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Study of the bilinear biquadratic Heisenberg model on a honeycomb lattice via Schwinger bosons

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ABSTRACT

We analyze the biquadratic bilinear Heisenberg magnet on a honeycomb lattice via Schwinger boson formalism. Due to their vulnerability to quantum fluctuations, non-conventional lattices (kagome, triangular and honeycomb for example) have been cited as candidates to support spin liquid states. Such states without long range order at zero temperature are known in one-dimensional spin models but their existence in higher dimensional systems is still under debate. Biquadratic interaction is responsible for various possibilities and phases as it is well-founded for one-dimensional systems. Here we have used a bosonic representation to study the properties at zero and finite low temperatures of the biquadratic term in the two-dimensional hexagonal honeycomb lattice. The results show an ordered state at zero temperature but much more fragile than that of a square lattice; the behavior at finite low temperatures is in accordance with expectations.

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1. Introduction

Non-conventional lattices in magnetic systems have received much attention in recent years. Traditional square lattices are well established and no surprises are expected. On the other hand, the non-conventional lattices are serious candidates to the so-called two-dimensional spin liquid phase. Spin liquids are disordered states of matter with power-law decay of spin–spin correlations and zero local magnetic moment. Such properties occur at zero temperature and the disorder is derived from quantum and not thermal fluctuations. These phases are known to exist in one-dimensional antiferromagnets but they still remain uncertain in higher dimensions. Most known two-dimensional ($2D$) magnetic materials have a Néel order at zero temperature ($T=0$) even though some unusual systems may be considered as candidates to present a spin liquid behavior. In three-dimensional magnetic systems, the existence of this state is even more unexpected due to stronger spin interactions.

One possible way to obtain a $2D$ spin liquid is through the presence of geometric frustration in some lattices. In the classical antiferromagnetic kagomé lattice, for example, it is impossible to align all neighbors spins and the ground state is highly degenerate. In addition, anisotropies together with longer range interactions (second and far nearest neighbors) contribute to disorder the

ground state, increasing the possibility of a spin liquid state. Although the properties at zero temperature are questionable, recent works indicate the occurrence of spin liquid states [1–9]. Even lattices without frustration have shown interesting possibilities as it is the case of hexagonal honeycomb lattice. The honeycomb is the two-dimensional lattice with the smallest coordination number (neighbors number) $z=3$. It is between the disordered one dimensional spin model with $z=2$ and the ordered (at zero temperature) square lattice with $z=4$. Thus, such a system may have larger vulnerability to quantum fluctuations, mainly for small spins, and it is a possible candidate to be a two-dimensional spin liquid. Nevertheless, recent works have shown a Néel order for the spin-1/2 Heisenberg antiferromagnet (AF) on honeycomb lattice [9,10], although weaker than the square lattice case. Furthermore, frustrated honeycomb models have revealed disordered ground states [12–16].

In the present work we are interested in the behavior of the biquadratic bilinear Heisenberg AF model in a hexagonal honeycomb lattice. It is well known that the Heisenberg Hamiltonian is one of the simplest model able to describe both the ferromagnetic and antiferromagnetic materials in any dimension. Here, in addition to the usual Heisenberg model, we consider a biquadratic term in such a way that the complete Hamiltonian is given by

$$H = \sum_{\langle i,j \rangle} [J_1(\mathbf{S}_i \cdot \mathbf{S}_j) + J_2(\mathbf{S}_i \cdot \mathbf{S}_j)^2], \tag{1}$$

where the sum is over nearest neighbors and the constants J_1 and J_2 define the bilinear and biquadratic couplings, respectively. It is important to highlight that we adopt $S=1$ once the biquadratic

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term makes sense only for $S > 1/2$. The $SU(2)$ spin rotation symmetry in Hamiltonian (1) is preserved and so we can expect Goldstone modes as lower energy excitations over the ground state. We consider the case $J_1 = 1$ (antiferromagnetic coupling) and $-J_1 \leq J_2 \leq J_1$ but it is also common to write $J_1 = \cos\theta$ and $J_2 = \sin\theta$. The one-dimensional case is well documented [17–19] and the various phases were already discovered. For $\theta = \pi$ one has the usual ferromagnet, while $\theta = 0$ corresponds to the usual Heisenberg antiferromagnetic system. In the range $\pi < \theta < 5\pi/4$, there is a stable ferromagnetic regime with long range order (LRO); for $-\pi/4 < \theta < \pi/4$ there is an antiferromagnetic phase with Haldane gap (spin-1) and, in the limit $\pi/4 < \theta < \pi/2$, there is a trimerized phase. Some points have exact solutions. For instance, the angles $\theta = \pm\pi/4$ can be solved by the Bethe ansatz and besides, the angle $\tan\theta = 1/3$ corresponds to AKLT Model. The two-dimensional case is more complicated and only some regions are known. Ivanov et al. [20,21] have shown a nematic phase for $\theta \gtrsim 5\pi/4$ by using a continuous model similar to the $O(3)$ nonlinear Sigma Model (the same result has been achieved by Chubukov using the Holstein–Primakoff representation [16]); for $5\pi/5 < \theta < 7\pi/4$ there is a dimerized ferromagnetic phase.

