Incommensurate phase of a triangular frustrated Heisenberg model studied via Schwinger-boson mean-field theory

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Received 28 February 2009, in final form 13 June 2009
Published 20 July 2009
Online at stacks.iop.org/JPhysCM/21/326005

Abstract

We study a triangular frustrated antiferromagnetic Heisenberg model with nearest-neighbor interactions $J_1$ and third-nearest-neighbor interactions $J_3$ by means of Schwinger-boson mean-field theory. By setting an antiferromagnetic $J_3$ and varying $J_1$ from positive to negative values, we disclose the low-temperature features of its interesting incommensurate phase. The gapless dispersion of quasiparticles leads to the intrinsic $T^2$ law of specific heat. The magnetic susceptibility is linear in temperature. The local magnetization is significantly reduced by quantum fluctuations. We address possible relevance of these results to the low-temperature properties of NiGa$_2$S$_4$. From a careful analysis of the incommensurate spin wavevector, the interaction parameters are estimated as $J_1 \approx -3.8755$ K and $J_3 \approx 14.0628$ K, in order to account for the experimental data.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In two-dimensional (2D) antiferromagnets, it was proposed the ‘geometrical frustration’ may enhance the quantum spin fluctuation and suppress the magnetic order to form a spin liquid [1]. In this context the triangular- and Kagomé-related lattices are studied extensively to seek a quantum spin liquid [2]. It turns out that the triangular lattice antiferromagnet with nearest-neighbor (NN) coupling exhibits $120^\circ$ magnetic order [3], while the Kagomé lattice antiferromagnet is still a controversial topic for intriguing exploring [4]. People resort to other interactions, such as longer range and multiple-spin exchange ones, to realize a quantum spin liquid [2]. Experimental evidence in favor of this long-predicted spin-liquid state have emerged in recent years², although many aspects are still elusive. The spin disorder at low temperatures found in the compound NiGa$_2$S$_4$, in which Ni spins ($S = 1$) form a stack of triangular lattices, aroused much attention [6–9]. The crystal structure of the material is highly 2D, since inter-layer interactions are quite weak. Intriguing low-temperature properties of this material include the $T^2$ law of specific heat, incommensurate short-range spin correlation and lack of divergent behavior of the magnetic susceptibility. A dominant third-nearest-neighbor (3-NN) antiferromagnetic (AFM) interaction $J_3$ could produce the incommensurate phase in a rough picture: four sublattices will form commensurate $120^\circ$ magnetic order separately if the NN interaction $J_1$ is zero, and the system will be driven into an incommensurate order if $J_1$ is gradually switched on. A first-principles calculation by Mazin [10] suggests a large 3-NN interaction $J_3$ and a negligible 2-NN interaction. $J_3$ is confirmed to be AFM, but the sign of $J_1$ has not yet been identified [10]. The classical
spin version of this model was studied in a Monte Carlo simulation [11], which provides some helpful information such as the incommensurability. Up to now, the quantum spin version of this model has not yet been studied very well. Besides the sign of $J_1$, many aspects of this model, either in agreement or disagreement with the experiment of NiGa$_2$S$_4$, need further clarification and treatment. In this paper we focus on the low-temperature properties of the quantum spin model and intend to make a contribution to this topic.

The Schwinger-boson mean-field theory (SBMFT) provides a reliable description for both quantum ordered and disordered antiferromagnets based on the picture of the resonant valence-bond (RVB) state [1, 12, 13]. As a merit, it does not prescribe any prior order for the ground state in advance, which should emerge naturally if the Schwinger bosons condence in the lowest energy states. For the Heisenberg antiferromagnets with NN couplings at zero temperature, it successfully captures the lowest energy states. For the Heisenberg antiferromagnets should emerge naturally if the Schwinger bosons condense in ordered antiferromagnets based on the picture of the resonant wavevector observed in the experiment. Our results suggests be in the small FM region to obtain the incommensurate wavevector.

