in the modified static CPA, too. Although dynamical fluctuations of spin and charge densities are artificially forbidden in the static approximation, it has been found against our expectation that the inequality $\Omega < \Omega_s$ does *not* always hold in the functional integral formalism under the Stratonovich–Hubbard transformation. Rather, we may say that a parameter J, which cannot be determined using the variational principle, should be chosen so as to satisfy the inequality. The modified static CPA introduced in this work is essentially the static approximation. However, it has some merits in comparison with the simple static CPA, as it gives grounds for the use of the variational principle and it reduces to the Hartree–Fock approximation in the limit of small U. We consider that our optimum determination of the parameter J has led not only to the removal of the arbitrariness in the theory but also to the remarkable improvement of the approximate theory compared with the use of the less accurate values of J.

In conclusion, we have investigated a few approximation methods in the functional integral formalism, where the Stratonovich–Hubbard transformation is used. It has been shown that the inequality $\Omega < \Omega_s$, which is essential to the use of the variational principle, does not always hold in the static approximation. Here, Ω and Ω_s are the thermodynamic potentials of the exact theory and the static approximation, respectively. Therefore, the so-called arbitrariness accompanying the Stratonovich–Hubbard transformation cannot, essentially, be removed in this approximation. The dynamical theory of the CPA, which is as completely free from the arbitrariness of the parameter J as the exact theory, has been given. In spite of the difficulty of the direct solution of the Soven equation, the perturbative treatment seems to give a meaningful result in this approximation. The modified static CPA, which is revised to include the effects of the dynamical fluctuation of spin and charge densities in part, is useful in the sense that it can be used for determining the value of the arbitrary parameter J by the variational method and reproduces the results of the Hartree–Fock approximation in the limit of small U. Moreover, this approximation is far more tractable than the dynamical CPA.

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