We can represent the biquadratic term as a function of spin and quadrupole operators (second-order spin moment)

$$(\mathbf{S}_i \cdot \mathbf{S}_j)^2 = \tfrac{1}{2}(\mathbf{Q}_i \cdot \mathbf{Q}_j) - \tfrac{1}{2}(\mathbf{S}_i \cdot \mathbf{S}_j) + \tfrac{4}{3}, \tag{2}$$

where Q_i operators are given by

$$Q_i^{(0)} = \frac{2(S_i^z)^2 - (S_i^x)^2 - (S_i^y)^2}{\sqrt{3}}, \tag{3}$$

$$Q_i^{(2)} = (S_i^x)^2 - (S_i^y)^2, \tag{4}$$

$$Q_i^{xy} = S_i^x S_i^y + S_i^y S_i^x, \tag{5}$$

$$Q_i^{yz} = S_i^y S_i^z + S_i^y S_i^z, \tag{6}$$

$$Q_i^{zx} = S_i^z S_i^x + S_i^x S_i^z. \tag{7}$$

The three spin operators together the five quadrupole operators form the generators of the $SU(3)$ Lie group. For the special case $J_1 = J_2$ one has the $SU(3)$ symmetric ferromagnetic model [22] while for $J_1 = 0$ one has the $SU(3)$ symmetric valence-bound antiferromagnet [23–25].

The usual methods applied to study systems in condensed matter physics are vast and diversified. In the current work we have adopted the Schwinger boson representation to develop the physics of the bilinear biquadratic Heisenberg model in a honeycomb lattice at both zero and low temperatures. The Schwinger formalism has some advantages over other bosonic representations (such as Holstein–Primakoff and Dyson–Maleev). Firstly, the holonomic constraint that fix the number of bosons can be implemented easily by a Lagrange multiplier. Secondly, there are not root terms and so we do not need to specify a preferential direction to the ground state as occur for the Holstein–Primakoff method. Therefore we are able to treat ordered and disordered phases, which are important in the search for a possible spin liquid state. Following the usual prospects, we have adopted the boson condensation at zero temperature to avoid the divergences of the theory and at low temperatures we have used approximations that, within the correct limits, provide coherent results. The paper is organized as follow: in Section 2 we developed the Schwinger bosons formalism; in Section 3, we present the results for zero temperature and finite low temperatures and, finally, the conclusions are exposed in the last Section 4.

2. Formalism

Commonly, the spin operators are defined by two $SU(2)$ Schwinger operators but, because the biquadratic term, we have considered the representation by $SU(3)$ Schwinger formalism. Thus, each spin operator is represented by three bosonic operators $a_{i,m}$, where i denotes the lattice sites and $m = -1, 0, 1$ specifies the eigenvalues of S_i^z. Accordingly, $a_{i,m}^\dagger|0\rangle$ creates a particle with z-component of spin ($S^z = m$) on site i (we denote the $|0\rangle$ state as the vacuum of the Fock space). The generators $F_i^{mn} = a_{i,m}^\dagger a_{i,n}$ form the $SU(3)$ Lie algebra and they obey the commutation relation $[F_i^{mn}, F_j^{pq}] = \delta_{i,j}(\delta_{n,p}F_i^{mq} - \delta_{m,p}F_i^{nq})$. As a function of the a operators, the spin operators are expressed by $S_i^+ = \sqrt{2}(a_{i,0}^\dagger a_{i,-1} + a_{i,1}^\dagger a_{i,0})$, $S_i^- = \sqrt{2}(a_{i,-1}^\dagger a_{i,0} + a_{i,0}^\dagger a_{i,1})$ and $S_i^z = a_{i,1}^\dagger a_{i,1} - a_{i,-1}^\dagger a_{i,-1}$. The bosonic operators keep the spin commutation relation and to fix $S_i^2 = S(S+1)$ we have to impose the local constraint $\sum_m a_{i,m}^\dagger a_{i,m} = S$. In order to symmetrize the spin and quadrupole operators, we apply a rotation over the a operators defining new operators b as follow:

$$b_{i1} = \frac{1}{\sqrt{2}}(a_{i,-1} - a_{i,1}), \tag{8}$$

$$b_{i2} = \frac{-i}{\sqrt{2}}(a_{i,-1} + a_{i,1}), \tag{9}$$

$$b_{i3} = a_{i,0}. \tag{10}$$

Therefore, the spin operators are written as

$$S_i^x = -i(b_{i2}^\dagger b_{i3} - b_{i3}^\dagger b_{i2}), \tag{11}$$

$$S_i^y = -i(b_{i3}^\dagger b_{i1} - b_{i1}^\dagger b_{i3}), \tag{12}$$

$$S_i^z = -i(b_{i1}^\dagger b_{i2} - b_{i2}^\dagger b_{i1}), \tag{13}$$

and the quadrupoles become

$$Q_i^{(0)} = \frac{1}{\sqrt{3}}(b_{i1}^\dagger b_{i1} + b_{i2}^\dagger b_{i2} - 2b_{i3}^\dagger b_{i3}), \tag{14}$$

$$Q_i^{(2)} = -(b_{i1}^\dagger b_{i1} - b_{i2}^\dagger b_{i2}), \tag{15}$$

$$Q_i^{xy} = -(b_{i1}^\dagger b_{i2} + b_{i2}^\dagger b_{i1}), \tag{16}$$

$$Q_i^{yz} = -(b_{i2}^\dagger b_{i3} + b_{i3}^\dagger b_{i2}), \tag{17}$$

$$Q_i^{zx} = -(b_{i3}^\dagger b_{i1} + b_{i1}^\dagger b_{i3}), \tag{18}$$

while the constraint holds the same. The biquadratic bilinear Heisenberg Hamiltonian as a function of b operators is expressed by

