

Title	Statistical diagonalization of the Hamiltonian with interaction in the Green function theory
Sub Title	
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Publisher	慶應義塾大学藤原記念工学部
Publication year	1970
Jtitle	Proceedings of the Fujihara Memorial Faculty of Engineering Keio University Vol.23, No.94/95 (1970.) ,p.123- 131
JaLC DOI	
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Notes	
Genre	Departmental Bulletin Paper
URL	https://koara.lib.keio.ac.jp/xoonips/modules/xoonips/detail.php?koara_id=KO50001004-00230095-0123

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Statistical Diagonalization of the Hamiltonian with Interaction in the Green Function Theory

(Received September 25, 1970)

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Abstract

A new method to obtain the knowledge for the ground state energy as well as one for the elementary excitation energy in an interacting many particle system is considered from the intuitive approach in the double time Green function theory. Using this method of approach the statistical diagonalization which may include properly the effects of temperature and other external fields can be performed when the Green functions are solved by an appropriate approximation, and the physical meaning of the results is considered. The application to the Heisenberg antiferromagnet is shown to lead the temperature and external magnetic field dependent results in the approximation of Tyablikov decoupling.

I. Introduction

The concept of elementary excitation is one of the most importance in the quantum theory of interacting many particles. In the previous paper¹⁾ we have treated the energy of spin wave excitation in the very low temperature region using the self-consistent linearization approach to the quantum mechanical equation of motion. In the present work we use the double time Green function approach²⁾ for an antiferromagnet, in order to calculate the mean total energy of the interacting particle system in addition to the excitation energy of quasi-particles. In this method of approach we can therefore further get the knowledge about the energy of the ground state.

As an illustrative example for the method, we consider first the following Hamiltonian,⁷⁾

$$\mathcal{H} = \omega a^+ a + \epsilon(ab + a^+ b^+), \quad (1-1)$$

where a , b , a^+ and b^+ are assumed to be the well-known Boson operators. Our

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approach may be applicable for other operators such as Fermion operators and Pauli operators with suitable modifications. Usually the above Hamiltonian can be diagonalized by the Bogolyubov transformation as in our previous treatment,¹⁾ in which operators a and b are expressed in terms of new Boson operators α and β ,

$$\left. \begin{aligned} a &= e\alpha + s\beta^\dagger \\ b &= s\alpha^\dagger + e\beta \end{aligned} \right\}. \quad (1-2)$$

The coefficients e and s are determined by the requirement that the Hamiltonian (1-1) may be diagonal in terms of α and β . Thus we obtain

$$\mathcal{H} = E_0 + \omega_1 \alpha^\dagger \alpha + \omega_2 \beta^\dagger \beta, \quad (1-3)$$

where E_0 means the energy of the ground state, and ω_1 and ω_2 are the elementary excitation energies of the quasi-particles of the type α and β respectively.

$$E_0 = \frac{1}{2}(-\omega + \sqrt{\omega^2 - 4\varepsilon^2}), \quad (1-4)$$

$$\omega_1 = \frac{1}{2}(\omega + \sqrt{\omega^2 - 4\varepsilon^2}), \quad (1-5)$$

and

$$\omega_2 = \frac{1}{2}(-\omega + \sqrt{\omega^2 - 4\varepsilon^2}). \quad (1-6)$$

In our previous paper we treated the problem along the view-point of the equation of motion in order to get the insight to the elementary excitation energies. We can solve the same problem with use of the double time Green function approach. We consider the Green functions $\langle\langle a(t); a^\dagger(t') \rangle\rangle$ and $\langle\langle b^\dagger(t); a^\dagger(t') \rangle\rangle$.³⁾ Solving the simultaneous coupled equations of motion for them in energy representation, we obtain the solutions,⁴⁾

