Large-Scale Numerical Evidence for Bose Condensation in the $S = 1$ Antiferromagnetic Chain in a Strong Field

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Abstract

Using the recently proposed density matrix renormalization group technique we show that the magnons in the $S = 1$ antiferromagnetic Heisenberg chain effectively behaves as bosons that condense at a critical field $h_c$. We determine the spin-wave velocity, $v = 2.49(1)$, as well as the gap $\Delta = 0.4107(1)J$. 75.10.-b, 75.10.Jm, 75.40.Mg
It is by now well established both experimentally \cite{2} and theoretically \cite{3-7} that the $S = 1$ antiferromagnetic chain has a gap, $\Delta$, to a triplet excitation above a singlet ground-state. Thus the magnetization, $M$, remains strictly zero up to a critical field $h_c = \Delta$. For the quasi-one-dimensional system NENP the critical field is found to be about 10T \cite{8} for a field applied along the symmetry axis. The behavior of $M(h)$ just above $h_c$ has been the subject of some theoretical work \cite{9-11}. The existing experimental results \cite{12} appear to be dominated by extraneous effects such as an off-diagonal alternating component of the gyromagnetic tensor \cite{13}, inter-chain coupling, anisotropies and impurities.

This problem can be solved using a boson quasi-particle model involving triplet magnons with repulsive interactions for parallel spins \cite{11}. This model predicts that $h_c = \Delta$. (We set the Bohr magneton and $g$-factors to one.) At this field the “rest-mass energy” of the magnons is exactly cancelled by their Zeeman energy and one-dimensional Bose condensation occurs. What prevents a catastrophe from occurring at $h_c$ is the inter-magnon repulsion which governs the behavior of $M(h)$ above $h_c$. To calculate $M(h)$ we need to calculate the energy, $E(M)$ of a very dilute system of $M$ polarized magnons in their ground-state. $M(h)$ is then found by inverting the equation: $h = dE/dM$. It was argued in Ref. \cite{11} that the behavior of $E(M)$ is the same as for a system of non-relativistic non-interacting fermions:

$$E = (\Delta - h)M + L \int_{-k_F}^{k_F} \frac{dk}{2\pi} \frac{v^2 k^2}{2\Delta}.$$  \hfill (1)

Here $v$ is the velocity, determined from the single magnon dispersion relation at low energies:

$$\omega(k) = \Delta + v^2 (k - \pi)^2/2\Delta + O([k - \pi]^3),$$  \hfill (2)

$L$ is the length of the system and $k_F$ is determined from the particle number:

$$M = L \int_{-k_F}^{k_F} \frac{dk}{2\pi} = Lk_F/\pi.$$  \hfill (3)

This gives, $E = M(\Delta - h) + (v\pi)^2 M^3/6\Delta L^2 + O(M^4)$ and hence

$$M/L = \sqrt{(h - \Delta)2\Delta/\pi v},$$  \hfill (4)

up to terms of higher order in $h - \Delta$. 

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This formula was first given based on a non-interacting fermion model of magnons [4]. It was later argued to also arise from an interacting boson model [11,12] sufficiently close to $h_c$, and hence to be exact. It is expected to be valid for very general short-range repulsive interactions between the spin-polarized magnons. It should hold for arbitrarily weak interactions for long enough chains. The reason is that when the average inter-magnon spacing is very large compared to the range of the repulsive interaction the multi-magnon wave-function, $\Psi_M(x_1, x_2, \ldots x_M)$, can be approximated by a free fermion (Bloch) wave-function multiplied by the sign function $\epsilon(x_1, x_2, \ldots x_M)$ which has the value $\pm 1$ and changes sign whenever two particles are interchanged of the following form

$$\Psi_M(x_1, x_2, \ldots x_M) = \frac{1}{\sqrt{M!}} \epsilon(x_1, x_2, \ldots x_M) \sum_{P(i_1, \ldots i_M)} \prod_{i=1}^{M} \psi_1(x_{i_1})\psi_2(x_{i_2})\ldots \psi_M(x_{i_M}) \text{sgn}P. \quad (5)$$

Here $P$ denotes the permutation and $\text{sgn}P$ the sign of the permutation. $\psi_i(x)$ is a single-particle non-interacting wave-function depending on the wave-vector $k_i$. $\Psi_M$ is symmetric as required by Bose statistics, is a solution of the non-interacting Schrödinger equation almost everywhere (ie. except where two or more particles intersect) and vanishes whenever two or more particles come together. As such it is expected to become exact in the dilute limit and hence to give exactly the magnetization as $h \to h_c$.