$$H = \sum_{\langle i,j \rangle} [(J_2 - J_1)\mathcal{A}_{ij}^\dagger \mathcal{A}_{ij} + J_1 : \mathcal{B}_{ij}^\dagger \mathcal{B}_{ij} :], \tag{19}$$

where we have introduced the bond operators $\mathcal{A}_{ij} = \sum_\mu b_{i\mu}b_{j\mu}$ and $\mathcal{B}_{ij} = \sum_\mu b_{i\mu}^\dagger b_{j\mu}$; the two points denote normal ordering and $\mu = 1, 2, 3$ (distinct from the index $m = -1, 0, 1$). The Hamiltonian is fourth order in b and we decouple it by the Hubbard–Stratonovich transform [26,27]

$$\Xi_{ij}^\dagger \Xi_{ij} \rightarrow \langle \Xi_{ij}^\dagger \rangle \Xi_{ij} + \langle \Xi_{ij} \rangle \Xi_{ij}^\dagger - \langle \Xi_{ij}^\dagger \rangle \langle \Xi_{ij} \rangle. \tag{20}$$

In above equation $\Xi_{ij} = \mathcal{A}_{ij}, \mathcal{B}_{ij}$, where we have adopted the mean field $A = \langle \mathcal{A}_{ij}^\dagger \rangle = \langle \mathcal{A}_{ij} \rangle$ and $B = \langle \mathcal{B}_{ij}^\dagger \rangle = \langle \mathcal{B}_{ij} \rangle$. Therefore, the second order mean field Hamiltonian is given by

$$H^{MF} = -\frac{3N}{2}[(J_2 - J_1)A^2 + J_1 B^2] - NS\lambda + \lambda \sum_{i\mu} b_{i\mu}^\dagger b_{i\mu}$$
$$+ \sum_{\langle i,j \rangle}[(J_2 - J_1)A(\mathcal{A}_{ij}^\dagger + \mathcal{A}_{ij}) + J_1 B(\mathcal{B}_{ij}^\dagger + \mathcal{B}_{ij})]. \tag{21}$$

The constraint $\sum_\mu b_{i\mu}^\dagger b_{i\mu} = S$ is implemented by a Lagrange multiplier λ_i on each site and we have adopted a constant mean field value $\lambda = \langle \lambda_i \rangle$. The λ parameter is similar to the chemical potential μ while the constraint $\sum_\mu b_{i\mu}^\dagger b_{i\mu} = S$ counts the bosons number on each site. The mean field values A, B and λ are determined by minimizing the Helmholtz free energy.

The honeycomb is a bipartite but not a Bravais lattice and so we have to treat each sublattice separately. The sublattices R and R' are hexagonal Bravais lattices and they are coupled by nearest neighbors interactions. After the Fourier transformation of the Schwinger bosons independently on each sublattice, we obtain

$$b_{i\mu} = \sqrt{\frac{2}{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_i} b_{\mathbf{k}\mu}, \quad i \in R \tag{22}$$

and

$$b_{j\mu} = \sqrt{\frac{2}{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_j} b'_{\mathbf{k}\mu}, \quad j \in R', \tag{23}$$

the Hamiltonian is written as

$$H^{\mathrm{MF}} = H_0 + \frac{1}{2} \sum_{\mathbf{k}} \sum_{\mu} [3(J_2 - J_1)A(b_{\mathbf{k}\mu}^\dagger b_{-\mathbf{k}\mu}^\dagger \gamma_{\mathbf{k}} + b_{\mathbf{k}\mu}'^\dagger b_{-\mathbf{k}\mu}^\dagger \gamma_{\mathbf{k}}^*)$$
$$+ 3J_1 B(b_{\mathbf{k}\mu}^\dagger b'_{\mathbf{k}\mu} \gamma_{\mathbf{k}} + b_{\mathbf{k}\mu}'^\dagger b_{\mathbf{k}\mu} \gamma_{\mathbf{k}}^*) + \lambda(b_{\mathbf{k}\mu}^\dagger b_{\mathbf{k}\mu} + b_{\mathbf{k}\mu}'^\dagger b'_{\mathbf{k}\mu}) + h.c.], \tag{24}$$

where $H_0 = -(3N/2)[(J_2 - J_1)A^2 + J_1 B^2] - NS\lambda$ are constant terms and $\gamma_{\mathbf{k}} = e^{i\varphi_{\mathbf{k}}}|\gamma_{\mathbf{k}}|$ is the structure factor

$$\gamma_{\mathbf{k}} = \frac{1}{3}\left[2\cos\frac{k_x}{2}\cos\frac{\sqrt{3}k_y}{2} + \cos k_x + 2i\sin\frac{k_x}{2}\cos\frac{\sqrt{3}k_y}{2} - i\sin k_x\right]. \tag{25}$$

