We present a finite size spin wave calculation on the Heisenberg antiferromagnet on the triangular lattice focusing in particular on the low-energy part of the excitation spectrum. For $s = 1/2$ the good agreement with the exact diagonalization and quantum Monte Carlo results supports the reliability of the spin wave expansion to describe the low-energy spin excitations of the Heisenberg model even in presence of frustration. This indicates that the spin susceptibility of the triangular antiferromagnet is very close to the linear spin wave result.

I. INTRODUCTION

The antiferromagnetic Heisenberg model represents the prototype of a quantum many body system where the Hamiltonian does not commute with the order parameter -the staggered magnetization-. Therefore, quantum fluctuations are important and may play a crucial role in the ground state properties of the system. In principle they might destroy the long-range order of the classical minimum energy configuration depending, basically, on the dimensionality and the topology of the system.

In two dimensions and for a triangular lattice, quantum fluctuations are also strongly enhanced by frustration so that Fazekas and Anderson argued the possible stabilization of a resonating valence bond (RVB) ground state, i.e., a state which does not break the $SU(2)$ symmetry of the Hamiltonian. However, after a long period of intensive theoretical and numerical investigations, no definite conclusion has been settled on the ground state properties of this system. In fact -unlike the antiferromagnet on the square lattice where there is a general consensus about the ordered nature of the ground state even for $s = 1/2$- in the frustrated cases the lack of exact analytical results is accompanied by difficulties in applying stochastic numerical methods, as their reliability is strongly limited by the well-known sign problem. A few years ago Bernu et al., with a deep analysis of the exact excitation spectra obtained for small clusters with the Lanczos technique, already evidenced an antiferromagnetic $120^\circ$ ordering in the ground state. Only very recently, however, quantum Monte Carlo (QMC) calculations have allowed to extrapolate to fairly large system sizes giving evidence of a quantum Néel order with the order parameter $m^\dagger$ reduced by about 59% from its classical value.

Assuming as established the long-range Néel order of the ground state, in this paper we address the reliability of the spin wave (SW) theory as an analytical tool to treat the Heisenberg antiferromagnet on the triangular lattice. To this purpose, we generalize to the latter model a previously developed SW theory specialized to finite size systems, and we study the low-lying excited states. We will show that the agreement with numerical results obtained by exact diagonalization and QMC is very good, thus confirming the effectiveness of SW theory in describing the ground state properties of the triangular Heisenberg model.

II. SPIN WAVE CALCULATION

Several attempts to generalize SW theory to finite sizes can be found in the literature. Here we will follow the method proposed in the mentioned Ref. which allows to deal with finite clusters avoiding the spurious Goldstone modes divergences in a straightforward way, and, in particular, without imposing any ad hoc holonomic constraint on the sublattice magnetization.

Assuming the classical $Q = (4\pi/3, 0)$ magnetic structure lying in the $x-y$ plane and applying the unitary transformation which defines a spatially varying coordinate system $(x'-y'-z')$ in such a way that the $x'$-axis coincides on each site with the local Néel direction, the transformed Heisenberg Hamiltonian reads:
\[ H = J \sum_{(i,j)} \left[ \cos (\mathbf{Q} \cdot (\mathbf{r}_j - \mathbf{r}_i)) (S_i^x S_j^x + S_i^y S_j^y) \\
+ \sin (\mathbf{Q} \cdot (\mathbf{r}_j - \mathbf{r}_i)) (S_i^x S_j^y - S_i^y S_j^x + S_i^z S_j^z) \right] \]  
(1)

where \( J \) is the (positive) exchange constant between nearest neighbors, the indices \( i, j \) label the points \( \mathbf{r}_i \) and \( \mathbf{r}_j \) on the \( N \)-site triangular lattice and the quantum spin operators satisfy \( |\mathbf{S}_i|^2 = s(s+1) \). Then, using Holstein-Primakoff transformation for spin operators to order \( 1/s \), \( S_i^x = s - a_i^\dagger a_i, S_i^y = \sqrt{2} (a_i^\dagger + a_i), S_i^z = i \sqrt{2} (a_i^\dagger - a_i) \), being \( a \) and \( a^\dagger \) the canonical creation and destruction Bose operators, after some algebra the Fourier transformed Hamiltonian results:

\[
H_{SW} = E_{cl} + 3J_s \sum_k \left[ A_k a_k^\dagger a_k + \frac{1}{2} B_k (a_k^\dagger a_{-k}^\dagger + a_k a_{-k}) \right] 
\]  
(2)

where \( E_{cl} = -3Js^2 N/2 \) is the classical ground state energy, \( A_k = 1 + \gamma_k/2, B_k = -3 \gamma_k/2, \gamma_k = [\cos (k_x) + 2 \cos (k_x/2) \cos (\sqrt{3} k_y/2)]/3 \) and \( \mathbf{k} \) is a vector varying in the first Brillouin zone of the lattice. The Hamiltonian \( H_{SW} \), can be diagonalized for \( k \neq 0, \pm Q \) introducing the well-known Bogoliubov transformation, \( a_k = u_k a_k^\dagger + v_k \alpha_{-k}^\dagger \), with

\[
u_k = \left( \frac{A_k + \epsilon_k}{2\epsilon_k} \right)^{1/2}, \quad v_k = -\text{sgn}(B_k) \left( \frac{A_k - \epsilon_k}{2\epsilon_k} \right)^{1/2}
\]  
(3)

where \( \epsilon_k = \sqrt{A_k^2 - B_k^2} \) is the SW dispersion relation. Such a diagonalization leads to

\[
H_{SW}^0 = E_{cl} + 3J_s \sum_{k \neq 0, \pm Q} (\epsilon_k - A_k) + \frac{3J_s}{2} \sum_{k \neq 0, \pm Q} \epsilon_k (a_k^\dagger a_k + \alpha_{-k}^\dagger \alpha_{-k}).
\]  
(4)

The Goldstone modes, instead, cannot be diagonalized with this transformation since they become singular for \( k = 0 \) and \( k = \pm Q \). For infinite systems such modes do not contribute to the integrals in Eq. (1), but in the finite case they are important and they must be treated separately. By defining the following Hermitian operators

\[
Q_x = \frac{i}{2} (a_0^\dagger a_0 - a_Q^\dagger a_Q - a_{-Q}^\dagger a_{-Q}),
Q_y = \frac{1}{2} (a_Q^\dagger a_0 + a_0^\dagger a_Q + a_{-Q}^\dagger a_{-Q}),
Q_z = i (a_0^\dagger a_0 - a_0),
\]  
(5)

such that, \([Q_\alpha, Q_\beta] = 0 \) and \([Q_\alpha, H_{SW}] = 0 \) for \( \alpha, \beta = x, y, z \), the contribution of the singular modes, \( H_{SM}, \) in Eq. (2) can be expressed in the form

\[
H_{SM} = -3J_sA_0 + 3J_s \frac{A_0}{2} [Q_x^2 + Q_y^2 + Q_z^2].
\]

Then, taking into account the fact that to the leading order in \( 1/s \), \( Q_\alpha = S^\alpha \sqrt{2/Ns} \), where \( S^\alpha \) are the components of the total spin, \( H_{SM} \) may be also rewritten in the more physical form

\[
H_{SM} = -3J_sA_0 + 3J_s \frac{A_0}{N} [(S^x)^2 + (S^y)^2 + (S^z)^2],
\]

which clearly favors a singlet ground state (for an even number of sites) being \( A_0 \) positive definite. This result is highly non trivial since we have recovered the Lieb-Mattis property which has not been demonstrated for non bipartite lattices. Actually, a similar result is obtained by solving exactly the three Fourier components \( k = 0, \pm Q \) of the Heisenberg model, however, our treatment allows to construct a formal expression for the SW ground state on finite triangular lattices which keeps the correct singlet behavior. In fact, starting from the usual SW ground
TABLE I. Ground state energy for the $s = 1/2$ Heisenberg antiferromagnet on the triangular lattice, as obtained within the finite size SW theory and with a QMC calculation. For $N = 36$ the exact value of the energy is $E_0/JN = -0.5604$.

