Large-S expansion for quantum antiferromagnets on a triangular lattice

# Large-$S$ expansion for quantum antiferromagnets on a triangular lattice

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**Abstract.** We report spin-wave results for the sublattice magnetization (to order $O(1/S^2)$) and two spin stiffnesses and susceptibilities (to order $O(1/S)$) for the two-dimensional triangular Heisenberg antiferromagnet. These stiffnesses and susceptibilities are used as input parameters in scaling functions for various observables. The scaling results for uniform susceptibility are compared with recent numerical data.

## 1. Introduction

In recent years, there has been significant interest in the theory of the low-temperature properties of frustrated quantum antiferromagnets in two dimensions (2D). Among these systems, antiferromagnets on a triangular lattice are perhaps the most popular objects, as there are several experimental realizations such as $VCl_2$, $VBr_2$, $C_6Eu$, $NaTiO_2$ etc [1]. Theoretical studies of such antiferromagnets go back to 1974 when Fasekas and Anderson [2] first suggested that for spin $S = \frac{1}{2}$, quantum fluctuations may be strong enough to destroy the classical 120° ordering of Heisenberg spins. Since then, there have been a number of numerical studies of the $S = 1/2$ antiferromagnet: some of them [3] do indicate the presence of well defined long-range order reduced by quantum fluctuations by nearly the same amount as predicted by non-interacting spin-wave theory [4], while others indicate a substantially smaller (if any) ordered moment [5, 6]. The latter, if true, would indicate that triangular antiferromagnets are very close to a quantum disordering transition. Recently, we considered [7] the low-temperature theory of frustrated antiferromagnets, similar in spirit to the low-$T$ theory of collinear antiferromagnets [8]. We described the general features of such a theory, and *assuming* the existence of deconfined spinons in the quantum disordered phase, derived a number of experimentally testable results for the uniform susceptibility, correlation length, dynamical structure factor, spin-lattice relaxation rates etc. We found that the behaviour of observables near the quantum transition is universal and depends only on a few input parameters at $T = 0$. The triangular antiferromagnet is likely to be located on the ordered side of the transition in which case input parameters are on-site magnetization ($N_0$), two spin stiffnesses, $\rho_\perp$ and $\rho_\parallel$, and two susceptibilities, $\chi_\perp$ and $\chi_\parallel$. The fact that one needs two stiffnesses is indeed a direct consequence of the well known fact that the macroscopic order parameter in triangular (and any other frustrated) antiferromagnets is given by a pair of mutually orthogonal unit vectors, $n_1$ and $n_2$, which specify a plane. The two stiffnesses then measure the energy cost of twists in the plane ($\rho_\parallel$) and perpendicular to

the plane of the order parameter ($\rho_\perp$). Two uniform susceptibilities, $\chi_\parallel$ and $\chi_\perp$, on the other hand, define the response of the antiferromagnet with infinitesimal anisotropy to uniform magnetic fields perpendicular and parallel to the plane of the order parameter, respectively. Note the inversion in the order of 'parallel' and 'perpendicular'—the susceptibility tensor $\chi_{\alpha,\beta}$ is defined with respect to a unit vector $m = n_1 \times n_2$ perpendicular to the plane of spin ordering [9, 10]:

$$\chi_{\alpha,\,\beta} = \chi_\perp \delta_{\alpha\beta} + (\chi_\parallel - \chi_\perp) m_\alpha m_\beta. \tag{1.1}$$

The two stiffnesses and susceptibilities are indeed related by spin-wave velocities $c_\perp^2 = \rho_\perp/\chi_\perp$, $c_\parallel^2 = \rho_\parallel/\chi_\parallel$.

The goal of the present paper is to calculate the five input parameters for triangular antiferromagnets in the expansion over the inverse spin $S$. This will allow us to make *quantitative* predictions in the deconfined spinon scenario on the behaviour of observables, and to compare scaling results with recent high-temperature series expansion studies of triangular antiferromagnets. We will also compare our result for sublattice magnetization, $N_0$, with recent series expansion [6] and other studies.

Although throughout the paper we will use a large-$S$ approach, our chief interest is in the case of $S = 1/2$ for which numerical studies have been performed. Indeed, for small $S$, the expansion parameter for spin-wave calculations is not small. However, as we will see below, the convergence of the perturbative series in $1/2S$ in triangular antiferromagnets is very good (as it is on the square lattice [11, 12]), and the $1/S$ expansion is likely to give quite accurate values of observables, even for $S = 1/2$.