Until very recently it has been essentially impossible to test this prediction by numerical simulations. The reason is that extremely long systems are required. To simulate the $M$-magnon problem in the dilute regime we need a length $L >> M\xi$ where $\xi \approx 6$ is the correlation length or the approximate range of the inter-magnon interaction. In practice it appears that $L \geq 30M$ is required. Before last year, the longest chains that had been studied accurately had $L = 32$ so good results were only available for a single magnon and it was impossible to study magnon interactions. This situation has now completely changed thanks to a breakthrough in the real-space renormalization group technique made by Steven White [1] which makes it quite feasible to study chains of length 100 or longer using a density matrix renormalization group (DMRG) approach. We will present results here on chains of length up to 100 containing up to three magnons. White and Huse [5] obtained related
numerical results independently. We analyze our results in a different way which establishes Eq. (4). Our results indicate quite convincingly that the lowest energy two or three magnon state has the form discussed above; namely the lowest-energy free fermion wave-function multiplied by the sign function. We establish this result in two ways. Firstly we study 

\[ S^z(x) = \sum_{j=1}^{M} \delta(x - \hat{x}_j), \]

where \( \hat{x}_j \) is the position operator for the j’th particle, showing that it has the expected form:

\[ \langle S^z(x) \rangle = M \int dx_2 dx_3 ... dx_M |\Psi_M(x, x_2, x_3, ... x_M)|^2. \]  

(6)

Secondly, we study the finite-size dependence of the energy of the multi-magnon ground-state, showing that it behaves as:

\[ E(M) \approx \sum_{i=1}^{M} \omega(k_i). \]  

(7)

Holding \( M \) fixed and taking \( L \to \infty \), the \( k_i \)'s are \( O(1/L) \) so the above formula gives \( E(M, L) = M(\Delta - h) + a(M)/L^2 \). The corrections to Eq. (7) from inter-magnon interactions are expected to be \( O(L^{-3}) \). This power of \( L \) can be most easily understood in the \( M = 2 \) case. The wave-function contains a \( L^{-1} \) normalization factor but is \( O(L^{-2}) \) over the entire region where the interaction is non-negligible since it vanishes proportional to \( k(x_1 - x_2) \) with \( k \) of \( O(L^{-1}) \). The power \( L^{-3} \) arises from squaring the wave-function and picking up a factor of \( L \) from the integral over the center-of-mass position. We verify that the corrections to Eq. (7) are indeed of this order.

The DMRG method does create certain technical problems because of the fact that implementing it optimally requires studying chains with open, rather than periodic boundary conditions. Such chains have \( S = 1/2 \) excitations localized near the ends which have been the subject of a number of experimental and theoretical studies [14]. For our purposes they are just a minor annoyance. They are also found to have repulsive interactions with the bulk magnons for parallel spins. Thus the magnon wave-functions essentially obey vanishing boundary conditions at the ends, with additional corrections of \( O(L^{-3}) \) to the energy, Eq. (7), from the magnon-end excitation interactions. We also considered more
general boundary conditions for the magnon wave-functions. These were found to change the energy only to $O(L^{-3})$ since they lead to negligible changes in the wave-function.

The DMRG method for open chains leaves only two good quantum numbers the total $S^z$ component, $S^z_T$, and the parity, $P$. These are conserved under iteration and it is therefore possible to work within a subspace defined by these two quantum numbers. We need to determine the parity for low-lying states with a given $S^z_T$. We shall only be concerned with chains of even length. For these chains the ground-state is a singlet with even parity, $0^+$. Above the ground-state is an exponentially low-lying triplet, $1^-$. In the thermodynamic limit the triplet and the singlet become degenerate and the ground-state four-fold degenerate. This spectrum can be seen to arise from the two $S = 1/2$ end-excitations forming either an odd parity singlet or an even parity triplet, in addition to an overall parity flip coming from the rest of the ground-state. This parity-flip can be understood from the valence bond solid state [7] where we draw two valence bonds emanating from each site. These valence bonds represent singlet contractions of pairs of $S = 1/2$’s so they have a directionality associated with them. When we make a parity transformation we flip the orientation of an odd number of valence bonds resulting in a $(-)$ sign. Thus, the parity, $P_E$, of a state with no magnons present is $(+)$ if the end excitations combine into the singlet and $(-)$ for the triplet. The parity of higher excited states, containing one or more magnons, is a product of three factors, $P_E P_{SW} P_m$. $P_m$ contains a contribution of $(-)$ from each magnon present. This is because the magnons are created and annihilated by the staggered magnetization operator, and this changes sign upon switching even and odd sublattices. $P_{SW}$ is the parity of the spatial wave-functions of the magnons. For instance, for a single magnon, the wave-functions, $\psi_i$, in Eq. (3) are $\psi_i = \sqrt{2/(L-1)} \sin k_i x$, $k_i = \pi n_i/(L-1)$, with $n_i$ odd for even parity and $n_i$ even for odd parity. We take $0 \leq x \leq L-1$ and parity will therefore take $x$ into $L-1-x$.