| $N$ | $E_{SW}/JN$ | $E_{QMC}/JN$ |
|-----|-------------|--------------|
| 36  | -0.5587     | -0.5581(1)   |
| 48  | -0.5504     | -0.5541(1)   |
| 108 | -0.5410     | -0.5482(1)   |
| $\infty$ | -0.5388 | -0.5458(1)   |

state, composed by the $120^\circ$ classical Néel order plus the zero point quantum fluctuations (i.e., zero Bogoliubov quasiparticles),

$$|0\rangle = \prod_{k \neq 0, \pm Q} u_k^{-1} \exp \left[ \frac{1}{2} \frac{\sum_{\alpha} a_\alpha^+ a_{\alpha - k}^+} {u_k} \right] |N\rangle$$

with $|N\rangle = \prod_i |S_i^x\rangle = s$, the corresponding singlet wavefunction is obtained by projecting $|0\rangle$ onto the subspace $S = 0$:

$$|\psi_{SW}\rangle = \int d\alpha \int d\beta \int d\gamma \ e^{iQ_\alpha + iQ_\beta + iQ_\gamma} |0\rangle$$

and reads $|\psi_{SW}\rangle \sim e^{-\alpha^+ a^+ a + \frac{1}{2} \sum_{\alpha} v_\alpha^2} |0\rangle$. In particular the singular modes have no contribution to the ground state energy while the computation of the order parameter (defined as in Ref.13) $m^1$, requires their remotion:

$$m^1 = \sqrt{\langle (S^x_0)^2 \rangle} = s - \frac{1}{N} \sum_{k \neq 0, \pm Q} v_k^2.$$  \hspace{1cm} (7)

Even for $s = 1/2$, the previous SW calculation predicts a very good quantitative agreement with exact results on small clusters ($N \leq 36$) of both ground state energy and sublattice magnetization. For larger lattice sizes (see Table I), a comparison of the SW predictions with the available QMC results also shows a surprisingly good agreement for the ground state energy which is conserved also with respect to the extrapolated values in the thermodynamic limit. Furthermore the QMC estimate of the order parameter in the thermodynamic limit $m_{QMC}^1 = 0.41(1)$ can be reasonably compared with the SW prediction $m_{SW}^1 = 0.478$. In the next sections we will also show that the low-energy spectra on finite sizes, calculated within the SW approximation, compare very accurately with the available numerical results. This agreement supports the numerical evidence for an ordered ground state in the present model.

### III. LOW-ENERGY SPIN WAVE SPECTRUM

In this section, we show how to construct the low-lying energy spectra $E(S)$ for finite systems. Following Ref.12, a magnetic field in the $z$-direction is added to stabilize the desired total spin excitation $S$,

$$\mathcal{H}_S = \mathcal{H}_{SW} - hS \sum_i S^z_i.$$  \hspace{1cm}

Classically, the new solution is the $120^\circ$ Néel order canted by an angle $\theta$ along the direction of the field $h$. In order to develop a SW calculation, a new rotation around $y'$-axis is performed on the spin operators and it can be proven that $\mathcal{H}_S$ takes the same form of Eq.(2) with renormalized coefficients $A_k$ and $B_k$:

$$A^h_k = 1 + \gamma_k \left[ \frac{1}{2} - \frac{3}{2} \frac{2h}{3J} \right] \quad B^h_k = -\frac{3}{2} \gamma_k \left[ 1 - \frac{2h}{3J} \right],$$

being $\frac{2h}{3J} = \sin \theta$. In the present case the only singular mode is $k = 0$ and its contribution is given by

$$\mathcal{H}_{SM} = -\frac{3JS}{2} A^h + 3J \frac{A^h}{N} (S^z - Ns \sin \theta)^2,$$

which now favors a value of $S^z$ consistent with the applied field, at the classical level. The Hellmann-Feynman theorem relates the latter quantities as it follows:
FIG. 1. SW (full dots and continuous line), exact (empty dots and dashed lines) and QMC (empty squares) low-energy spectra as a function of $|S^2| = S(S+1)$ for $N = 12, 27, 36, 144$ and $s = 1/2$.