## 2. $1/S$ expansion

### 2.1. Bose Hamiltonian

We now turn to a description of the calculations. We consider here the model with interactions between nearest neighbours:

$$\mathcal{H} = J \sum_{l,\Delta} S_l \cdot S_{l+\Delta}. \tag{2.1}$$

The procedure of doing the $1/S$ expansion is rather standard and involves several steps which include (i) the transformation from spin operators to bosons via Holstein–Primakoff, Dyson–Maleev, or some other transformation, (ii) the diagonalization of the quadratic form in bosons, and (iii) the use of a standard perturbative technique for Bose liquids to treat the interaction between spin waves. Non-interacting spin waves have energy which scales as $S$, while the interaction vertex involving $m$ bosons scales as $S^{2-m/2}$; this gives rise to an expansion in powers of $1/S$ for anharmonic contributions, similar to that in a weakly interacting Bose gas.

Another important issue, related to the $1/S$ expansion, is the number of Bose fields which one has to introduce in order to keep track of the whole spin-wave spectrum, not just the low-energy modes. This is important because quantum fluctuations are not divergent in 2D, and the $1/S$ expansion involves sums over the whole Brillouin zone. In the general case, the number of different Bose fields is equivalent to the number of magnetic sublattices. However, in several special cases, a multisublattice magnetic configuration can be transformed into a one-sublattice ferromagnetic one by applying a uniform twist on the

coordinate frame. In this situation, the spin-wave spectrum has no gaps at the boundaries of the reduced Brillouin zone and one can describe all excitations by a single bosonic field, as in the case of a ferromagnet. Obviously, the triangular antiferromagnet in a zero magnetic field is an example of such special behaviour: the 120° ordering becomes a ferromagnetic one in the twisted coordinate frame with a pitch $Q = (4\pi/3, 4\pi/\sqrt{3})$. We will therefore use a one-sublattice description of triangular antiferromagnet whenever possible. This indeed substantially simplifies the calculations.

We start with the transformation from spin operators to bosons. The choice of the transformation is indeed only a matter of convenience, and the final results are independent of the way in which bosons are introduced. Nevertheless, there are several possibilities extensively discussed in the literature [13]. We found it most convenient to use here the conventional Holstein–Primakoff transformation because it preserves the Hermitian properties of the Hamiltonian. We therefore use

$$S_z = S - a^\dagger a \qquad S^+ = \sqrt{2S - a^\dagger a}\ a \qquad S^- = a^\dagger \sqrt{2S - a^\dagger a}. \qquad (2.2)$$

Substituting this transformation into (2.1), expanding the radical, and restricting to only cubic and quartic anharmonic terms, we obtain after some algebra

$$\mathcal{H} = \mathcal{H}_0 + 3JS(\mathcal{H}_2 + \mathcal{H}_3 + \mathcal{H}_4) \qquad (2.3)$$

where $\mathcal{H}_0 = -\frac{3}{2}JS^2N$ is the classical ground state energy, and other terms are

$$\mathcal{H}_2 = \sum_k A_k a_k^\dagger a_k + \frac{B_k}{2}(a_k^\dagger a_{-k}^\dagger + a_k a_{-k})$$

$$\mathcal{H}_4 = \frac{1}{16S} \sum a_1^\dagger a_2^\dagger a_3 a_4 \left[ 4(v_{1-3} + v_{2-3}) + v_1 + v_2 + v_3 + v_4 \right]$$

$$- 2\left( a_1^\dagger a_2^\dagger a_3^\dagger a_4 + a_4^\dagger a_3 a_2 a_1 \right)(v_1 + v_2 + v_3)$$

$$\mathcal{H}_3 = i\sqrt{\frac{3}{8S}} \sum (a_1^\dagger a_2^\dagger a_3 - a_3^\dagger a_2 a_1)(\bar{v}_1 + \bar{v}_2). \qquad (2.4)$$

Here $i \equiv k_i$, and

$$v_k = \frac{1}{3}\left( \cos k_x + 2\cos\frac{k_x}{2}\cos\frac{k_y\sqrt{3}}{2} \right) \qquad \bar{v}_k = \frac{2}{3}\sin\frac{k_x}{2}\left( \cos\frac{k_x}{2} - \cos\frac{k_y\sqrt{3}}{2} \right). \qquad (2.5)$$

