Method of effective potential for quantum Heisenberg ferromagnet theory

E.V.Podivilov
Institute of Automation & Electrometry,
Novosibirsk, 630090, Russia

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Abstract

Self-consistent temperature dependence of the average magnetization in quantum Heisenberg ferromagnet is obtained as a first approximation of perturbation theory on an inverse radius by application of the functional method for quantum ferromagnet. The experimental data are compared with the theoretical results for EuO ferromagnet. A quantitative agreement is observed between theoretical and experimental results outside interval near Curie temperature. The theory is of critical behavior in the vicinity of Curie temperature $T_c$. Theoretical $T_c$ value itself is agreed with the experimental one with an accuracy of several percents.

1 Introduction

The functional representation of a partition function allows to extend the application of the approximate methods to the problem of the statistical physics. Convenience and naturalness of the functional representation resulted in numerous attempts to extend this method to the Heisenberg quantum ferromagnet model (see [1, 2, 3, 4]). A method proposed in [3] makes it possible to write an expression for the partition function of a magnet in the asymmetric phase in the explicit closed form of an integral over two number
fields — a neutral field and a charged field. The charged field $\Psi$ corresponds to the elementary excitations of magnet. The neutral field $\rho$ corresponds to the average spin magnitude. Erroneous interpretation of global effects in [3] was corrected in [5].

The partition function may be considered as a generating functional of averages of the spin operators. Accordingly the closed expression for the partition function allows to calculate approximately different averages of spin operators, using small parameter $1/z$ — the inverse range of the interaction.

A problem of the average spin calculation can be formulated within the scope of the functional formalism as a minimum of the effective potential $W_{\text{eff}}(\rho)$ problem [7]. We will calculate $W_{\text{eff}}(\rho)$ in the first order in $1/z$. Minimizing $W_{\text{eff}}(\rho)$, we will next obtain the average magnetization $M(T)$ as a function of the temperature. Such a way of considering it allows to avoid the emergence of the fictitious divergences presented in the direct diagram expansion. The comparison between theoretical relationship $M(T)$ and experimental one for the ferromagnet EuO demonstrates that they are in close agreement, just as magnitudes of Curie’s temperature with an accuracy of a few percents.

2 Generating functional of averages of the spin operators

The model of the Heisenberg quantum ferromagnet is based upon the Hamiltonian

$$\hat{H} = -\frac{1}{2} \sum_{i,j} \hat{S}_i J_{ij} \hat{S}_j,$$

(1)

where $J_{ij}$ — is the matrix of the exchange interaction between neighboring spins $\hat{S}_i$ which are located at the lattice sites $\vec{r}_i$. If the interaction of spins with external magnetic field is taken into account the partition function can be written as:

$$Z[\vec{h}_i(t)] = \text{Tr} \exp \left( -\beta \hat{H} + \int_0^\beta \text{d}t \vec{h}_i(t) \hat{S}_i \right),$$

2
where the symbol $T$ denotes time ordering and $\vec{h}_i(t)$ is the external field at lattice site $\vec{r}_i$. For the operator $\exp(-\epsilon \hat{H})$ a Gaussian transformation

$$
\exp(-\epsilon \hat{H}) = \int \prod_i \sqrt{\frac{\epsilon d\phi_i}{2\pi}} (\det J_{ij})^{-1/2} \exp \left( -\sum_{ij} \vec{\phi}_i J_{ij}^{-1} \vec{\phi}_j \epsilon / 2 + \vec{\phi}_i \hat{S}_i \epsilon \right) + O(\epsilon^2)
$$

can be performed to within terms $\sim \epsilon^2$. Thus, writing $\exp(-\beta \hat{H}) = (\exp(-\epsilon \hat{H}))^{\beta/\epsilon}$, with $\epsilon \to 0$, we arrive at an expression for the partition function in the following form

$$
Z[\vec{h}_i(t)] = N \int \prod_i D\phi_i(t) \exp \left( -\frac{1}{2} \int_0^\beta dt \sum_{ij} \vec{\phi}_i(t) J_{ij}^{-1} \vec{\phi}_j(t) \right) \times \prod_i \text{Tr} T \exp \left( \int_0^\beta dt \left[ \vec{\phi}_i(t) + \vec{h}_i(t) \right] \hat{S} \right),
$$

