Variational Theory of the Heisenberg Ferromagnet

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Under the assumption of the existence of model Hamiltonian, the variational theory which is proposed by Sawada is applied to the Heisenberg Ferromagnet. The spontaneous magnetization at one and two dimensions does not exist, and the Curie temperature at three dimensions agrees with that of molecular field theory. In low temperature regions the temperature dependence of spin wave energy agrees with that of Bloch's calculations.

§ 1. Introduction

Since the random phase approximation of Tjabrikov's theory, there have appeared many papers to try to improve the random phase approximation using the Green's function with untrivial decoupling procedures and they have gained various qualitative solutions.

In the whole temperature region, the random phase approximation gives comparatively satisfactory results. But in low temperature regions the energy of the spin wave is proportional to the magnetization $\sigma$ which has a temperature dependence $T^{\sigma/2}$, so that the temperature dependence of the spin wave energy is proportional to $T^{\sigma/2}$. This result is different from $T^{\sigma/2}$ of magnon approximation of Dyson's work.

We must especially take notice of the decoupling of correlation functions of spin systems. Unfortunately, there is no guiding principles of decoupling procedure at present, and we base our theory on the variational principle, namely the free energy minimum or at least stationary.

Adopting the Dyson Hamiltonian which is described by Bose particles gained by the Dyson-Maleev transformation of the spin operator and using the Hartree-Fock approximation which satisfies the variational principle, Bloch has gained results which are consistent with Dyson's results in low temperature regions.

Although the temperature dependence of spin wave energy of her result shows a correct $T^{\sigma/2}$ dependence, the result showed an antisymmetric relation of magnetization $\sigma$ for an external magnetic field $H$, i.e. $\sigma(H) = -\sigma(-H)$ is not satisfied and the phase transition is not of second order but of first order.

Therefore the Boson approximation which changes from spin operators to Bose operators is not appropriate in high temperature regions.

The variational theory of the Heisenberg model which leaves spin operators as it is, is only the molecular field theory. But molecular field theory shows
that the spontaneous magnetization exists at all dimensions and does not predict
the existence of a spin wave, so that this theory is not sufficient physically in
spite of satisfying the free energy minimum.

It is not obvious whether the R.P.A. and other Green’s function theory us­ing
the decoupling method satisfy the variational principle.

Using a new variational theory which is proposed by Sawada, we obtain
results as follows.

In low temperature regions the temperature dependence of spin wave energy
agrees with that of Bloch’s results and spontaneous magnetization does not exist
at one and two dimensions, and the Curie temperature is to coincide with that
of molecular field theory, and an antisymmetric relation \( \sigma(H) = -\sigma(-H) \) is
satisfied. The spurious \( T^3 \) term of spontaneous magnetization in low tempera­
ture regions has appeared. Our solutions agree with the results of Mubayi and
Lange which were gained by using the decoupling method of the Green’s func­tion
for two-dimensional Heisenberg ferromagnet.

In § 2, the formulation is presented and in § 3 the low temperature expan­sion
of the spontaneous magnetization and spin wave energy are calculated. In
§ 4 the Curie temperature and the critical index \( \beta \) are obtained.

### § 2. Formalism

The Heisenberg model can be described by a Hamiltonian,

\[ \mathcal{H} = -g \mu H \sum_f S_f^z - \sum_{f,m} I(f - m) S_f \cdot S_m, \]

where \( S_f \) is the spin operator of an electron situated at the lattice site \( f \), \( I(f - m) \) is the exchange integral which we shall assume to be positive, \( g \) is Lande
\( g \) factor, \( \mu \) is the Bohr magneton and \( H \) is the external magnetic field.

In the case \( S = 1/2 \), the spin operators can be expressed in terms of Pauli
operators,

\[ S_f^z = S_f^x + i S_f^y = 0, \]
\[ S_f^x = S_f^+ - i S_f^- = b_f^+, \]
\[ S_f^y = \frac{1}{2} - b_f^+ b_f^-, \]

which satisfy the commutation relations

\[ [b_f, b_m^+] = \delta_{fm} (1 - 2n_f) = \delta_{fm} \sigma_f, \]
\[ [b_f, b_m] = 0 \quad \text{and} \quad [b_f^+, b_m^+] = 0. \]