In Hamiltonian (24), the two sublattices are still coupled and differently from the square lattice, the structure factor for honeycomb lattice is not real. We solve these two difficulties defining new operators $b_{\mathbf{k}\mu} = (e^{i\varphi_{\mathbf{k}}/2}/\sqrt{2})(ic_{\mathbf{k}\mu}^I + c_{\mathbf{k}\mu}^{II})$ and $b'_{\mathbf{k}\mu} = (e^{-i\varphi_{\mathbf{k}}/2}/\sqrt{2})(-ic_{\mathbf{k}\mu}^I + c_{\mathbf{k}\mu}^{II})$. The new bosons $c_{\mathbf{k}}$ satisfy all commutation relations and the Hamiltonian is written as

$$H^{\mathrm{MF}} = H_0 + \frac{1}{2}\sum_{\mathbf{k}} \beta_{\mathbf{k}}^{I\dagger} \tilde{H}^I \beta_{\mathbf{k}}^I + \frac{1}{2}\sum_{\mathbf{k}} \beta_{\mathbf{k}}^{II\dagger} \tilde{H}^{II} \beta_{\mathbf{k}}^{II}, \tag{26}$$

with $\beta_{\mathbf{k}}^{s\dagger} = (c_{\mathbf{k}1}^{s\dagger}, c_{\mathbf{k}2}^{s\dagger}, c_{\mathbf{k}3}^{s\dagger}, c_{-\mathbf{k}1}^s, c_{-\mathbf{k}2}^s, c_{-\mathbf{k}3}^s)$, where $s = I, II$, while the matrices are $\tilde{H}^I = (\lambda - 3J_1 B|\gamma_{\mathbf{k}}|)\sigma_0 \otimes I_{3\times 3} + 3(J_2 - J_1)A|\gamma_{\mathbf{k}}|\sigma_x \otimes I_{3\times 3}$ and $\tilde{H}^{II} = (\lambda + 3J_1 B|\gamma_{\mathbf{k}}|)\sigma_0 \otimes I_{3\times 3} + 3(J_2 - J_1)A|\gamma_{\mathbf{k}}|\sigma_x \otimes I_{3\times 3}$ (here σ_i are the Pauli matrices). H^{MF} can be diagonalized by a canonical Bogoliubov transformation

$$c_{\mathbf{k}\mu}^I = \cosh\theta_{\mathbf{k}}^I \alpha_{\mathbf{k}\mu}^I + \sinh\theta_{\mathbf{k}}^I \alpha_{-\mathbf{k}\mu}^{I\dagger} \tag{27}$$

$$c_{\mathbf{k}\mu}^{II} = \cosh\theta_{\mathbf{k}}^{II} \alpha_{\mathbf{k}\mu}^{II} + \sinh\theta_{\mathbf{k}}^{II} \alpha_{-\mathbf{k}\mu}^{II\dagger}. \tag{28}$$

We choose $\theta_{\mathbf{k}}^I$ and $\theta_{\mathbf{k}}^{II}$ so that the non-diagonal terms vanish. It is achieved by

$$\tanh 2\theta_{\mathbf{k}}^I = -\frac{\lambda - 3J_1 B|\gamma_{\mathbf{k}}|}{3(J_2 - J_1)A|\gamma_{\mathbf{k}}|}, \tag{29}$$

$$\tanh 2\theta_{\mathbf{k}}^{II} = -\frac{\lambda + 3J_1 B|\gamma_{\mathbf{k}}|}{3(J_2 - J_1)A|\gamma_{\mathbf{k}}|}. \tag{30}$$

Once diagonalized, H^{MF} gives the eigenvalues of energy

$$E_I = \sqrt{(\lambda - 3J_1 B|\gamma_{\mathbf{k}}|)^2 - (3A(J_2 - J_1)|\gamma_{\mathbf{k}}|)^2} \tag{31}$$

$$E_{II} = \sqrt{(\lambda + 3J_1 B|\gamma_{\mathbf{k}}|)^2 - (3A(J_2 - J_1)|\gamma_{\mathbf{k}}|)^2}. \tag{32}$$

The mean field equations are $\partial F/\partial A$, $\partial F/\partial B$ and $\partial F/\partial \lambda$, where the Helmholtz free energy F is

$$F = H_0 + \frac{3}{\beta}\sum_{\mathbf{k}}\left\{\ln\left[\sinh\left(\frac{\beta E_I}{2}\right)\right] + \ln\left[\sinh\left(\frac{\beta E_{II}}{2}\right)\right]\right\}, \tag{33}$$

yielding the integral self-consistent equations

$$S + \frac{3}{2} = \frac{3}{2N}\sum_{\mathbf{k}}\left[\coth\left(\frac{\beta E_I}{2}\right)\frac{\lambda - 3J_1 B|\gamma_{\mathbf{k}}|}{E_I} + \coth\left(\frac{\beta E_{II}}{2}\right)\frac{\lambda + 3J_1 B|\gamma_{\mathbf{k}}|}{E_{II}}\right], \tag{34}$$

$$A = -\frac{3}{2N}\sum_{\mathbf{k}}\left[\coth\left(\frac{\beta E_I}{2}\right)\frac{3A(J_2 - J_1)}{E_I} + \coth\left(\frac{\beta E_{II}}{2}\right)\frac{3A(J_2 - J_1)}{E_{II}}\right]|\gamma_{\mathbf{k}}|^2 \tag{35}$$

and

$$B = \frac{3}{2N}\sum_{\mathbf{k}}\left[\coth\left(\frac{\beta E_{II}}{2}\right)\frac{\lambda + 3J_1 B|\gamma_{\mathbf{k}}|}{E_{II}} - \coth\left(\frac{\beta E_I}{2}\right)\frac{\lambda - 3J_1 B|\gamma_{\mathbf{k}}|}{E_I}\right]|\gamma_{\mathbf{k}}|. \tag{36}$$

As it is well known, one- and two-dimensional systems can have LRO only at zero temperature and this implies an abrupt change at $T = 0$. Indeed, when the temperature approaches absolute zero, the bosons condensate at a zero energy state and the self-consistent equations diverge. This inconvenience is surmounted by separating the divergent term of the sum and introducing a new parameter (the condensate density) as it is done in the Bose-Einstein condensate. For finite temperatures such problem does not exist and the equations can be solved customarily. Obviously, the self-consistent equation cannot be solved exactly and numeric methods or approximations are usually applied. In the next section we will present the results for both $T = 0$ and low finite temperatures.