The substitution put forward by Kolokolov in [3]

$$
\phi_i^+ = J_{ij} \rho_j - h_i^+, \\
\phi_i^- = \psi_i^+ - h_i^-,
$$

rearranges the ordered operator exponential [3] to the explicitly specified operator

$$
\hat{A}(\beta) = T \exp \left( \int_0^\beta dt \left[ \vec{\phi}(t) + \vec{h}(t) \right] \hat{S} \right) = \exp(\psi^- (\beta) \hat{S}^+) \times \exp \left( \hat{S}^z \int_0^\beta dt \tilde{\rho}(t) \right) \exp \left( \hat{S}^- \int_0^\beta \psi^+(t) \exp \left( \int_0^t \tilde{\rho}(t') \, dt' \right) \, dt \right) \times \exp(-\psi^- (0) \hat{S}^+),
$$

where index $i$ is omitted.
\[ \tilde{\rho}_i = J_{ij} \rho_j - 2 \psi_i^- \psi_i^+ , \quad \hat{S}^\pm = \hat{S}^x \pm i \hat{S}^y. \]

Thus, regarding \( \psi^\pm(t) \) and \( \rho(t) \) as new integration variables, we can calculate the trace of the T-exponential (\( \tilde{\mathcal{T}} \)) explicitly and obtain a closed functional representation for \( Z[\vec{h}] \). We have for the arbitrary spin magnitude \( S \)

\[
\text{Tr} \hat{A}(\beta) = \sum_{l=0}^{2S} \left[ \left( \psi^- (\beta) - \psi^- (0) \right) \int_0^\beta dt \psi^+ (t) \exp \left( \int_0^t \tilde{\rho}(t') dt' \right) \right] \left[ g_l \left( \int_0^\beta \tilde{\rho}(t) dt \right) \right],
\]

\[
g_0(\xi) = \sum_{m=-S}^{S} e^{m \xi} , \quad g_l(\xi) = \sum_{m=-S}^{S} P_1 \times \ldots \times P_l e^{m \xi},
\]

\[
P_l = S(S + 1) - (m + l)(m + l - 1).
\]

The authors of \( [5] \) showed that it is necessary to use the initial conditions \( \psi_i^- (0) = 0 \) in order to transform from the original variables to the new integration variables (\( \psi^\pm \)). With this conditions and in the discretization of the transformation (\( \psi^\pm \))

\[
\frac{d\psi^- (t)}{dt} = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left( \psi^- (t + \epsilon) - \psi^- (t) \right)
\]

the Jacobian of the transformation is equal to the constant. Hence follows a functional representation for \( Z[\vec{h}] \)

\[
Z[\vec{h}] = N \int \prod_i D\rho_i D\psi_i^- D\psi_i^+ \exp (-\Gamma_l - \Gamma_n),
\]

\[
\Gamma_n = \sum_i - \ln \left( \sum_{l=0}^{2S} \left[ \psi_i^- (\beta) \int_0^\beta dt \psi_i^+ (t) \exp \left( \int_0^t \tilde{\rho}_i(t') dt' \right) \right] \right) \left[ g_l \left( \int_0^\beta \tilde{\rho}_i(t) dt \right) \right],
\]

\[
\Gamma_l = \int_0^\beta dt \sum_{ij} \frac{1}{2} \left[ \rho_i J_{ij} \rho_j - 2 \rho_i h_i^z + h_i^z J_{ij}^{-1} h_j^z \right] + 2 \left[ \left( \psi_i^+ - h_i^- \right) J_{ij}^{-1} \left( \frac{d\psi_j^-}{dt} - h_j^+ - \psi_j^- J_{jk} \rho_k + (\psi_j^-)^2 \psi_j^+ \right) \right].
\]

This partition function may be considered as a generating functional of averages of the spin operators:

\[
< \hat{S}_i^z(t) > = \lim_{\hat{n} \to 0} \frac{\delta \ln \left( Z[\vec{h}] \right)}{\delta h_i^z(t)} = < \rho_i(t) >.
\]
### Effective potential of field $\rho$

In order to obtain the field $\rho$ effective potential, we must integrate over fields $\psi^\pm$. We cannot perform this integration exactly, however it can be made approximately over parameter $1/z = \sum_j J_{ij}^2 / (\sum_j J_{ij})^2 = \sum_k \bar{J}_k^2 / \bar{J}_0^2$, where $\bar{J}_k$ is the Fourier transform of the exchange matrix $J_{ij} = J(\vec{r}_i - \vec{r}_j)$ ($J_0 = J(\vec{k} = 0)$, $\sum_k \bar{J}_k = 0$).

