Finite-size spectrum, magnon interactions, and magnetization of $S=1$ Heisenberg spin chains

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We report on density-matrix renormalization-group and analytical work on $S=1$ antiferromagnetic Heisenberg spin chains. We study the finite-size behavior within the framework of the nonlinear σ model. We study the effect of magnon-magnon interactions on the finite-size spectrum and on the magnetization curve close to the critical magnetic field, determine the magnon scattering length, and compare it to the prediction from the nonlinear σ model.

I. INTRODUCTION

Since Haldane pointed out the difference between integer spin and half integer spin Heisenberg chains,¹ the richness of the physics in the Heisenberg model has attracted much attention. The $S=1$ antiferromagnetic Heisenberg chain is gapped¹ and the magnitude of the gap has been accurately computed.^{2,3} With open boundary conditions (OBC's), the Hamiltonian:

$$H = \sum_{j=1}^{L-1} \mathbf{S}_j \cdot \mathbf{S}_{j+1}, \quad (1.1)$$

gives low-energy effective $S=1/2$ spins localized near the chain ends whose interaction decreases exponentially with system size, resulting in an exponentially low-lying excited state.⁴⁻⁹

Many low-energy features of the model can be understood using an approximate mapping onto the nonlinear σ model (NL σ M). In particular, the low-lying excited states are constructed from a triplet of interacting bosons (magnons). There are various types of predictions from the NL σ M for the behavior of $S=1$ chains that have been tested to varying extents numerically or experimentally. Some of the predictions are not really specific to the NL σ M but would follow from any relativistic quantum field theory with a triplet of massive particles. These include the relativistic dispersion relation,¹⁰ exponential temperature (T) dependence of the susceptibility and Bose condensation transition at a critical magnetic field.^{11,12} A qualitative prediction specific to the NL σ M is the absence of bound states. Quantitative predictions, following from the details of the magnon interactions, have also been made concerning the two-¹³ and three-¹⁴ magnon contributions to the neutron-scattering cross section. However, perhaps mainly because these contributions are so small, they have, so far, not been extensively tested numerically or experimentally. A numerical test of the *equal time* correlation function is discussed in Ref. 24.

In this paper we present numerical results on low-lying states of the spin chain with both open and periodic boundary conditions using the density-matrix group (DMRG)

technique.¹⁵ We keep $m=800$ states in our DMRG calculations. The biggest truncation error is 10^{-8} and the largest system size is $L=200$. These results are used to study the interactions of the edge spins with each other and with bulk magnons, as well as the interactions of two magnons with each other. In particular, we determine numerically one parameter which characterizes the low-energy magnon interactions, the scattering length for two parallel spin magnons. We deduce how this single parameter determines finite-size corrections to the $S=2$ two-magnon state with both periodic and open boundary conditions. We also show that the same parameter determines the leading correction to the square-root singularity of the magnetization at the (lower) critical field and generalize these results to finite T and length L . Numerical results on all these quantities give a consistent value for the magnon scattering length of the $S=1$ chain, of about -2 lattice constants or about $-\xi/3$ where ξ is the correlation length. On the other hand, the exact S matrix for the NL σ M gives a scattering length of $-2\xi/\pi$, roughly twice as large. Thus, the NL σ M does not fair well in this quantitative comparison to the $S=1$ chain. This is perhaps not terribly surprising given that the mapping only becomes exact, at low energies, at large S . Better agreement could be expected for larger S or for $S=1$ with a (nonfrustrating) ferromagnetic next-nearest-neighbor coupling added to decrease the bare coupling constant in the NL σ M. This rather poor agreement suggests that other predictions of the NL σ M, such as the two-¹³ and three-¹⁴ magnon contributions to the neutron-scattering cross section may not be very accurate either.

The L dependence of the single magnon energy for open chains has been found to behave as $1/L$ for medium chain length and as $\Delta + O(1/L^2)$ for long chain length.¹⁶ In this paper we will show that those two behaviors for different range of lengths have a unified expression $\sqrt{\Delta^2 + v^2 \sin^2 \pi/(L+2)}$.

With periodic boundary conditions (PBC's) finite-size corrections to the ground state and single magnon energies are exponentially small but, as we show, the lowest two-magnon state (with $S=2$) has energy:

$$E_{2P} - E_{0P} = 2 \sqrt{\Delta^2 + v^2 \sin^2 \frac{\pi}{L-2a}}. \quad (1.2)$$

We will use the physical quantities obtained for $S=1$ spin chains in previous studies $\Delta=0.4105$ and $v=2.49$. Note that the Lorentz invariant dispersion relation $E=\sqrt{\Delta^2+(vk)^2}$ has been modified by the replacement:

$$k \rightarrow \sin k. \quad (1.3)$$

(Throughout this paper we use wave vectors shifted by π so that the minimum energy single magnon excitation occurs at $k=0$.) This modification only affects the expansion in $1/L$ at $O(1/L^4)$. To order $1/L^2$, this is just the energy of two free magnons with wave vectors $\pm \pi/L$. The fact that these wave vectors are nonzero and different reflects the hard-core boson approximation in which the wave function is approximated by a free fermion (Bloch) wave function, multiplied by a sign function to correct the statistics. The antisymmetric nature of the Bloch wave function requires the use of two different wave vectors. Periodic boundary conditions then requires them to be odd multiples of $\pm \pi/L$. a is a new parameter which we introduce, the magnon-magnon scattering length. This leads to an $O(1/L^3)$ correction:

$$E_{2p}-E_{0p} \approx 2\Delta + \frac{1}{\Delta} \left(\frac{v\pi}{L} \right)^2 + \left(\frac{4a}{\Delta L} \right) \left(\frac{v\pi}{L} \right)^2 + O(1/L^4). \quad (1.4)$$

The replacement of k by $\sin k$ is not derived here but is just an empirical improvement which reflects the presence of a lattice. In particular, if we ignore Δ this gives the standard spin-wave theory formula. It gives a fairly good fit to the magnon dispersion relation over a large range of k ,¹⁷ although it fails badly near $k=\pi$ (that is $k=0$ before the wave-vector shift).

