Finite-size effects in Heisenberg antiferromagnets

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A system which exhibits antiferromagnetic order in the thermodynamic limit will, generically, have a symmetric ground state when the volume is finite. In this case the leading size dependence of various observables is controlled by soft magnons. The precise form of the finite-size corrections is worked out, and it is claimed that the expressions so obtained will be useful for the analysis of results obtained by Monte Carlo simulations or by exact diagonalization.

I. INTRODUCTION

Spontaneous symmetry breaking plays a central role in the physics of large systems. The basic characteristics of this phenomenon remain unchanged, although applications vary from energy scales of order 10^{-4} eV in the context of magnetism, to energy scales of order 10^{25} eV in the context of grand unification. In many cases all the low-energy and low, momentum properties of a system are fixed, up to a few parameters, by the pattern of breaking a continuous symmetry. These few parameters constitute all that is left dependent on the microscopic dynamics. Different microscopic systems which have identical values for these parameters would be indistinguishable in the low-energy, low-momentum regime.

In this paper we shall be mainly concerned with two-dimensional quantum-spin models defined on a square lattice. We assume that the ground state exhibits antiferromagnetic order and that the staggered magnetization is not a constant of motion. The relevance of such systems to the physics of materials which exhibit high-temperature superconductivity has been extensively discussed in the literature before.[1]

The large-distance, long-time behavior of all these systems is described, up to a normalization, by a nonlinear sigma model in three Euclidean dimensions. At zero temperature this model has two unknown parameters which have to be extracted from the microscopic physics.[2] To relate the predictions of such an effective theory to low-energy, low-momenta properties of the original model one additional parameter is needed. We thus concentrate on three parameters: Two appear in the effective Euclidean action and the third relates the physical staggered magnetization, as felt by scattered neutrons for example, to the expectation value of the order parameter in the effective model. All our work is at zero temperature. The effects of small temperatures can be incorporated later;[2] we do not expect additional microscopic information to be necessary for the description of the leading effects.

The first step is to give precise microscopic definitions of the parameters. Subsequently we address the practical question of how to calculate these parameters from a given microscopic Hamiltonian. Since it would be unrealistic to expect the microscopic model to be exactly soluble, and judging from the experience with the 2D Heisenberg antiferromagnet, good and reliable approximation methods may not be available due to the absence of a small expansion parameter, we concentrate here on "safe" numerical techniques. Although we have mainly exact diagonalization in mind, much of what we have to say is relevant for properly interpreting Monte Carlo data as well.

The major obstacle to the employment of numerical methods is the relative smallness of the systems investigated. Our main observation is that the leading size dependence of the observables of these systems is governed by the same three parameters we discussed before and is universal otherwise. We suggest therefore the following strategy for investigating small systems.

First assume that spontaneous symmetry breakdown would occur if the system were infinite. Using the complete arsenal of our understanding of the physics of this phenomenon we derive the form of the finite-size contributions to the ground-state average of the staggered magnetization squared, and also the leading effects on the low-lying spectrum.[3] These formulas predict a definite form of the finite-size effects (shape and volume dependence). The numerical values of the corrections also depend on the three parameters we discussed above. Once the correct finite-size dependence is numerically observed, one can conclude that the original assumption about the occurrence of spontaneous symmetry breaking in the infinite system is indeed correct. Moreover one can extract numerical values for the three parameters of interest.

Although our derivations are not fully rigourous we believe that our finite-size formulas are exact. In this paper we focus on obtaining these formulas. On the basis of preliminary investigations we can state that we have good reasons to believe that the finite-size formulas will prove to be of practical use in the interpretation of numerical data on Heisenberg antiferromagnetics obtained either by exact diagonalization or by Monte Carlo simulations. We shall provide a simple explanation for why such asymptotic formulas might work for even the smallest systems imaginable. As our formulas are universal their use is by no means limited to pure spin models.

The importance of a correct treatment of finite-size effects in this context was realized first by Huse and by

Reger and Young.[4] Some qualitative ideas have been presented recently by Gross, Sánchez-Velasco, and Siggia.[5] Our own work presented below has been done independently of theirs following analogous developments in high-energy physics.[6] We have been informed that D. Fisher is also working on similar questions but know no details about the work.[7]

The plan of the paper is as follows: Since we would like to exploit as much as possible the approximate relativistic invariance of the soft magnon sector we start our paper (Sec. II) with a brief but self-contained review of the physics of a fully relativistic $(2+1)$-dimensional field theory.[8] We then proceed to the case of interest and show how approximate relativistic invariance leads us to specific limiting forms for some matrix elements (Sec. III). The unknown constants in these formulas are the relevant low-energy parameters we are interested in. Next we relate the staggered magnetization to these parameters (Sec. IV). We employ a method of proof which is familiar in the context of the techniques reviewed in Sec. II. In Sec. V we present a finite-size theorem giving the leading asymptotic correction to the ground state expectation value of the square of the finite-volume staggered magnetization. We then proceed in Sec. VI to study the finite-size effects on the low-lying spectrum of the system. This is the first instance that the overall scale of the Hamiltonian is of importance. In Sec. VII we summarize our results. The Appendix contains a calculation of the universal shape dependence of the asymptotic correction presented in Sec. V. There we also show that the spin wave expansion for the nearest-neighbor antiferromagnet seems to indicate that the asymptotic formulas are strikingly effective numerically, even for very small systems.

II. RELATIVISTIC PION PHYSICS

Since the order parameter is not a constant of motion, hydrodynamic considerations lead us to expect a linear dispersion for soft spin waves. This is known to be true in the spin wave expansion and is very likely correct to any order in this expansion. The linearity of the dispersion means that at large distances and large times the system has an approximate relativistic invariance. The relevant group is the $2+1$ Lorentz group, whose algebra is the same as that of $SL(2,R)$. By analytically continuing to imaginary times the invariance group becomes SO(3) and the two-dimensional relativistic quantum field theory becomes a classical Euclidean three-dimensional one.

Spontaneous symmetry breaking has been studied extensively in the framework of relativistic quantum field theory.[8] This will prove to be useful for our investigations so we would like to briefly review the definitions of the the low-energy, low-momentum parameters there. For conciseness we discuss a definite model, the O(3) $2+1$ linear sigma model. The Minkowsky action is given by

$$S=\int d^3x\,[\tfrac{1}{2}(\partial_\mu\Phi_0)^2+\tfrac{1}{2}\mu_0^2\Phi_0^2-\tfrac{1}{4}\lambda_0(\Phi_0^2)^2]\ . \tag{1}$$

The parameters and fields are unrenormalized. The theory can be renormalized and has a limit free of any ultraviolet divergences. The three-component renormalized scalar field Φ develops (in some regime) a nonzero expectation value and spontaneous breakdown occurs. The SO(3) group is broken down to $SO(2)\cong U(1)$. Since two generators are broken one expects a doubly degenerate spectrum of pions with zero mass. The velocity of light is always set to unity.

