On the nature of the order parameter in quantum antiferromagnets

Joseph Reger

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On the nature of the order parameter in quantum antiferromagnets

Joseph D. Reger

Institut fur Physik, Universität Mainz, D-6500 Mainz, Germany

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Abstract. — The first moments of the magnetization m_z of the $d = 2$, $S = \frac{1}{2}$ quantum Heisenberg antiferromagnet with nearest neighbor interactions on the square lattice are computed for $T = 0$ via path integral Monte Carlo Simulations. The results for the ratio $R = \langle m_z^4 \rangle / \langle m_z^2 \rangle^2$ show a cross-over at a system size of $N \approx 100$ to the classical behavior, $\lim_{N \to \infty} R = 9/5$. This supports the arguments that the long range order in the ground state is reached by a spontaneous symmetry breaking, just as in the classical case.

1. Introduction.

It seems that an agreement has been reached in the literature on the existence of long range order in the ground state of the two-dimensional nearest neighbor $S = \frac{1}{2}$ isotropic antiferromagnetic quantum Heisenberg model on the square lattice, e.g. [1-8], and probably on all regular unfrustrated lattices in two dimensions [9]. The question has a long history and the interest in it has been revived recently by the discovery of the new high-T_c materials.

More precisely, the consensus is that the quantum fluctuations, althrough they reduce the long range order in the ground state, are not strong enough to completely destroy it. There is no consent however, on the precise value of the magnetization at $T = 0$ (although a clear majority favors about 60% of the classical value), or on the mechanism by which the long range order is built up. Some reports of computer simulations quote rather low numerical values, but this discrepancy stems from a numerical factor which is omitted with the argument that the usual (classical) symmetry breaking scenario is not applicable here [3]. This is because the order parameter vector will have fluctuations in its *length* for quantum mechanical reasons, as it has been argued subsequently [10]. In this case one would not be permitted to anticipate in finite systems the effects of spontaneous symmetry breaking in the usual way [3]. In a different study it has been even explicitely argued that the long range order is reached without symmetry breaking [4].

Symmetry breaking occurs, of course, in the thermodynamic limit only. Hence, the correct definition of the order parameter in finite systems simulates the effect of spontaneous symmetry breaking by applying an infinitesimal symmetry breaking field, taking the thermodynamic limit *in the presence of the field* and letting this field tend to zero as the last step. unfortunately, this procedure is impractical for most systems because the range of sizes that can be studied is too small. One argues instead, that for large systems without external fields the distribution of the order parameter vector will be strongly peaked at a particular value of the magnitude, but otherwise rotationally invariant. The application of an external field, provided it is infinitesimal, will merely fix the direction of the order parameter vector. Therefore the magnitude of the order parameter is the correct measure of order in finite systems.

It has been pointed out recently [10] that this argument is only valid if implicit assumptions about the lack of fluctuations in the magnitude of the order parameter vector are fulfilled. The authors of [10] argue that they are *not* fulfilled for quantum *anti*ferromagnets. This would place quantum antiferromagnets into a different class from quantum ferromagnets and classical magnets.

The issue raised has both theoretical and practical importance. Firstly, if the quantum antiferromagnet is so different, it is difficult to understand the apparently excellent agreement with spin wave theory [2, 8, 11], as well as the mounting evidence that this system's behavior is essentially classical [12-14]. Secondly, if the order parameter is not a classical vector and the conventional symmetry breaking scenario is not applicable, it is very difficult to interpret the results of the Monte Carlo simulations, which supply rotationally invariant correlation functions of one component of the order parameter only [5, 9], typically the magnetization m_z. The results of the simulations and the spin wave theory are in good agreement with the experimental results [9].

The purpose of the present study was to test the violation of the above mentioned assumptions in the two-dimensional nearest neighbor $S = \frac{1}{2}$ isotropic antiferromagnetic quantum Heisenberg model on the square lattice. We follow the proposition of [10] and study the ratio of moments of the magnetization distribution

$$R = \frac{\langle m_z^4 \rangle}{\langle m_z^2 \rangle^2}$$

If the order parameter $\mathbf{m} = (m_x,\ m_y,\ m_z)$ is a classical vector of fixed length and has an isotropic distribution, then in 3 dimensions one obtains $R = 9/5$ by performing two simple integrals in spherical coordinates.

The previous results for R, that showed a monotonic increase with increasing system size to a value of about 1.9 and led to the conclusion that the classical value of $9/5 = 1\,8$ will not be reached, were obtained from simulations on very small systems ($N \le 20$). Since this behavior was surprising and the issue raised very important, it was clearly of interest to check whether the above trend continues for much larger system sizes.

2. The method.

The simulations were carried out using the world-line path integral Monte Carlo technique, as described in earlier work [5, 9]. The computations were quite demanding, since it is more difficult to determine higher moments of the order parameter with comparable statistical errors than lower moments. Fortunately, however, one does not need very high accuracy to find the correct *trend* of the data as a function of system size.

Hence, no attempt has been made to obtain smaller *statistical* errors in the final estimates than sufficient to establish the right trend. The inherent *systematic* errors of the method due to finite temperature and finite Trotter-dimension in the simulation were kept under control in the same fashion as described by [5, 9]. The simulations were performed for lattice sizes of 2×2, 4×4,

8×8, 10×10 and 12×12. The temperature T used upto linear system size $L = 10$ was $T = 0.1$, a value that guarantees temperature independent ($T = 0$) results for these system sizes. For $L = 12$ the value $\beta = T^{-1} = 15$ was used. The number of "time slices" were between 100 and 200, for $L = 12$ between 100 and 400. Several different values were used to perform a quadratic fit, from which the extrapolated value for infinite Trotter-dimension was obtained. For the largest system size 500000 MCS/spin were needed, out of which 200000 MCS/spin were discarded for equilibration. 5-7 MC runs were averaged to estimate statistical errors.