Finally we discuss the physical meanings of the results. As the incommensurability. Up to now, the quantum spin $\lambda$ model falls as the incommensurability. Up to now, the quantum spin $\lambda$ model falls

\[ H_{\text{eff}} = \sum_k \phi_k^2 + M(k)\phi_k + \varepsilon_0, \]

(4)

where $\phi_k^2 = (a_k^\dagger b_k^\dagger a_{-k}^\dagger b_{-k})$. $M(k) = \epsilon(k)\sigma_0 \otimes \sigma_0 + \Delta(k)\sigma_y \otimes \sigma_y$, $\epsilon(k) = \lambda - J_1 F \sum \cos k^{(i)}$, $\Delta(k) = J_1 A \sum \sin k^{(i)} + J_2 \Pi \sum \sin^2 k^{(i)}$, $\varepsilon_0 = 3 N_\lambda(-J_1 F^2 + J_2 A^2 + J_3 \Pi^2) - N_\lambda(35 + 1)$ and $\otimes$ means the Kronecker product, $\sigma_0$ is a $2 \times 2$ unit matrix and $\sigma_y, \sigma_z$ are Pauli matrices, $k^{(i)} = k_x, k_y$, respectively. The Matsubara Green functions are defined as

\[ G(k, \tau) = -(T \phi_k(\tau) \phi_k^\dagger), \]

(5)

where $\tau$ is the imaginary time and $\phi(k) = e^{iH_n} \phi_k e^{-iH_n}$. All physical quantities can be expressed in terms of the matrix elements of the Green function.

The Matsubara Green function in Matsubara frequency $\omega_n = 2n\pi/\beta$ ($n$ is an integer for bosons) can be worked out as

\[ G(k, i\omega_n) = \frac{i\omega_n \sigma_z \otimes \sigma_0 - \epsilon(k)\sigma_0 \otimes \sigma_0 + \Delta(k)\sigma_y \otimes \sigma_y}{(i\omega_n)^2 - \omega^2(k)}, \]

(6)

For the distribution of $\omega_n$, the two degenerate spectra of the quasi-particles can be readily read out:

\[ \omega(k) = \sqrt{\epsilon^2(k) - \Delta^2(k)}. \]

(7)

The mean-field equations are obtained by the constraint and the introduced mean fields. We omit the details and only present the results here:

\[ \frac{1}{N_A} \sum_k (1 + 2n_B[\omega(k)]) \frac{\epsilon(k)}{\omega(k)} = 2S + 1, \]

(8a)

\[ \frac{1}{6N_A} \sum_k (1 + 2n_B[\omega(k)]) \frac{\epsilon(k) \sum \cos k^{(i)}}{\omega(k)} = F, \]

(8b)

\[ \frac{1}{6N_A} \sum_k (1 + 2n_B[\omega(k)]) \frac{\Delta(k) \sum \sin k^{(i)}}{\omega(k)} = A, \]

(8c)

\[ \frac{1}{6N_A} \sum_k (1 + 2n_B[\omega(k)]) \frac{\Delta(k) \sum \sin^2 k^{(i)}}{\omega(k)} = \Pi, \]

(8d)

where $n_B[\omega(k)] = [e^{\omega(k)/k_B T} - 1]^{-1}$ is the Bose–Einstein distribution function. In the thermodynamical limit $N_A \to \infty$, the momentum sum is replaced by an integral, $(1/N_A) \sum_k \to (1/A_{BZ}) \int d^2 k$, $A_{BZ} = 8\pi^2/\sqrt{3}$. If the Schwinger-boson condensation occurs at $k^*$, a condensation term should be extracted in the momentum sumnation of the first equation, equation (8a):

\[ 2S + 1 = \rho_0 + \int \frac{d^2 k}{A_{BZ}} (1 + 2n_B[\omega(k)]) \frac{\epsilon(k)}{\omega(k)}, \]

(9)

where the density of condensates:

\[ \rho_0 = \frac{1}{N_A} \sum_k (1 + 2n_B[\omega(k^*)]) \frac{\epsilon(k^*)}{\omega(k^*)}. \]

(10)
gapless nodal points occur at $k^*$, where $k^* = \pm (k^*/2, \sqrt{3}k^*/2)$ with $k^* = 0.158\pi$. The blue hexagon denotes the first Brillouin zone. See more details in the text.

![Figure 1](image1.png)

**Figure 1.** The gapless spectrum with nodal points. To compare with the experiment, we choose the parameter $J_1/J_3 = -0.2756$, so that the gapless nodal points occur at $k^* = \pm (k^*/2, \sqrt{3}k^*/2)$ with $k^* = 0.158\pi$. The blue hexagon denotes the first Brillouin zone. See more details in the text.

The zero-temperature static spin structure factor at the parameter $J_1/J_3 = -0.2756$. The blue hexagon denotes the first Brillouin zone. See more details in the text.