Changing in the Hamiltonian from spin operators to Pauli operators, we get

\[ \mathcal{H} = \varepsilon_0 + \sum_f (J(0) + g \mu H) n_f - \sum_{f,m} I(f - m) b_f^+ b_m - \sum_{f,m} I(f - m) n_f m_m, \]

where
Now we assume the existence of model Hamiltonian $H_0$ which satisfies the following equation

$$[b_f, H_0] = \sum E_f b_f.$$  

(7)

According to Sawada's paper\(^3\), using the model Hamiltonian, we obtain the variational model free energy

$$F = -\frac{1}{\beta} \ln \text{Tr} e^{-\beta H_0} \leq F_{\text{mod}} = -\frac{1}{\beta} \ln \text{Tr} e^{-\beta H_0} + \text{Tr} e^{-\beta H_0} (\mathcal{H} - H_0) / \text{Tr} e^{-\beta H_0}.$$  

(8)

We define the variational Hamiltonian

$$\delta H_\lambda = \lambda \sum |l\rangle \langle l| \beta (E_l - E_m)(G)_{lm} \langle m|,$$

(9)

where $\lambda$ is the small constant, $|l\rangle$ is the eigenstate of the model Hamiltonian $H_0$ and

$$(G)_{lf} = G_{lf} + G_{fl},$$

(10)

where

$$G_{lf} = -e^{\beta H_0} \frac{1}{2} (b_l^+ b_f + b_fb_l^+) e^{-\beta H_0} - e^{\beta H_0} \frac{1}{2} (b_l^+ b_f + b_f b_l^+) e^{\beta H_0},$$

$$(G)_{lf} = e^{\beta H_0} b_l^+ e^{-\beta H_0} b_f e^{\beta H_0} + e^{\beta H_0} b_f e^{-\beta H_0} b_l^+ e^{\beta H_0}.$$  

(11)

The requirement of stationarity of free energy under the change from $H_0$ to $H_0 + \delta H_\lambda$ requires

$$\delta F_{\text{mod}} = \left\langle -\int e^{\beta H_0} \delta H_\lambda e^{-\beta H_0} d\beta (H - H_0) \right\rangle = 0, \quad \langle \delta H_\lambda \rangle = 0.$$  

(12)

where $\langle \cdots \rangle$ is defined by

$$\langle \cdots \rangle = \text{Tr} (e^{-\beta H_0} \cdots) / \text{Tr} e^{-\beta H_0}.$$  

Substituting (9), (10) and (11) into (12), we get

$$\langle [b_f, [\mathcal{H} - H_0], b_t^+] \rangle + \langle [b_f, [\mathcal{H} - H_0, b_t^+]] \rangle = 0.$$  

(13)

Now we consider the following equation:

$$A_{fl} = \langle [b_f, [\mathcal{H} - H_0], b_t^+] \rangle - \langle [b_f, [\mathcal{H} - H_0, b_t^+]] \rangle = \langle [\mathcal{H} - H_0, [b_f, b_t^+]] \rangle.$$  

(14)