Finally, $A_k$ and $B_k$ are given by

$$A_k = 1 + \frac{v_k}{2} \qquad B_k = -\frac{3}{2}v_k. \qquad (2.6)$$

At $S = \infty$, anharmonic terms are absent and $\mathcal{H}_2$ can be diagonalized by a standard Bogolubov transformation

$$a_k = l_k(c_k + x_k c_{-k}^\dagger) \qquad (2.7)$$

with

$$l_k = \left(\frac{A_k + E_k}{2E_k}\right)^{1/2} \qquad x_k = -\frac{B_k}{|B_k|}\left(\frac{A_k - E_k}{A_k + E_k}\right)^{1/2} \tag{2.8}$$

and

$$E_k = (A_k^2 - B_k^2)^{1/2} = ((1 - \nu_k)(1 + 2\nu_k))^{1/2}. \tag{2.9}$$

The diagonalization yields

$$\mathcal{H}_1 = \sum_k E_k c_k^\dagger c_k. \tag{2.10}$$

It follows from equation (2.9) that the excitation spectrum of the ideal gas of magnons has three zero modes, as indeed it should. Two of these modes are at $k = \pm Q$ where $Q = (4\pi/3, 4\pi/\sqrt{3})$ is the ordering momentum in a triangular antiferromagnet, and the third is at $k = 0$ and describes soft fluctuations of total magnetization. The expansion near zero modes gives two spin-wave velocities

$$c_\perp = c_{\pm Q} = \frac{3\sqrt{3}}{2\sqrt{2}} J S a \tag{2.11}$$

$$c_\parallel = c_{k=0} = \frac{3\sqrt{3}}{2} J S a. \tag{2.12}$$

The ratio of the two at $S = \infty$ is $c_\parallel/c_\perp = \sqrt{2}$. This was also obtained in other approaches [10].

The infinite-$S$ spin-wave results can be also used to get the first quantum correction to on-site magnetization [4]. Indeed, $\langle a^\dagger a \rangle$ in (2.2) is nothing but the density of particles which is finite due to the anomalous term in the quadratic form. From (2.7) and (2.8), we have $\langle a_k^\dagger a_k \rangle = (A_k - E_k)/2E_k$, and therefore non-interacting spin waves reduce the sublattice magnetization to

$$\langle S \rangle = S\left(1 - \frac{1}{2S}\sum_k \frac{A_k - E_k}{E_k}\right) = S\left(1 - \frac{0.522}{2S}\right). \tag{2.13}$$

We next consider corrections to equations (2.11) and (2.13) due to the interactions between spin waves. We will follow the same line of reasoning as for square-lattice antiferromagnets. However, the presence of cubic terms makes the analysis considerably more involved.

We start with the spin-wave velocity renormalization.

## 2.2. Spin-wave velocity

Our goal is to obtain the leading $1/S$ renormalization of spin-wave excitations. For this we consider first-order self-energy corrections due to quartic anharmonicities and second-order corrections due to cubic anharmonicities (recall that cubic terms have the overall factor $S^{1/2}$). The corrections due to quartic terms are easy to compute, because of leading order in $1/S$, one can get away with simple one-loop diagrams. Equivalently, one can simply decouple the fourfold term in equation (2.4) by making possible pair averaging. The quadratic form allows for non-zero normal $\langle a_k^\dagger a_k \rangle$ and anomalous $\langle a_k a_{-k} \rangle$ pair products of Bose particles, and the decoupling changes $A_k$ and $B_k$ to

$$\bar{A}_k = \left(1 + \frac{\nu_k}{2}\right)\left(1 + \frac{1}{2S} - \frac{1}{2S}\sum_p \frac{1}{E_p}\left(1 + \frac{\nu_p}{4} + \nu_p^2\right)\right) - \frac{3}{8S}\sum_p \frac{\nu_p}{E_p}(1 - 4\nu_p) \qquad (2.14)$$

$$\bar{B}_k = -\frac{3}{2}\nu_k\left(1 + \frac{1}{2S} - \frac{1}{2S}\sum_p \frac{1}{E_p}\left(1 + \frac{\nu_p}{4} - \nu_p^2\right)\right) + \frac{3}{8S}\sum_p \frac{\nu_p}{E_p}. \qquad (2.15)$$

A simple inspection then shows that the renormalized spectrum $(\bar{E}_k = (\bar{A}_k^2 - \bar{B}_k^2)^{1/2})$ still keeps a zero mode at $k = 0$, but acquires a finite gap at $k = \pm Q$:

$$E_Q^2 = -\frac{9}{8S}\sum_p \frac{\nu_p(1 - \nu_p)}{E_p}. \qquad (2.16)$$

This finite gap is indeed an artifact of using only quartic terms, and cubic anharmonicities should restore the correct structure of the spectrum, as we demonstrate below.