Let us expand the nonpolynomial part of action $\Gamma_n$ (8) in a series in powers of $\psi^- \psi^+$ and extract all the $\Gamma$ terms at $\vec{h} = 0$, which are linear functions of $\psi^\pm$

\[
\Gamma^1 = \int_0^\beta dt \sum_{ij} \frac{1}{2} \rho_i(t) J_{ij} \rho_j(t) + 2 \psi_i^+(t) J_{ij}^{-1} \left( \frac{d\psi^-_j}{dt} - \psi^-_j(t) J_{jk} \rho_k(t) \right) + \int_0^\beta dt \sum_i 2b(\rho_i^0(\beta)) \left( \psi_i^+(t) \psi_i^-(t) - \psi_i^-(\beta) \psi_i^+(t) \exp(\rho_i^0(t)) n_0(\rho_i^0(\beta)) \right) - \sum_i g_0(\rho_i^0(\beta)),
\]

(10)

where $b(\xi) = d \ln(g_0(\xi))/d\xi$ is Brillouin function. The contributions from the other terms of $\Gamma$ are small in the inverse range of interaction, because these terms include two and more sums of $(J_{ij})^2$. Hence in a zero approximation on $1/z$ follows:

1. The saddle-point value $\rho$ is determined by equation

\[
\langle S^z \rangle \approx \langle \vec{p} \rangle = b(\beta J_0 \vec{p}),
\]

(11)

which agree with mean field theory equation.

2. The Fourier transform of the longitudinal correlator $K_k$ takes the form

\[
K_k(t, t') = \langle (\rho_k(t) - \bar{\rho})(\rho_k(t') - \bar{\rho}) \rangle = -J_k^{-1} \delta(t - t') \approx \frac{b(\beta J_0 \vec{p})}{1 - \beta J_k b'(\beta J_0 \vec{p})},
\]

(12)
where $\bar{\rho} = \frac{1}{M} \sum \rho_i = \rho(\bar{k} = 0)$ is the average value of the field $\rho_i$, $M$ — number of lattice sites.

3. The bare propagator of the field $\psi^\pm$ in the Fourier representation has the form

$$G_{\vec{k}}(t, t') = \langle \psi^-_{\vec{k}}(t) \psi^+_{\vec{k}}(t') \rangle > \sim \frac{J}{2} \left( \theta(t - t') + (n_{\vec{k}} + 1) \left[ \exp(J_{\vec{k}} t) - 1 \right] \right) \times \exp(\omega_{\vec{k}}(t - t')),$$

$$n_{\vec{k}} = \frac{1}{\exp(\omega_{\vec{k}} / \beta) - 1}, \quad \omega_{\vec{k}} = J_0 \bar{\rho} - J_{\vec{k}} \beta, \quad b = b(\beta J_0 \bar{\rho}), \quad \theta(0) = 1,$$

where $\theta(t)$ — theta function.

4. The transverse correlator in the Fourier representation has the following form

$$K^-_{\vec{k}}(t, t') = 4J_{\vec{k}}^{-2} < \phi^-_{\vec{k}}(t) \phi^+_{\vec{k}}(t') > \sim -2J_{\vec{k}}^{-1} \delta(t - t') \approx 2b \left( n_{\vec{k}} + 1 - \theta(t - t') \right) \exp(\omega_{\vec{k}}(t - t')).$$

Let us remind that we impose the zero initial conditions $\psi^-(0) = 0$ on the $\psi(t)$ field, then the propagator is of the $G_{\vec{k}}(0, t') = 0$ property and is nonperiodical. Function $\omega_{\vec{k}}$ does not approach zero value at $\vec{k} = 0$ for an arbitrary value of $\bar{\rho}$. However, if $\bar{\rho}$ is defined by (11) in the zero approximation on $1/\bar{z}$, the Goldstone symmetry will be restored ($\omega(0) = 0$).