For $f \neq l$, from the commutation relation (3), we obtain

$$A_{fl} = 0.$$  

(15)
For \( f = l \), we have
\[
A_{ff} = -2 \langle [\mathcal{H} - H_0, n_f] \rangle = -2 \langle [\mathcal{H}, n_f] \rangle.
\] (16)
Here we have used the relation
\[
\text{Tr} (e^{-\beta H_0} n_f) = \text{Tr} (e^{-\beta H} n_f).
\]
Substituting (4) into (16), we have
\[
A_{ff} = -2 \left\{ \sum_m I(f-m) \langle b_f^+ b_m \rangle - \sum_m I(m-f) \langle b_m^+ b_f \rangle \right\}.
\]
From the translational symmetry, we obtain
\[
A_{ff} = 0.
\] (17)
Consequently, from (15) and (17), we get \( A_{fl} = 0 \) for arbitrary indices \( l \) and \( f \). So, we have
\[
\langle [b_f, \mathcal{H} - H_0], b_l^+ \rangle = 0.
\] (18)
Inserting (4) and (7) into (18), we obtain
\[
\langle \sigma \rangle E_{fl} = \delta_{fl} \langle \sigma \rangle (J(0) + g \mu H) - \sigma I(f-l) + 2 \delta_{fl} \sum_m I(l-m) \langle b_f^+ b_m \rangle
- 2I(f-l) \langle b_f^+ b_f \rangle - 2 \delta_{fl} J(0) \langle n \rangle + 2 \langle n \rangle I(f-l)
+ 4 \delta_{fl} \sum_m I(f-m) \langle n_f n_m \rangle - 4 I(f-l) \langle n_f n_f \rangle.
\] (19)
Here we have used the translational symmetry and the equivalence of all lattice sites, i.e. \( \langle n_f \rangle = \langle n \rangle \) and \( I(f-l) \langle b_f^+ b_f \rangle = I(f-l) \langle b_f^+ b_f \rangle \) because \( I(0) = 0 \).
Using the translational symmetry of the lattice, \( E_{fl} \), \( \langle b_f^+ b_l \rangle \) and \( \langle n_f n_l \rangle \) etc. depend only on the difference of lattice vector \( f - l \) respectively, we change to the Fourier components in these variables
\[
E_{fl} = \frac{1}{N} \sum_q \epsilon_q e^{iq(f-l)}, \text{ etc.}
\] (20)
The Kronecker symbol \( \delta_{fl} \) can also be written in the form
\[
\delta_{fl} = \frac{1}{N} \sum_q e^{iq(f-l)}.
\] (21)
Substituting (5), (19) and (21) into (20), we get
\[
\epsilon_q = g \mu H + (J(0) - J(q)) \left( 1 - \frac{2n}{\sigma} \right) + \frac{2}{N \sigma}
\times \sum_p (J(p) - J(p-q)) \langle b^+ b \rangle_p + \frac{4}{N \sigma} \sum_p (J(p) - J(p-q)) \langle nn \rangle_p. \] (22)
From the fluctuation-dissipation theorem, we obtain
Restricting ourselves to the nearest neighbour interaction approximation, we get
\[ \sum_p (J(p) - J(p - q)) \langle nn \rangle_p = \frac{J(0) - J(q)}{J(0)} \sum_p J(p) \langle nn \rangle_p, \]
(24)
where
\[ \langle nn \rangle_p = \sum \langle n_f n_i \rangle e^{-i(p_f - i)}, \]
and
\[ \langle b^+ b \rangle_q = \sum \langle b^+_f b_i \rangle e^{-q(f - i)}. \]

In order to calculate \( \sum J(p) \langle nn \rangle_p \), we consider the following identity:
\[ \sum_f \langle b^+_f [b_f, H] \rangle = (\mu H + J(0)) \sum_f n_f - \sum_{P, m} I(f - m) \langle b^+_f b_m \rangle \]
\[ - 2 \sum_{P, m} I(f - m) \langle n_m n_f \rangle. \]
(25)

In order to calculate the left-hand side of (24), we consider the following equation.
From (18),
\[ \sum_f \langle [b_f, \mathcal{H} - H_0] b^+_f \rangle = \sum_f \langle b^+_f [b_f, \mathcal{H} - H_0] \rangle. \]

Changing to the Fourier transform
\[ b_i = \frac{1}{N} \sum_p b_p e^{ip_i}, \quad b^+_i = \frac{1}{N} \sum_p b^+_p e^{-ip_i}, \]
(27)
we get
\[ \sum_p \langle [b_p, \mathcal{H} - H_0] b^+_p \rangle = \sum_p \langle b^+_p [b_p, \mathcal{H} - H_0] \rangle \]
\[ = \sum_p \langle [b_p, \mathcal{H} - H_0] e^{-\beta H_0} b^+_p e^{\beta H_0} \rangle, \]
(28)
where indices \( f, l, i, \ldots \) denote the configuration space and \( p, q, \ldots \) denote the momentum space.

Using the Fourier transform of (7), i.e.
\[ [b_p, H_0] = \epsilon_p b_p, \]
(29)
we obtain
\[ \sum_p \langle [b_p, \mathcal{H} - H_0] b^+_p \rangle = \sum_p \langle b^+_p [b_p, \mathcal{H} - H_0] b^+_p \rangle e^{-\beta p}. \]
(30)

Consequently we get the following equation:
\[ \sum_f \langle b^+_f [b_f, \mathcal{H} - H_0] \rangle = \sum_p \langle b^+_p [b_p, \mathcal{H} - H_0] \rangle = 0, \]
(31)
Substituting (7) and (25) into (31), taking the Fourier component and using (23), we get
\[
\sum_p \sigma \epsilon_p f(p) = N \langle n \rangle (g \mu H + J(0)) - \sum_p J(p) \langle b^* b \rangle_p - 2 \sum_p J(p) \langle nn \rangle_p.
\]