The charges generating the global SO(3) are Q^α:

$$[Q^\alpha,Q^\beta]=i\epsilon^{\alpha\beta\gamma}Q^\gamma\ . \tag{2}$$

Relativistic invariance and the global symmetry imply the existence of local three-vector currents $J_\mu^\alpha(x)$ that are conserved,

$$\partial^\mu J_\mu^\alpha(x)=0\ , \tag{3}$$

and satisfy $Q^\alpha=\int d^2x\,J_0^\alpha(x,t)$, with $dQ^\alpha/dt=0$ as a result of (3).

The action of the Q's on the renormalized Φ's is given by

$$[Q^\alpha,\Phi^\beta]=i\epsilon^{\alpha\beta\gamma}\Phi^\gamma\ . \tag{4}$$

Note that Eq. (2) fixes the overall normalization of the currents J but the normalization of the field Φ is not fixed by (4).

The symmetry is spontaneously broken in some regime of couplings. One chooses traditionally the breaking to single out the third direction in isospace and writes $\Phi=(\pi,\sigma)$, where π^i $(i=1,2)$ are the two pion fields which create Goldstone particles.

The scatterings of soft pions are governed by one energy scale, the pion constant f. It is defined as follows: Let $|\pi^i(q)\rangle$ be pion one-particle states of three-momentum $\mathbf{q}$. Masslessness implies $q_0^2=|\mathbf{q}|^2$. The relativistic normalization is chosen such that the projection on the one-particle pion space has the relativistic invariant phase-space measure $2\,d^3q\,\delta(q^2)\Theta(q_0)=d^2q/|\mathbf{q}|$:

$$\langle\pi^i(\mathbf{q})|\pi^j(\mathbf{q}')\rangle=(2\pi)^2\delta^{ij}|\mathbf{q}|\delta^2(\mathbf{q}-\mathbf{q}')\ . \tag{5}$$

The occurrence of spontaneous symmetry breakdown means that only Q^3 is a "good" operator in the Hilbert space: $Q^{1,2}$ are not, because they generate rotations in isospin space which try to change the direction of the vacuum. The local currents $J_\mu^{1,2}$ are acceptable, however, as long as we do not integrate over all space. Clearly they create the pion states when acting on the vacuum. The constant f is defined by

$$\langle 0|J_\mu^i(x)|\pi^j(k)\rangle=if\exp(-i\mathbf{k}\cdot\mathbf{x})\delta^{ij}k_\mu\ . \tag{6}$$

There μ takes the values 0,1,2, and $k\cdot x=k_0x_0-\mathbf{k}\cdot\mathbf{x}$ with $k_0=|\mathbf{k}|$. Relativistic invariance, analyticity, and group theory fix the structure of (6) up to the dimensional constant f. f is one of the parameters we shall be interested in later.

The normalization of the field Φ is usually fixed by some convention. Once this is done one has

$$\langle 0|\pi^i(x)|\pi^j(k)\rangle=Z\delta^{ij}\exp(-i\mathbf{k}\cdot\mathbf{x})\ . \tag{7}$$

Again, up to the constant Z, the structure of (7) is fixed by general considerations.

Current algebra techniques[7] then lead to the following formula:

$$\langle 0|\sigma|0\rangle = fZ \ . \tag{8}$$

Z shall be our second parameter. A sum rule analogous to Eq. (8) will be derived later on, giving the relation between our parameters and the average staggered magnetization.

The third parameter we need has to do with the fact that the velocity of light, which has been set to unity above, has a physical meaning in the application we have in mind. It is worthwhile to keep in mind that the first two parameters depend only on the ground state (and therefore are insensitive to a scaling up or down of the Hamiltonian), while c, the velocity of the sound, is a spectral property which does scale with the Hamiltonian.

III. THE IDENTIFICATION OF LOW-ENERGY PARAMETERS

Both in the relativistic framework and in that of classical statistical physics finite-size effects for systems which would undergo spontaneous breaking for infinite volumes have been investigated recently. It is these developments which we are going to exploit below. Before doing that we would like to introduce our parameters without going to the infinite ultraviolet cutoff limit (zero lattice spacings). Here we follow Ref. 6.

We imagine having a general local Hamiltonian defined on an infinite square lattice with sites denoted by $\mathbf{x}$ and directions (1,2) by μ:

$$\mathcal{H} = J\sum_{x,\mu}(\mathbf{S}_x\cdot\mathbf{S}_{x+\mu}) + J_2\sum_{x,\mu\neq\nu}(\mathbf{S}_x\cdot\mathbf{S}_{x\pm\mu\pm\nu}) + \cdots \ , \tag{9}$$

where

$$[\mathbf{S}_x^\alpha,\mathbf{S}_y^\beta] = \delta_{x,y}\epsilon^{\alpha\beta\gamma}\mathbf{S}_x^\gamma \ , \qquad S_x^2 = \tfrac{3}{4} \ . \tag{10}$$

We assume that the couplings in H are such that spontaneous breakdown will occur with the simplest antiferromagentic order:

$$\langle 0|S_x^3|0\rangle = (-1)^{\|\mathbf{x}\|}\mathcal{S} \ , \tag{11}$$

where $\|\mathbf{x}\| \equiv x_1 + x_2$

This means that in our model not only was the global internal symmetry broken but also the lattice translation group was broken to the even subgroup [translations by $\mathbf{a}=(a_1,a_2)$ with a_1+a_2 even]. This introduces some complications which one avoids as follows: Introduce the Holstein-Primakoff transformation from the spin variables to bosonic creation annihilation operators subjected to a constraint:

$$\begin{gathered} S_x^\pm = S_x^1 \pm iS_x^2 \ , \\ S_x^+ = \frac{1+(-1)^{\|\mathbf{x}\|}}{2}\sqrt{1-n_x}\,a_x + \frac{1-(-1)^{\|\mathbf{x}\|}}{2}a_x^\dagger\sqrt{1-n_x} \ , \\ n_x = a_x^\dagger a_x, \quad 0\le n_x\le 1 \ , \\ [a_x,a_y^\dagger]=\delta_{x,y}, \quad [a_x,a_y]=0 \ , \\ S_x^- = (S_x^+)^\dagger, \quad S_x^3 = (-1)^{\|\mathbf{x}\|}(\tfrac{1}{2}-n_x) \ . \end{gathered} \tag{12}$$

It is easy to see that when expressed in terms of the a's, $\mathcal{H}$ is still translationally invariant, and (11) is now

$$\langle 0|n_x|0\rangle = \tfrac{1}{2} - \mathcal{S} \ . \tag{13}$$

Therefore we have now full translational invariance; what we have lost is the explicit SO(3) invariance of H. In particular the unbroken U(1) is less obvious now. One should note that our translations, generated by U_μ with

$$U_\mu^\dagger a_x U_\mu = a_{x+\mu} \ , \tag{14}$$

are not the same as the natural translations associated with H when written in terms of the spin operators. Nevertheless products of even numbers of U_μ are generating translations for the $\mathbf{S}$ variables too.