By substituting $\Gamma^1$ for $\Gamma_n + \Gamma_l$ and integrating (14) over $\psi^\pm$, we obtain the partition function in the first approximation on $1/\bar{z}$.

$$Z = N \int \prod_i D\rho_i \exp(-W^1(\rho_i)), \quad (15)$$

where up to a constant $W^1(\rho_i)$ has the form $\Gamma^1$ in which the bare propagator (13) is substituted for $\psi^-(t)\psi^+(t')$. It can be pointed out that $W^1(\rho_i)$ also determines a longitudinal correlator, whose infrared behavior was examined in low-temperature limit in [5].
Let us perform the Fourier transformation of field $\rho_i$ and expand $W^1$ into a series in $\rho(\vec{k} \neq 0)$. It is enough to hold the quadratic terms in $\rho(\vec{k} \neq 0)$ only within the first order in $1/z$. By integrating over $\rho(\vec{k} \neq 0)$, we obtain the effective potential $W^1(\overline{\rho})$. The saddle-point value $\overline{\rho}$ is determined in the first approximation on $1/z$ by minimizing the effective potential $W^1(\overline{\rho})$:

$$\overline{\rho} = b - \sum_{\vec{k}} (1 - \beta J_\vec{k} b')(n_\vec{k} - n_0) + \frac{b''}{2} \sum_{\vec{k}} \frac{\beta J_\vec{k}}{1 - \beta J_\vec{k} b'},$$

(16)

This equation was obtained in [6] by spin diagram technique application, wherein (16) was concerned as the approximation to (11). Within the scope of our approach the equation (16) means the equation in the saddle-point value $\rho$ in the effective potential, so there is a need to solve (16) exactly for calculation $\langle S^z \rangle = \overline{\rho}$. The temperature dependence of the $S^z(T)$ at $S^z \to 0$ can be found analytically. Magnetization $S(T)$ approaches zero as a square

$$S(T) = A \left( T^1_c - T \right)^{-\frac{1}{2}}$$

(17)

at temperature $T^1_c$

$$T^1_c = T^0_c \left[ 1 - \frac{1}{12b'(0)} \left( \frac{T^0_c}{T^1_c} \right)^2 \sum_{\vec{k}} \frac{J^2_\vec{k}}{J_0^2} + \frac{5b'''(0)}{6b'(0)} \sum_{\vec{k}} \frac{J_\vec{k}}{T^1_c - b'(0) J_\vec{k}} \right],$$

(18)

$$T^0_c = b'(0) J_0 = \frac{S(S+1)}{3} J_0,$$

which is the critical temperature value in the first approximation on $1/z$.

For the illustration of the results obtained, let us compare magnetization-temperature relationship (16) with that obtained in experiment. We have pick Heisenberg ferromagnet EuO as a standard for comparison. Its structure (FCC — face-centered cubic lattice), exchange integral values for interaction between neighboring spins $J1 = 1.212^0K$ (12 neighbors) and $J2 = 0.238^0K$ (6 neighbors), magnetization-temperature relationship $S(T)$ and Curie’s temperature $T_c = 69.15^0K$ were examined carefully in experiments [8]. In EuO the magnitude of spin is equal to $S = 7/2$ and the perturbation theory parameter is $\sum_{\vec{k}} J_\vec{k}^2 / J_0^2 = 1/14$, $J_0 = 15.97^0K$. The figure illustrates experimental relation between temperature and magnetization $S(T)$ (points) and relation given by mean field theory equation (11) (curve 2) and
given by equation (16) (curve 3) which were calculated by computer. Similar comparison between theoretical results obtained by spin diagram technique and experimental data on EuO and EuS were made in [4]. The jump of curve 3 at 65° K determines critical region. The method of steepest descent with the help of which the equation (16) was obtained, does not work in the critical region. It means that dependence $S(T)$ specified by (17) breaks down over critical region in the vicinity of $T_c$. However, $T_c$ itself can be obtained exactly, since the effective potential dependence $W(\rho)$ changes qualitatively at $T = T_c$. For $T < T_c$ function $W(\rho)$ has two minimums at $\rho = \pm \rho$, and for $T > T_c$ function $W(\rho)$ has one minimum at $\rho = 0$. Hence, calculating effective potential at each following order of perturbation theory on $1/z$, we can obtain more exact equation in magnetization as well as critical temperature value.

It is significant that the critical behavior which is characteristic to the phase transitions of the second kind in the method of effective potential is conserved in the perturbation theory. Therefore, in spite of inapplicability of our approach near $T_c$, it nevertheless does not disturb the qualitative picture of the phenomenon.

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