There are several ways to deal with the cubic terms: one can either calculate the effective fourfold vertex produced by two triple vertices [14, 15], and then use the decoupling procedure, or one can transform to quasiparticles (i.e., diagonalize the quadratic form) considering first only quartic corrections, and then calculate the renormalization of the excitation spectrum due to cubic terms in the second-order perturbation theory. Below we use the second approach which is technically advantageous. We therefore first transform from particle operators $(a_k)$ to quasiparticles $(c_k)$ using equation (2.7), but with $\bar{A}_k$ and $\bar{B}_k$ instead of $A_k$ and $B_k$. The bare Hamiltonian then keeps the form of equation (2.10) with $\bar{E}_k$ instead of $E_k$. On the other hand, the structure of cubic vertices becomes more involved after the transformation to quasiparticles, and instead of equation (2.4) we obtain

$$\mathcal{H}_3 = i\sqrt{\frac{3}{32S}}\sum \left[ c_1^\dagger c_2^\dagger c_3 \Phi_1(1, 2; 3) + \frac{1}{3}c_1^\dagger c_2^\dagger c_3^\dagger \Phi_2(1, 2, 3)\right] + \text{HC}. \qquad (2.17)$$

The vertex functions $\Phi_1$ and $\Phi_2$ are given by

$$\Phi_1(1, 2; 3) = \frac{\tilde{\Phi}_1(1, 2; 3)}{\sqrt{\bar{E}_1 \bar{E}_2 \bar{E}_3}} \qquad \Phi_2(1, 2, 3) = \frac{\tilde{\Phi}_2(1, 2, 3)}{\sqrt{\bar{E}_1 \bar{E}_2 \bar{E}_3}} \qquad (2.18)$$

where

$$\tilde{\Phi}_1(1, 2; 3) = \bar{\nu}_1 f_-^{(1)}(f_+^{(2)} f_+^{(3)} + f_-^{(2)} f_-^{(3)}) + \bar{\nu}_2 f_-^{(2)}(f_+^{(1)} f_+^{(3)} + f_-^{(1)} f_-^{(3)})$$
$$+ \bar{\nu}_3 f_-^{(3)}(f_+^{(1)} f_+^{(2)} - f_-^{(1)} f_-^{(2)})$$

$$\tilde{\Phi}_2(1, 2, 3) = \bar{\nu}_1 f_-^{(1)}(f_+^{(2)} f_+^{(3)} - f_-^{(2)} f_-^{(3)}) + \bar{\nu}_2 f_-^{(2)}(f_+^{(1)} f_+^{(3)} - f_-^{(1)} f_-^{(3)})$$
$$+ \bar{\nu}_3 f_-^{(3)}(f_+^{(1)} f_+^{(2)} - f_-^{(1)} f_-^{(2)})$$

and

$$f_{\pm}^{(i)} = (\bar{A}_i \pm \bar{B}_i)^{1/2}. \tag{2.19}$$

The self-energy diagrams to order $1/S$ are shown in figure 1. We see that cubic terms give rise to both normal and anomalous self-energy parts so that the dispersion relation again has the form typical for a $2 \times 2$ problem:

$$(\omega + \Sigma_a(k, \omega))^2 = (\bar{E}_k + \Sigma_s(k, \omega))^2 - (\Sigma_{+,+}(k, \omega))^2 \tag{2.20}$$

where $\Sigma_{s,a}(k, \omega) = \frac{1}{2} (\Sigma_{+,-}(k, \omega) \pm \Sigma_{+,-}(-k, -\omega))$. However, it is not difficult to check that $\Sigma_{-,-} \sim \Sigma_{+,+} \sim 1/S$ and therefore anomalous self-energy terms contribute to the excitation energy only to order $1/S^2$, while to order $1/S$ a solution of equation (2.20) is simply $\omega = \tilde{E}_k$ where

$$\tilde{E}_k^2 = \bar{E}_k^2 + 2\bar{E}_k \Sigma_{+,-}(k, \bar{E}_k). \tag{2.21}$$