$$\left. \begin{aligned} \langle\langle a; a^\dagger \rangle\rangle_E &= \frac{1}{2\pi} \left\{ \frac{\omega + \sqrt{\omega^2 - 4\varepsilon^2}}{2\sqrt{\omega^2 - 4\varepsilon^2}} \cdot \frac{1}{E - \frac{1}{2}(\omega + \sqrt{\omega^2 - 4\varepsilon^2})} \right. \\ &\quad \left. + \frac{-\omega + \sqrt{\omega^2 - 4\varepsilon^2}}{2\sqrt{\omega^2 - 4\varepsilon^2}} \cdot \frac{1}{E - \frac{1}{2}(\omega - \sqrt{\omega^2 - 4\varepsilon^2})} \right\} \\ \langle\langle b^\dagger; a^\dagger \rangle\rangle_E &= -\frac{\varepsilon}{2\pi\sqrt{\omega^2 - 4\varepsilon^2}} \left\{ \frac{1}{E - \frac{1}{2}(\omega + \sqrt{\omega^2 - 4\varepsilon^2})} - \frac{1}{E - \frac{1}{2}(\omega - \sqrt{\omega^2 - 4\varepsilon^2})} \right\} \\ &= \langle\langle a; b \rangle\rangle_E. \end{aligned} \right\} \quad (1-7)$$

In the solutions (1-7) for the Green functions, namely in the expressions for $\langle\langle a; a^\dagger \rangle\rangle_E$ and $\langle\langle b^\dagger; a^\dagger \rangle\rangle_E$, what kind of poles in the equations (1-7) does correspond to the

elementary excitation energy? In the limiting case of the non-interacting Hamiltonian, $\mathcal{H} \rightarrow \omega a^\dagger a$, ($\varepsilon \rightarrow 0$), the pole of the $\langle\langle a; c \rangle\rangle_E$ type Green function becomes equal to the elementary excitation energy ω and the pole of the $\langle\langle a^+; c' \rangle\rangle_E$ type one tends to correspond to the negative of the elementary excitation energy. The operators c and c' are some operators which are not commutable with a and $a^\dagger$, respectively. This change of sign is determined by the fact that we consider the N -particle state with use of $N+1$ -particle state for the Green function of type $\langle\langle a; c \rangle\rangle_E$ and for the type $\langle\langle a^+; c' \rangle\rangle_E$ with use of $N-1$ -particle state, as was pointed out in our previous treatment for the equation of motion approach.^{1),5)}

We can extend this method of consideration to the case of the Green functions for the interacting particle system. In the equation (1-7), the second term for the Green function $\langle\langle a; a^+ \rangle\rangle_E$ becomes zero as the interaction constant ε tends to zero. Let us consider ε -term in the Hamiltonian (1-1) be the small perturbation, so we can obtain the diagonalized Hamiltonian in terms of new Boson operators α and β , which coincide with a and b in the zeroth order approximation by the transformation (1-2). Then we can expect the following relation holds,

$$\begin{aligned} \langle\langle a; a^+ \rangle\rangle_E = & \langle\langle \alpha; \alpha^+ \rangle\rangle_E \times \text{coefficient of order } \varepsilon^0 \\ & + \langle\langle \beta^+; \beta \rangle\rangle_E \times \text{coefficient of order } \varepsilon^1. \end{aligned} \quad (1-8)$$

Thus the pole of the term which has the coefficient of order ε^0 in the equation (1-7) for $\langle\langle a; a^+ \rangle\rangle_E$ corresponds to the elementary excitation energy of the quasi-particle of type α , and the other pole of the term which has the coefficient of order ε^1 corresponds to the negative of the excitation energy of the quasi-particles of type β . This consideration gives us the correct expression for the excitation energy from the solution (1-7), that is,

$\omega_1 = \frac{1}{2}(\omega + \sqrt{\omega^2 - 4\varepsilon^2})$ from the pole of the first term to the solution $\langle\langle a; a^+ \rangle\rangle_E$, and
 $\omega_2 = \frac{1}{2}(-\omega + \sqrt{\omega^2 - 4\varepsilon^2})$ from the negative of pole of the second term to the solution $\langle\langle a; a^+ \rangle\rangle_E$.