For the case of open boundary conditions (OBC's), we derive the following formulas for the L dependence of the energies of the lowest energy states of spin $S=0,1,2,3$:

$$\begin{aligned} E_0 &= e_0(L-1) + \Delta_b - \frac{3J_{eff}}{4} \exp\left(-\frac{L-1}{\xi}\right), \\ E_1 &= e_0(L-1) + \Delta_b + \frac{J_{eff}}{4} \exp\left(-\frac{L-1}{\xi}\right), \\ E_2 - E_1 &= \sqrt{\Delta^2 + v^2 \sin^2 \frac{\pi}{L-2a_b}}, \\ E_3 - E_1 &= \sqrt{\Delta^2 + v^2 \sin^2 \frac{\pi}{L-2a_b-a}} \\ &\quad + \sqrt{\Delta^2 + v^2 \sin^2 \frac{2\pi}{L-2a_b-a}}. \end{aligned} \quad (1.5)$$

We use the previously obtained parameters: $e_0 = -1.401484$ and $\Delta_b = -0.193166$. J_{eff} , a_b , and a are parameters. Their magnitude will be determined by fitting Eqs. (1.5) to DMRG data later in Sec. III. The terms with these parameters will be derived in later sections. The exponentially small terms in $E_{0,1}$ arise from the interaction between the effective $S=1/2$ edge excitations. E_2-E_1 is the single magnon energy. Note that it is approximately $\sqrt{\Delta^2+(vk)^2}$ with $k=\pi/(L-2a_b)$ up to corrections of $O(1/L^4)$. This is simply the energy of a free massive particle in a box with an interaction at the boundaries producing a scattering length

a_b . The formula for E_3-E_1 gives the lowest energy two-magnon state. Note that the second wave vector occurring here is twice as large. This reflects the hard-core boson approximation. The appropriate value of this second wave-vector is again determined from consideration of the boundary interactions and contains the same boundary scattering length a_b . The same intermagnon scattering length a appears as in the periodic case. These formulas are only expected to be completely correct up to $O(1/L^3)$. The same empirical replacement of k by $\sin k$ has been made.

The magnetization per unit length, at $T=0$, $L=\infty$, close to the critical field is given by

$$M/L = \frac{1}{\pi v} \left[\sqrt{2\Delta(H-\Delta)} - \frac{8\Delta a}{3\pi v} (H-\Delta) \right]. \quad (1.6)$$

(We adopt units where $g\mu_B=1$.) The square-root singularity was proposed by Tsvelik,¹¹ using an approximate fermionic representation for the $S=1$ chain. It was later argued¹² to be the universal behavior of bosons with repulsive interactions, and therefore, to be an exact result for integer spin chains. The linear correction to this formula was derived by Okunishi *et al.*¹⁸ recently by assuming a δ -function interaction between magnons, $c\delta(x_i-x_j)$, with a replaced by

$$a \rightarrow -v^2/\Delta c. \quad (1.7)$$

We argue here that this formula obtains for *any* short-range interaction (which does not produce bound states), the details of the interaction determining the scattering length.

The scattering length is defined by the behavior of the (symmetric) scattering phase shift in the limit of zero wave vector. For a symmetric wave function describing the relative motion of two particles, the long distance behavior is written in terms of the phase shift, $\delta(k)$ as:

$$\psi(x) \rightarrow \sin[k|x| + \delta(k)]. \quad (1.8)$$

For general short-range potentials with no bound states in the limit $k \rightarrow 0$:

$$\delta(k) \rightarrow -ak. \quad (1.9)$$

We note that the scattering length can be positive or negative. An infinite hard-core potential gives a positive scattering length equal to the core size. On the other hand, a repulsive δ -function potential gives a negative scattering length given by Eq. (1.7).

We also derive the generalization of Eq. (1.6) at low temperature T and large L in order to fit recent Monte Carlo results.¹⁹ We obtain a consistent value of a of about -0.34ξ from all three fits, as mentioned above. However, using a product wave-function renormalization-group method to calculate the magnetization, Okunishi *et al.* obtained a considerably larger value, $a \approx -0.54\xi$, which is closer to the prediction of the NL σ M. From the viewpoint of the renormalization-group treatment of the one-dimensional Bose condensation transition,²⁰ we may regard a as the leading irrelevant coupling constant. Although its value is nonuniversal, many different quantities can be expressed in terms of it. Thus it plays a similar role to one over the Kondo temperature in the Kondo problem.

The boundary scattering length, a_b , resulting from the interaction of bulk magnons with the chain end and the ef-

fective $S=1/2$ degree of freedom residing there, is found to have a value of approximately -1 lattice constants.

In the next section we discuss the simpler case of periodic boundary conditions, deriving the wave functions and energies for dilute bosons with short-range interactions in terms of the scattering length and obtaining the scattering length for the NL σ M. We compare Eq. (1.2) to DMRG results to determine a . In Sec. III we discuss the case of open boundary conditions, deriving Eqs. (1.5) and comparing them to DMRG results, obtaining a_b and a consistent value of a . In Sec. IV we discuss the magnetization, deriving Eq. (1.6) and its finite T and L generalizations, comparing to Monte Carlo results and again obtaining a consistent value of a .