We therefore need to evaluate here only the normal component of the self-energy. The analytical expression for $\Sigma_{+,-}$ is

$$\Sigma_{+,-}(k, \bar{E}_k) = -\frac{3}{16S} \sum \left( \frac{|\Phi_1(1, 2; k)|^2}{\bar{E}_1 + \bar{E}_2 - \bar{E}_k} + \frac{|\Phi_2(1, 2, k)|^2}{\bar{E}_1 + \bar{E}_2 + \bar{E}_k} \right). \tag{2.22}$$

To leading order in $1/S$ we can indeed use non-renormalized values for $A_k, B_k, E_k$ in the RHS of (2.22).
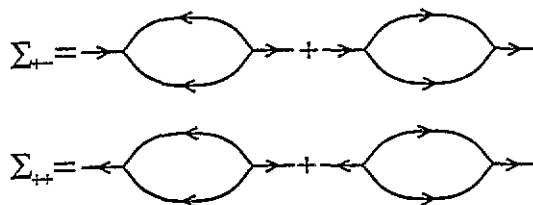


**Figure 1.** Second-order self-energy corrections to magnon propagators due to cubic vertices. Notice that cubic terms always produce anomalous self-energy terms.

We first demonstrate that $\tilde{E}_k$ has a true zero mode at $k = Q$. For this we need to evaluate $\Sigma_{+,-}(Q, \bar{E}_Q)$. We found the following equality to be quite useful in the calculation

$$\sqrt{3}\, \bar{v}_{q\pm Q/2} = (A_{q\pm Q/2} + B_{q\pm Q/2}) - (A_{q\mp Q/2} - B_{q\mp Q/2}). \tag{2.23}$$

Substituting (2.23) into the expressions for the vertex functions and using $A_Q = B_Q = \frac{3}{4}$, we obtain after simple algebra

$$\tilde{\Phi}_1(1, 2; Q) = \tilde{\Phi}_2(1, 2, Q) = \frac{(E_1 + E_2)}{\sqrt{2}} (f_+^{(1)} f_+^{(2)} - f_-^{(1)} f_-^{(2)}). \tag{2.24}$$

Substituting, then, the vertex functions into the formula for the self-energy we obtain using (2.19)

$$\Sigma_{+,-}(Q, E_Q) = \frac{1}{2E_p} \frac{9}{8S} \sum_p \frac{\nu_p(1 - \nu_p)}{E_p}. \tag{2.25}$$

Finally, upon substituting this result into equation (2.21) and using (2.16) for $\bar{E}_Q$, we find that the gap in the excitation spectrum disappears as it should.

Our next step is to expand $\bar{E}_k$ and $\Sigma_k$ near the zero modes, and obtain the corrections to the spin-wave velocities to order $1/S$. The expansion near $k = 0$ is quite straightforward because $\tilde{\Phi}_1(1, 2; k)$ and $\tilde{\Phi}_2(1, 2, k)$ both scale as $k$ at small $k$, and one can therefore safely neglect $E_k$ in the denominators in (2.22). Doing the algebra, we obtain the renormalized spin-wave velocity at $k \approx 0$ in the form

$$\tilde{c}_{\parallel} = c_{\parallel} \left(1 + \frac{1}{2S} - \frac{1}{3S} \sum \frac{Q_k^2}{E_k} \left(\frac{5}{2} - Q_k^2 + \frac{3}{8} (9 - 4Q_k^2) \Lambda_k\right)\right) \tag{2.26}$$

where

$$Q_k^2 = \sin^2 \frac{k_x}{2} + \sin^2 \frac{k_x + \sqrt{3}k_y}{4} + \sin^2 \frac{k_x - \sqrt{3}k_y}{4}$$

$$\Lambda_k = -\frac{1}{3} + \left(\sin^4 \frac{k_x}{2} + \sin^4 \frac{k_x + \sqrt{3}k_y}{4} + \sin^4 \frac{k_x - \sqrt{3}k_y}{4}\right) \bigg/ Q_k^4.$$

Numerical integration then gives

$$\tilde{c}_{\parallel} = c_{\parallel} \left(1 - \frac{0.115}{2S}\right). \tag{2.27}$$

The structure of the expansion near $k = \pm Q$ is more involved and we refrain from presenting the analytical expression for the spin-wave velocity. Numerically, we obtained

$$\tilde{c}_{\perp} = c_{\perp} \left(1 + \frac{0.083}{2S}\right). \tag{2.28}$$

Comparing (2.27) and (2.28), we observe that quantum fluctuations tend to diminish the difference between the two spin-wave velocities. This is consistent with our $1/N$ result in [7] that the relative difference between $\tilde{c}_{\perp}$ and $\tilde{c}_{\parallel}$ should disappear at the quantum-critical point. We will use (2.27) and (2.28) below and now proceed with the calculations of sublattice magnetization.

