Frustrated Honeycomb Heisenberg Antiferromagnet:

A Schwinger Boson Approach

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Abstract

We analyze the frustrated Heisenberg antiferromagnet defined on a honeycomb lattice using a Schwinger-boson mean-field theory. The spin-wave velocity and the susceptibility are presented as functions of the strength of the frustrating interaction for spin $S = \frac{1}{2}$, and the dynamic structure factor is calculated for various temperatures and frustrations. For large $S$, we find an increased Néel stability with respect to the classical case.
INTRODUCTION

The two-dimensional Heisenberg antiferromagnet has received much attention during the last years. One of the reasons for this new interest stems from the discovery of high-$T_c$ superconductors, which has encouraged comprehensive investigations of the model defined on a square lattice. In particular, there is now convincing evidence that it has a Néel ordered ground state for nearest-neighbor interactions even for spin $S = \frac{1}{2}$ [1]. For the honeycomb lattice, however, the situation is less clear. The special features of this lattice make it more intricate and it has so far been paid less attention.

The honeycomb lattice is bipartite and has a Néel state as its classical ground state. However, since it has the smallest possible two-dimensional coordination number ($z = 3$), quantum fluctuations are expected to be larger than for a square lattice. Hence, it can be used for analyzing whether quantum fluctuations may destroy antiferromagnetic long-range order (AF LRO) in higher dimensions than one. There are strong indications though that this is not the case, even for $S = \frac{1}{2}$. Extrapolations of finite-lattice diagonalizations [2] and of Monte Carlo simulations [3], as well as first-order corrections to spin-wave theory [4] and series expansions around the Ising limit [5] all give a finite, albeit much reduced, Néel-order parameter. The AF LRO at $T = 0$ is also found in our approach.

Another property of the honeycomb lattice is that it is not a Bravais lattice, i.e., translational invariance of the full lattice is broken for any type of state. Hence, for a transition from magnetic disorder at finite temperatures to Néel order at $T = 0$, the spatial symmetry is not reduced as for the square lattice. Our treatment here should therefore be possible to extend to a Kagomé lattice, which is neither a Bravais- nor a bipartite lattice. The non-Bravais character has also led to a more exotic speculation, namely that the model possesses a Haldane gap if it fails to be Néel-ordered [6]. However, as just mentioned, several results are not in favor of this possibility.

After our corroboration of the stability of the Néel state on the honeycomb lattice at $T = 0$, it is of course interesting to consider the behavior under frustrating interactions.
How will the thermodynamic parameters change, what will happen to the dynamic structure factor, and when will the Néel state finally break down?

In this paper we calculate several thermodynamic parameters and investigate effects of frustration of the spin-$\frac{1}{2}$ case. For this purpose we employ the Schwinger-boson mean-field theory (SBMFT), which has proved successful in incorporating quantum fluctuations [7] and which two of us have used for an investigation of frustration in the square case [8]. In particular, we report results for the spin-wave velocity and transverse susceptibility, with and without frustration, at zero temperature. We also calculate the dependence of frustration for the mass of spin-wave excitations at low temperature.

While the weak-frustration limit is well-defined and well-behaved both in spin-wave theory and SBMFT, the case of strong frustration close to the classical critical frustration is more complicated. For the square lattice, for example, the location of the Néel boundary has been an issue of considerable interest and it is not settled yet. In the present paper we present results for the honeycomb Néel boundary using SBMFT, linear spin-wave theory (LSWT), and a mapping to the nonlinear $\sigma$ model with SBMFT parameters calculated here for $S = \frac{1}{2}$. The qualitative differences between the various methods are the same as for the square lattice.

Finally, we present calculations of the dynamic structure factor, which allows for a detailed study of the nature of the spin-wave excitations. In particular, we probe the excitations around the antiferromagnetic Bragg peak and their dependence on frustration and temperature.