\[
\langle S_z^2 \rangle = -\frac{1}{Ns} \frac{\partial}{\partial h} E(h)
\]

\[
= s \frac{2h}{\varepsilon^2 3J} \left[ 1 + \frac{1}{2Ns} \sum_{k \neq 0} \gamma_k \sqrt{\frac{A^h_k + B^h_k}{A^h_k - B^h_k}} \right]
\]

where

\[
E(h) = E_{cl} - \frac{1}{2}(sh)^2 \frac{2N}{3^2 J} - 3Js \frac{N}{2} + \frac{3Js}{2} \sum_k \epsilon^h_k.
\] (8)

and $\epsilon^h_k = \sqrt{(A^h_k)^2 - (B^h_k)^2}$. In particular, the expansion to order $(sh)^2$ of the two first terms in Eq.(8) for $h \to 0$ gives the classical perpendicular susceptibility $\chi_{cl} = 1/9J$, while taking the whole expression the known SW result $\chi_{SW}/\chi_{cl} = 1 - 0.449/2s$ is recovered. Finally, in order to evaluate the energy spectrum $E(S)$ of the $s = 1/2$ case, a Legendre transformation $E(S) = E(h) + hsS$ has to be performed. The advantage of this expression is that $E(S)$ can be computed within our framework for any size of the lattice and, in particular, in the thermodynamic limit. Of course our SW spectra are biased by the underlying classical Néel order which is invariant under the point group $C_{3v}$ and under translations of the magnetic sublattices.

A. Comparison with numerical results

The occurrence of symmetry breaking in the ground state for $N \to \infty$ can be evidenced from the structure of the finite size energy spectra. In particular, it is well known that when long-range order is present in the thermodynamic limit, the low-lying excited states of energy $E(S)$ and spin $S$ are predicted to behave as the spectrum of a free quantum rotator (or quantum top)

\[
E(S) - E_0 \propto \frac{S(S+1)}{N},
\] (9)

as long as $S \ll \sqrt{N}$. Fig. 1 shows $E(S)$ vs $S(S+1)$ calculated within the SW theory compared with the exact (for $N \leq 36$) and QMC (for $S = 3$, up to $N = 144$) results, being the two last also consistent with the above mentioned spatial symmetries of the classical Néel state 4. Remarkably SW theory turns out to be efficient to reproduce the low-energy spectrum in the whole range of sizes. Furthermore, we can extend our calculation to the thermodynamic limit and observe easily the collapse of a macroscopic number of states with different $S$ to the ground state as $N \to \infty$. This clearly gives rise to a broken $SU(2)$ symmetry ground state, as expected within the SW framework.
FIG. 2. Size dependence of $\frac{1}{2}\chi_L$ (a) and of $\frac{1}{2}\chi_L/2 - \frac{1}{2}\chi_L$ (b) obtained according to Eq. (10) using the $(s = 1/2)$ SW excitation spectra. The continuous line is a quadratic fit for $L < 18$ in (a) and a guide for the eye in (b).

B. Spin susceptibilities and anomalous finite size effects

Whenever the quantum top law (9) is verified, the quantity

$$[2\chi_S]^{-1} = NE(S)[S(S+1)]^{-1},$$

should approach the physical inverse susceptibility $1/2\chi_{SW}$ for infinite size and for any spin excitation $S \ll N$. This feature is clearly present in the SW theory and it is shown in Fig. 2(a) where the $1/2\chi_S$ is plotted for $S = L \equiv \sqrt{N}$ and approaches the predicted value ($1/2\chi_{SW} = 8.167$), even if the correct asymptotic scaling $1/2\chi_L = 1/2\chi_{SW} + a/L + b/L^2$ turns out to be satisfied only for very large sizes ($L \geq 36$). Such feature is also shared by the Heisenberg antiferromagnet on the square lattice where a similar SW analysis has allowed to account for the anomalous finite size spectrum resulting from an accurate QMC calculation. Furthermore, similarly to the latter case, a non-monotonic behavior of $\frac{1}{2}\chi_L/2 - \frac{1}{2}\chi_L$ (Fig. 2(b)), which should extrapolate to 0 as $1/L$ according to the quantum top law, persists also in presence of the frustration within the SW approximation and is likely to be a genuine feature of the Heisenberg model.