## 2.3. Sublattice magnetization

We have shown above that to leading order in $1/S$, the correction to sublattice magnetization comes already from non-interacting magnons (equation (2.13)). Here we obtain the next term in the expansion in $1/S$, which is also the leading $1/S$ correction to the density of particles. We again have to consider both quartic and cubic terms, since they contribute at

the same order to $\sum_k \langle a_k^\dagger a_k \rangle$. As before, quartic terms only renormalize the coefficients in the quadratic form, and hence change the expression for the density of particles to

$$\sum_k \langle a_k^\dagger a_k \rangle = -\frac{1}{2} + \frac{1}{2} \sum_k \frac{\bar{A}_k}{\bar{E}_k} \tag{2.29}$$

where $\bar{A}_k$ and $\bar{E}_k$ are given by (2.14) and (2.15). In explicit form

$$\frac{1}{2} \sum_k \frac{\bar{A}_k}{\bar{E}_k} = \frac{1}{2} \sum_k \frac{1 + \nu_k/2}{E_k} - \frac{9}{32S} \sum_p \frac{\nu_p^2}{E_p} \sum_q \frac{\nu_q}{E_q} - \frac{9}{32S} \sum_p \frac{\nu_p(1 - \nu_p)}{E_p} \sum_q \frac{\nu_q(1 - \nu_q)}{E_q^3}. \tag{2.30}$$

We see that the very last term behaves near $q = Q$ as $|q - Q|^{-3}$ which makes the integral over $q$ divergent. The divergence is indeed an artificial one and should disappear when we add the contributions of the cubic terms.

To see how cubic terms modify (2.29), we express the density of particles in terms of the quasiparticle operators using (2.7) and (2.8):

$$\sum_k \langle a_k^\dagger a_k \rangle = -\frac{1}{2} + \frac{1}{2} \sum_k \frac{\bar{A}_k}{\bar{E}_k} - \sum_k \frac{\bar{B}_k}{\bar{E}_k} \langle c_k c_{-k} \rangle + \sum_k \frac{\bar{A}_k}{\bar{E}_k} \langle c_k^\dagger c_k \rangle. \tag{2.31}$$

The first two terms are just the renormalized spin-wave terms. The third correction is related to the anomalous self-energy term in figure 1. Performing the frequency summation in this term, we obtain

$$-\sum_k \frac{\bar{B}_k}{\bar{E}_k} \langle c_k c_{-k} \rangle = -\frac{9}{32S} \sum_k \frac{\nu_k}{E_k^3} \Psi_k \tag{2.32}$$

where

$$\Psi_k = \sum \frac{1}{E_1 E_2} \frac{\tilde{\Phi}_1(1,2;k)\tilde{\Phi}_2(1,2,-k)}{E_1 + E_2 + E_k}. \tag{2.33}$$

Finally, the last term in (2.31) contains the density of quasiparticles. This density is finite to order $1/S$ because among cubic non-linearities, there is the term which describes simultaneous emission of three spin waves. Evaluating the expectation value of $\langle c_k^\dagger c_k \rangle$ by the usual means, we obtain

$$\sum_k \frac{\bar{A}_k}{\bar{E}_k} \langle c_k^\dagger c_k \rangle = \frac{3}{16S} \sum_k \frac{1 + \nu_k/2}{E_k^2} \Upsilon_k \tag{2.34}$$

where

$$\Upsilon_k = \sum \frac{1}{E_1 E_2} \frac{|\tilde{\Phi}_2(1,2,k)|^2}{(E_1 + E_2 + E_k)^2}. \tag{2.35}$$

We first show that the total expression for the density of particles is free from divergencies. Simple inspection of equations (2.32)–(2.35) shows that the divergent contributions from the cubic terms (namely, $1/E^3$ and $1/E^2$ terms in (2.32) and $1/E^2$ terms in (2.34) ) come from the region $k \approx Q$, where $\Psi$ and $\Upsilon$ tend to constant values. For these $k$, we again use (2.23), substitute it into the vertex functions, and after some simple algebra obtain

$$\Psi_k = -(1 - \nu_Q) \sum_p \frac{\nu_p(1 - \nu_p)}{E_p} - E_k \Upsilon_Q + O(E_k^2). \tag{2.36}$$