Next we search for the terms E_0 in the diagonalized Hamiltonian (1-3). Averaging the equation (1-3) over a grand canonical ensemble,

$$\begin{aligned} \langle \mathcal{H} \rangle = & E_0 + \omega_1 \langle \alpha^\dagger \alpha \rangle + \omega_2 \langle \beta^\dagger \beta \rangle \\ = & \omega \langle a^\dagger a \rangle + \varepsilon \{ \langle ab \rangle + \langle b^\dagger a^\dagger \rangle \}. \end{aligned} \quad (1-9)$$

The same result was intended to get from the knowledge of our solutions for the Green function (1-7). The correlation function of the type $\langle \alpha^\dagger \alpha \rangle$ means the average number of the quasi-particles and has the factor $1/(\exp \beta \omega_i - 1)$. ($i=1$ or 2 ; $\beta=1/kT$) We notice that the terms which do not contain the factor like this in the expression for the Green function contribute to the ground state energy. According to the

spectrum theorem in the theory of double time Green function, the average number $\langle a^+ a \rangle$ is obtained from the Green function $\langle\langle a; a^+ \rangle\rangle_E$. Thus the term in the Green functions whose pole is equal to the elementary excitation energy gives the factor $1/(\exp \beta \omega_i - 1)$ for the correlation function. ($i=1$, or 2) The other terms in the Green functions may give the factor $1/(\exp -\beta \omega_i - 1) = -1 - 1/(\exp \beta \omega_i - 1)$. We pick up those terms in the Green functions whose pole is the negative of the elementary excitation energy and substitute -2π times the coefficient of this term for the corresponding term in the Hamiltonian, thus the ground state energy E_0 can be obtained. The correspondence means;

$\langle\langle a; a^+ \rangle\rangle$ corresponds to $a^+ a$ term,

$\langle\langle b; a \rangle\rangle$ corresponds to ab terms,

and so on. Thus in order to obtain E_0 , we may use the following intuitive substitutions.

$$\left. \begin{aligned} a^+ a &\rightarrow \frac{\omega - \sqrt{\omega^2 - 4\varepsilon^2}}{2\sqrt{\omega^2 - 4\varepsilon^2}}, \\ ab (= a^+ b^+) &\rightarrow -\frac{\varepsilon}{\sqrt{\omega^2 - 4\varepsilon^2}}. \end{aligned} \right\} \quad (1-10)$$

We may therefore obtain the expression,

$$E_0 = \omega \times \frac{\omega - \sqrt{\omega^2 - 4\varepsilon^2}}{2\sqrt{\omega^2 - 4\varepsilon^2}} - 2\varepsilon \times \frac{\varepsilon}{\sqrt{\omega^2 - 4\varepsilon^2}} = \frac{1}{2}(-\omega + \sqrt{\omega^2 - 4\varepsilon^2}). \quad (1-11)$$

This result agrees exactly with that due to the Bogolyubov transformation (1-4). Though we can't directly get the knowledge about the wave functions, this method seems to be useful because we may have some insight to the quasi-particle and the energy of the ground state directly. Furthermore, we can also diagonalize the interacting Hamiltonian approximately when the equations of motion for the Green functions can be solved by an appropriate decoupling approximation. The exact results in this section does not give us the results which depend upon the temperature and other external parameters, for the Hamiltonian does not contain the fourth order interaction terms. In the next section we will apply this method to an antiferromagnet and obtain the temperature and field dependent results.

II. Application to the Heisenberg Antiferromagnet

One of the reasons why we decide to choose up an antiferromagnet as an example of the above mentioned method and to treat it with our method of approach, is that we can apply this method in a straightforward way in the lowest approximation to get the reasonable result. In the very low temperature region, we previously have got the spin wave energy or the elementary excitation energy.¹⁾ Now

we consider the double time Green function approach for an antiferromagnet by the Tyablikov decoupling approximation which seems to be a good approximation for wide temperature regions. The Hamiltonian for an antiferromagnet is

$$\mathcal{H} = 2|J| \sum_{\langle l, m \rangle} \mathbf{S}_l \cdot \mathbf{S}_m - g\mu_B H \left(\sum_l S_l^z + \sum_m S_m^z \right), \quad (2-1)$$