II. DILUTE BOSONS AND THE NONLINEAR σ MODEL

Following the derivation of the NL σ M for large S from the Heisenberg model,^{1,21} we first define

$$\mathbf{S}_{2i-1} = -S\vec{\phi}_i + \mathbf{I}_i, \quad \mathbf{S}_{2i} = S\vec{\phi}_i + \mathbf{I}_i, \quad i=1 \quad \text{to} \quad L/2, \quad (2.1)$$

for a chain of L sites. $\vec{\phi}$ and $\mathbf{I}$ represent the low-energy Fourier modes of the spin operators with wave vectors near π and 0, respectively. Starting from Eq. (1.1) we obtain a continuum NL σ M Hamiltonian:

$$\mathcal{H} = \int_0^L dx \left[\frac{1}{S} \mathbf{I}^2 + \frac{S}{4} \left(\frac{d\vec{\phi}}{dx} \right)^2 \right] + \dots \quad (2.2)$$

This gives a velocity of $2S$ and a coupling constant $g=2/S$. The nonlinear constraints and commutation relations give the corresponding Lagrangian:

$$\mathcal{L} = \frac{1}{2g} \partial_\mu \vec{\phi} \cdot \partial^\mu \vec{\phi}, \quad (2.3)$$

with the constraint $\vec{\phi}^2=1$. (We have set the effective “velocity of light” v to one.) The spectrum of this field theory is known to consist of only a triplet of massive bosons, created by the fields, $\vec{\phi}$, and their multiparticle scattering states. There are no bound states. The boson mass is exponentially small in the coupling constant, g ; it results from nonperturbative effects. A simpler Lagrangian which is expected to have qualitatively similar physics is the ϕ^4 model in which the constraint on $\vec{\phi}$ is relaxed:

$$\mathcal{L} = \frac{1}{2} \partial_\mu \vec{\phi} \cdot \partial^\mu \vec{\phi} - \frac{\Delta^2}{2} \vec{\phi}^2 - \frac{\lambda}{4} \vec{\phi}^4. \quad (2.4)$$

This model also has a triplet of massive bosons and presumably no bound states for $\lambda>0$ (repulsive interactions). Of course, the details of the boson interactions will be somewhat different in the two models. However, the single boson energy, $\sqrt{\Delta^2 + v^2 k^2}$, for Δ the renormalized mass, is independent of the interactions and simply reflects Lorentz invariance and the stability of the single boson excitation.

We now consider the low-energy states of a dilute gas of bosons, all with $S^z=+1$ such that the average spacing is much greater than the Compton wavelength of the boson, $\xi=v/\Delta$. A great deal of universality occurs in this limit. In particular since the bosons in these states have small wave

vectors, $k \ll \xi^{-1}$, the usual nonrelativistic approximation to the dispersion relation is adequate:

$$\epsilon(k) \approx \Delta + \frac{v^2 k^2}{2\Delta}. \quad (2.5)$$

This implies that the behavior will not depend on the Lorentz invariance of the underlying field theory. This is an important point because the $S=1$ chain is only approximately Lorentz invariant. Nevertheless, it contains stable bosonic magnons whose dispersion relation is given by Eq. (2.5) for small k . (Note that we have shifted the wave vectors in the spin chain problem by π .) This follows from the assumption that the dispersion relation is an even function of k analytic near $k=0$ and defines the parameters Δ and v . Due to spin conservation, the low-energy states under consideration are completely stable against decaying into states involving bosons of other spin polarizations, so they may be integrated out. At low energies, the effect of all processes involving creation and annihilation of virtual particles, as given, for example by the Feynman diagram expansion of the ϕ^4 theory, may be boiled down to a simple nonrelativistic effective Hamiltonian, written in first quantized notation as

$$H_N = -\frac{1}{2m} \sum_{i=1}^N \frac{d^2}{dx_i^2} + \sum_{i,j} V(x_i - x_j). \quad (2.6)$$

Here $m \equiv \Delta/v^2$ (the Einstein relation) and V is some effective short-range interaction. We emphasize that the exact form of V is unknown in all cases except for the weak-coupling limit of the ϕ^4 model where it is simply a repulsive δ function. We *do* know that it is such as not to produce any bound states and we expect its range to be roughly ξ . We may indirectly infer its properties, in the case of the NL σ M, from the low-energy S matrix which is known exactly. Nothing is known, *a priori* about the effective potential for the $S=1$ chain, but we may indirectly deduce some of its properties from numerical simulations. Importantly, in the dilute limit the spectrum only depends very weakly on the detailed form of V .