Since $[\mathcal{H},U_\mu]=0$ we can diagonalize $\mathcal{H}$ and U_μ simultaneously, and eigenstates of U_μ are labeled by a crystal momentum $\mathbf{k}_\mu$ with $|\mathbf{k}_\mu|<\pi$:

$$U_\mu|\mathbf{k}\rangle = e^{i\mathbf{k}_\mu}|\mathbf{k}\rangle \ . \tag{15}$$

We assume our infinite system was approached by considering a sequence of finite systems having a total even number of sites. Hence we may consider the operator $Q=\sum_x(-1)^{\|\mathbf{x}\|}n_x$ which commutes with H and has zero ground-state expectation value. However, if we insist in diagonalizing the U_μ's we cannot diagonalize Q too, because $U_\mu^\dagger Q U_\mu = -Q$. Q is the generator of the unbroken U(1).

In our language Goldstone's theorem does not promise two degenerate magnon states per momentum but only one. The doubling of magnon states will occur by the expected halving of the Brillouin zone. The magnon states are defined as those states giving a pole to $(1/\mathcal{H}-z)P_\mathbf{k}$ where $P_\mathbf{k}$ projects on total momentum k. The location of the pole is at $\epsilon_\mathbf{k}$ and we expect $\epsilon_\mathbf{k}\approx c|\mathbf{k}|$ for $\mathbf{k}\to\mathbf{0}$ and $\epsilon_\mathbf{k}\approx c|\mathbf{k}-\mathbf{T}|$ for $\mathbf{k}\to T=(\pi,\pi)$. We are only interested in the magnon states of very low energy. Using (12) and translational invariance we can write

$$\begin{aligned} \langle 0|S_\mathbf{x}^+|\mathbf{k}\rangle &= A_\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{x}} + B_\mathbf{k}e^{i(\mathbf{k}+\mathbf{T})\cdot\mathbf{x}} \ , \\ \langle 0|S_\mathbf{x}^-|\mathbf{k}\rangle &= A_\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{x}} - B_\mathbf{k}e^{i(\mathbf{k}+\mathbf{T})\cdot\mathbf{x}} \ , \end{aligned} \tag{16}$$

where $\mathbf{k}\cdot\mathbf{x}=\mathbf{k}_1\mathbf{x}_1+\mathbf{k}_2\mathbf{x}_2$. The one-magnon states are normalized by $\langle\mathbf{k}|\mathbf{k}'\rangle=(2\pi)^2\delta^2(\mathbf{k}-\mathbf{k}')$.

There must be a degeneracy in the one-magnon sector reflecting the unbroken U(1). Since the degeneracy must be compatible with halving the Brillouin zone and the latter is obtained by identifying $\mathbf{k}$ with $\mathbf{k}+\mathbf{T}$, we expect that there exists a unitary operator V which satisfies $[V,H]=0$ and $V|\mathbf{k}\rangle \propto |\mathbf{k}+\mathbf{T}\rangle$. We shall argue now that

$$V=\exp[-(i\pi/2)Q] \ . \tag{17}$$

It is easy to see that V commutes with all even translations. V does not commute with odd translations. However V is an element of the unbroken U(1) group and the one-magnon subspace provides a representation of this group. Therefore V maps one-magnon states into linear combinations of one-magnon states. In conclusion $\langle\mathbf{k}|V|\mathbf{k}'\rangle$ may be nonzero only for $\mathbf{k}-\mathbf{k}'=\mathbf{0}$ or $\mathbf{T}$, and in the invariant subspace spanned by a given $|\mathbf{k}\rangle$ and $|\mathbf{k}+\mathbf{T}\rangle$ V is represented by

$$\begin{aligned} V|\mathbf{k}\rangle &= a|\mathbf{k}\rangle + b|\mathbf{k}+\mathbf{T}\rangle \ , \\ V|\mathbf{k}+\mathbf{T}\rangle &= a'|\mathbf{k}\rangle + b'|\mathbf{k}+\mathbf{T}\rangle \ . \end{aligned} \tag{18}$$

Using the commutation relations of V and U_μ one can show that

$$\begin{aligned} V^\dagger|\mathbf{k}\rangle &= a|\mathbf{k}\rangle - b|\mathbf{k}+\mathbf{T}\rangle \ , \\ V^\dagger|\mathbf{k}+\mathbf{T}\rangle &= a'|\mathbf{k}\rangle - b'|\mathbf{k}+\mathbf{T}\rangle \ . \end{aligned} \tag{19}$$

Imposing unitarity we obtain that in the $\{|\mathbf{k}\rangle,|\mathbf{k}+\mathbf{T}\rangle\}$ space V is represented by

$$V = \begin{bmatrix} a & b \\ -b^* & a \end{bmatrix} .$$

Since Q is an integral quantum number, the eigenvalues of V must be ± 1, $\pm i$. The one-magnon space should contain states with $Q=\pm 1$, so V cannot be proportional to the unit matrix ($b=0$). Combining these requirements we conclude that $a=0$ and $b=e^{i\phi}$. Going back to (19) we obtain $V|\mathbf{k}\rangle = e^{i\phi}|\mathbf{k}+\mathbf{T}\rangle$ and $V^\dagger|\mathbf{k}+\mathbf{T}\rangle = -e^{i\phi}|\mathbf{k}\rangle$ leading to $\phi=\pm i\pi/2$ or $b=\pm i$. By redefining (if necessary) V via a sign change in Q we finally conclude

$$\begin{aligned} V|\mathbf{k}\rangle &= i|\mathbf{k}+\mathbf{T}\rangle \ , \\ V^\dagger|\mathbf{k}+\mathbf{T}\rangle &= -i|\mathbf{k}\rangle \ . \end{aligned} \tag{20}$$

V therefore unitarily implements the expected degeneracy in the one-magnon spectrum. Diagonalizing V and all the even translations would give two degenerate magnon states with momenta taking values in the halved Brillouin zone. Using the commutation relations between V and $S_x^\pm$,

$$V S_x^\pm V^\dagger = \pm i S_x^\pm \ , \tag{21}$$

we can derive a kinematical relationship between the amplitudes in (16) ($A_\mathbf{k} = -B_{\mathbf{k}+\mathbf{T}}$):

$$\langle 0|S_x^\pm|\mathbf{k}\rangle = A_\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{x}} \pm A_{\mathbf{k}+\mathbf{T}} e^{i(\mathbf{k}+\mathbf{T})\cdot\mathbf{x}} \ . \tag{22}$$