Inserting (22) and (24) into (32), solving \( \sum_p J(p) \langle nn \rangle_p \), and substituting it into (22), we get
\[
\epsilon_q = g \mu H + (J(0) - J(q)) / K,
\]

where
\[
K = 1 + \frac{2}{N} \sum_p J(0) - J(p) f(p) = \frac{1}{N} \sum_p \text{cth} \frac{\beta \epsilon_p}{2} - \frac{1}{NJ(0)} \sum_p J(p) \text{cth} \frac{\beta \epsilon_p}{2}.
\]

From (23), the relative magnetization is obtained by
\[
\frac{1}{\sigma} = \frac{1}{N} \sum_p \text{cth} \frac{\beta \epsilon_p}{2}.
\]

Substituting (35) into (34), we obtain the spin wave energy
\[
\epsilon_q = g \mu H + \sigma (J(0) - J(q)) \left(1 - \frac{1}{N J(0)} \sum_p J(p) \text{cth} \frac{\beta \epsilon_p}{2}\right).
\]

These solutions (35) and (36) clearly satisfy the antisymmetric relation \( \sigma(H) = -\sigma(-H) \), and the renormalization factor of the spin wave energy is added in contrast with Tjablikov's solutions. Expanding the denominator of Eq. (36) to the second powers of \( \sigma \), we find that it agrees with the Callen results 5 which are gained by choosing the parameter as \( \alpha = \sigma \).

Equations (35) and (36) agree with the result of Mubayi and Lange 6 which are gained by using the decoupling method of the Green's function theory.

\section{Low temperature expansion}

From (35), we have
\[
\sigma = 1 / (1 + 2P) = 1 - 2P + 4P^2 + \ldots,
\]

where
\[
P = \frac{1}{N} \sum_p f(p) = \frac{1}{N} \sum_n \sum_p e^{-(n+1) \beta \epsilon_p} = \epsilon \left(\frac{3}{2}\right) (\theta K)^{3/2} + \frac{3\pi}{4} (\theta K)^{5/2} + \frac{33}{32} \epsilon \left(\frac{7}{2}\right) (\theta K)^{7/2} + \ldots,
\]

where
\[ \theta = \frac{T}{4\pi J}, \quad \frac{\alpha}{2} = \sum_a e^{-\eta a J/4} / (\eta)^{3/2}, \]

and

\[ K = 1 + 2\pi z \left( \frac{5}{2} \right) \theta^{5/3} + \ldots. \quad (39) \]

Substituting (39) into (33), we have

\[ \varepsilon_\mu = g\mu H + (J(0) - J(p)) \left( 1 - 2\pi z \left( \frac{5}{2} \right) \theta^{5/3} + \ldots \right) \quad (40) \]

and

\[ P = 2 \left[ \frac{3}{2} \right] \theta^{5/3} + 3\pi z \left( \frac{5}{2} \right) \theta^{5/3} + 33 \pi^2 z \left( \frac{7}{2} \right) \theta^{7/3} + 3\pi z \left( \frac{3}{2} \right) z \left( \frac{5}{2} \right) \theta^{5/3} + \ldots. \quad (41) \]

The spin wave energy (40) agrees with the result of Bloch's boson approximation which satisfies the variational principle, namely, the Hartree-Fock theory.

If we adopt the second term of \( \sigma \) in (37), i.e. \( \sigma = 1 - 2P \), which corresponds to the boson approximation, the magnetization agrees with Dyson's results.

If we do not take the boson approximation, \( \sigma \) is given by

\[ \sigma = 1 - 2 \left\{ \frac{3}{2} \right\} \theta^{5/3} + 3\pi z \left( \frac{5}{2} \right) \theta^{5/3} + 33 \pi^2 z \left( \frac{7}{2} \right) \theta^{7/3} + 3\pi z \left( \frac{3}{2} \right) z \left( \frac{5}{2} \right) \theta^{5/3} + \ldots. \quad (42) \]

This result contains the spurious \( T^3 \) term. This term will disappear if we take the higher order approximation. This spurious \( T^3 \) term, in general, has appeared only for spin 1/2, and the correction term of the dynamical interaction \( T^{2(s(s+1))/2} \) has appeared for higher spin \( S \).