For a chain with open boundary conditions the lowest lying state of a given magnetization, $M$, will have $M = m+1$, where $m$ is the number of magnons present and the additional term, 1, corresponds to the end excitations forming a triplet. In order to minimize the inter-magnon repulsion, the wave-function for large $L$ takes the Bloch form of Eq. (3), with $\psi_i$ as
above and \( n_i = i \), in order to satisfy vanishing boundary conditions. Thus Eq. (8) becomes

\[
E_{m+1}(L) - E_1(L) = (\Delta - h)m + \frac{(v\pi)^2}{2\Delta(L - 1)^2} \sum_{i=1}^{m} n_i^2 + O(L^{-3}), \quad n_i = i.
\]

We test this formula below for \( m = 1, 2 \) and 3.

The \( 1^- \) state becomes degenerate with the ground-state in the thermodynamic limit and we shall therefore view this state as the reference state and calculate energy gaps with respect to this state and not \( 0^+ \), as already implied in Eq. (8). We have calculated the gap as a function of chain length between this state and three of the low lying states using density matrices of the size \( 243 \times 243 \) keeping 81 eigenvectors of these matrices at each iterations. For each of these states we have also calculated \( \langle S_z \rangle \) and \( \langle S_i \cdot S_{i+1} \rangle \) along a \( L = 100 \) site chain using a finite lattice method [1]. For a discussion of the numerical procedure we refer the reader to Ref. [1]. A brief summary of our results is shown in Table I.

The lowest lying \( M = m + 1 = 2 \) state corresponds to a state with the end excitations in the \( 1^- \) state and one magnon present. This state has therefore parity (+) since \( P_E = (-), P_{SW} = (+) \) and \( P_m = (-) \). We approximate the wave-function as consisting of two factors existing in different Hilbert spaces. A factor from the end excitations and a factor, \( \Psi_m \), corresponding to the \( m \)-magnon wave-function. From the above discussion we see that for a single magnon the magnon part of the wave-function, \( \Psi_m \), becomes \( \Psi_1 = \sqrt{\frac{2}{L-1}} \sin k_1 x \), \( n_1 = 1 \). From Eq. (8) we then see that \( \langle S_i^z \rangle >_{2^+} - \langle S_i^z \rangle >_{1^-} = \frac{2}{L-1} \sin^2 k_1 x \), which is shown as the solid line in Fig. I. Here the subtraction of \( \langle S_i^z \rangle >_{1^-} \) essentially removes any contribution from the end-excitations. In Fig. I we show \( \langle S_i^z \rangle >_{2^+} - \langle S_i^z \rangle >_{1^-} \). An excellent agreement is evident. Also shown in Fig. I is the local bond energy \( e_i^{21} = \langle S_i \cdot S_{i+1} \rangle >_{2^+} - \langle S_i \cdot S_{i+1} \rangle >_{1^-} \). The dilute boson model predicts an energy density, \( e(x) \simeq \Delta \sum_{j=1}^{m} \delta(x - \hat{x}_j) \) ignoring the \( O(L^{-2}) \) kinetic energy. Therefore \( e(x) \) should be proportional to \( S^z(x) \) in Eq. (9), the proportionality factor being the gap, \( \Delta \). In Fig. I this prediction is shown as the dotted line. From Eq. (8) we can now extract values for the gap, \( \Delta \), and the velocity, \( v \). The fit of \( \Delta_{21}(L) = E_{2^+}(L) - E_{1^-}(L) \) to Eq. (8) is excellent, and we obtain \( \Delta_{21}(L) = 0.4107(1) + 74.7(4)(L - 1)^{-2} + O([L - 1]^{-3}), \)
with $\chi^2 = 4.55$. We see that $\Delta = 0.4107(1)$, $v = 2.49(1)$. The value of $\Delta$ is in excellent agreement with what was previously obtained [13]. The value of $v$ is in good agreement with the value $v = 2.46$ that can be extracted from exact diagonalization [3], and the value $v \sim 2.36$ obtained from $1/S$ expansions [15]. It is also in good agreement with the experimental results on NENP [16], $v \sim 2.45$. The coefficient, $74.7(4)$, in front of the $(L - 1)^{-2}$ term, that determines $v$, differs marginally from what was obtained by White [1], (67.9), due to the use of a different polynomial form.