It is worthwhile to compare (22) to (6) and (7). Clearly we do not have exact relativistic invariance and the equivalents of the parameters f and Z should be obtained from the limiting behavior of $A_\mathbf{k}$ as $\mathbf{k}\to\mathbf{0}$ and as $\mathbf{k}\to\mathbf{T}$. There are two points to remember now: (1) Our states are not relativistically normalized, and (2) the local field representing the current J_μ is the same as the local field representing the fields π. The normalization issue is easily resolved: In order to be compatible with (5) we choose

$$|\mathbf{k}\rangle_R = \left[\frac{\omega_\mathbf{k}}{c}\right]^{1/2} |\mathbf{k}\rangle \ . \tag{23}$$

The second point deserves a little more discussion: $S_x^\pm$ really gives us the zero component of $J_\mu(x)$ ($\mu=0$) because their sum over all sites give us the "broken" charges. The other components of J (the space components) can be obtained by calculating $dS_2^\pm/dt$ from H and imposing the local conservation law (3). Equation (6) now implies that the J_μ piece of (22) is hidden in the amplitude which vanishes as $\mathbf{k}\to\mathbf{0}$. We conclude that $\omega_\mathbf{k}^{1/2} A_\mathbf{k}$ should go as $|\mathbf{k}|$ as $\mathbf{k}\to\mathbf{0}$.

$$A_\mathbf{k} \to \kappa_2 |\mathbf{k}|^{1/2} \quad \text{as } \mathbf{k}\to\mathbf{0} \ . \tag{24}$$

The π-field piece of (22) is obtained when the amplitudes multiplied by $\omega^{1/2}$ go to a constant as $\mathbf{k}\to\mathbf{T}$. We are led therefore to

$$A_\mathbf{k} \to \frac{\kappa_1}{|\mathbf{k}-\mathbf{T}|^{1/2}} \quad \text{as } \mathbf{k}\to\mathbf{T} \ . \tag{25}$$

Although we have not proven rigourously the functional dependences in (24) and (25) they hold in the spin wave approximation and we believe them to be exact. Equations (24) and (25) replace Eqs. (6) and (7). The two parameters κ_1 and κ_2 replace f and Z. They do not depend on the overall scale of H. The derivation of (22) from (16) replaced the group theoretical δ factors in Eqs. (6) and (7).

The third parameter is c defined by

$$\epsilon_\mathbf{k} \equiv \omega_\mathbf{k} \sim c|\mathbf{k}| \quad \text{as } \mathbf{k}\to\mathbf{0} \ . \tag{26}$$

IV. THE STAGGERED MAGNETIZATION

The purpose here is to derive the analogue of Eq. (8). This will give the staggered magnetization in terms of κ_1 and κ_2.

We start from

$$[S_x^+, S_y^-] = 2S_x^3 \delta_{x,y} \ . \tag{27}$$

We take the ground-state expectation value of (27), then sum over y and insert a complete set of intermediate states:

$$2\mathcal{S}(-1)^{\|\mathbf{x}\|} = \sum_y \sum_{\mu^n} \int \frac{d^2k_n}{(2\pi)^2} [\langle 0|S_x^+|n\rangle\langle n|S_y^-|0\rangle - \langle 0|S_y^-|n\rangle\langle n|S_x^+|0\rangle] \ . \tag{28}$$

Here $|n\rangle \equiv |k_n;\mu_n\rangle$ is a state of total crystal momentum k_n, and μ^n is a complete set of other quantum numbers.

Using the basic form of $S_x^\pm$ we can exploit translational invariance to write

$$\langle 0|S_x^\pm|n\rangle = \tilde{A}_n e^{i\mathbf{k}\cdot\mathbf{x}} \pm \tilde{B}_n e^{i(\mathbf{k}+\mathbf{T})\cdot\mathbf{x}} \ . \tag{29}$$

Upon insertion in (28) we obtain

$$\mathcal{S} = \frac{1}{2} \sum_{\mu^n} \int d^2k_n \{(\tilde{A}_n^* \tilde{B}_n + \tilde{B}_n^* \tilde{A}_n)[\delta^2(k_n) + \delta^2(k_n+T)]\} \ . \tag{30}$$

Very much in the spirit of soft pion physics we expect only the one-magnon states to have sufficient phase space (contained in the matrix elements $\tilde{A}_n$ and $\tilde{B}_n$) to overcome the δ functions and contribute to the integral. We get

$$\mathcal{S} = -\frac{1}{2}\left(\lim_{k\to 0} + \lim_{k\to T}\right)(A_k^* A_{k+T} + A_{k+T}^* A_k) \ . \tag{31}$$

Choosing the phases of the states $|k\rangle$ so that the A_k are real, we end up with

$$\mathcal{S}=-2\lim_{k\to 0}(A_k A_{k+T}) . \tag{32}$$

Using (29) and (25) we have

$$\mathcal{S}=-2\kappa_1\kappa_2 , \tag{33}$$

and this is the formula we were after. We believe that it is exact.

V. THE FINITE-SIZE THEOREM

Until now we were working strictly in the infinite-volume limit. Now we consider our model defined on a rectangular region of a two-dimensional square lattice. The sides of the rectangle are L_1 and L_2 in lattice units. Both L_1 and L_2 are taken to be even, and periodic boundary conditions are imposed. Another case is discussed at the end of this section. We define $L^2 \equiv L_1 L_2$ and concentrate on the following quantity:

$$M_L^2=\frac{1}{L^2}\sum_{0\le x_\mu \le L_\mu -1}(-1)^{\|\mathbf{x}\|}\,{}_L\langle 0|\mathbf{S}_x\cdot\mathbf{S}_0|0\rangle_L . \tag{34}$$

Momentum space is now discrete with $\mathbf{k}_s = 2\pi(s_1/L_1, s_2/L_2)$. We introduce a Fourier decomposition of the two point-function:

$${}_L\langle 0|\mathbf{S}_\mathbf{x}\cdot\mathbf{S}_0|0\rangle_L=\frac{1}{L^2}\sum_{0\le s_\mu\le L_\mu-1}\frac{e^{i\mathbf{k}_s\mathbf{x}}}{X_s} . \tag{35}$$

We assume that in the infinite-L limit spontaneous symmetry breakdown occurs. Therefore we should separate the $s=T$ term from the sum:

$${}_L\langle 0|\mathbf{S}_\mathbf{x}\cdot\mathbf{S}_0|0\rangle_L=\frac{(-1)^{\|\mathbf{x}\|}}{L^2X_T}+\frac{1}{L^2}\sum_{s\ne T}\frac{e^{i\mathbf{k}_s\mathbf{x}}}{X_s} . \tag{36a}$$

Setting $x=(0,0)$ we get

$$\tfrac{3}{4}=\frac{1}{L^2X_T}+\frac{1}{L^2}\sum_{s\ne T}\frac{1}{X_s} , \tag{36b}$$

which leads to

$$(-1)^{\|\mathbf{x}\|}\,{}_L\langle 0|\mathbf{S}_\mathbf{x}\cdot\mathbf{S}_0|0\rangle_L=\tfrac{3}{4}+\frac{1}{L^2}\sum_{s\ne T}\frac{e^{i\mathbf{k}_{s+T}\mathbf{x}}-1}{X_s} . \tag{36c}$$

We wish now to make the following claim: Suppose we calculate X_s and let $L_{1,2}\to\infty$ with a fixed ratio, also changing s such that k_s is kept fixed at a value q. q is assumed to differ from 0 and T. The claim is the X_s approaches a limit $x(q)$ and that the corrections are vanishing faster than $1/L$. At most we expect them to go as $\log^\gamma L/L^2$.