where μ_B is the Bohr magneton, g the Landé g -factor and H is the externally applied magnetic field, which is assumed to be along the z -direction. Operators $\mathbf{S}_l$ and $\mathbf{S}_m$ refer to spin operators in units of $\hbar$ at plus lattice site l and minus lattice site m , respectively. The notation $|J|$ represents the negative exchange integral for the nearest neighbour coupling. In the following we use the subscripts l , f , and g , to indicate the plus lattice site and m , h , and i to indicate the minus lattice site respectively. We assume that the nearest neighbours of the plus lattice site (or minus lattice site) are the members of the minus lattice site (or plus lattice site).

To simplify the problem, we consider only about the case $S = \frac{1}{2}$, and reexpress the Hamiltonian (2-1) using Pauli operators,

$$\left. \begin{aligned} \mathbf{S}_l^+ &= b_l, & \mathbf{S}_l^- &= b_l^+, \\ S_l^z &= \frac{1}{2} - b_l^+ b_l, \\ \mathbf{S}_m^+ &= a_m^+, & \mathbf{S}_m^- &= a_m, \\ S_m^z &= -\frac{1}{2} + a_m^+ a_m. \end{aligned} \right\} \quad (2-2)$$

These operators satisfy the following commutation relations.

$$\left. \begin{aligned} [b_l, b_l^+] &= 2 \left(\frac{1}{2} - b_l^+ b_l \right) \delta_{l, l'}, \\ [b_l, b_{l'}] &= [b_l^+, b_{l'}^+] = 0, \\ b_l^2 &= b_l^{+2} = 0, & b_l b_l^+ + b_l^+ b_l &= 1, \\ [b_l, a_m] &= [b_l, a_m^+] = [b_l^+, a_m] = [b_l^+, a_m^+] = 0, \end{aligned} \right\} \quad (2-3)$$

and the same commutation relations for operators a_m . Using these operators, the Hamiltonian becomes

$$\begin{aligned} \mathcal{H} &= -\frac{1}{4} N |J| z + (z|J| + g\mu_B H) \sum_l b_l^+ b_l + (z|J| - g\mu_B H) \sum_m a_m^+ a_m \\ &\quad + |J| \sum_{\langle l, m \rangle} (b_l^+ a_m^+ + b_l a_m) - 2|J| \sum_{\langle l, m \rangle} b_l^+ b_l a_m^+ a_m. \end{aligned} \quad (2-4)$$

Following Tyablikov's procedure for a ferromagnet,⁶⁾ we construct the commu-

tator,

$$[b_f, \mathcal{H}] = (z|J| + g\mu_B H)b_f + |J| \sum a_m^\dagger - 2|J| \sum b_f^\dagger b_f a_m - 2|J| \sum b_f a_m^\dagger a_m, \quad (2-5)$$

and then we get

$$\sum_f b_f^\dagger [b_f, \mathcal{H}] = (z|J| + g\mu_B H) \sum_f b_f^\dagger b_f + |J| \sum_{\langle f, m \rangle} b_f^\dagger a_m^\dagger - 2|J| \sum_{\langle f, m \rangle} b_f^\dagger b_f a_m^\dagger a_m. \quad (2-6)$$

After substitution of this expression (2-6) for the Hamiltonian (2-4), and with use of the relation $i\dot{b}_f = [b_f, \mathcal{H}]$, we obtain,

$$\begin{aligned} \mathcal{H} = & -\frac{1}{4}N|J|z + \sum_f \left(b_f^\dagger i \frac{db_f}{dt} \right) \\ & + (z|J| - g\mu_B H) \sum_m a_m^\dagger a_m + |J| \sum_{\langle l, m \rangle} b_l a_m. \end{aligned} \quad (2-7)$$