The lowest lying 2-magnon state has parity $(-)$ since $P_E = (-), P_{SW} = (+), P_m = (+)$ and total magnetization $M = m + 1 = 3$. The magnon part of the wave-function is $\Psi_2 = \frac{2}{L-1} [\sin k_1 x_1 \sin k_2 x_2 - \sin k_1 x_2 \sin k_2 x_1] \epsilon(x_1, x_2)$ with $n_1 = 1$, $n_2 = 2$. Note that under parity $x_i \rightarrow L - x_i - 1$, $\sin k_1 x_i$ is even, $\sin k_2 x_i$ is odd and $\epsilon(x_1, x_2)$ is odd resulting in $P_{SW} = (+)$. We now obtain $< S_i^z >_{3^-} - < S_i^z >_{1^-} = \frac{2}{L-1} \{\sin^2 k_1 x + \sin^2 k_2 x\}$, which is shown as the solid line in Fig. 2. The dotted line represents the theoretical prediction for the local bond energy which is also shown in Fig. 2. Again we fit $\Delta_{31}(L) = E_{3^-}(L) - E_{1^-}(L)$ to Eq. (8) and we obtain $\Delta_{31}(L) = 0.823(1) + 359(5)(L - 1)^{-2} + O([L - 1]^{-3})$. The constant term should be $2\Delta$ in good agreement with the value of $\Delta$ obtained above. Since in this case we expect $n_1 = 1$, $n_2 = 2$ and therefore $\sum n_i^2 = 5$, the coefficient in front of the $(L - 1)^{-2}$ term should be 5 times greater than what we found for the $2^-$ level. Clearly this is the case: we obtain $\sum n_i^2 = 4.80(6)$, and the only values of $n_i$ consistent with our results are indeed $n_1 = 1$, $n_2 = 2$.

The three magnon state with $M = m + 1 = 4$ has parity $(+)$ by the same arguments as above. The wave-function now has 6 terms and we obtain $< S_i^z >_{4^+} - < S_i^z >_{1^-} = \frac{2}{L-1} \{\sin^2 k_1 x + \sin^2 k_2 x + \sin^2 k_3 x\}$, with $n_1 = 1$, $n_2 = 2$, $n_3 = 3$. This expression is shown as the solid line in Fig. 3 along with the numerical results for $< S_i^z >_{4^+} - < S_i^z >_{1^-}$ and the local bond energy $< S_i \cdot S_{i+1} >_{4^+} - < S_i \cdot S_{i+1} >_{1^-}$. The dotted line is the prediction for the local bond energy. Again good agreement is evident between theory and the numerical results is seen. Fitting the energy gap to Eq. (8) we find that the $(L - 1)^{-2}$ term now has a coefficient of 1030(150). Thus in this case, if we use the value of $v$ determined above,
∑n_i^2 = 14(2). This is only consistent with the values n_1 = 1, n_2 = 2, n_3 = 3. The DMRG method works progressively worse for states with higher magnetization and the agreement between the theory and the numerical results is therefore not as spectacular for this state as for the states previously discussed.

In summary we find that the numerical results are in excellent agreement with Eq. (8) with \( v = 2.49(1), \Delta = 0.4107(1) \). The magnons behave as bosons with repulsive interactions among themselves and with the end excitations. The lowest energy state for given \( M \) has the Bloch form of Eq. (5), implying the validity of Eq. (4).

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REFERENCES

[1] S. R. White, Phys. Rev. Lett. 69, 2863 (1992).

[2] W. J. L. Buyers, R. M. Morra, R. L. Armstrong, M. J. Hogan, P. Gerlach, and K. Hirikawa, Phys. Rev. Lett. 56, 371 (1986); J. P. Renard, M. Verdaguer, L.P. Regnault, W. A. C. Erkelens, J. Rossat-Mignod, and W. G. Stirling, Europhys. Lett. 3, 945 (1988).