Using Eqs. (27) and (28), we calculate the mean field double boson operators

$$\langle b_{i\mu}^\dagger b_{j\mu}\rangle = \frac{1}{N}\sum_{\mathbf{k}} e^{-i\mathbf{k}\Delta\mathbf{r}}\left[\cosh 2\theta_{\mathbf{k}}^I\left(n_{\mathbf{k}}^I + \frac{1}{2}\right) + \cosh 2\theta_{\mathbf{k}}^{II}\left(n_{\mathbf{k}}^{II} + \frac{1}{2}\right)\right] - \frac{1}{2}\delta_{ij} \tag{37}$$

$$\langle b_{i\mu} b_{j\mu}\rangle = \frac{1}{N}\sum_{\mathbf{k}} e^{-i\mathbf{k}\Delta\mathbf{r}}\left[-\sinh 2\theta_{\mathbf{k}}^I\left(n_{\mathbf{k}}^I + \frac{1}{2}\right) + \sinh 2\theta_{\mathbf{k}}^{II}\left(n_{\mathbf{k}}^{II} + \frac{1}{2}\right)\right] \tag{38}$$

for i and j belonging to the same sublattice and

$$\langle b_{i\mu}^\dagger b_{j\mu}\rangle = \frac{1}{N}\sum_{\mathbf{k}} e^{-i\mathbf{k}\Delta\mathbf{r}} e^{-i\varphi_{\mathbf{k}}}\left[-\cosh 2\theta_{\mathbf{k}}^I\left(n_{\mathbf{k}}^I + \frac{1}{2}\right) + \cosh 2\theta_{\mathbf{k}}^{II}\left(n_{\mathbf{k}}^{II} + \frac{1}{2}\right)\right] \tag{39}$$

$$\langle b_{i\mu} b_{j\mu}\rangle = \frac{1}{N}\sum_{\mathbf{k}} e^{-i\mathbf{k}\Delta\mathbf{r}} e^{-i\varphi_{\mathbf{k}}}\left[\sinh 2\theta_{\mathbf{k}}^I\left(n_{\mathbf{k}}^I + \frac{1}{2}\right) + \sinh 2\theta_{\mathbf{k}}^{II}\left(n_{\mathbf{k}}^{II} + \frac{1}{2}\right)\right] \tag{40}$$

for i and j in different sublattices. The phase angle $\varphi_{\mathbf{k}}$ is the same as that which appears in the structure factor (Eq. (25)), whilst the boson densities are given by

$$n_{\mathbf{k}}^t = \langle \alpha_{\mathbf{k}\mu}^{t\dagger} \alpha_{\mathbf{k}\mu}^t \rangle = \frac{1}{e^{\beta E_t} - 1} \tag{41}$$

with $t = I, II$. All others mean field quantities are null.

3. Results

When the temperature decreases to zero, a phase transition takes place and one of the energies of the spectrum vanishes, characterizing a boson condensation. Therefore, the self-consistent equations diverge and there are not more solutions for the

parameters A, B and λ. According to Takahashi and Arovas [28–31], the non-existence of solutions is related to a spontaneous broken symmetry, since Schwinger formalism is invariant over $SU(2)$. At finite temperatures, there are solutions for any dimension and the system is disordered, i.e., there is not long range order (at zero temperature, there are solutions only for the one-dimensional case). Here, the condensation occurs for E_I if $J_1 > 0$ and E_{II} otherwise. The ground state is therefore ordered and the lowest excitation energies are the massless Goldstone modes. Expanding for small k, the dispersion relations (31) and (32) assume a relativist form

$$E_I = \sqrt{\Delta_I^2 + \mathbf{k}^2 c_I^2} \quad \text{and} \quad E_{II} = \sqrt{\Delta_{II}^2 + \mathbf{k}^2 c_{II}^2}, \tag{42}$$

with the gap energies

$$\Delta_I = \sqrt{(\lambda - 3J_1 B)^2 - (3(J_1 - J_2)A)^2}, \tag{43}$$

$$\Delta_{II} = \sqrt{(\lambda + 3J_1 B)^2 - (3(J_1 - J_2)A)^2}, \tag{44}$$

while the spin-wave velocities are given by

$$c_1 = \sqrt{\frac{1}{2}(3J_1 B - 9J_1^2 B^2 + 9(J_1 - J_2)^2 A^2)}, \tag{45}$$

$$c_2 = \sqrt{\frac{1}{2}(-3J_1 B - 9J_1^2 B^2 + 9(J_1 - J_2)^2 A^2)}. \tag{46}$$

The spin-wave velocities as a function of J_2 ($J_1 = 1$) are plotted in Fig. 1. A similar behavior is observed for the frustrated honeycomb Heisenberg system [12], where there is a linear decreasing of the spin-wave velocity as a function of the second-nearest neighbors exchange coupling. For $J_2 \geq 0.65$, the c_2 spin-wave velocity is null whilst the point where $c_1 = 0$ is beyond the limits considered.