We consider the following two types of Green functions,

$$G_1 = \langle\langle b_f; b_g^\dagger \rangle\rangle \quad \text{and} \quad G_2 = \langle\langle a_h^\dagger; b_g^\dagger \rangle\rangle \quad (2-8)$$

and construct the equations of motion for them in energy representation,

$$\left. \begin{aligned} EG_1(E) = & \frac{\sigma}{2\pi} \delta_{f,g} + (z|J| + g\mu_B H)G_1(E) + |J| \sum_\delta \langle\langle a_{f+\delta}^\dagger; b_g^\dagger \rangle\rangle_E \\ & - 2|J| \sum_\delta \langle\langle (b_f^\dagger b_f a_{f+\delta}^\dagger + b_f a_{f+\delta}^\dagger a_{f+\delta}); b_g^\dagger \rangle\rangle_E, \\ EG_2(E) = & -(z|J| - g\mu_B H)G_2(E) - |J| \sum_\delta \langle\langle b_{h+\delta}; b_g^\dagger \rangle\rangle_E \\ & + 2|J| \sum_\delta \langle\langle (b_{h+\delta} a_h^\dagger + b_{h+\delta}^\dagger b_{h+\delta} a_h^\dagger); b_g^\dagger \rangle\rangle_E, \end{aligned} \right\} \quad (2-9)$$

where δ means the nearest neighbour vectors and

$$\sigma = 1 - 2\langle b_f^\dagger b_f \rangle = 1 - 2\langle a_h^\dagger a_h \rangle. \quad (2-10)$$

The last terms in the equations (2-9) may be evaluated by Tyablikov's decoupling approximation,⁶⁾ although we expect that it does not give the correct temperature expansion for the very low temperature region but it offers good temperature dependence over wider temperature region.

$$\begin{aligned} & \langle\langle (b_f^\dagger b_f a_{f+\delta}^\dagger + b_f a_{f+\delta}^\dagger a_{f+\delta}); b_g^\dagger \rangle\rangle_E \\ & \rightarrow \langle b_f^\dagger b_f \rangle \langle\langle a_{f+\delta}^\dagger; b_g^\dagger \rangle\rangle_E + \langle a_{f+\delta}^\dagger a_{f+\delta} \rangle \langle\langle b_f; b_g^\dagger \rangle\rangle_E, \end{aligned} \quad (2-11)$$

$$\begin{aligned} & \langle\langle (b_{h+\delta} a_h^\dagger + b_{h+\delta}^\dagger b_{h+\delta} a_h^\dagger); b_g^\dagger \rangle\rangle_E \\ & \rightarrow \langle a_h^\dagger a_h \rangle \langle\langle b_{h+\delta}; b_g^\dagger \rangle\rangle_E + \langle b_{h+\delta}^\dagger b_{h+\delta} \rangle \langle\langle a_h^\dagger; b_g^\dagger \rangle\rangle_E. \end{aligned} \quad (2-11')$$

Considering the translational symmetry of the crystal, it is convenient to treat the Green functions in the reciprocal space. Introducing the Fourier transformation;

$$\text{and} \quad \left. \begin{aligned} G_{1\nu} &= \frac{2}{N} \sum G_1 \exp i(f-g) \cdot \nu, \\ G_{2\nu} &= \frac{2}{N} \sum G_2 \exp i(h-g) \cdot \nu, \end{aligned} \right\} \quad (2-12)$$

we obtain the solutions in our decoupling approximation,

$$\left. \begin{aligned} G_{1\nu} &= \frac{1}{2} \cdot \frac{\sigma}{2\pi} \left\{ \frac{1+1/\sqrt{1-\gamma_\nu^2}}{E-g\mu_B H-z|J|\sigma\sqrt{1-\gamma_\nu^2}} - \frac{1-1/\sqrt{1-\gamma_\nu^2}}{E-g\mu_B H+z|J|\sigma\sqrt{1-\gamma_\nu^2}} \right\}, \\ G_{2\nu} &= -\frac{1}{2} \cdot \frac{\sigma}{2\pi} \frac{\gamma_\nu}{\sqrt{1-\gamma_\nu^2}} \left\{ \frac{1}{E-g\mu_B H-z|J|\sigma\sqrt{1-\gamma_\nu^2}} - \frac{1}{E-g\mu_B H+z|J|\sigma\sqrt{1-\gamma_\nu^2}} \right\}, \end{aligned} \right\} \quad (2-13)$$

where $\gamma_\nu = \frac{1}{z} \sum_\delta \exp i\nu \cdot \delta$, is the quantity which plays a role as a coupling constant ε in the previous section.