**THE MODEL**

The honeycomb lattice can be viewed as composed of two interlacing triangular sublattices. Each site has its three nearest neighbors on the other sublattice and its six second-nearest neighbors on its own sublattice, whereas the third-nearest neighbors are again on the opposite sublattice. With positive exchange couplings, the nearest-neighbor interac-
tions classically lead to a Néel-ordered ground state, which is frustrated by the interactions within the sublattices. In our study of the frustrated quantum Heisenberg antiferromagnet, we consider the $J_1$-$J_2$ model

$$
\mathcal{H} = J_1 \sum_{r,\alpha} S_r \cdot S_{r+\alpha} + J_2 \sum_{R,\beta} S_R \cdot S_{R+\beta} \quad ,
$$

with $J_1, J_2 \geq 0$. The first sum runs over all sites $r$ of one sublattice and over the three nearest-neighbor vectors $\alpha$. The next sum, on the other hand, runs over all lattice sites $R$ and three of the six second-nearest-neighbor vectors $\beta$. We have chosen

$$
\alpha_1 = \frac{\sqrt{3}}{2} e_x + \frac{1}{2} e_y \quad ,
$$

$$
\alpha_2 = -\frac{\sqrt{3}}{2} e_x + \frac{1}{2} e_y \quad ,
$$

$$
\alpha_3 = -e_y \quad ,
$$

and

$$
\beta_1 = \frac{\sqrt{3}}{2} e_x - \frac{3}{2} e_y \quad ,
$$

$$
\beta_2 = \frac{\sqrt{3}}{2} e_x + \frac{3}{2} e_y \quad ,
$$

$$
\beta_3 = -\sqrt{3} e_x \quad ,
$$

and units where the (nearest-neighbor) lattice constant equals 1. These vectors are depicted in Fig. 1.

The Schwinger-boson approach for the honeycomb lattice is similar to the one on the square lattice. However, as the former is not a Bravais lattice, complex phases enter geometric factors and it is necessary to treat the sublattices separately. In the following, we give the main formulas for SBMFT on a honeycomb lattice, which are to be compared with the corresponding formulas for the square case (Eqs. (4)–(12) in Ref. [8]). The spin operators $S_R$ at each lattice site are replaced by two species of Schwinger bosons $b^\dagger_{\mu R}$ ($\mu = 1, 2$) via

$$
S_R = \frac{1}{2} b^\dagger_{\mu R} \sigma_{\mu} b_{\nu R} \quad ,
$$

(4)
with the local constraints $b_{\mu R}^\dagger b_{\mu R} = 2S$. Here $\sigma = (\sigma^x, \sigma^y, \sigma^z)$ is the vector of Pauli matrices, and summation over repeated (Greek) indices is implied. The spins on one sublattice are rotated by $\pi$ around the $y$-axis, which leads us to the following Hamiltonian:

$$\mathcal{H} = -J_1 \sum_{r,\alpha} \mathcal{W}_{r,\alpha}^A + J_2 \sum_{R,\beta} \mathcal{W}_{R,\beta}^B + \sum_R \lambda_R [b_{\mu R}^\dagger b_{\mu R} - 2S] ,$$

where we have included the local constraints with Lagrange multipliers $\lambda_R$ at each site. The expression for the summands is

$$\mathcal{W}_{R,\delta}^\chi = \frac{1}{2} : \chi_{R,\delta}^\dagger \chi_{R,\delta} : - S^2 ,$$

with $\chi_{R,\delta}$ any of the two link operators

$$\mathcal{A}_{R,\delta} \equiv b_{1 R}^\dagger b_{1 R+\delta} + b_{2 R}^\dagger b_{2 R+\delta} ,$$

$$\mathcal{B}_{R,\delta} \equiv b_{1 R}^\dagger b_{1 R+\delta} + b_{2 R}^\dagger b_{2 R+\delta} .$$

The mean-field theory is finally generated by the Hartree-Fock decoupling

$$: \chi_{R,\delta}^\dagger \chi_{R,\delta} : \to \chi_{R,\delta}^\dagger \langle \chi_{R,\delta} \rangle + \langle \chi_{R,\delta}^\dagger \rangle \chi_{R,\delta} - \langle \chi_{R,\delta}^\dagger \rangle \langle \chi_{R,\delta} \rangle ,$$

where the link fields $Q_1 \equiv \langle A_{r,\alpha} \rangle$ and $Q_2 \equiv \langle B_{R,\beta} \rangle$ are taken to be uniform and real. In our mean-field treatment, we replace the local Lagrange multipliers $\lambda_R$ by a single parameter $\lambda$.