[3] F. D. M. Haldane, Phys. Lett. 93A, 464 (1983); R. Botet and R. Julien, Phys. Rev. B 27, 613, (1983); R. Botet, R. Julien, and M. Kolb, Phys. Rev. B 28, 3914 (1983); M. Kolb, R. Botet, and R. Julien, J. Phys. A 16 L673 (1983); M. P. Nightingale and H. W. J. Blöte, Phys. Rev. B 33, 659 (1986); H. J. Schulz and T. A. L. Ziman, Phys. Rev. B 33, 6545 (1986).

[4] M. Takahashi, Phys. Rev. Lett. 62, 2313 (1989).

[5] S. R. White and D. A. Huse, to be published.

[6] M. Takahashi to be published.

[7] For a review see I. Affleck, J. Phys. Cond. Matt. 1, 3047 (1989).

[8] Y. Ajiro, T. Goto, H. Kikuchi, T. Sakakibara, and T. Inami, Phys. Rev. Lett. 63, 1424 (1989); K. Katsumata, H. Hori, T. Takeuchi, M. Date, A. Yamagishi, and J. P. Renard, Phys. Rev. Lett. 63 (1989).

[9] A. M. Tsvelik, Phys. Rev. B 42, 10499 (1990).

[10] K. Nomura and T. Sakai, Phys. Rev. B 44, 5092 (1991); T. Sakai and M. Takahashi, Phys. Rev. B 43, 13383 (1991).

[11] I. Affleck, Phys. Rev. B 43 3215 (1991).

[12] K. Katsumata, H. Hori, T. Takeuchi, M. Date, A. Yamagishi and J.P. Renard, Phys.
Rev. Lett. 63, 86 (1989); Y. Ajiro, T. Goto, H. Kikuchi, T. Sakakibara and T. Inami, Phys. Rev. Lett. 63, 1424 (1989).

[13] M. Chiba, Y. Ajiro, H. Kikuchi, T. Kubo, and T. Morimoto, Phys. Rev. B 44, 2838 (1991).

[14] T. Kennedy, J. Phys. Cond. Matt. 2, 5737 (1990); M. Hagiwara, K. Katsumata, I. Affleck, B. I. Halperin, and J.-P. Renard, Phys. Rev. Lett. 65, 3181 (1990); S. J. Glarum, S. Geschwind, K. M. Lee, M. L. Kaplan, and J. Michel, Phys. Rev. Lett. 67, 1614 (1991).

[15] D. V. Kveshchenko and A. V. Chubukov, Sov. Phys. JETP 66, 1088 (1987).

[16] S. Ma, C. Broholm, D. H. Reich, B. J. Sternlieb, and R. W. Erwin, Phys. Rev. Lett. 69, 3571 (1992).
TABLES

**TABLE I.** The spectrum of the $L=100$ open $S=1$ antiferromagnetic Heisenberg chain.

| $S^P_T$ | $-E$    |
|---------|---------|
| $1^-$   | 138.940086 |
| $2^+$   | 138.522461 |
| $3^-$   | 138.08557  |
| $4^+$   | 137.603    |


FIGURES

FIG. 1. The open circles represent $< S_i^z >_{2+} - < S_i^z >_{1-}$. The solid line is the expression given in the text. Also shown, by triangles, is $< \mathbf{S}_i \cdot \mathbf{S}_{i+1} >_{2+} - < \mathbf{S}_i \cdot \mathbf{S}_{i+1} >_{1-}$. The dotted line is the prediction for this local bond energy.

FIG. 2. The open circles represent $< S_i^z >_{3-} - < S_i^z >_{1-}$. The solid line is the expression given in the text. Also shown, by triangles, is $< \mathbf{S}_i \cdot \mathbf{S}_{i+1} >_{3-} - < \mathbf{S}_i \cdot \mathbf{S}_{i+1} >_{1-}$. The dotted line is the prediction for this local bond energy.

FIG. 3. The open circles represent $< S_i^z >_{4+} - < S_i^z >_{1-}$. The solid line is the expression given in the text. Also shown, by triangles, is $< \mathbf{S}_i \cdot \mathbf{S}_{i+1} >_{4+} - < \mathbf{S}_i \cdot \mathbf{S}_{i+1} >_{1-}$. The dotted line is the prediction for this local bond energy.