By using the same approximation, the solutions for the Green functions

$$G_3 = \langle\langle b_f; a_i \rangle\rangle \quad \text{and} \quad G_4 = \langle\langle a_h^+; a_i \rangle\rangle, \quad (2-14)$$

can be obtained.

$$\left. \begin{aligned} G_{3\nu} &= -\frac{1}{2} \frac{\sigma}{2\pi} \frac{\gamma_\nu}{\sqrt{1-\gamma_\nu^2}} \left\{ \frac{1}{E-g\mu_B H-z|J|\sigma\sqrt{1-\gamma_\nu^2}} - \frac{1}{E-g\mu_B H+z|J|\sigma\sqrt{1-\gamma_\nu^2}} \right\}, \\ G_{4\nu} &= -\frac{1}{2} \frac{\sigma}{2\pi} \left\{ \frac{1-1/\sqrt{1-\gamma_\nu^2}}{E-g\mu_B H-z|J|\sigma\sqrt{1-\gamma_\nu^2}} + \frac{1+1/\sqrt{1-\gamma_\nu^2}}{E-g\mu_B H+z|J|\sigma\sqrt{1-\gamma_\nu^2}} \right\}. \end{aligned} \right\} \quad (2-15)$$

From the first expression of the solutions (2-13), we obtain

$$\begin{aligned} &\langle\langle b_f(t); b_g^+(t') \rangle\rangle \\ &= \frac{\sigma}{2\pi} \frac{2}{N} \sum_\nu \int \frac{E-g\mu_B H+\sigma z|J|}{(E-g\mu_B H)^2-(z|J|\sigma\sqrt{1-\gamma_\nu^2})^2} \exp i[(f-g) \cdot \nu - E(t-t')] dE \end{aligned} \quad (2-16)$$

and differentiating with respect to t , we get

$$\begin{aligned} &\left\langle\left\langle i \frac{db_f}{dt}; b_g^+(t') \right\rangle\right\rangle \\ &= \frac{\sigma}{2\pi} \frac{2}{N} \sum_\nu \int \frac{E(E-g\mu_B H+\sigma z|J|)}{(E-g\mu_B H)^2-(z|J|\sigma\sqrt{1-\gamma_\nu^2})^2} \exp i[(f-g) \cdot \nu - E(t-t')] dE. \end{aligned} \quad (2-17)$$

We see then the Green function $G_\nu = \frac{2}{N} \sum \left\langle\left\langle i \frac{db_f}{dt}; b_g^+ \right\rangle\right\rangle e^{i(f-g) \cdot \nu}$ in reciprocal space are given by

$$\begin{aligned} G_\nu &= \frac{1}{2} \frac{\sigma}{2\pi} \left\{ (g\mu_B H+z|J|\sigma\sqrt{1-\gamma_\nu^2}) \frac{1+1/\sqrt{1-\gamma_\nu^2}}{E-g\mu_B H-z|J|\sigma\sqrt{1-\gamma_\nu^2}} \right. \\ &\quad \left. + (g\mu_B H-z|J|\sigma\sqrt{1-\gamma_\nu^2}) \frac{1-1/\sqrt{1-\gamma_\nu^2}}{E-g\mu_B H+z|J|\sigma\sqrt{1-\gamma_\nu^2}} \right\}. \end{aligned} \quad (2-18)$$

If we take for the ordered antiparallel spin state, i.e., the Néel state to be zeroth order approximate ground state and for the quantity γ_ν to be a coupling constant in our treatment, we can find the elementary excitation energies according to the method previously described.