After Fourier-transforming the Schwinger bosons independently on each sublattice,

$$b_{\mu R} = \frac{1}{\sqrt{N/2}} \sum_k e^{-ik \cdot R} a_{\mu k} ,$$

$$b_{\mu R'} = \frac{1}{\sqrt{N/2}} \sum_k e^{ik \cdot R'} a'_{\mu k} ,$$

with $R$ and $R'$ on different sublattices, we use a (complex) Bogoliubov transformation

$$a_{\mu k} = e^{-i\varphi_k} \cosh \vartheta_k c_{\mu k} + \sinh \vartheta_k c_{\mu k}^\dagger ,$$

$$a'_{\mu k} = e^{-i\varphi_k} \cosh \vartheta_k c'_{\mu k} + \sinh \vartheta_k c'_{\mu k}^\dagger ,$$

to diagonalize the resulting Hamiltonian by choosing $\varphi_k$ and $\vartheta_k$ properly. This yields free bosons with dispersion relation

6
\[ \omega_k = \sqrt{(\lambda + 3J_2Q_2\gamma_{2,k})^2 - \frac{3}{2} J_1Q_1\gamma_{1,k}^2} , \]  

where the geometrical factors are given by

\[ \gamma_{1,k} = \frac{1}{3} \sum_{\alpha} e^{ik \cdot \alpha} , \]  
\[ \gamma_{2,k} = \frac{1}{3} \sum_{\beta} \cos(k \cdot \beta) . \]  

The mean-field equations are the minimization equations for the free energy:

\[ \int \frac{d^2k}{A} \cosh(2\vartheta_k)(n_k + \frac{1}{2}) - (S + \frac{1}{2}) = 0 , \]  
\[ \int \frac{d^2k}{A} \sinh(2\vartheta_k)|\gamma_{1,k}|(n_k + \frac{1}{2}) - \frac{1}{2} Q_1 = 0 , \]  
\[ \int \frac{d^2k}{A} \cosh(2\vartheta_k)\gamma_{2,k}(n_k + \frac{1}{2}) - \frac{1}{2} Q_2 = 0 , \]

with \( A = \frac{8\pi^2}{(3\sqrt{3})} \) the area of the reciprocal unit cell of a sublattice, \( n_k = [\exp(\beta \omega_k) - 1]^{-1} \) being the Bose occupation number and

\[ \tanh(2\vartheta_k) = \frac{\frac{3}{2} J_1Q_1|\gamma_{1,k}|}{\lambda + 3J_2Q_2\gamma_{2,k}} . \]  

Solving the mean-field equations yields values for \( Q_1, Q_2, \) and \( \lambda, \) and also the opportunity to determine thermodynamic quantities at finite temperatures.

In two dimensions there can be LRO only at zero temperature. This means that exactly at \( T = 0 \) there is an abrupt phase transition, and we must be careful when reducing \( T \) to zero. As the AF LRO corresponds to a condensation of the Schwinger bosons, we obtain the mean-field equations at \( T = 0 \) from Eqs. (13) by the replacement

\[ \frac{n_k}{\omega_k} \to S^*\delta^{(2)}(k) , \]

where \( S^* \) is a new unknown quantity measuring the Bose condensate. On the other hand, we can now determine \( \lambda \) from \( Q_1 \) and \( Q_2, \) as there is no gap in the spin-wave spectrum (\( \omega_{k=0} = 0 \) in (11)) at \( T = 0. \)
THERMODYNAMIC PARAMETERS

For small \( k \) the dispersion relation (11) takes a relativistic form: \( \omega_k = c\sqrt{(mc)^2 + |k|^2} \), with the spin-wave velocity \( c \) being

\[
c = \frac{3}{2} \sqrt{\frac{1}{2} J_1^2 Q_1^2 - 2J_2 Q_2 (\lambda + 3J_2 Q_2)} ,
\]

and a mass \( m \) in the energy gap \( \Delta = mc^2 \) of the spin-wave excitations:

\[
\Delta = mc^2 = \sqrt{(\lambda + 3J_2 Q_2)^2 - (\frac{3}{2} J_1 Q_1)^2} .
\]