In this dilute limit we may construct the many body wave functions following the construction of Lieb and Liniger for the δ -function Bose gas.²² This follows because we may ignore the possibility of more than two particles being within a distance ξ of each other simultaneously so we only have to consider two-particle scattering processes. In the most likely case where all particles are far from each other compared to ξ , we may write the N -body wave-function as a sum of plane waves. Considering the case $x_1 < x_2 \dots < x_N$, we write

$$\psi(x_1, \dots, x_N) \approx \sum_P A(P) P \exp \left(i \sum_{j=1}^N k_j x_j \right), \quad (2.7)$$

for some set of wave vectors, k_j . Here P permutes the k_j 's and the sum is over all permutations. ψ is determined for other orderings of the x_i from the symmetry of the wave function following from Bose statistics. By considering what happens when two particles approach each other, we can see that

$$A(Q) = -A(P) e^{i2\delta[(k_i - k_j)/2]}. \quad (2.8)$$

Here the two permutations P and Q differ by the interchange of only 1 pair, i and j and $\delta(k)$ is the even channel phase shift defined by the two-body problem with potential $V(x)$. The Hamiltonian for this problem, where we consider only the relative motion of a pair of particles, defining $x=x_1-x_2$, is

$$H = -\frac{1}{m} \frac{d^2}{dx^2} + V(x). \quad (2.9)$$

(Note that the reduced mass, $m/2$ occurs here.) The even wave functions, at distances $|x| \gg \xi$ take the form of Eq. (1.8), defining $\delta(k)$. In general, the coefficients $A(P)$ in Eq. (2.7) are just products of the factor in Eq. (2.8) over all elementary permutations corresponding to P . By considering again, a region where all the particles are far apart, so $V \approx 0$, we see that

$$E \approx \frac{1}{2m} \sum_j k_j^2. \quad (2.10)$$

Periodic boundary conditions then determine the k_j 's, which must all be different from each other, from the N equations:

$$(-1)^{N-1} e^{-ik_j L} = \exp \left(i \sum_{s=1}^N 2\delta[(k_s - k_j)/2] \right), \quad \text{all } j. \quad (2.11)$$

We emphasize that this result only holds in the dilute limit when all the k_j 's are small. Thus we are only interested in the phase shift for small k . It is easy to see that

$$\delta(k) \rightarrow -ak, \quad (2.12)$$

for some constant a at small k , $k \ll 1/\xi$. This follows from observing that in this limit, in the region $\xi \ll |x| \ll 1/k$, the wave function obeys approximately the zero energy, zero potential Schrödinger equation:

$$-\frac{1}{m} \frac{d^2}{dx^2} \psi(x) = 0. \quad (2.13)$$

The even solutions have the form

$$\psi \propto |x| - a. \quad (2.14)$$

Matching this with $\sin[k|x| + \delta(k)]$ at large $|x|$ then determines $\delta \approx -ak$. By analogy with the standard definition in three dimensions, we refer to a as the scattering length. We discussed it briefly in Sec. I. We generally expect it to be of $O(\xi)$.

It is perhaps worth remarking here that, with our definition of phase shift, it takes the value $\pi/2$ for all k for $V=0$ since the symmetric wave functions are then $\cos kx$. In this noninteracting case Eq. (2.14) is not valid. The fact that $\delta(k) \rightarrow 0$ at $k \rightarrow 0$ for any short-range repulsive interaction, no matter how weak, represents a sort of infrared singularity of one-dimensional single-particle quantum mechanics. It is basically this singularity which is responsible for the fact that, in the dilute limit, the many-body wave function for interacting bosons reduces to that of free fermions times an antisymmetric sign function.¹² A related observation is that $\delta(k)=0$ implies the k_j must all be different since otherwise the wave function of Eqs. (2.7), (2.8) would vanish.

FIG. 1. Excitation energy of two-magnon states with PBC, $E_{2P} - E_{0P}$. The fitting equation is Eqs. (1.5). $\xi = v/\Delta$ is used in the figure, and the $1/L^3$ coefficients is -1200 .

In general, it is nontrivial to solve Eq. (2.11), requiring numerical methods. However, in the small- k limit, where Eq. (2.12) applies, it is easy. Since the phase shift for the δ -function potential and the hard-core potential have this form at low k , we simply recover the low density, low k limit of those problems.²² In that limit, Eq. (2.11) can be written

$$k_j(L - Na) + a \sum_s k_s = \pi n_j, \quad \text{all } j, \quad (2.15)$$

where the integers, n_j are all even, for N odd and all odd for N even. In the case $N=2$ the lowest energy solution of Eq. (2.15) is

$$k_1 = -k_2 = \frac{\pi}{L - 2a} \quad (2.16)$$

and the energy is

$$E \approx \frac{1}{m} \left(\frac{\pi}{L - 2a} \right)^2 \approx \frac{1}{m} \left(\frac{\pi}{L} \right)^2 + \frac{4a}{mL} \left(\frac{\pi}{L} \right)^2. \quad (2.17)$$

This is fitted to our DMRG results for the excitation energy of the lowest state with $S^z=2$ with PBC's in Fig. 1. A $1/L^3$ is clearly discernible and gives an estimate of the intermagnon scattering length:

$$a \approx -0.34\xi \quad (2.18)$$

We emphasize that a negative scattering length does not imply an attractive interaction. In particular, as mentioned in Sec. I, a repulsive δ -function interaction gives $a < 0$.