$$\left. \begin{aligned} \omega_{\nu 1} &= z|J|\sigma\sqrt{1-\gamma_\nu^2} + g\mu_B H, \\ \omega_{\nu 2} &= z|J|\sigma\sqrt{1-\gamma_\nu^2} - g\mu_B H. \end{aligned} \right\} \quad (2-19)$$

The elementary excitation energies of the quasi-particles with wave number ν are $\omega_{\nu 1}$ and $\omega_{\nu 2}$ respectively. They depend on temperature and external magnetic field through the quantity σ , that is, the relative magnetization. At the absolute zero of temperature 0°K, $\sigma=1$, then the energies of elementary excitation,

$$\omega_{\nu 2}^1 = z|J|\sqrt{1-\gamma_\nu^2} \pm g_B H$$

agree with the results which are obtained previously.¹⁾ The temperature dependence of the excitation energies is given approximately by the equation (2-19) over the wide range of temperatures although they are expected to have yet incorrect form for the low temperature expansion.³⁾

Next, we search for the ground state energy E_0 by the substitution for the Hamiltonian (2-7) taking into consideration the minor change due to our use for Pauli operators instead of Boson operators as in the previous treatment;

$$\begin{aligned} a_h b_f &\rightarrow \frac{2}{N} \sum_\nu \left\{ -\frac{\sigma}{2} \frac{\gamma_\nu}{\sqrt{1-\gamma_\nu^2}} \right\} \exp i(h-f) \cdot \nu, \\ a_m a_h^\dagger &\rightarrow \frac{2}{N} \sum_\nu \frac{\sigma}{2} (1 + 1/\sqrt{1-\gamma_\nu^2}) \exp i(m-h) \cdot \nu, \\ b_g^\dagger i \frac{db_f}{dt} &\rightarrow \frac{2}{N} \sum_\nu \left\{ -\frac{\sigma}{2} (g\mu_B H - z|J|\sigma\sqrt{1-\gamma_\nu^2}) \left(1 - \frac{1}{\sqrt{1-\gamma_\nu^2}} \right) \exp i(f-g) \cdot \nu \right\}, \end{aligned}$$

to get finally,

$$E_0 = -\frac{1}{4} N |J| z + \frac{1}{2} \sigma (1 + \sigma) \sum_\nu z |J| (\sqrt{1-\gamma_\nu^2} - 1). \quad (2-20)$$

III. Discussions

Since the macroscopic value σ varies with temperature and external magnetic field, the ground state energy E_0 (2-20) depends upon these parameters through it. At the absolute zero of temperature, 0°K, we get

$$E_0(0) = -\frac{1}{4} N |J| z + \sum_\nu z |J| (\sqrt{1-\gamma_\nu^2} - 1),$$

which agree with the result previously obtained.¹⁾ At the Néel temperature we

expect $\sigma=0$ and may obtain the result,

$$E_0(T_N) = -\frac{1}{4}N|J|z,$$

which coincides with the energy for the Néel state, though we may expect that our quasi-particle approximation becomes invalid near the Néel temperature. Our result shows that the ground state energy as well as the elementary excitation energies varies with the temperature and the external magnetic field. These effects are expected to be statistical in origin and seem to have some interesting meaning. If we consider the quasi-particle due to the elementary excitation, it seems reasonable that the averaged fundamental state in which there are no quasi-particles present at finite temperature, i.e., the ground state as we have called, has the character which depends upon the surrounding effects. We have to consider our system along the statistical point of view. There exist particles a , and b , interacting one another even at the absolute zero of temperature. The true ground state means the unified and averaged state in which the virtual particles are being created and destructed and the dressed particles α_v^0 and β_v^0 have the elementary excitation energies ω_{v1}^0 , and ω_{v2}^0 respectively. At the finite temperatures the dressed particles may be excited thermally, and we may expect the ground state energy $E_0(T)$ and the elementary excitation energies ω_{v1}^T and ω_{v2}^T may have some changes due to the effects of surroundings. Our method of approximation goes along the above consideration.

Eventually this type of diagonalization may be suitable for inquiring into the macroscopic actual nature at any temperature and in the external field.

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