Considering positive values of J_1, the condensation occurs for E_I and then $\Delta_I = 0$ while Δ_{II} is finite. After separating the divergent terms, the self-consistent equations are written in the continuous limit as

$$\rho = \left(S + \frac{3}{2}\right) - \frac{3}{2} \int \frac{d^2 \mathbf{k}}{2\sigma} \left[\frac{\lambda - 3J_1 B|\gamma_{\mathbf{k}}|}{E_I} + \frac{\lambda + 3J_1 B|\gamma_{\mathbf{k}}|}{E_{II}}\right], \tag{47}$$

$$A = \rho - \frac{3}{2} \int \frac{d^2 \mathbf{k}}{2\sigma} \left[\frac{3A(J_2 - J_1)|\gamma_{\mathbf{k}}|^2}{E_I} + \frac{3A(J_2 - J_1)|\gamma_{\mathbf{k}}|^2}{E_{II}}\right] \tag{48}$$

and

$$B = -\rho + \frac{3}{2} \int \frac{d^2 \mathbf{k}}{2\sigma} \left[-\frac{(\lambda - 3J_1 B|\gamma_{\mathbf{k}}|)|\gamma_{\mathbf{k}}|}{E_I} + \frac{(\lambda + 3J_1 B|\gamma_{\mathbf{k}}|)|\gamma_{\mathbf{k}}|}{E_{II}}\right], \tag{49}$$

where ρ is a new parameter that measures the boson condensate and $\sigma = 8\pi/3\sqrt{3}$ is the first Brillouin zone area.
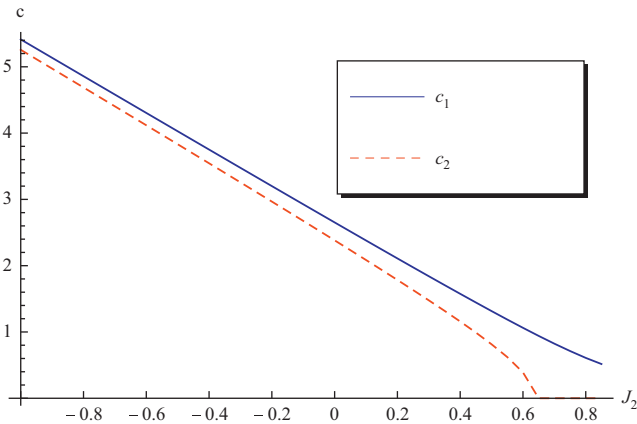
Fig. 1. Almost linear decreasing behavior of spin-wave velocities c_1 and c_2.
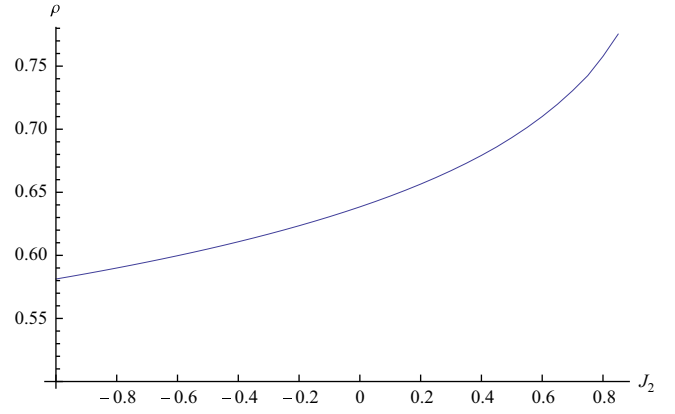
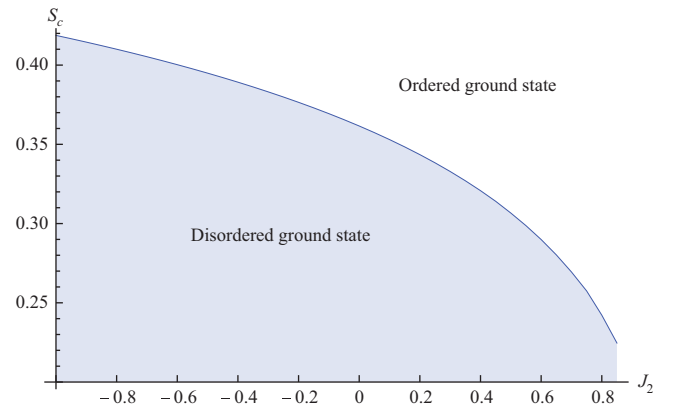**Fig. 2.** The boson density condensate as a function of J_2.

Fig. 3. The critical spin value separates the region with an ordered ground state from that with a disordered ground state.

The condensate density is plotted in Fig. 2. For $J_2 = 0$ we have the pure Heisenberg antiferromagnet, in which the condensate density is approximately 0.64. As expected, ρ is smaller than the corresponding one for the square lattice (approximately 80% smaller [31]). The condensate density increases as J_2 increases (with an almost linear behavior in the range $-1 \leq J_2 \leq 0.2$). Comparing with the spin-wave velocity graphics in Fig. 1 we can see that the increasing condensate density (and consequently the ordering) occurs together a decreasing of the spin-wave velocities. This is expected since the spin-wave is responsible for disordering the ground state and then, a larger velocity implies in higher disorder. Therefore the honeycomb lattice holds a long range order at $T=0$ but due to the small coordination number this ordering is weaker than that of the square lattice case.