This claim is similar to a property conjectured to hold for the classical nonlinear sigma model in three dimensions.[9] The basis of it is the fact that global invariants [like the left-hand side of (36) after Fourier transformation] have the property that they are less infrared singular in the spin wave expansion than other quantities. For example, although the staggered magnetization of the one-dimensional spin chain would suffer from infrared divergences in the spin wave expansion, global invariants would not.[10] In the equivalent classical case (now in two-dimensions) this infrared finiteness is known to hold to any order in the spin wave expansion.[10] It is very plausible to expect the same to be true in the quantum one-dimensional case. When we go to higher dimensions, only the momenta summed over change but not the structure of the higher-order corrections in the spin wave expansion. Smaller phase space at low momenta will soften the infrared divergences, and by power counting, we expect a quantity that was infrared finite in $d=1$ to approach its infinite-volume limit faster than $1/L$ in $d=2$. Note only do we expect this to hold to any order in the spin wave expansion; we expect this to be an exact result unspoiled by nonperturbative corrections.

The above claim implies that if $x(q)$ has singularities of such a nature that replacing X_s by $x(k_s)$ in the calculation of M_L^2 and then taking the infinite-volume limit induces corrections of order $1/L$; then we may, to leading order, neglect corrections which come about because X_s is not equal to $x(k_s)$. In other words we have, up to and including order $1/L$ corrections,

$$M_L^2\equiv\tfrac{3}{4}-\frac{1}{L^2}\sum_{s\ne T}\frac{1}{X_s}\approx\frac{3}{4}-\frac{1}{L^2}\sum_{s\ne T}\frac{1}{x(k_s)} . \tag{37}$$

The main point here is that in the last term all the finite-size dependence is explicit, as the function $x(q)$ has no size dependence left. $x(q)$ is a property of the infinite volume model. $x(q)$ has a singularity at $q=T$, as we know from the analysis of the infinite-volume case: $x(q)\sim x_0|q-T|$, $q\to T$.

It is this singularity which gives all the leading finite-size corrections in (37). We get

$$M_L^2=\tfrac{3}{4}-\int\frac{d^2k}{(2\pi)^2}\frac{1}{x(k)}-\frac{\alpha(\rho^2)}{x_0L}+O\left[\frac{\log^\gamma L}{L^2}\right] . \tag{38}$$

The shape function $\alpha(\rho^2)$ is universal and defined as follows: Let $f(k)$ be a periodic function of k_μ (under $k_\mu\to k_\mu+2\pi$). We assume that $f(k)\ge 0$ everywhere and that f is smooth everywhere except at $k=T$, where it also vanishes; $f(k)/|k-T|\to 1$ as $k\to T$. f does not vanish anywhere else in the first Brillouin zone. Then $\alpha(\rho^2)$ is well defined by

$$\alpha(\rho^2)=\lim_{\substack{L\to\infty\\ L_1=L\rho\\ L_2=L\rho^{-1}}}\left[L\left[\frac{1}{L^2}\sum_{s\ne T}\frac{1}{f(k_s)}-\int_{0\le k_\mu\le 2\pi}\frac{d^2k}{(2\pi)^2}\frac{1}{f(k)}\right]\right] . \tag{39}$$

Going back now to (38) we easily identify

$$\mathcal{S}^2=\lim_{L\to\infty}M_L^2=\tfrac{3}{4}-\int\frac{d^2k}{(2\pi)^2}\frac{1}{x(k)} , \tag{40}$$

and by (33) $\mathcal{S}^2$ also equals $4\kappa_1^2\kappa_2^2$. All that is left to do is to identify x_0. This can be done at $L=\infty$, where we have from (35)

$$\langle 0|\mathbf{S}_x\cdot\mathbf{S}_0|0\rangle=(-1)^{\|\mathbf{x}\|}\mathcal{S}^2+\int\frac{d^2k}{(2\pi)^2}\frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{x(k)} . \tag{41}$$

For large x we get the following asymptotics

$$(-1)^{\|\mathbf{x}\|}\langle 0|\mathbf{S}_x\cdot\mathbf{S}_0|0\rangle\sim\mathcal{S}^2+\frac{1}{2\pi x_0}\frac{1}{|\mathbf{x}|}+\cdots \quad \text{as } |\mathbf{x}|\to\infty . \tag{42}$$

We use now $\mathbf{S}_x\cdot\mathbf{S}_0=S_x^3S_0^3+\frac{1}{2}[S_x^+S_0^-+S_x^-S_0^+]$ and insert intermediate states, assuming as usual that the only the one-magnon states are needed for leading large distance asymptotics. This leads to the identification

$$\frac{1}{x_0}=2\kappa_1^2 . \tag{43}$$

Our final finite-size formula is given by

$$M_L^2=4\kappa_1^2\kappa_2^2-2\kappa_1^2\frac{\alpha(\rho^2)}{L}+O\left[\frac{\log^\gamma L}{L^2}\right] \tag{44}$$

with $\alpha(\rho^2)$ defined in (39). In the Appendix we show how to calculate $\alpha(\rho^2)$ in an efficient way.

The restriction to periodic boundary conditions has forced L_1 and L_2 to be even separately. While it is obvious that the absence of frustration in a finite volume would require that L_1L_2 be even we should be able to deal with a case where L_1 is even (say) and L_2 is odd. This can be done by using skewed periodic boundary conditions. These boundary conditions are defined by writing the two-dimensional system in a notation appropriate for a one-dimensional chain with periodic boundary condition. For the nearest-neighbor case we would write

$$\mathcal{H}=J\sum_{i=0}^{L_1L_2-1}(\mathbf{S}_i\cdot\mathbf{S}_{i+1}+\mathbf{S}_i\cdot\mathbf{S}_{i+L_2}) . \tag{45}$$

The nomenclature "skewed periodic boundary conditions" becomes clear if we write

$$\begin{aligned} &i=x_1+L_1x_2 ,\\ &0\le i\le L_1L_2-1 ,\\ &0\le x_1\le L_1-1 ,\\ &0\le x_2\le L_2-1 , \end{aligned} \tag{46}$$

leading to

$$\begin{aligned} &\mathcal{H}=J\sum_{x_1=0}^{L_1-1}\sum_{x_2=0}^{L_2-1}(\mathbf{S}_{(x_1,x_2)}\cdot\mathbf{S}_{(x_1+1,x_2)}+\mathbf{S}_{(x_1,x_2)}\cdot\mathbf{S}_{(x_1,x_2+1)}) ,\\ &\mathbf{S}_{(x_1,x_2)}=\mathbf{S}_{(x_1,x_2+L_2)} ,\\ &\mathbf{S}_{(x_1+L_1,x_2)}=\mathbf{S}_{(x_1,x_2+1)} . \end{aligned} \tag{47}$$

Working out the momentum space associated with these boundary conditions one can convince oneself that formula (44) still holds. There is no frustration for L_2 odd because only spins separated by an odd number of bonds are coupled in (45).