Substituting further this expression into (2.32) and comparing the result with the divergent piece in (2.30), we find that the $1/E^3$ contributions from cubic and quartic terms, and the $1/E^2$ contributions from the two cubic terms cancel each other, so that the $1/S$ correction to the density of particles is finite, as it of course should be. We then performed numerical computation of the $1/S$ terms in (2.31) and obtained

$$\langle S \rangle = \left( S - 0.261 + \frac{0.027}{(2S)} \right). \tag{2.37}$$

For $S = 1/2$, equation (2.37) yields $\langle S \rangle \approx 0.266$, which is close to half the classical value. A very similar result was obtained earlier by Miyake [16], who calculated the on-site magnetization to order $1/S^2$ by evaluating numerically the response to a staggered magnetic field. His estimate for the $1/S^2$ correction is however somewhat smaller than ours (0.01 instead of 0.027). In any event, $1/S^2$ terms are rather small and can hardly change substantially the lowest-order spin-wave result for the magnetization [4]. We therefore found no support for the recent claim based on series expansion analysis [6] that the value of magnetization is substantially lower than the spin-wave prediction. Note, in passing, that for a square-lattice antiferromagnet, the first anharmonic correction to $\langle S \rangle$ is exactly zero [17]. Indeed, cubic terms are absent from the square-lattice antiferromagnet, and $1/S$ corrections due to quartic terms do not change the shape of the quasiparticle spectrum (that is, $\bar{A}_k/\bar{E}_k = A_k/E_k$ ). The next-to-leading-order correction in the square-lattice case has been calculated and found to be very small [17].

## 2.4. Uniform susceptibility

Now we calculate, to order $1/S$, the response of a triangular antiferromagnet to an external magnetic field, i.e., transverse and longitudinal susceptibilities. For classical spins, the two susceptibilities can easily be obtained by minimizing the ground state energy. This yields $\chi_\perp = \chi_\parallel = 2/9\sqrt{3}Ja^2$ where $a$ is the interatomic spacing ($a^2\sqrt{3}/2$ is the unit cell volume). As in the bulk of the paper, we define $\chi_\perp$ and $\chi_\parallel$ without the gyromagnetic ratio $g\mu_B/\hbar$. We see that the two susceptibilities are equal in the classical limit [18]. This degeneracy in the response to a magnetic field in a 2D triangular antiferromagnet has attracted some attention in the past as an example of the 'order from disorder' phenomenon [18–22]. For our present purposes, it is sufficient to observe that the degeneracy is a purely classical effect. It is not related to the symmetry properties of a quantum system and therefore should be broken by quantum fluctuations.

Technically, the computations in a finite field are more involved because the transverse field breaks the 120° ordering in the basal plane. In this case, a transformation to a twisted coordinate frame is no longer advantageous because Umklapp processes also contribute to

order $1/S$. It is then more convenient to introduce a separate Bose field for each of three sublattices. For the longitudinal response, the 120° ordering in the basal plane is preserved and a one-sublattice description with no Umklapp terms is still valid. However, one has to be careful in this case as well, because in the presence of a field, the excitation spectrum is no longer an even function of $k$. This is consistent with the fact that time reversal symmetry in a magnetic field requires that in changing $k \to -k$ in the spectrum, one has to change simultaneously the sign of $H$.

The corrections to the susceptibility tensor to order $1/S$ were computed by Golosov and one of us [21]. We refrain from presenting the details of the calculations and list here only the results. To order $1/S$, they are (notice that the definitions of $\chi_\perp$ and $\chi_\parallel$ in [21] are interchanged compared to ours):

$$\chi_\perp = \frac{2}{9\sqrt{3}Ja^2}\, Z_\perp^\chi \qquad \chi_\parallel = \frac{2}{9\sqrt{3}Ja^2}\, Z_\parallel^\chi \tag{2.38}$$

where

$$Z_\parallel^\chi = \left(1 + \frac{1}{2S}\sum_k \frac{v_k(1-v_k)}{E_k}\right) = 1 - \frac{0.449}{2S} \tag{2.39}$$

and

$$Z_\perp^\chi = \left(1 - \frac{1}{2S}\sum_k \frac{v_k(1+2v_k)}{E_k} + \frac{3}{2S}\sum_k \frac{v_k^2}{E_{k_1}+E_{k_2}}\frac{(f_-^{(1)}\,f_-^{(2)})^2}{E_{k_1}E_{k_2}}\right) = 1 - \frac{0.285}{2S} \tag{2.40}$$

where $f^{(i)} \equiv f^{(k_i)}$ were defined in (2.19). Note that contrary to the situation in a stacked 3D triangular antiferromagnet where $\chi_\parallel > \chi_\perp$, the transverse (in-plane) susceptibility in the 2D case turns out to be larger than the longitudinal one; this gives rise to an unconventional phase diagram in a magnetic field which has been discussed several times in the literature [18–21].