The simulations were carried out on a multi-processor Transputer machine containing 88 processors (T800/20). The existing code [5] was parallelized using geometrical decomposition in the Trotter-dimension (this is the obvious choice, since it is an order of magnitude larger than the space-like dimensions). In this scheme the processors are connected into a ring topology to comply with periodic boundary conditions and the adjacent processors update the spin variables in neighboring blocks of "time slices". One needs rather sophisticated communication between the processors to ensure detailed balance. Despite of this, an overall parallel efficiency of 80% could be achieved.

3. Results.

The results are shown in figure 1. The ratio of moments $\langle m_z^4 \rangle / \langle m_z^2 \rangle^2$ is plotted against $1/N$ Some of the data of [10] (upto $N = 20$) are also included (open circles). Note that the x-axis is $1/N$ in contrast to [10] where $1/N^2$ is used, which is justified for the infinite range Lieb-Mattis model only. The present choice enables one to plot all the available data in a single figure. Clearly, the conclusion is not influenced by this choice in any way.

For small system sizes we reproduce the results of [10], where available. The ratio is monotonically increasing upto $N = 64$. For larger system sizes it decreases again and approaches the classical limit of 9/5. The error bars in the latter region are shown.

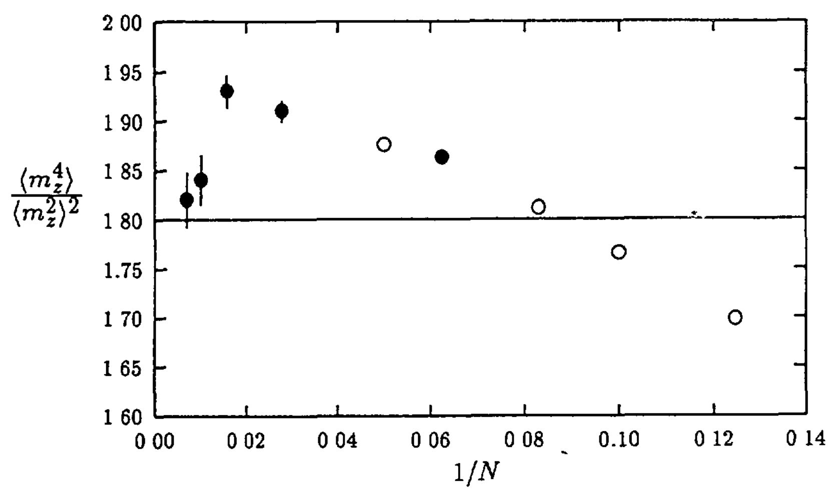

Fig. 1. — The ratio of moments $R = \langle m_z^4 \rangle / \langle m_z^2 \rangle^2$ of the magnetization of the nearest neighbor $S = 1/2$ Heisenberg antiferromagnet on the square lattice *versus* $1/N$ Some of the results of [10] are also included (open circles). A cross-over to the classical value of 9/5 is observed for $N \approx 100$ The error bars are shown in this region only.

4. Discussion.

The non-monotonic behavior of R is somewhat unusual and has to be contrasted with the results for the Lieb-Mattis model [15], which does *not* exhibit this behavior, but rather converges monotonically to the classical value [10]. The Lieb-Mattis model is, however, an *infinite range* Heisenberg model. It has been studied in detail, the exact solution is known [16]. One can explicitly examine its finite size behavior and find the following [16, 17]: There is spontaneous symmetry breaking in the thermodynamic limit, where at $T = 0$ all states with different values of the total spin become degenerate. The same scenario has been demonstrated for the infinite range XY-model [18]. The ratio R can be easily computed analytically [17]. It approaches the classical value monotonically from below, in agreement with the results of the simulations [10]. Moreover, one can derive the distribution function of the magnetization $P(m_z)$, which is uniform since the ground state has long range order. The *only* finite size effect in $P(m_z)$ is the discreteness of the possible values of m_z, but all values have the same weight, i.e. the distribution is sharp for all sizes.

On the other hand it is obvious that in the *short range* model there will be an *additional* finite size effect: The rounding of the shape of $P(m_z)$ for smaller system sizes. This has also been explicitly demonstrated in simulations, see figure 10 of [9]. There is a presumably complicated interplay between the two effects, which can lead to the cross-over behavior found in figure 1. In the thermodynamic limit $P(m_z)$ becomes sharp and the classical value of R is restored. It is clear that all states with arbitrarily large angular momentum are contained in the ground state in this case, too (for numerical evidence see [19]). The ground state of the model is a symmetry broken state.

A detailed understanding of the non-monotonic behavior of R, however, is still missing and is clearly an interesting question.

5. Conclusion.

In conclusion, the above results show that the nature of the order parameter in quantum antiferromagnets is indeed classical in the sense that the fluctuations in its magnitude disappear in the thermodynamic limit, in other words the order parameter $\mathbf{m}$ is an isotropically distributed classical vector. It is correct to think about the spontaneous symmetry breaking in this model in the same fashion as in classical spin systems: in finite systems the rotationally invariant expression of the order parameter (magnitude) is the appropriate measure of order.

Hence, in this respect, the quantum Heisenberg antiferromagnet belongs to the same class of models as the quantum ferromagnetic Heisenberg model, as well as the classical counterparts. This result is in agreement with other studies which find that, although this is a quantum system, its behavior is essentially classical [12-14].

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