We have calculated the spin-wave velocity \( c \) at \( T = 0 \) with the zero-temperature formalism and by extrapolation from finite \( T \). The results of the two methods are the same within the accuracy of the extrapolation, and they are shown in Fig. 3 together with the result for LSWT. Without frustration one can compare our result with the first-order SWT (FSWT) obtained from \( 1/S \)-corrections to LSWT. In fact, they give exactly the same result

\[
c = 1.2098417 * c_{LSWT} = 1.2832309 J_1 .
\]

Next we consider the gap, or the mass \( m \). As in the square case [1], without frustration it behaves like \( m \propto \exp(-\text{const}/T) \) as \( T \to 0 \). For fixed temperatures the mass (\( = \)the gap) varies along with frustration. As can be seen in Fig. 3, it increases nearly exponentially with frustration, in analogy with the square case.

Our last thermodynamic parameter is the uniform transverse susceptibility \( \chi_\perp \). To calculate this, we first obtain the rotational average \( \bar{\chi} \) at finite \( T \) from the static structure factor \( S_{xx}(q = 0, t = 0) \) by

\[
\bar{\chi} = \frac{1}{{k_B}T} S_{xx}(q = 0, t = 0) ,
\]

where

\[
S_{xx}(q = 0, t = 0) = \frac{2}{3} \int \frac{d^2k}{A} n_k (n_k + 1) .
\]
Here, the factor $\frac{2}{3}$ has been inserted on the right-hand side of \( (20) \) to make up for the mean-field treatment of the local constraints [7]. Second, we extrapolate $\bar{\chi}$ down to $T = 0$, and use that at $T = 0$ the longitudinal susceptibility $\chi_\parallel \equiv 0$, so that $\chi_\perp = \frac{2}{3} \bar{\chi}$. The result is shown in Fig. 4, where one can also see that the LSWT is independent of frustration. The extrapolation scheme reduces the precision of the $T = 0$ values. For a test, we have evaluated the exact SBMFT result at $T = 0$ with no frustration by using a formula obtained for the square lattice [9], with integrals calculated for the honeycomb lattice [4]. It reads

$$\chi_\perp = 0.3997332/6J_1,$$

(21)

to be compared with our extrapolation $\chi_\perp = (0.41\pm 0.01)/6J_1$. Two other results to compare with are the FSWT result [4] $\chi_\perp = 0.274/6J_1$ and the series result [5] $\chi_\perp = 0.454/6J_1$, which shows that the SBMFT gives a result close to the one obtained by a series expansion [5].

**STABILITY OF THE NÉEL STATE**

The classical Néel order vanishes as the frustration $\alpha \equiv J_2/J_1$ reaches the critical value $\alpha_{cl} = 1/6$, above which each triangular sublattice becomes ordered and totally decoupled from the other sublattice.

The LSWT correction to the classical Néel boundary for the square lattice was obtained by Chandra and Douçot [10] by finding the frustration at which the sublattice magnetization vanishes. A repetition of their calculation reduces the Néel stability also in the honeycomb case, as shown in Fig. 4. The square-case reduction was soon challenged by modified spin-wave theory calculations (a theory very similar to SBMFT) in Refs. [11] and by SBMFT results [12], which instead pointed to an increase of the Néel region. The discrepancy between SWT and SBMFT-like theories has later been argued to exist only in LSWT, and should vanish in FSWT through the cancellation of two logarithmic divergences [13–15]. Indeed, for large $S$, FSWT and SBMFT give the same magnetization [14]. There seems to be general consensus that for large $S$ there is a stabilization of Néel order beyond the classical Néel boundary: quantum fluctuations stabilize a state which is classically forbidden.
We have also calculated the Neel boundary by using our $T = 0$ mean-field equations. This was done by determining the frustration at which the Bose condensate amplitude $S^*$, and hence the sublattice magnetization, vanishes. This curve is also presented in Fig. 5. As in the square case, it is stabilized beyond the classical region, and enhances the Néel stability even for $S = \frac{1}{2}$. However, in this latter limit of $S = \frac{1}{2}$, the phase boundary obtained by the large-$S$ theories can be trusted less. The most extensive exact diagonalizations of the $J_1 - J_2$ model with extrapolations to the thermodynamic limit indeed reduces the Néel stability [16].

