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Modifying the Spin Diagram Technique for Describing Quantum Magnets with Strong Fluctuations

T. A. Val'kova[a] and V. V. Val'kov[b, c]
[a]Siberian Federal University, Krasnoyarsk, 660041 Russia
[b]Kirensky Institute of Physics, Russian Academy of Sciences, Siberian Branch, Krasnoyarsk, 660036 Russia
[c]Siberian State Aerospace University, Krasnoyarsk, 660014 Russia
e-mail: vvv@iph.krasn.ru

Abstract—Using the diagram technique for spin operators, the exact representations for quantum magnets are obtained that express the Green's functions via the components of mass operator $\Sigma^{\alpha\beta}$, end factors L and Q, and the Larkin- and Dyson-irreducible part T_{irr}^{--}. The elementary excitation spectrum and mean magnetization are calculated accurate to the first-order contributions on the parameter r_0^{-3} by the self-consistent field method.

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INTRODUCTION

The properties of quantum magnets with strong fluctuations have been discussed in many scientific works. The problem for discussion is the difficulty of describing these systems by traditional methods. In this work, we show that modifying the spin operator diagram technique (SODT) [1] allows us to obtain a regular procedure for calculating the spectral and thermodynamic properties of anisotropic quantum magnets.

EXPERIMENTAL

We describe the effective Hamiltonian for a quantum magnet in the form

$$H = -\sum_f S_f^z - \sum_{fm}\left\{I_{fm}^{\perp} S_f^z S_m^z + I_{fm} S_f^+ S_m^- + \xi_{fm}\left(S_f^+ S_m^+ + S_f^- S_m^-\right)\right\}, \quad (1)$$

where we introduce the following notations:

$$I_{fm} = \frac{1}{2}\left(I_{fm}^{\parallel} + I_{fm}^{\perp}\right), \quad \xi_{fm} = \frac{1}{4}\left(I_{fm}^{\parallel} - I_{fm}^{\perp}\right). \quad (2)$$

If parameters $I_{fm}^{\parallel}$, $I_{fm}^{\perp}$, and ξ_{fm} are independent, Eq. (1) corresponds to the *XYZ* model. Then, in the momentum representation,

$$I_q = \frac{1}{2}\left(\tilde{I}_q^x + \tilde{I}_q^y\right), \quad \xi_q = \frac{1}{4}\left(\tilde{I}_q^x - \tilde{I}_q^y\right), \quad I_q^{\perp} = \tilde{I}_q^z. \quad (3)$$

The use of the Hamiltonian in this form allow us to describe not only anisotropic ferromagnetic systems, but also the anisotropic two-sublattice antiferromagnets (AFMs) in a zero external magnetic field.

Unlike the isotropic Heisenberg model, there is in this case an additional interaction related to parameter ξ_{fm}. This makes us introduce Green's matrix function

$$\hat{K}(f\tau;\, m\tau') = \begin{pmatrix} K^{++}(f\tau;\, m\tau'), & K^{+-}(f\tau;\, m\tau') \\ K^{-+}(f\tau;\, m\tau'), & K^{--}(f\tau;\, m\tau') \end{pmatrix}, \quad (4)$$

$$K^{\alpha\beta}(f\tau;\, m\tau') = -\frac{1}{2}\left\langle T_\tau\, \tilde{S}_f^{\alpha}(\tau)\, \tilde{S}_m^{\beta}(\tau')\right\rangle, \quad (5)$$

where $(\alpha,\ \beta = +,\ -)$.

In Equation (5), T_τ is the operator of the chronological ordering by time variable τ $(0 \le \tau \le \delta)$, $\delta = 1/T$ (where T is the temperature) and the operators are written in the so-called Heisenberg representation

$$\tilde{S}_f^{\alpha}(\tau) = e^{\tau H}\, S_f^{\alpha}\, e^{-\tau H}. \quad (6)$$