The exact S matrix has been conjectured for the $O(n)$ NL σ M based on factorization of m -particle scattering and various consistency conditions and checked against the $1/n$ expansion.²³ The three possible states of a single magnon are labeled by a vector index $i=1, 2, 3$ so that $|A_i\rangle \propto \phi^i|0\rangle$. $O(3)$ symmetry then implies that the S matrix takes the form:

$$\begin{aligned} {}_{ik}S_{jl} &\equiv \langle A_j(p'_1)A_l(p'_2), \text{ out } | A_i(p_1)A_k(p_2), \text{ in } \rangle \\ &= \delta(p_1 - p'_1) \delta(p_2 - p'_2) [\delta_{ik} \delta_{jl} \sigma_1(\theta) + \delta_{ij} \delta_{kl} \sigma_2(\theta) \\ &\quad + \delta_{il} \delta_{jk} \sigma_3(\theta)] + (i \leftrightarrow k, p_1 \leftrightarrow p_2). \end{aligned} \quad (2.19)$$

Here the momenta of the particles are labeled by the rapidities θ_a :

$$vp_a = \Delta \sinh \theta_a, \quad (2.20)$$

and in Eq. (2.19) the σ_i 's are expressed as functions of

$$\theta \equiv \theta_1 - \theta_2. \quad (2.21)$$

These functions are given by

$$\begin{aligned} \sigma_1(\theta) &= \frac{2\pi i \theta}{(\theta + \pi i)(\theta - 2\pi i)}, \\ \sigma_2(\theta) &= \frac{\theta(\theta - \pi i)}{(\theta + \pi i)(\theta - 2\pi i)}, \\ \sigma_3(\theta) &= \frac{-2\pi i(\theta - \pi i)}{(\theta + \pi i)(\theta - 2\pi i)}. \end{aligned} \quad (2.22)$$

The S matrix for scattering of two spin-up particles is obtained by using

$$|A_+(p)\rangle = (|A_1(p)\rangle + i|A_2(p)\rangle)/\sqrt{2}, \quad (2.23)$$

giving

$$\begin{aligned} &\langle A_+(p'_1)A_+(p'_2), \text{out} | A_+(p_1)A_+(p_2), \text{in} \rangle \\ &= -\delta(p_1 - p'_1)\delta(p_2 - p'_2) \frac{1 + i\theta/\pi}{1 - i\theta/\pi} \\ &\quad - \delta(p_2 - p'_1)\delta(p_1 - p'_2) \frac{1 - i\theta/\pi}{1 + i\theta/\pi}. \end{aligned} \quad (2.24)$$

This determines the phase shift:

$$e^{2i\delta[(p_1 - p_2)/2]} = \frac{1 + i\theta/\pi}{1 - i\theta/\pi}. \quad (2.25)$$

Now letting $p_1 - p_2 \rightarrow 0$, we obtain the exact scattering length of the NL σ M, for two spin-up magnons:

$$a_{NL\sigma M} = -2v/\Delta\pi = -2\xi/\pi, \quad (2.26)$$

roughly twice as large as the value determined numerically for the $S=1$ Heisenberg model.

This calculation can also be repeated for two magnons in a state of total spin $S=1$ or $S=0$. The $S=1$ states are produced from the ground state by the low wave-vector components of the lattice spin operators. We obtain the scattering lengths for spin- S from the NL σ M:

$$\begin{aligned} a^2 &= -2\xi/\pi, \\ a^1 &= -\xi/\pi, \\ a^0 &= \xi/\pi. \end{aligned} \quad (2.27)$$

For the $S=0$ case, where the wave function is again symmetric with respect to the spatial coordinates, Eqs. (2.16) and (2.17) still apply with a replaced by a^0 . The $S=1$ case is a bit different because now the wave function must be antisymmetric with respect to the spatial coordinates since it is antisymmetric with respect to the spin indices. In this case we obtain the wave vectors for the lowest energy states:

$$k_1 \approx 0, \quad k_2 \approx \pm 2\pi/(L - a^1), \quad (2.28)$$

and the energy:

$$E'_{1P} - E_{0P} \approx 2\Delta + \frac{1}{2m} \left(\frac{2\pi}{L} \right)^2 + \frac{1}{m} \left(\frac{2\pi}{L} \right)^2 \frac{a^1}{L}. \quad (2.29)$$

FIG. 2. Ratio of the coupling energy of two edge $1/2$ spins in ground state and edge excited state. Here energy ratio $[E_1 - e_0(L-1) - \Delta_b]/[E_0 - e_0(L-1) - \Delta_b]$ vs $1/(L-1)$ is plotted. The dashed line is $-1/3$.

III. OPEN BOUNDARY CONDITIONS

While a periodic integer spin chain has an excitation gap which depends only weakly on L , in the case of OBC there are low-lying edge excitations. These correspond to effective $S=1/2$ spins localized at the two ends of the chain which are coupled to the bulk degrees of freedom. An effective field theory is given by the NL σ M with Neumann boundary conditions,

$$d\vec{\phi}/dx = 0, \quad (x=0, L), \quad (3.1)$$

coupled to the $S=1/2$ spins, $\mathbf{S}_1$ and $\mathbf{S}_2$. In general, one expects a coupling to both the staggered and uniform magnetization density at the chain ends.²⁴

$$\begin{aligned} H &= H_{\text{bulk}} + \lambda_s [\vec{\phi}(0) \cdot \mathbf{S}_1 + (-1)^L \vec{\phi}(L) \cdot \mathbf{S}_2] \\ &\quad + \lambda_u [\mathbf{I}(0) \cdot \mathbf{S}_1 + \mathbf{I}(L) \cdot \mathbf{S}_2]. \end{aligned} \quad (3.2)$$

Integrating out the bulk field, $\vec{\phi}$ gives an effective exponentially small interaction, between the end spins proportional to λ_s^2 .

$$J_{\text{eff}} \propto \lambda_s^2 e^{-L/\xi}. \quad (3.3)$$

This leads to the splitting between the lowest singlet and triplet states in Eq. (1.5) which can simply be thought of as formed from the two $S=1/2$ end excitations. The singlet (triplet) state of the two $S=1/2$'s has lowest energy for L even (odd). (We only consider L even here.) We check the formulas in Eq. (1.5) for E_0 and E_1 in Figs. 2 and 3. Because J_{eff} is exponentially small, it becomes smaller than our numerical error for the longest chain lengths that we have studied. Therefore, we do not show data for these chain lengths in Figs. 2 and 3 since it would be meaningless. This problem does not occur for the other energy differences that we consider which only involve finite-size effects scaling as powers of $1/L$.