\( \text{§ 4. Curie temperature and critical index} \)

In the limits \( \sigma \to 0 \) and \( H/\sigma \to 0 \) of (35), the Curie temperature is gained by

\[ 1/\sigma = \frac{1}{N} \sum_p \text{cth} \frac{\beta \varepsilon_p}{2} \]

\[ = \frac{2}{N\beta} \sum_p \frac{1}{\sigma (J(0) - J(p))} \left[ 1 - \frac{\sigma}{N} \sum_q J(q) \text{cth} \frac{\beta \varepsilon_q}{2} \right] = \frac{2}{\sigma\beta} F(-1) B, \quad (43) \]

where

\[ F(-1) = \frac{1}{N} \sum \frac{1}{J(0) - J(p)} \]

and

\[ B = 1 - \frac{\sigma}{N} \sum_q J(q) \text{cth} \frac{\beta \varepsilon_q}{2} = 1 - \frac{\sigma}{N} \sum_q \frac{2BJ(q)}{J(0) \beta \sigma (J(0) - J(q))}, \quad (44) \]
Calculating $B$ from (44) and substituting it into (44), we get
\[
\beta_c J = 0.33
\]
which agrees with the Curie temperature of molecular field that satisfies the variational principle.

The spontaneous magnetization of molecular field approximation exists at one, two and three dimensions but in our solution (35), following the results of Mubayi and Lange, the spontaneous magnetization does not exist at one and two dimensions.

Substituting (45) into (43), the temperature dependence of magnetization $\sigma$ at $T < T_c$ is given by
\[
\sigma \propto (T_c - T)^{-1/2}.
\]
Thus the critical index $\beta$ is equal to 1/2.

§ 5. Discussion

In this paper we assumed the existence of model Hamiltonian $H_0$ and use the variational theory. But the existence of $H_0$ is not trivial and we do not know the way of proving of the existence of model Hamiltonian. The physical meaning of the approximation of decoupling method of the double time Green's function is not clear, so that the qualitatively different solutions for the spin system which was gained by the decoupling procedure of the Green's function must be selected by the variational principle.

If $H_0$ exists, our theory is variational theory which contains the correlation effects at finite temperature. Therefore the results of the Green's function theory, if it is correct, may be consistent with the results of our variational theory.

Finally we consider the relation of the sum rules of the spectral function\(^7\). Consider the function defined by
\[
A_{ij}(\omega) = \left< [b_i(\omega), b_j^+] \right>.
\]
From the definition, we get the following equations:
\[
\int \frac{d\omega}{2\pi} e^{-\omega t} A_{ij}(\omega) = \left< [e^{\lambda_1 x_1} b_i e^{-\lambda_2 x_1}, b_j^+] \right>,
\]
\[
\int \frac{d\omega}{2\pi} e^{-\omega t} A_{ij}(\omega) e^{\beta\omega} - 1 = \left< b_j^+ e^{\lambda_1 x_1} b_i e^{-\lambda_2 x_1} \right>.
\]
Putting $t = 0$, in (48) and the first derivative of $t$ in (48), we get the following sum rules.
\[
\int \frac{d\omega}{2\pi} A_{ij}(\omega) = \left< [b_i, b_j^+] \right> = \delta_{ij} \sigma, \quad \int \frac{d\omega}{2\pi} A_{ij}(\omega) e^{\beta\omega} - 1 = \left< b_i^+ b_j \right>,
Using (23) and (33), the spectral function of our solution is given by

\[
A_\omega(\omega) = \delta(\omega - \epsilon_p),
\]

where

\[
A_{ij} = \frac{1}{N} \sum_p A_p \epsilon_p \delta(i-j).
\]

Substituting (50) into (49), we find the following sum rules satisfied by our solutions:

\[
\int \frac{d\omega}{2\pi} A_{ij}(\omega) = \delta_{ij} \delta, \quad \int \frac{d\omega}{2\pi} e^{i\omega} A_{ij}(\omega) = \langle b_i^+ b_j \rangle,
\]

\[
\int \frac{d\omega}{2\pi} e^{i\omega} A_{ij}(\omega) = \langle [b_i, \mathcal{H}], b_j^+ \rangle
\]

and

\[
\frac{1}{N} \sum_i \int \frac{d\omega}{2\pi} e^{i\omega} A_{ii}(\omega) = \sum_i \langle b_i^+ [b_i, \mathcal{H}] \rangle.
\]

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1) For example, see
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