As it is well known, the two-dimensional square lattice presents LRO for all spin values $S > S_c \approx 0.19$. Writing the magnetization as $m_s = S + \frac{3}{2} - \frac{3}{2} \int \left(\frac{\lambda - 3J_1 B}{E_I} + \frac{\lambda + 3J_1 B}{E_{II}}\right) \frac{d^2 \mathbf{k}}{2\sigma}$ we determine the critical value of the spin S_c for which $m_s \to 0$ for the honeycomb lattice. The results are shown in Fig. 3. The S_c curve separates the region with an ordered ground state from the one with a disordered ground state. Similar to the square lattice case, on the honeycomb lattice the disordered ground state is inaccessible to all physical values of spins. Using Eqs. (37) and (38) we obtain the mean value $\langle \mathbf{S}_i \cdot \mathbf{S}_i \rangle \approx 2.5$ for all values of J_2. It is greater than the expected value $S(S+1)=2$ by a factor of approximately 3/2. Such factor also appears in the equations obtained by Arovas and Auerbach [29] and this discrepancy arises because we imposed the constraint only on the average. The problem can be solved through a pertubative expansion in low order. The Fourier

transform $S(\mathbf{q})$ of the two-point function $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ is as follow:

$$S(\mathbf{q}) = -\frac{6}{4} + \frac{3}{N} \sum_{\mathbf{k}} \left\{ \left[\cosh(2\theta_{\mathbf{k}+\mathbf{q}}^I - 2\theta_{\mathbf{k}}^I) \left(n_{\mathbf{k}+\mathbf{q}}^I + \frac{1}{2} \right) \left(n_{\mathbf{k}}^I + \frac{1}{2} \right) \right. \right.$$
$$+ \cosh(2\theta_{\mathbf{k}+\mathbf{q}}^{II} - 2\theta_{\mathbf{k}}^{II}) \left(n_{\mathbf{k}+\mathbf{q}}^{II} + \frac{1}{2} \right) \left(n_{\mathbf{k}}^{II} + \frac{1}{2} \right) \left] [1 + e^{\varphi_{\mathbf{k}+\mathbf{q}} - \varphi_{\mathbf{k}}}] \right.$$
$$+ [1 - e^{\varphi_{\mathbf{k}+\mathbf{q}} - \varphi_{\mathbf{k}}}] \left[\cosh(2\theta_{\mathbf{k}+\mathbf{q}}^I + 2\theta_{\mathbf{k}}^{II}) \left(n_{\mathbf{k}+\mathbf{q}}^I + \frac{1}{2} \right) \left(n_{\mathbf{k}}^{II} + \frac{1}{2} \right) \right.$$
$$\left. \left. + \cosh(2\theta_{\mathbf{k}+\mathbf{q}}^{II} + 2\theta_{\mathbf{k}}^I) \left(n_{\mathbf{k}+\mathbf{q}}^{II} + \frac{1}{2} \right) \left(n_{\mathbf{k}}^I + \frac{1}{2} \right) \right] \right\}. \tag{50}$$

The static uniform susceptibility $\chi = S(\mathbf{0})/3T$ is therefore

$$\chi = T^{-1} \frac{2}{N} \sum_{\mathbf{k}} [n_{\mathbf{k}}^I (n_{\mathbf{k}}^I + 1) + n_{\mathbf{k}}^{II} (n_{\mathbf{k}}^{II} + 1)]. \tag{51}$$

Similar equations were obtained by Takahashi [30] for an anti-ferromagnetic system in a square lattice.

For $T \neq 0$ the energies (31) and (32) are finite and we have no divergences in the self-consistent equations. Eqs. (34), (35) and (36), therefore, can be solved using numeric methods but we have adopted an approximation following Yoshida [32]. Matching Eqs. (34) and (47) we got

$$\rho = \frac{3}{2} \int \frac{d^2\mathbf{k}}{2\sigma} \left[\frac{\lambda - 3J_1 B |\gamma_{\mathbf{k}}|}{E_I} \coth\left(\frac{\beta E_I}{2} \right) + \frac{\lambda + 3J_1 B |\gamma_{\mathbf{k}}|}{E_{II}} \coth\left(\frac{\beta E_{II}}{2} \right) \right]$$
$$- \frac{3}{2} \int \frac{d^2\mathbf{k}}{2\sigma} \left[\frac{\lambda_0 - 3J_1 B_0 |\gamma_{\mathbf{k}}|}{E_{0,I}} + \frac{\lambda_0 - 3J_1 B_0 |\gamma_{\mathbf{k}}|}{E_{0,II}} \right], \tag{52}$$

where the "0" index indicates the solutions at zero temperature. The above equation is solved in the low temperature limit. We separate the integral in two regions: the first one is a circle around the origin of radius k_M and the other is the remaining area of the Brioullin zone. The radius is chosen such that the thermal energy is much lower than the spin-wave energy, i.e. $T \ll ck_M$ ($k_B = 1$) where the spin-wave velocity c refers to c_1 or c_2. In principle, the superior value for k_M is much smaller than 1 and it should be chosen so that the energies can be approximated by $E_I = \sqrt{\Delta_I^2 + \mathbf{k}^2 c_I^2}$ and $E_{II} = \sqrt{\Delta_{II}^2 + \mathbf{k}^2 c_{II}^2}$. For $k_M = 1$ the error between the exact and approximate energy is around 10%, which allow us to assign $k_M \sim 0.1$ as a reasonable limit. Thus, we can estimate k_M for temperatures not too small. At zero temperature, we have $E_{0,I} = kc_{0,I}$ (massless gap mode) and $E_{0,II} = \sqrt{\Delta_{0,II}^2 + \mathbf{k}^2 c_{0,II}^2}$. Inside the first region $\beta E_{II} \approx \beta \Delta_{II}^2 \gg 1$ and so $\coth(\beta E_{II}/2) \approx 1$ whilst E_I is gapped and $\coth(\beta E_I/2)$ holds without more approximations. In the external region, $k > k_M$, the spin-wave energies are not too small to be approached by the relativistic dispersion relation; meanwhile the cotangent terms (at low temperatures) are taken as unitary. With these considerations and after some work, the density condensate is calculated as