IV. CONCLUDING REMARKS

In conclusion, we have applied a previously developed finite size spin wave theory to the Heisenberg model on the triangular lattice. Comparison for the case $s = 1/2$ of the low-energy part of the spin wave spectra with the exact and the more recent quantum Monte Carlo results reveals a very good agreement.

The accuracy of our results on finite sizes indicates that spin wave theory is a reliable analytical approximation to describe the ground state properties of the present model in the thermodynamic limit $N \to \infty$. In particular the effectiveness of the spin wave theory in reproducing the finite size spectrum strongly suggests that the value of the spin susceptibility should be very close to the spin wave prediction. This represents the main finding of this paper. Furthermore we have found, to order $1/s$, anomalous finite size effects for the spin susceptibilities for $s = 1/2$, similar to the case of the square lattice.

Finally, this study provides further support to the recent numerical evidences about the existence of long-range Néel order in the ground state of the present frustrated model.
This work was supported in part by INFM (PRA HTCS), MURST (COFIN97) and Fundación Antorchas (A.E.T.). It is a pleasure to acknowledge stimulating discussions with C. Lhuillier, M. Capone, M. Calandra, F. Becca, A. Parola, G. Santoro, V. Tognetti and L. O. Manuel.

1 P. Fazekas and P. W. Anderson, Philos. Mag. 30, 423 (1974).
2 V. Kalmeyer and R. B. Laughlin, Phys. Rev. Lett. 59, 2095 (1987).
3 D.A. Huse and V. Elser, Phys. Rev. Lett. 60, 2531 (1988).
4 R. Singh and D. Huse, Phys. Rev. Lett. 68, 1766 (1992).
5 N. Elstner, R. R. P. Singh, and A. P. Young, Phys. Rev. Lett. 71, 1629 (1993).
6 K. Yang, L. K. Warman, and S. M. Girvin, Phys. Rev. Lett. 70, 2641 (1993).
7 Th. Jolicoeur and J. C. Le Guillou, Phys. Rev. B 40, 2727 (1989).
8 S. J. Miyake, J. Phys. Soc. Jpn. 61, 983 (1992).
9 L. O. Manuel, A. E. Trumper and H. A. Ceccatto, Phys. Rev. B 57, 8348 (1998).
10 P. Azaria, B. Delamotte and D. Mouhanna, Phys. Rev. Lett. 70, 2483 (1993).
11 P. W. Leung and K. J. Runge, Phys. Rev. B 47, 5861 (1993).
12 B. Bernu, C. Lhuillier, and L. Pierre, Phys. Rev. Lett. 69, 2590 (1992); B. Bernu, P. Lecheminant, C. Lhuillier, L. Pierre, Phys. Rev. B 50, 10048 (1994).
13 A. Chubukov, S. Sachdev, and T. Senthil, J. Phys.: Condens. Matter 6, 8891 (1994).
14 L. Capriotti, A. E. Trumper, and S. Sorella, Phys. Rev. Lett. 82, 3899 (1999).
15 Q. F. Zhong and S. Sorella, Europhys. Lett. 21, 629 (1993).
16 M. Takahashi, Phys. Rev. B 40, 2494 (1989).
17 J. E. Hirsch and S. Tang, Phys. Rev. B 40, 4769 (1989).
18 E. Lieb and D. Mattis, J. Math. Phys. 3, 749 (1962).
19 C. Lavalle, S. Sorella and A. Parola, Phys. Rev. Lett. 80, 1746 (1998).
20 In order to perform a faithful comparison, we have computed the spin wave energy $E(S)$ using the same clusters of the numerical results, i.e., with periodic boundary conditions and all the spatial symmetries of the infinite lattice that do not frustrate the classical Néel order (see for details Ref. [2]).