From the diagram representation of the Green's function, we obtain the exact representation for the matrix components of the Fourier image of the Green's function:

$$K^{++}(q,\, i\omega_n) = \frac{\left(1 - 2\xi_q T_{\text{irr}}^{--}\right) + 2\xi_q Q^+ Q^-}{\Delta(q,\, i\omega_n)},$$

$$K^{+-}(q,\, i\omega_n) = \frac{\left(L^+ + I_q T_{\text{irr}}^{--}\right)\Sigma^{--} + \left(i\omega_n + \varepsilon - Q^- I_q - \Sigma^{+-}\right)Q^+}{\Delta(q,\, i\omega_n)},$$

$$K^{-+}(q,\ i\omega_n) = \frac{\left(L^- + I_q T_{\mathrm{irr}}^{--}\right)\Sigma^{--} + \left(-i\omega_n + \varepsilon - Q^+ I_q - \Sigma^{-+}\right)Q^-}{\Delta(q,\ i\omega_n)}, \quad (7)$$

$$K^{--}(q,\ i\omega_n) = \frac{1}{\Delta(q,\ i\omega_n)}\Big\{\left(i\omega_n + \varepsilon - \Sigma^{+-}\right)\left(-i\omega_n + \varepsilon - \Sigma^{-+}\right) + \left(Q^+Q^- - T_{irr}^{--}\Sigma^{--}\right)\left(2\xi_q + \Sigma^{++}\right)\Big\} + L^+L^-\Sigma^{--} + L^+Q^-\left(-i\omega_n + \varepsilon - \Sigma^{-+}\right) + L^-Q^+\left(i\omega_n + \varepsilon - \Sigma^{+-}\right)\Big\}.$$

Here, the quantity $\Delta(q,\ i\omega_n)$ is determined as

$$\begin{aligned}\Delta(q,\ i\omega_n) &= \left(1 - 2\xi_q T_{irr}^{--}\right)\Big\{\left(i\omega_n - \varepsilon + \Sigma^{-+}\right) \times \left(i\omega_n + \varepsilon - \Sigma^{+-}\right) + \left(2\xi_q + \Sigma^{++}\right)\Sigma^{--}\Big\}\\ &+ \left[\left(L^+ + L^-\right)I_q + 2\xi_q L^+L^- + I_q^2 T_{irr}^{--}\right]\Sigma^{--}\\ &+ \left(4\xi_q^2 - I_q^2 + 2\xi_q\Sigma^{++}\right)Q^+Q^-\\ &+ \left(I_q + 2\xi_q L^-\right)\left(i\omega_n + \varepsilon - \Sigma^{+-}\right)Q^+\\ &+ \left(I_q + 2\xi_q L^+\right)\left(-i\omega_n + \varepsilon - \Sigma^{-+}\right)Q^-.\end{aligned} \quad (8)$$

For the sake of brevity, in (7) and (8) we omit arguments q and $i\omega_n$, on which T_{irr}^{--}, $\Sigma^{\alpha\beta}$, $L^{\pm}$, and $Q^{\pm}$ depend, and introduce the notations

$$L^+ \equiv L(q,\ i\omega_n);\quad L^- \equiv L(-q,\ -i\omega_n);$$
$$Q^+ \equiv L(q,\ i\omega_n); Q^- \equiv L(-q,\ -i\omega_n).$$

The dispersion equation for the excitation spectrum is obtained by the analytical continuation to the real axis with sequential putting the obtained expression to zero:

$$\Delta\left(q,\ i\omega_n \to \omega + i\delta\right) = 0. \quad (9)$$

A one-loop approximation was used in any specific calculation. Associating the obtained analytical expressions with the diagram series, we arrive at the collective excitation spectrum

$$\begin{aligned}E_k^2 &= \left\{1 + \frac{2b_0'}{N}\sum_q \frac{\left(I_k - I_{k-q}^{\perp}\right)\left(I_q - I_{k-q}^{\perp}\right) - 4\xi_k\xi_q}{\left(1 - b_0' I_{k-q}^{\perp}/T\right)\left(E_k^2 - \omega_{0q}^2\right)}\right\}\omega_{0q}^2\\ &+ 2\left[\varepsilon_{0q}\left(I_0^{\perp} - I_k\right) - 4b_0\xi_k^2\right]\sigma^{(1)} + \frac{2}{N}\\ &\times \sum_q \frac{\varepsilon_{0k}\Phi(q,k) + 4b_0\xi_k\xi_q\left[H + b_0\left(I_0^{\perp} - I_{k-q}^{\perp}\right)\right]}{\omega_{0q}}\\ &\times\left(\frac{1}{2} + n_q\right) + \frac{2b_0'}{N}\sum_q \frac{\Phi(q,k)\Phi(k,q) + 4\xi_k\xi_q\left(\varepsilon_0 - b_0 I_{k-q}^{\perp}\right)^2}{\left(1 - b_0' I_{k-q}^{\perp}/T\right)\left(E_k^2 - \omega_{0q}^2\right)},\end{aligned} \quad (10)$$

where

$$\begin{aligned}\Phi(q,k) &= \varepsilon_{0q}\left(I_q - I_{k-q}^{\perp}\right) + 4b_0\xi_q^2,\\ \varepsilon_{0q} &= H + b_0\left(I_0 - I_q^{\perp}\right),\\ \varepsilon_0 &= H + b_0 I_0^{\perp},\quad \omega_{0q} = \sqrt{\varepsilon_{0q}^2 - 4b_0^2\xi_q^2},\\ n_q &= \left[\exp\left(\omega_{0q}/T\right) - 1\right]^{-1}.\end{aligned} \quad (11)$$