$$\rho = \frac{6\pi(\lambda - 3J_1 B)T}{\sigma c_I^2} \left[\ln \sinh\left(\frac{\sqrt{\Delta_I^2 + \mathbf{k}_M^2 c_I^2}}{2T} \right) - \ln \sinh\left(\frac{\Delta_I}{2T} \right) \right]$$
$$- \frac{3\pi(\lambda_0 - 3J_1 B_0)|\mathbf{k}_M|}{\sigma c_{0,I}}, \tag{53}$$

which, at low temperature limit, yields $\Delta_I(T) = Te^{-\kappa T}$ with $\kappa = \rho\sigma c_I^2 / 6\pi(\lambda - 3J_1 B)$. In Fig. 4 we show the gap energy Δ_I as a function of the temperature for three different exchange constants J_2 and in Fig. 5, $\ln \Delta_I$ is shown as a function of J_2 for $T = 0.15$. The finite gap result agrees with the Mermin–Wagner theorem.
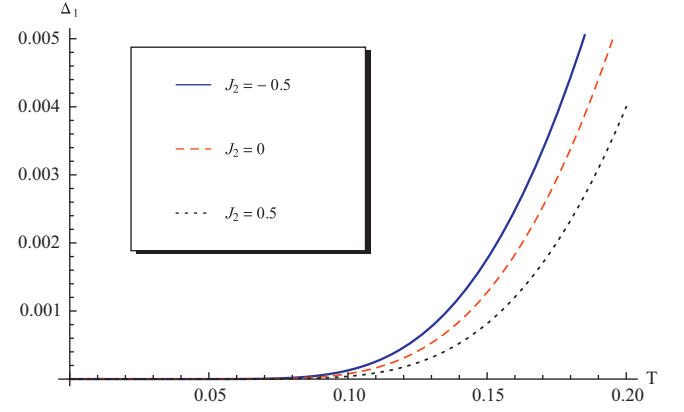

Fig. 4. The gap energy Δ_I as a function of temperature for some values of J_2 ($\Delta_{II} = 0$ in the considered limits).
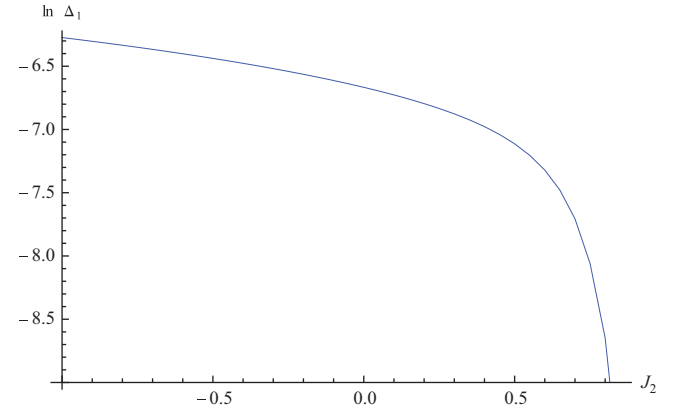

Fig. 5. The decreasing behavior of $\ln \Delta_I$ as a function of J_2 for $T = 0.15$.

4. Conclusions

Using the Schwinger boson formalism we have studied the bilinear biquadratic Heisenberg model at zero and low temperatures. We have shown that, inside the considered limits of J_2 (the biquadratic coupling), the ground state at zero temperature remains ordered. By considering the boson condensation, we have shown that the degree of order in a honeycomb lattice is between 58% (for $J_2 = -1$) and 78% (for $J_2 = 1$), which is weaker than that observed for the square lattice (which is 81%), as expected. Therefore, even with a smaller coordination number ($z = 3$), the quantum fluctuations in the honeycomb lattice are not sufficient to create a two-dimensional spin liquid state. Our approach is not appropriate for $|J_2| > 1$; however, the asymptotic behavior of the negative values of J_2 (Fig. 2) suggests the absence of a disordered phase in the limit $J_2 \ll -1$ while for $J_2 > 1$ the system seems to be strongly ordered. We have also shown that the ordered ground state exists for all physical spin values. The superior value of spin for a phase with $\langle m \rangle = 0$ is around 0.42 and it occurs when $J_2 = -1$. Above the ground state, the low energy excitations are massless Goldstone modes with relativist dispersion relation, since there is a spontaneous broken symmetry. The spin-wave velocities decrease almost linearly as a function of J_2 (Fig. 1) and c_2 vanishes when $J_2 \approx 0.65$ (c_1 vanishes for $J_2 > 1$, outside the limit considered). Analyzing the condensate density graphic, one can see that the slow spin-wave velocity corresponds to a more ordered system (higher condensation). Although the Schwinger formalism is not the best way to treat finite temperatures, we have found consistent results. At low temperatures, the ground state is disordered and the excitations have a gap that increases with the temperature ($\Delta \propto Te^{-\kappa T}$) as dictated by the Mermin–Wagner theorem.

Acknowledgments

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