Before closing we should address the question of whether (44) works in practice. Using the value of $\alpha(1)$ calculated in the Appendix and the slope we extracted from the data of Reger and Young[4] we were able to obtain an estimate of κ_1 which agreed well with the value obtained to leading order in the spin wave expansion of the Heisenberg antiferromagnet.

VI. THE LOW-LYING SPECTRUM

We proceed to find a way to extract the sound velocity c from a finite-size effect. For too-small systems it is impractical to get in the low-momentum regime and see the linear dispersion for the magnons directly. We shall present a method we expect to work better in practice.

In the previous section we established

$$M_L^2\equiv\frac{3}{4}-\frac{1}{L^2}\sum_{s\ne T}\frac{1}{X_s}\approx\frac{3}{4}-\frac{1}{L^2}\sum_{s\ne T}\frac{1}{x(k_s)} . \tag{48}$$

For $L\to\infty$ we have

$$X_T\sim\frac{1}{4L^2\kappa_1^2\kappa_2^2} \quad \text{as } L\to\infty . \tag{49}$$

For any value of $s\ne T$ one can replace X_{s+T} by $x(k_{s+T})$ but for $s=T$ this would be incorrect. Motivated by the expected form in a relativistic theory we use the following approximation for X:

$$\begin{aligned} &X_{s+T}\approx[x^2(k_s+T)+X_T^2]^{1/2} ,\\ &(-1)^{\|\mathbf{x}\|}\langle 0|\mathbf{S}_x\cdot\mathbf{S}_0|0\rangle\approx\frac{1}{L^2}\sum_s\frac{e^{ik_sx}}{[x^2(k_s+T)+X_T^2]^{1/2}} . \end{aligned} \tag{50}$$

We expect this approximation to be acceptable for large values of $|\mathbf{x}|$; for those we can use $x(k_s+T)\propto x_0|k_s|$. Going now to unequal times we have

$$ {}_L\langle 0|(-1)^{\|\mathbf{x}\|}\mathbf{S}_x(t)\cdot\mathbf{S}_0(0)|0\rangle_L \approx\frac{1}{L^2}\sum_s\frac{e^{ik_sx-i\omega_{k_s}t}}{[x^2(k_s+T)+X_T^2]^{1/2}} . \tag{51}$$

$\omega_k\approx c|k|$ for $k\ne0$ (51) is adequate for large $|x|$ and large t. Relativistic invariance, however, now forces

$$\omega_{k_s}=\frac{c}{x_0}(x_0^2k_s^2+X_T^2)^{1/2} . \tag{52}$$

X_T plays the role of a mass and (52) is simply the famous relation $E=(m^2c^4+p^2c^2)^{1/2}$. This should be interpreted to mean that one magnon states have an effective mass in finite volumes given by (Planck's constant has been set to unity throughout, $h/2\pi=1$):

$$m_{\text{eff}}=\frac{X_T}{x_0c} . \tag{53}$$

The energy of a zero momentum one magnon state is then separated from the ground state by a gap ΔE given by

$$\Delta E=m_{\text{eff}}c^2=\frac{cX_T}{x_0}=\frac{c}{2L^2\kappa_2^2} . \tag{54}$$

Since there are two such one-magnon states with $Q=\pm1$ we have identified two low-lying states at momentum T.

However, in a finite volume the ground state is a singlet with respect to the total magnetization and all the states must have integral magnetization because of the evenness of the number of lattice sites. So we are forced to conclude that we have identified a triplet which is the lowest-lying excited state in our system. The energy gap is given by Eq. (54). The third member of the triplet has $Q=0$ and is not excited when $\sum_x(-1)^x \mathbf{S}_x$ acts on the ground state.

We now approach the problem of identifying the lowest portion of the spectrum in the finite box from a different point of view.[3,11] In a very large box the lowest-lying spectrum of the system, assuming spontaneous symmetry breaking at infinite volume, must represent the slow precession of the order parameter in time. This precession freezes at infinite volume and it has been argued a long time ago already that the levels participating in the precesion are separated from the ground state by gaps going like the inverse volume.[12]

The tower of low-lying states (all are below the softest magnon of nonzero momentum) collapse onto the ground state where the volume is taken to infinity. Since we need to produce in this limit a continuous infinity of states distinguished by different orientations of a global order parameter (a classical variable in the limit) the tower must contain an infinite number of finite dimensional representations of the SO(3) global symmetry group.

We seek now an effective Hamiltonian $\mathcal{H}_{\text{eff}}$ which describes this tower of states. $\mathcal{H}_{\text{eff}}$ governs the time development of the global order parameter, in our case the staggered magnetization. We can imagine getting $\mathcal{H}_{\text{eff}}$ by iterating a renormalization group transformation which integrates out all spin modes with momentum different from T. The fixed point which controls the form of $\mathcal{H}_{\text{eff}}$ must be the same which controls the nonlinear sigma model viewed as a quantum system.[11] This implies that $\mathcal{H}_{\text{eff}}$ has the following form:

$$\begin{aligned} &\mathcal{H}_{\text{eff}}=\gamma \mathbf{L}^2+E_g \ , \\ &[L^\alpha, L^\beta]=i\epsilon^{\alpha\beta\gamma}L^\gamma \ . \end{aligned} \tag{55a}$$

The single relevant unknown in $\mathcal{H}_{\text{eff}}$ is the parameter γ. The spectrum of $\mathcal{H}_{\text{eff}}$ is given by

$$E_l=\gamma l(l+1)+E_g, \quad l=0,1,2,\ldots \tag{55b}$$

with a degeneracy of $2l+1$ per level. E_g is the ground-state energy. Comparing with (54) we get, using $l=0$ and $l=1$,

$$\begin{aligned} &\gamma=\frac{c}{4L^2\kappa_2^2} \ , \\ &\mathcal{H}_{\text{eff}}-E_g=\frac{c}{4L^2\kappa_2^2}\mathbf{L}^2 \ . \end{aligned} \tag{56}$$

Therefore, if we know already κ_2 and identify a few lower l states in a finite system, we can obtain the last of our parameters, namely c.