![Figure 2](image2.png)

**Figure 2.** The zero-temperature static spin structure factor at the parameter $J_1/J_3 = -0.2756$. The blue hexagon denotes the first Brillouin zone. See more details in the text.

Our numerical solution demonstrates the condensation occurs at zero temperature for spin $S > S_C$, where $S_C$ varies with the ratio of $J_3/J_1$. Since we have $S_C < 0.172$ in our concerned range of the ratio of $J_3/J_1$, we will always consider condensations in the following discussions. The condensation terms in the next three mean-field equations, equations (8b)–(8d), should also be extracted carefully. It is noticeable the per site ground-state energy can be simplified by utilizing the mean-field equations:

$$E_0/N_A = \frac{1}{N_A} \left( \sum_k \omega(k) + \varepsilon_0 \right) = -3J_1(A^2 - F^2) - 3J_1\Pi^2.$$  

(11)

### 3. The incommensurate phase solution

The mean-field equations are solved numerically at zero temperature. For our purpose, we set $S = 1$ in the calculation in order to compare the result with the related experiment, although the qualitative conclusion is spin-independent, but the quantitative results vary with the values of spin. One fact that should be noticed is that the mean fields $F$ and $A$ could not exist simultaneously [14], so the number of mean-field equations can be reduced from 4 to 3 in both $J_1 > 0$ and $J_1 < 0$ regions. In the two regions, we found the system falls into the incommensurate phases with gapless excitations.

The quasiparticle’s spectra become gapless at the nodal points, say $k^* = (k^*_x, k^*_y) = \pm (k^*/2, \sqrt{3}k^*/2)$ (e.g. see figure 1). Near the nodal points, the spectrum is linear in $|k - k^*|$

$$\omega(k) \approx \alpha |k - k^*| + O(|k - k^*|^2).$$  

(12)

At a finite temperature, a gapful spectrum will develop asymptotically as $\Delta_{gap} = c_1 e^{-S/T}$ with constants $c_1$ and $c_2$, which coincides with the Mermin–Wagner theorem [13]. The incommensurate order at zero temperature of the system is signaled by the divergence in the static spin structure factor:

$$\chi_S(q) = \frac{1}{N_A} \sum_k \frac{1}{2} [P(k+q)Q(k) - R(k+q)R(k)].$$  

(13)

where $P(k) = [\epsilon(k)/\omega(k) + 1]/2$, $Q(k) = [\epsilon(k)/\omega(k) - 1]/2$, $R(k) = \Delta(k)/[2\omega(k)]$. Because the spectra is gapless at $k^*$, $\omega(k^*) = 0$, $\chi_S(q)$ becomes divergent at $q^* = 2k^*$ (see figure 2):

$$\chi_S(q^*) = \frac{1}{16} N_A \rho_0^2.$$  

(14)

as it is proportional to the number of lattice sites $N_A$. The local magnetization will be reduced significantly due to strong

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6 Introduction of both $F$ and $A$ mean fields can be found in [14]. Here we find that if one supposes both $F$ and $A$ are nonzero at the same time, then an inconsistent result will be induced. This fact is very useful when one solves the equations. The merit of retaining both mean fields is that quite a good ground-state energy value can be produced.
quantum fluctuations:

\[ m \approx \sqrt{\chi_S(k^*)} = \frac{\rho_0}{4\sqrt{1 - \cos q^*}} \]  

where the factor 2 comes from the degeneracy of the quasiparticle spectra. As a result, a \( T^2 \) law of specific heat follows apparently:

\[ C_V/N_A \approx \frac{6\sqrt{3}\zeta(3)k_B^3}{\pi^2a^2J_3^2}T^2, \]  

where \( \zeta(3) = 1.202 \). If one supposes that the \( T^2 \) law of specific heat of NiGa2S4 is ascribed to the gapless incommensurate phase, a numerical estimation, \( J_1 \approx -3.8755 \) K and \( J_3 \approx 14.0628 \) K, could be obtained.