The lowest $S=2$ state is obtained by polarizing the two end spins and then adding one $S^z=1$ magnon. When the end spins are polarized, the λ_u term produces an effective boundary potential energy acting on the magnons. We may describe this by adding an effective boundary potential for the magnons. Thus the nonrelativistic N -body Hamiltonian of Eq. (2.6) gets modified to

FIG. 3. Coupling constant for edge spins. Here $\ln(E_1 - E_0)/(L-1)$ vs $1/(L-1)$ is plotted. The straight fitting line is $\ln(E_1 - E_0)/(L-1) = -1/\xi + c'/(L-1)$, where $\xi=6$ and $c'=2/3$ is taken from Ref. 16.

$$H_N = -\frac{1}{2m} \sum_{i=1}^N \frac{d^2}{dx_i^2} + \sum_{\langle i,j \rangle} V(x_i - x_j) + \sum_{i=1}^N [V_b(x_i) + V_b(L - x_i)], \quad (3.4)$$

where $0 \leq x_j \leq L$ with the Neumann boundary condition:

$$\partial_j \psi(x_1, x_2, \dots, x_N) = 0, \quad (x_j = 0, L). \quad (3.5)$$

We expect $V_b(x)$ to be some short-range function [with range of $O(\xi)$]. It is not *a priori* clear whether V_b is attractive or repulsive. However, the absence of boundary bound states that is evident from earlier numerical work²⁵ indicates that it is repulsive.

For low-energy multimagnon states only the scattering length a_b , produced by V_b is relevant to the spectrum. This has the effect of modifying the low-energy single magnon wave functions, at distances large from the boundaries compared to ξ , to the form

$$\psi(x) \approx \sin[k(x - a_b)] \propto \sin[k(L - a_b - x)]. \quad (3.6)$$

Consistency of these expressions quantizes the wave vectors:

$$k_j = \pi j / (L - 2a_b), \quad j = 1, 2, 3, \dots \quad (3.7)$$

The effective chain length becomes $L - 2a_b$. It is now clear that our results are quite robust against variations in how the effective Hamiltonian is written. For instance, it does not matter whether we impose the Neumann b.c. at $x=0$ or $x=1$. Such differences can be absorbed into the scattering length. We also note that $\langle S_z^2 \rangle$ exhibits period π oscillations upon which are superimposed long wavelength variations which can be interpreted in terms of the magnon wave function.²⁵ The boundary scattering length can be determined from the additional energy to add one $S^z = 1$ magnon to the polarized end spins, giving the third of Eqs. (1.5). This gives a $1/L^3$ term:

$$E_2 - E_1 \approx \Delta + \frac{1}{2m} \left(\frac{\pi}{L} \right)^2 + \frac{2}{m} \frac{a_b}{L} \left(\frac{\pi}{L} \right)^2. \quad (3.8)$$

Fitting to this expression, as shown in Fig. 4, we obtain

$$a_b \approx -1. \quad (3.9)$$

FIG. 4. Single magnon energy with OBC's. Here $(E_2 - E_1)^2$ vs $\sin^2 \pi/(L+2)$ is plotted. The boundary scattering length, $a_b \approx -1$ is obtained. The straight fitting line shows a better fit at short chain lengths resulting from the replacement of k by $\sin k$.

This is equivalent to imposing vanishing boundary conditions on a chain of length $L+2$. We remark that there is no simple derivation that we know of for this result. Presumably the value of a_b depends on the (integer) magnitude of the spin and other details of the microscopic Hamiltonian. We note that a somewhat better fit is obtained in Fig. 4 by the replacement $k \rightarrow \sin k$.

We now consider the spin-polarized two-magnon wave function in the presence of the polarized end spins, with $S^z = 3$. The effect of the boundary potential is simply to fix the effective size of the chain at $L - 2a_b \equiv L'$ with an effective vanishing boundary condition. The two-magnon wave function, with wave vectors k_1 and k_2 can then be written in terms of the magnon-magnon phase shift, $\delta(k)$. This wave function is made from linear combinations of the periodic two-magnon wave functions discussed in Sec. II with wave vectors (k_1, k_2) , $(k_1, -k_2)$, $(-k_1, k_2)$, and $(-k_1, -k_2)$. Two different magnon-magnon phase shifts occur

$$\delta_{\pm} \equiv \delta[(k_1 \pm k_2)/2], \quad (3.10)$$

for $x_1 < x_2$, this wave function, constructed to obey $\psi(0, x_2) = 0$, is given by

$$\begin{aligned} \psi(x_1, x_2) = & e^{i(k_1 x_1 + k_2 x_2)} - e^{i[(k_2 x_1 + k_1 x_2) + 2\delta_-]} - e^{i(-k_1 x_1 + k_2 x_2)} \\ & + e^{i[(k_2 x_1 - k_1 x_2) - 2\delta_+]} + [-e^{i(k_1 x_1 - k_2 x_2)} \\ & + e^{i[(-k_2 x_1 + k_1 x_2) + 2\delta_+]} + e^{-i(k_1 x_1 + k_2 x_2)} \\ & - e^{-i[(k_2 x_1 + k_1 x_2) - 2\delta_-]}] e^{2i(\delta_- - \delta_+)}. \end{aligned} \quad (3.11)$$