The triplet state has been seen already by Tang and Hirsch.[13] Their interpretation of the state is different from ours. As is clear from our discussion in this paper, this state is, in our opinion, entirely expected if the most conventional picture of spontaneous symmetry breaking with antiferromagnetic long-range order is assumed to occur at infinite volume.

What are the properties of the tower of states we would expect to hold approximately? Since the magnitude of $\psi\equiv\sum_x(-1)^{\|x\|}\mathbf{S}(x)$ is expected to fluctuate much faster than the orientation it can be taken as fixed at its average for time scales of the order L^2. So only the orientation of $\psi,\tilde{\psi}$ is a dynamical variable and $\mathbf{L}$ is the conjugate momentum. The wave functions should therefore be given by

$$\phi_{lm}(\psi)=Y_{l,m}(\tilde{\psi})F(\psi^2) \ . \tag{57}$$

For very large volumes we ought to have

$$F(\psi^2)=\delta(\psi^2-\mathcal{S}^2) \ . \tag{58}$$

Let us calculate the distribution of ψ^3 for the ground state:

$$\begin{aligned} \mathcal{P}(\psi^3)d\psi^3&=\mathcal{N}\int d^3\psi\,\delta(\psi^2-\mathcal{S}^2) \\ &=\mathcal{N}d\psi^3\int d\psi^2 d\psi^1\delta((\psi^1)^2+(\psi^2)^2-\mathcal{S}^2+(\psi^3)^2) \\ &=a\Theta((\psi^3)^2-\mathcal{S}^2) \ . \end{aligned} \tag{59}$$

In particular we find

$$\langle(\psi^3)^2\rangle_g=\tfrac{1}{3}\mathcal{S}^2 \tag{60}$$

as expected. For the $l=1$ state we take the $m=1$ component to get

$$\phi_{1,1}=\mathcal{N}\frac{\psi^3}{|\psi|}\delta(\psi^2-\mathcal{S}^2) \ , \tag{61}$$

leading to

$$\langle(\psi^3)^2\rangle_{1,1}=\tfrac{3}{5}\mathcal{S}^2 \ . \tag{62}$$

This leads to

$$\frac{\langle(\psi^3)^2\rangle_{1,1}}{\langle(\psi^3)^2\rangle_g}=\tfrac{9}{5}=1.8 \ , \tag{63}$$

in good agreement with the measurement of Tang and Hirsch.[13]

This supports our feeling that we understand well the finite-size effects in the systems under consideration and that even very small systems may provide us with accurate and detailed information about the infinite-volume limit.

The tower of states is a generic feature for any system which undergoes spontaneous symmetry breakdown and has a nonconserved global order parameter. The special feature here is that if one employs the definition of translations which is naturally associated with the spin operators the order parameter carries momentum T. Since in a finite volume spontaneous breakdown does not occur, this momentum is a good quantum number without halving the Brillouin zone. Therefore we know that the states of the tower at level l will carry momentum lT. In other words even l states have zero momentum while odd l states have a total momentum equal to T.

Another way to estimate c is to consider the size dependence of the ground-state energy E_g, in the finite volume. Since the tower of states are spaced at gaps of order $1/L^2$ they would contribute shifts of order $1/L^2$ to the ground-state energy. As we shall see later the zero-point energies of the magnons give a shift of $O(1/L)$ and therefore a leading contribution. We have two magnons per state of reduced momentum p (p and $p+T$ identified). The zero-point contribution is a Casimir energy given by

$$\frac{E_g}{L^2}-\lim_{L\to\infty}\left[\frac{E_g}{L^2}\right]=\frac{1}{2L^2}\sum_s \omega_{k_s}-\tfrac{1}{2}\int_{|k_\mu|<\pi}\frac{d^2k}{(2\pi)^2}\omega_k \ . \tag{64}$$

In (64) we went back to using the full Brillouin zone and therefore we have only one magnon per state.

Consider now a function f as defined above, Eq. (39). We define

$$\beta(\rho^2)=\lim_{\substack{L\to\infty\\ L_1=L\rho\\ L_2=L\rho^{-1}}}\frac{1}{2}\left[L^3\left[\sum_{s\neq T}f(k_s)-\int_{0\le k_\mu\le\pi}\frac{d^2k}{(2\pi)^2}f(k)\right]\right] . \tag{65}$$

$\beta(\rho^2)$ is easily calculated by the same methods as those of the Appendix. For example,

$$\beta(1)=-0.719 \ . \tag{66}$$

Remembering the factor of 2 needed because ω_k vanishes twice (unlike f) we obtain

$$\frac{E_{g,L}}{L^2}=\lim_{L\to\infty}\frac{E_{g,L}}{L^2}+\frac{2c}{L^3}\beta(\rho^2) \ . \tag{67}$$

For $\rho=1$ we can compare with the measurement of Gross *et al.*[5] In their normalization the coefficient of the L^{-3} term is -9.14 ± 0.05. This gives $c=6.36\pm0.03$.

Judging by their absolute value of the energies we conclude that their numbers really correspond to $J=4$. Oguchi's spin wave analysis[14] would give, for $J=4$

$$c=4\sqrt{2}(1+0.158+\cdots)\approx 6.55 \ . \tag{68}$$

The agreement is quite good.

We are not sure whether (67) is indeed an exact result theoretically. In practice we see that it works quite well.

VII. SUMMARY

Let us summarize the main results. Using the Holstein-Primakoff variables the momentum is defined in such a way that translational invariance is not broken by antiferromagnetic order. Working at infinite volume we define the parameters κ_1, κ_2, and c:

$$\langle 0|S_x^+|k\rangle=\begin{cases}\kappa_2|k|^{1/2}e^{ikx}-\dfrac{\kappa_1}{|k|^{1/2}}e^{i(k+T)x}, & k\to 0\ ,\\[2ex] \dfrac{\kappa_1}{|k-T|^{1/2}}e^{ikx}+\kappa_2|k-T|^{1/2}e^{i(k+T)x}, & k\to T\ ,\end{cases} \tag{69a}$$

$$\omega_k=\begin{cases}c|k|, & k\to 0\ ,\\ c|k-T|, & k\to T\ .\end{cases}$$

One has then (still at infinite volume)

$$\mathcal{S}=-2\kappa_1\kappa_2$$

$$(-1)^{\|x\|}\langle 0|\mathbf{S}_x\cdot\mathbf{S}_0|0\rangle\sim\mathcal{S}^2+\frac{2\kappa_1^2}{\pi|x}|+O\left[\frac{\log^\gamma|x|}{|x|^2}\right] \quad \text{as } |x|\to\infty\ . \tag{69b}$$

Hence κ_1,κ_2 are closely related to the stiffness ρ_s.

Equations (69a) and (69b) give the precise definition of the constants κ_1, κ_2 and c as parameters characterizing the infinite volume systems. It is customary to represent the low-momentum and low-energy behavior of a system with Goldstone bosons by an effective Lagrangian. To leading order in the momenta and frequencies the response of the original system to slowly varying and slowly fluctuating external sources is given by coupling the same sources to the effective Lagrangian and solving the associated Euler-Lagrange equations. To this order, by definition, loop corrections coming from the effective Lagrangian are not be included. Therefore, the parameters in the effective Lagrangian include all the renormalization effects of the original, microscopic Hamiltonian.