In another approach, we use a mapping to the nonlinear $\sigma$ model with quantum corrected thermodynamic parameters for the frustrated spin-$\frac{1}{2}$ antiferromagnet on a square lattice [17,8]. The method considerably reduces the Néel stability in that case. In Ref. [17] the formulas for the honeycomb lattice were also given, but at that time the quantum corrections were not known. Using the values obtained here, these formulas yield that already without frustration the bare coupling $\tilde{g}_0$ of the nonlinear $\sigma$ model exceeds the fixed point value $g_c$,$$
abla g_0 = (8\pi\sqrt{3})^{1/2} \frac{c_{\text{LSWT}}}{c_{\text{SBMFT}}} \chi_{\text{LSWT}} \approx 13.64 > g_c = 4\pi \approx 12.57 ,$$assuming the hydrodynamic relation $\rho = \chi c^2$. This means that the model is in its massive, disordered state, and that for $S = \frac{1}{2}$ there is no Néel order even without frustration. This result contradicts the ones obtained previously, and most likely this method underestimates the Néel stability. Therefore, the result obtained in Ref. [8] for the critical frustration on the square lattice is most probably too low as well, although we believe the tendency of a reduced Néel stability for $S = \frac{1}{2}$ to be valid both on the square and the honeycomb lattice.

To sum up, qualitatively SBMFT and LSWT give the same Néel boundaries as on the square lattice, while the effective-action method underestimates the Néel stability for $S = \frac{1}{2}$. For $S$ large, the SBMFT phase boundary probably can be trusted, but much work remains to be done to determine the disordered phase transition for the $S = \frac{1}{2}$ honeycomb antiferromagnet.
Finally we examine the spin dynamics by means of the dynamic structure factor $S(q, \omega)$. For $T \neq 0$ there is no LRO, but local Néel order still supports spin-waves with not too-long wavelengths. For finite temperatures, the structure factor is rotationally invariant and can be written as

$$S_{xx}(q, t) = \sum_{R, R'} e^{iq \cdot (R - R')} \langle S_R^x(t) S_{R'}^x(0) \rangle ,$$  \hspace{1cm} (23)$$

where $R$ and $R'$ run over all lattice sites. Notice that since $R - R'$ is not always a multiple of the lattice vectors $\beta$, this is not a spatial Fourier transform as it is for a Bravais lattice. The (time) Fourier transform is a sum of two terms

$$S_{xx}(q, \omega) = \int dt \ e^{i\omega t} S_{xx}(q, t) = S_1(q, \omega) + S_2(q, \omega) ,$$  \hspace{1cm} (24)$$

which evaluate to

$$S_1(q, \omega) = \frac{1}{2} \int \frac{d^2k}{A} \frac{(f_{k,k+q} + 1)}{2} n_k(n_{k+q} + 1) \delta(\omega_k - \omega_{k+q} + \omega) ,$$  \hspace{1cm} (25a)$$

$$S_2(q, \omega) = \frac{1}{4} \int \frac{d^2k}{A} \frac{(f_{k,k+q} - 1)}{2} (n_k + \Theta(\omega))(n_{k+q} + \Theta(\omega)) \delta(\omega_k + \omega_{k+q} - |\omega|) ,$$  \hspace{1cm} (25b)$$

where

$$f_{k,k+q} = \cosh(2\vartheta_k) \cosh(2\vartheta_{k+q}) - \cos(\varphi_k - \varphi_{k+q}) \sinh(2\vartheta_k) \sinh(2\vartheta_{k+q}) ,$$  \hspace{1cm} (26)$$

$\Theta(\omega)$ is the Heavyside step function, and $\varphi_k$ is the phase of $\gamma_{1,k}$. The non-Bravais character of the honeycomb lattice is reflected by the non-zero value of $\varphi_k$.