The wave function for $x_2 < x_1$ is obtained by interchanging x_1 and x_2 in order to enforce the symmetry required by Bose statistics. Imposing $\psi(x_1, L') = 0$ then requires

$$\begin{aligned} e^{ik_2 L'} &= e^{-ik_2 L' + 2i(\delta_- - \delta_+)}, \\ e^{ik_1 L' + 2i\delta_-} &= e^{-ik_1 L' - 2i\delta_+}. \end{aligned} \quad (3.12)$$

Now using the small- k approximation to $\delta(k)$ gives the conditions

$$\begin{aligned} 2k_2(L' - a)k_2 &= 2\pi n_2, \\ 2k_1(L' - a)k_1 &= 2\pi n_1. \end{aligned} \quad (3.13)$$

Thus the allowed wave vectors are

FIG. 5. Two-magnon excitation behavior for $S=1$ open chain. Here $(E_3 - E_2)^2$ vs $\sin^2 2\pi/(L+2)$ is plotted. The straight line is $(E_3 - E_2)^2 = \Delta^2 + v^2 \sin^2 2\pi/(L+2)$ without any behavior of magnon-magnon interaction included.

$$k_i = \frac{\pi n_i}{L - 2a_b - a}. \quad (3.14)$$

The lowest energy state has $n_1 = 1$, $n_2 = 2$. Figure 5 shows that the second magnon has momentum $k_2 = 2\pi/L$ with $n_2 = 2$. [The n_i must be different in order for the wave function of Eq. (3.11) not to vanish.] Setting $a_b = -1$, its energy is given by the last of Eq. (1.5). As can be seen from Fig. 6, good agreement with this formula is obtained with a value of the magnon-magnon scattering length:

$$a \approx -0.32\xi. \quad (3.15)$$

This appears consistent, within the numerical error, with the result $a \approx -0.34\xi$ obtained with PBC's.

We also comment briefly on finite-size energies of two magnon states with other spin quantum numbers. This would certainly be the simplest to study using PBC's so that there are no end spins to worry about. An alternative approach, following White and Huse,² would be to consider OBC's but to add extra $S=1/2$ variables at the edges of the system so as to cancel the effect of the edge excitations. The boundary scattering length will depend on the details of the boundary couplings. The contribution of the magnon-magnon interaction energy to the two-magnon states can again be expressed in terms of the scattering length for the appropriate spin channel, a^S . It can be seen that the wave vectors are still given by Eq. (3.14) with the appropriate value of a for both

FIG. 6. Two-magnon excitation energy for OBC's. Here $E_3 - E_2 - \sqrt{\Delta^2 + v^2 \sin^2 2\pi/(L+2)}$ vs $1/L^3$ is plotted. The fitting curve goes to zero linearly as $1/L^3 \rightarrow 0$. The coefficient of the cubic term determines the scattering length, $a \approx -0.32\xi$.

symmetric ($S=0,2$) and antisymmetric ($S=1$) wave functions. Thus the energy, to $O(1/L^3)$ in all cases is given by

$$E_{SO} - E_{00} \approx 2\Delta + \frac{5}{2m} \left(\frac{\pi}{L'} \right)^2 + \frac{5}{m} \left(\frac{\pi}{L'} \right)^2 \frac{a^S}{L}, \quad (3.16)$$

where $L' = L - 2a_b$ and a_b is the appropriate boundary scattering length.

DMRG results on two-magnon energies of various S were reported by White and Huse. They found repulsive interaction energy for $S=0,2$ but attractive for $S=1$. This is completely consistent with our approach. They did not use unequal wave vectors for the two magnons in their definition of the interaction energy, in the even S case. Thus their positive interaction energy is presumably of $O(1/L^2)$ and just reflects the effective Fermi statistics of the dilute Bose system, i.e., the requirement of unequal wave vectors. The attractive interaction energy in the $S=1$ channel corresponds to a negative a^1 . They only present data for $L=60$, but if we assume that the $1/L^3$ term is dominating at that value of L we extract a value, $a^1 \approx -0.43\xi$, about 30% larger in magnitude than the NL σ M prediction.

IV. MAGNETIZATION

We now consider wave functions, with periodic boundary conditions, containing an arbitrary number N , of magnons, assuming that the density and all wave vectors are small compared to $1/\xi$. To solve Eq. (2.15) for the k_j 's for a general low-energy N -particle state we now use the fact that the density is low, $Na/L \ll 1$ and $a \sum_s k_s \ll k_j L$. Hence, in the lowest order approximation:

$$k_j \approx k_{j0} \equiv \pi n_j / L (n_j \text{ even for } N \text{ odd, } n_j \text{ odd for } N \text{ even}). \quad (4.1)$$

The dimensionless expansion parameter is na where n is the density, N/L . Hence we may expand the k_j in powers of a . The leading correction is $k_j = k_{j0} + \delta k_j$, where

$$\delta k_j = \frac{Na}{L} k_{j0} - \frac{a}{L} \sum_s k_{s0}. \quad (4.2)$$

The energy of this state is approximately

$$\begin{aligned} E &\approx \frac{1}{2m} \sum_j [k_{j0}^2 + 2k_{j0} \delta k_j] \\ &= \frac{1}{2m} \sum_j k_{j0}^2 + \frac{a}{2mL} \sum_{\langle i,j \rangle} (k_{i0} - k_{j0})^2. \end{aligned} \quad (4.3)$$