## 2.5. Spin stiffness

With the values of the two spin-wave velocities and spin susceptibilities at hand, we are now in a position to calculate the spin stiffnesses. To order $1/S$ they are

$$\rho_\perp = \chi_\perp c_\perp^2 = \frac{\sqrt{3}}{4}JS^2 Z_\perp^\rho \qquad \rho_\parallel = \chi_\parallel c_\parallel^2 = \frac{\sqrt{3}}{2}JS^2 Z_\parallel^\rho \tag{2.41}$$

where

$$Z_\perp^\rho = 1 - 0.119/2S \qquad Z_\parallel^\rho = 1 - 0.679/2S. \tag{2.42}$$

## 3. Conclusions

In this paper, we calculated in the $1/S$ expansion the $T = 0$ parameters of a 2D Heisenberg antiferromagnet on a triangular lattice. The two spin stiffnesses and susceptibilities were calculated to first order in $1/S$, while sublattice magnetization was calculated up to $O(1/S^2)$. We found that numerically, the $1/S^2$ correction to the magnetization is rather small even for $S = 1/2$ so that one may hope that already the first order in the $1/S$ expansion yields quite accurate results for all spin values. We expect the same to be true for stiffnesses and susceptibilities. The application of our $1/S$ results to $S = 1/2$ then yields $\chi_\perp = 0.09/Ja^2$, $\chi_\| = 0.07/Ja^2$, $\rho_\perp = 0.09J$, $\rho_\| = 0.07J$. We also found $N_0 = 0.266$ which is about a half of the classical value. Both the on-site magnetization and the spin stiffnesses are smaller than in a square-lattice antiferromagnet, where $N_0 = 0.3$ and $\rho_s = 0.18J$ [23]. However, the difference in magnetization is relatively small, and for stiffness it is mostly associated with geometrical factors. We therefore cannot conclude from our results that triangular antiferromagnets are much closer to quantum disordering transition than square-lattice ones, as has been recently suggested [6].

Finally, for comparisons with experimental and numerical results at finite $T$, when long-range order is absent, it is convenient to introduce the effective stiffness and susceptibility averaged over all three spatial directions:

$$\rho = \frac{2}{3}\rho_\perp + \frac{1}{3}\rho_\|  \qquad \chi = \frac{2}{3}\chi_\perp + \frac{1}{3}\chi_\|. \tag{3.1}$$

Application of $1/S$ results yields

$$\rho = \frac{1 - 0.399/2S}{\sqrt{3}} \, JS^2 tqs \chi = \frac{2}{9\sqrt{3}Ja^2} \, (1 - 0.339/2S). \tag{3.2}$$

For $S = 1/2$, we then have $\rho = 0.087J$, $\chi = 0.085/Ja^2$.

In a separate publication [7], we obtained the scaling expressions for various observables near the critical point (in the quantum-critical region) with $\rho$ and $\chi$ as input parameters. In particular, for the uniform susceptibility we obtained

$$\chi_u(T) = \left(\frac{g\mu_B}{\hbar}\right)^2 \left[0.86\chi + 0.145\frac{k_B T}{c^2}\right] \tag{3.3}$$

where $c^2 = \rho/\chi$. Substituting the values of $\chi$ and $\rho$ into (3.3), we obtain for $S = 1/2$

$$\chi_u(T) = \left(\frac{g\mu_B}{\hbar a}\right)^2 \frac{1}{J} \left[0.07\chi + 0.14\frac{k_B T}{J}\right]. \tag{3.4}$$

The temperature dependence of $\chi_u$ was recently studied in high-temperature series expansions [24]. The data show that $\chi_u$ obeys a Curie–Weiss law at high $T$, passes through a maximum at $T \approx 0.4J$, and then falls. Numerical data are available only over a relatively small temperature region below the maximum. Nevertheless, we fitted the data by a dependence linear in $T$, as in equation (3.4), and found $0.13 \pm 0.03$ for the slope and around 0.06 for the intercept—both results are in reasonable agreement with our theoretical expression. The comparison with other observables is considered at some length in [7].

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