With allowance for the quantum fluctuations, the magnetization of the subsystem is defined as

$$\begin{aligned}\sigma &= b_0 + \frac{1}{1 - b_0' I_0^{\perp}/T}\\ &\times\left\{\frac{1}{2N}\sum_q \frac{\omega_{0q} - \varepsilon_{0q}}{\omega_{0q}} - \frac{1}{N}\sum_q\left(\frac{\varepsilon_{0q}}{\omega_{0q}}n_q - n_\varepsilon\right)\right.\\ &\left.+ \frac{b_0'}{TN}\sum_q \frac{I_q\varepsilon_{0q} + 4b_0\xi_q^2}{\omega_{0q}}\left(\frac{1}{2} + n_q\right) + \frac{b_0''}{2TN}\sum_q \frac{I_q^2}{1 - b_0' I_0^{\perp}/T}\right\},\end{aligned} \quad (12)$$

where $n_\varepsilon = \left[\exp(\varepsilon/T) - 1\right]^{-1}$.

According to (10), for an easy-plane ferromagnet in the temperature range $0 \geq T \geq T_C$, when I_k, $I_k^{\perp}$, and ξ_k are interrelated (see [2]) as $I_k^{\perp} = I_k - 2\xi_k$, in zero magnetic field we have $E_k \to 0$ at $k \to 0$. Using the expression for the spectrum, it can easily be seen that the gap in the collective excitation spectrum tends to zero for an easy-plane AFM. It should be considered that when the AFM is described via an anisotropic ferromagnet, allowance is made the Brillouin zone extended relative to the antiferromagnetic case. For example, in the zero approximation by r_0^{-3}, the AFM spectrum is described by the formula

$$\omega_q^0 = b_0\sqrt{\left(I_0^x - I_q^z + J_0^x - J_q^z\right)\left(I_0^x - I_q^x + J_0^x + J_q^z\right)}. \quad (13)$$

In the first order by r_0^{-3}, the spectrum of this AFM is specified by expression (10), if $I_q, I_q^{\perp}$, and ξ_q stand for the following combinations of the initial exchange integrals:

$$\begin{aligned}I_q &= \frac{1}{2}\left(I_q^z + I_q^x + J_q^z - J_q^x\right),\quad I_q^{\perp} = I_q^x + J_q^x,\\ \xi_q &= \frac{1}{4}\left(I_q^z - I_q^x + J_q^z + J_q^x\right).\end{aligned} \quad (14)$$

For the easy-axis AFM, we obtain

$$\omega_q^0 = b_0\sqrt{\left(I_0^z - I_q^x + J_0^z - J_q^x\right)\left(I_0^z - I_q^x + J_0^z + J_q^x\right)}.. \quad (15)$$

The renormalized spectrum of the easy-axis AFM is described by the same formula but with different expressions for parameters $I_q, I_q^{\perp}$, and ξ_q :

$$I_q = I_q^x,\quad I_q^{\perp} = I_q^z + J_q^z,\quad \xi_q = \frac{1}{2}J_q^x. \quad (16)$$

CONCLUSIONS

A spin operator diagram technique has been developed that applies to systems with zero quantum fluctuations.

Analysis of the diagram series structure allowed us to obtain an explicit representation for Green's spin function using the components of the mass operator, normal $Q(\vec{q};i\omega_n)$ and anomalous ($L(\vec{q};i\omega_n)$ end factors, and the irreducible Larkin and Dyson parts of Green's function $T_{\text{irr}}^{--}(\vec{q};i\omega_n)$.

Using a self-consistent field in the first order by r_0^{-3}, the renormalized collective excitation spectrum for a quantum magnet with developed zero fluctuations was calculated. The obtained expressions enable us to analyze the effect of frustrated couplings on the physical characteristics of a quantum magnet with the strong quantum fluctuations.

A correction for spontaneous magnetization caused by quantum fluctuations has been obtained that can be applied over a wide range of temperatures.

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