The two terms $S_1$ and $S_2$ correspond to different physical processes and give rise to two distinct peaks in the structure factor. In neutron-scattering terms, the first term $S_1$ describes a simple scattering process of a neutron against a spin-wave, while the other term, $S_2$, corresponds to a scattering process where two spin waves are created or annihilated. (However, this double-peak structure may be difficult to resolve experimentally at low temperatures. At higher temperatures the $S_2$ peak may be too small and smeared out to be detected.)
Our results are presented in two series of plots in Figs. 6 and 7 for $q$ close and parallel to the Néel ordering vector

$$q_0 = \left(\frac{2\pi}{\sqrt{3}}, \frac{2\pi}{3}\right).$$  

(Compare with plots for the square case in Ref. [12].) All (but one) contain two “peaks”, where one stems from $S_1$ and the other from $S_2$ as indicated in Fig. 6a.

In Fig. 6, $T = \frac{1}{5}J_1$ (constant) and we vary frustration (6a: $J_2/J_1 = 0$ and 6b: $J_2/J_1 = 0.1 < \text{critical frustration}$). Near the ordering vector we get “overdamped” spin-waves that turn into a magnetic Bragg peak as $T$ is lowered. Outside this region, we have the normal spin-wave dispersion ($S \propto \delta(\omega - c|q|)$). Note that $S_2$ has a small gap in the dispersion. (It is actually a double gap, as two spin waves are created.) The gap increases along with frustration, as can be seen when comparing Figs. 6a and 6b. (The increase of the gap with frustration has also been depicted in Fig. 3.) Above the gap, SWT-type dispersion is back to normal.

In Fig. 7, $J_2/J_1 = 0.22 > \text{the critical frustration}$. Being on the disordered side of the critical frustration, there is no Bragg peak at $T = 0$. This remedies the divergencies in the structure factor and makes it possible to calculate the structure factor at zero temperature within our formalism. In Fig. 7a the results for $T = 0$ are shown. Here, the $S_1$-peak has vanished since there are no thermally excited spin-waves to scatter against. The $S_2$ process still gives a peak due to creation of spin-wave pairs. At a temperature increase, the $S_1$ peak reappears as can be seen in Fig. 7b.

**CONCLUSIONS**

SBMFT works well for calculating thermodynamic properties for the Heisenberg antiferromagnet on a honeycomb lattice, although this is not a Bravais lattice. For $S = \frac{1}{2}$, the spin-wave velocity and the transverse susceptibility both decrease slowly with frustration, while the excitation gap grows nearly exponentially with increasing frustration. For large $S$
AF LRO is found to be stabilized beyond the classical boundary. The case of small $S$ calls for further investigation. Finally, the dynamic structure factor shows a double-peak structure with a gap for finite temperatures. In general, the qualitative behavior is the same as for the square lattice.

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FIGURES

FIG. 1. Honeycomb lattice with one of the two triangular sublattices marked. The vectors $\alpha$ and $\beta$ point to the nearest neighbors and half the number of second-nearest neighbors of a site, respectively.

FIG. 2. The $T = 0$ spin-wave velocity vs frustration $J_2/J_1$ for $S = \frac{1}{2}$. The full line shows the SBMFT result and the dashed line the LSWT result.

FIG. 3. The logarithm of the mass vs frustration for SBMFT at temperature $T = \frac{1}{5}J_1$ and $S = \frac{1}{2}$.

FIG. 4. The $T = 0$ uniform transverse susceptibility vs frustration for $S = \frac{1}{2}$. The full and dashed lines correspond to SBMFT and LSWT, respectively.

FIG. 5. The inverse of the critical spin $S_c$ as a function of frustration. The lines show the LSWT and the SBMFT result. They coincide for $J_2 = 0$ and for $J_2/J_1 = 1/6$ at the classical point $S = \infty$. Note the Néel stability beyond the classical value in the SBMFT case.

FIG. 6. The dynamic structure factor at a low temperature $T = \frac{1}{5}J_1$ close to the ordering vector $q_0$. In (a) the frustration is $J_2/J_1 = 0$, and in (b) it is $J_2/J_1 = 0.1 < \text{critical frustration}$. The peak corresponding to $S_2$ has a gap (starts at finite $\omega$) which increases with frustration.

FIG. 7. The dynamic structure factor for $J_2/J_1 = 0.22$, which is a value above the critical frustration. In (a) the result for $T = 0$ is shown, while in (b) we have $T = \frac{1}{20}J_1$. Note that the $S_1$ peak has vanished in (a) due to the lack of thermally excited spin waves.