We now consider the ground-state energy in the limit $L \rightarrow \infty$ with a nonzero but small density, n . The values of k_{j0} occupy the "Fermi sea," $|k| < k_F$ where k_F is determined from the density:

$$n = \int_{-k_F}^{k_F} \frac{dk}{2\pi} = \frac{k_F}{\pi}. \quad (4.4)$$

The ground-state energy, to $O(a)$ is then

FIG. 7. Magnetization curve for $S=1$ chain near critical field $H_c = \Delta$. (The exchange constant and $g\mu_B$ are set equal to 1.) For infinite length and at $T=0$, we plot it as given in Eq. (4.7). The full line has included the leading-order contribution of magnon-magnon interactions. The dashed line is a reference line for comparison and it is for free hard-core boson approximation.

$$E_0(n)/L = (\Delta - H)n + \int_{-k_F}^{k_F} \frac{dk}{2\pi} \frac{k^2}{2m} + \frac{a}{2m} \int_{-k_F}^{k_F} \frac{dk}{2\pi} \int_{-k_F}^{k_F} \frac{dk'}{2\pi} (k - k')^2. \quad (4.5)$$

Here we have included the Zeeman term, $-Hn$ in the energy; H is the applied magnetic field. Performing the integrals gives

$$E_0(n)/L = (\Delta - H)n + \frac{\pi^2 n^3}{6m} + \frac{a\pi^2 n^4}{3m}. \quad (4.6)$$

This represents an expansion of the energy in powers of the density. The first term which depends on the interactions is the $O(n^4)$ term. Minimizing E_0 with respect to n gives the density or magnetization per unit length:

$$M(H)/L = n \approx \frac{1}{\pi v} \left[\sqrt{2\Delta(H - \Delta)} - \frac{8a\Delta}{3\pi v} (H - \Delta) \right]. \quad (4.7)$$

In Fig. 7 we plot M/L vs H from Eq. (4.7) with and without the interaction ($a = -0.34\xi$ or $a=0$). The leading-order correction due to the magnon-magnon interaction is obvious around magnetization $M/L = 0.02$.

This finite density correction can be generalized to finite temperature T , as was observed by Okunishi²⁶ in the special case of the δ -function interaction. The correction to the free energy of lowest order in density is given by including thermal occupation numbers in the second term of Eq. (4.5):

$$\Delta F/L = \frac{a}{2m} \int \frac{dk_1 dk_2}{4\pi^2} n_F(k_1) n_F(k_2) (k_1 - k_2)^2. \quad (4.8)$$

Note that it is the *Fermi* distribution function which appears, rather than the Bose function. This simply follows from the

FIG. 8. Magnetization curve for $S=1$ chain near critical field $H_c = \Delta$, with length $L=100$ and at temperature $kT=1/100$. The full line has included the leading-order contribution of magnon-magnon interaction. The dashed line is a reference line for comparison and it is for the free hard-core boson approximation. The dots are the Monte Carlo results (Ref. 19).

condition that the k_j should all be distinct so that there is an effective occupation number for each momentum which can be 0 or 1 only. $n_F(k)$ is evaluated at finite T and H , then the magnetization is obtained by the usual thermodynamic formula, $\partial F/\partial H = -M$. In order to compare with recent Monte Carlo data on the magnetization for the $S=1$ chain, it is useful to also generalize our formulas to finite length, L with periodic boundary conditions. There is a slight subtlety in doing so because the allowed wave vectors of the magnons alternate between $k = 2\pi n/L$ ("even wave vectors") for an odd number of magnons and $k = 2\pi(n + 1/2)/L$ ("odd wave vectors") for an even number. This follows from the sign change of the wave function each time one magnon passes another one. However, this is easily dealt with exactly by inserting appropriate factors of

$$(-1)^N = e^{i\pi \sum_k n_k}, \quad (4.9)$$

into the partition function trace. This effectively gives the chemical potential an imaginary part, essentially converting fermion occupation numbers into boson ones. For $a=0$, the partition function is given by

$$Z^0 = (1/2)[Z_{Fe}^0 - 1/Z_{Be}^0 + Z_{Fo}^0 + 1/Z_{Bo}^0]. \quad (4.10)$$

Here Z_{Fe}^0 denotes the partition function for free fermions with even wave vectors; Z_{Bo}^0 denotes the partition function for bosons with odd wave vectors, etc. Note that *inverse* boson partition functions occur. The thermal average of the second term in Eq. (4.3) becomes

$$\Delta F = \frac{1}{2Z^0} \frac{a}{2m} \left\{ \sum_{k_1, k_2}^e (k_1 - k_2)^2 \left[Z_{Fe}^0 n_F(k_1) n_F(k_2) - \frac{1}{Z_{Be}^0} n_B(k_1) n_B(k_2) \right] + \sum_{k_1, k_2}^o (k_1 - k_2)^2 \left[Z_{Fo}^0 n_F(k_1) n_F(k_2) + \frac{1}{Z_{Bo}^0} n_B(k_1) n_B(k_2) \right] \right\}, \quad (4.11)$$

where the first sum is over even wave vectors and the second is over odd wave vectors. The resulting magnetization curve

is plotted in Fig. 8. Note the smoothing of the singularity at the critical field due to a finite T and the oscillations due to a finite L . We use the interaction parameter, $a \approx -0.34\xi$, obtained from the ground-state numerical data so there are no free parameters in drawing Fig. 8. The agreement with the Monte Carlo data,¹⁹ at the same length and temperature, $L = 100$, $T = 1/100$ is remarkable.

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