4. Discussions

Before ending this paper, we point out that the zero-field susceptibility for this incommensurate phase is linear in temperature:

\[ \chi_M/N_A \approx \frac{\sqrt{3}(g\mu_B)^2k_B}{2\pi^2a^2J_3^2}T. \]  

Using the parameters noted above, we find that it is \( \chi_M \approx 2.77 \times 10^{-4}T \) (emu mol\(^{-1}\)), which is not in agreement with the experimental data of NiGa2S4. \( J_M \approx A + BT \) with \( A \approx 0.009 \) (emu mol\(^{-1}\)) and \( B \approx 0 \) below 10 K [6]. The Monte Carlo study also shows the classical version of this model only produces a single peak in the specific heat [11]. These facts indicate that the model in equation (1) could not account for all mysteries in NiGa2S4. Thus, the solution shows the model equation (1) with AFM \( J_3 \) and FM \( J_1 \) has captured the main features for an incommensurate correlation in NiGa2S4, but it is still oversimplified as the minimal model for all low-temperature properties of NiGa2S4. A biquadratic interaction might be a good candidate for reproducing a finite susceptibility at zero temperature. In the absence of the 3-NN interactions, a biquadratic term can induce a quadrupolar order and totally suppress the spin order. The \( T^2 \) law of specific heat is also intact when quadrupolar order sets in [17–19]. It will be interesting to see how the incommensurate spin correlation will be influenced by the biquadratic interactions.

Acknowledgments

This work was supported by the COE-SUG grant (no. M58070001) of NTU and the Research Grant Council of Hong Kong under grant no. HKU 703804.

References

[1] Anderson P W 1973 Mater. Res. Bull. 8 153
[2] Fazekas P and Anderson P W 1974 Phil. Mag. 30 423
[3] Anderson P W 1987 Science 235 1196
[4] For a review see Misguich G and Lhuillier C 2003 Frustrated Spin Systems ed H T Diep (Singapore: World Scientific)
[5] Huse D A and Elser V 1988 Phys. Rev. Lett. 60 2531
[6] Berven B, Lhuillier C and Pietro L 1992 Phys. Rev. Lett. 69 2590
[7] Caprilli L, Trumper A E and Sorella S 1999 Phys. Rev. Lett. 82 3899
[8] Lee P A 2008 Science 321 1306
[5] Broholm C, Aeppli G, Espinosa G P and Cooper A S 1990
Phys. Rev. Lett. 65 3173
Mendels P, Bert F, de Vries M A, Olariu A, Harrison A, Duc F,
Trombe J C, Lord J, Amato A and Baines C 2007 Phys. Rev.
Lett. 98 077204
Helton J S, Maian K, Shores M P, Nyiko E A, Bartlett B M,
Yoshida Y, Takano Y, Suslov A, Qi Y, Chung J-H,
Nocera D G and Lee Y S 2007 Phys. Rev. Lett. 98 107204

[6] Nakatsuji S, Nambu Y, Tonomura H, Sakai O, Jonas S,
Broholm C, Tsunetsugu H, Qiu Y and Maeno Y 2005
Science 309 1697

[7] Nakatsuji S, Tonomura H, Onuma K, Nambu Y, Sakai O,
Maeno Y, Macaluso R T and Chan J Y 2007 Phys. Rev. Lett.
99 157203

[8] Nakatsuji S, Nambu Y, Onuma K, Jonas S, Broholm C and
Maeno Y 2007 J. Phys.: Condens. Matter 19 145232

[9] Yaouanc A, Dalmas de Réotier P, Chapuis Y, Marin C,
Lapertot G, Cervellino A and Amato A 2008 Phys. Rev. B
77 092403

[10] Mazin I I 2007 Phys. Rev. B 76 140406(R)
[11] Tamura R and Kawashima N 2008 J. Phys. Soc. Japan
77 103002
[12] Arovas D P and Auerbach A 1988 Phys. Rev. B 38 316
Auerbach A and Arovas D P 1988 Phys. Rev. Lett. 61 617
[13] Auerbach A 1994 Interacting Electrons and Quantum
Magnetism (New York: Springer)

[14] Gazza C J and Ceccatto H A 1993 J. Phys.: Condens. Matter
5 L135
[15] Shen S Q and Zhang F C 2002 Phys. Rev. B 66 172407
[16] Li P and Shen S Q 2004 New J. Phys. 6 160
[17] Tsunetsugu H and Arikawa M 2006 J. Phys. Soc. Japan
75 083701
Tsunetsugu H and Arikawa M 2007 J. Phys.: Condens. Matter
19 145248
[18] Lauchli A, Mila F and Penc K 2006 Phys. Rev. Lett.
97 087205
[19] Li P, Zhang G M and Shen S Q 2007 Phys. Rev. B 75 104420