The effective Lagrangian is written in terms of a unit-length three-component vector field $\Omega(x)$. This field has two degrees of freedom representing the magnons. In standard notation, at zero temperature the effective Lagrangian is given by

$$L=\frac{\rho_s}{2}\int dt\sum_x\left[\frac{1}{c}(\partial_t\Omega)^2-\sum_\mu[\Omega(x)-\Omega(x+\mu)]^2\right] . \tag{70}$$

The fluctuations in the original staggered magnetization (connected correlations) can be identified, at low energy and momentum, within the rule described above, with those of $\mathbf{\Omega}(x)$. There is a normalization factor in this correspondence with $(-1)^{\|x\|}\mathbf{S}_x$ mapping into $z^{1/2}\mathbf{\Omega}(x)$. This leads to $\kappa_2^2=2\rho_s$ and $\kappa_1^2=z/(8\rho_s)$. The parameter c in L is identical to that in Eq. (69a).

Consider now the system with the same Hamiltonian as above but now defined on a finite rectangular $L_1\times L_2$ lattice with periodic (even L_1, even L_2) or skewed periodic (even L_1, odd L_2) boundary conditions. For $L_1,L_2\to\infty$ with $L_1/L_2=\rho^2$ fixed and $\rho^2\neq 0,\infty$, one has the following asymptotic formulas:

$$\frac{1}{L_1L_2}\sum_{x\in\text{box}}(-1)^{\|x\|}{}_L\langle 0|\mathbf{S}_x\cdot\mathbf{S}_0|0\rangle_L \sim \mathcal{S}^2-2\kappa_1^2\frac{\alpha(\rho^2)}{L}+O\left[\frac{\log^\gamma(L_1L_2)}{L_1L_2}\right] \quad \text{as } L_{1,2}\to\infty \ , \tag{71}$$

with $\alpha(\rho^2)$ calculated in the Appendix. The lowest excited states of the system in the box have the following spectrum (and degeneracies $g_l=2l+1$):

$$E_l\approx E_g+\frac{c}{4L^2\kappa_2^2}l(l+1) \ . \tag{72}$$

Here E_g is the ground-state energy and $L^2\equiv L_1L_2$. Using the "normal" definition of momentum the states at level l carry momentum T or O depending on whether l is even or odd.

We also discussed the possibility that the volume dependence of the ground state can be used to obtain c via the following formula:

$$\frac{E_{g,L}}{L^2}=\lim_{L\to\infty}\frac{E_{g,L}}{L^2}+\frac{2c}{L^3}\beta(\rho^2) \ , \tag{73}$$

with $\beta(\rho^2)$ defined in (65). Good agreement between numerical results and spin wave theory was observed.

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APPENDIX

In this appendix we shall first calculate $\alpha(\rho^2)$ and then we shall try to estimate at what sizes would one have a reasonable chance to see the asymptotic correction to M_L^2. The latter question will be addressed in the spin wave expansion which, although by itself not necessarily reliable, could very well provide a good indication for the relative significance of finite size effects. The calculation of $\beta(\rho^2)$ will be only briefly outlined.

Let f be a function of periodic under $k_\mu\to k_\mu+2\pi$ which vanishes nowhere except at $k=T$. For any $k\neq T$ $f(k)$ is smooth and, we have

$$\frac{f(k)}{|k-T|}\to 1 \quad \text{as } k\to T \ . \tag{74}$$

We want to evaluate the leading correction to the quantity $\mathcal{S}_L$:

$$\mathcal{S}_L=\frac{1}{L_1L_2}\sum_{s\neq T}\frac{1}{f(k_s)} \ , \qquad k_s\equiv 2\pi(s_1/L_1,s_2/L_2) \ . \tag{75}$$

The sum extends over $0\le s_\mu\le L_\mu-1$. We rewrite $\mathcal{S}_l$ as

$$\mathcal{S}_L=\lim_{\Delta\to 0+}\left[\frac{1}{L^2}\sum_s\frac{1}{[f^2(k_s)+\Delta^2]^{1/2}}\frac{1}{L^2\Delta}\right] . \tag{76}$$

Starting from (76) and using Poisson's formula one easily establishes ($L^2=L_1L_2$)

$$\mathcal{S}_L=\int_{0\le k_\mu\le 2\pi}\frac{d^2k}{(2\pi)^2}\frac{1}{f(k)}+\frac{1}{L}\int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{\pi}}\left[\int_{0\le q_\mu\le 2\pi L_\mu}\frac{d^2q}{(2\pi)^2}\exp[-\tau^2L^2f^2(q_1/L_l,q_2/L_2)]\sum_{\mathbf{m}\neq 0}e^{i\mathbf{m}\cdot\mathbf{q}}-1\right] . \tag{77}$$

With our information on f we derive

$$\alpha(\rho^2)=\int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{\pi}}\left[\frac{1}{4\pi\tau^2}\sum_{\mathbf{m}}{}'\exp\left[-\frac{\rho^2m_1^2}{4\tau^2}-\frac{m_2^2}{4\tau^2\rho^2}\right]-1\right] . \tag{78}$$

Employing some Θ-function identities Eq. (78) can be put in the following form:

$$\alpha(\rho^2)=-\frac{2}{\pi}\left[1-\sum_{\mathbf{m}\neq 0}\int_1^\infty dt\, e^{-\pi t^2(\rho^2m_1^2+\rho^{-2}m_2^2)}\right] . \tag{79}$$

The evaluation of $\alpha(\rho^2)$ can be done now on a calculator. Using

$$Q(\xi)\equiv\int_\xi^\infty\frac{d\tau}{\sqrt{2\pi}}e^{-(1/2)\tau^2}\sim\frac{1}{\sqrt{2\pi}}\frac{e^{-(1/2)\xi^2}}{\xi}\left[1-\frac{1}{\xi^2+2}+\frac{1}{(\xi^2+2)(\xi^2+4)}-\frac{5}{(\xi^2+2)(\xi^2+4)(\xi^2+6)}+\frac{9}{(\xi^2+2)(\xi^2+4)(\xi^2+6)(\xi^2+8)}+\cdots\right] , \tag{80}$$

we need to sum only a few terms in the expansion

$$\alpha(\rho^2)=-\frac{2}{\pi}\left[1-\sum_{\mathbf{m}\neq 0}\frac{1}{R(\mathbf{m})}Q(\sqrt{2\pi}R(\mathbf{m}))\right], \qquad R^2(\mathbf{m})\equiv\rho^2m_1^2+\rho^{-2}m_2^2 . \tag{81}$$

Our results are

ρ^2	$\alpha(\rho^2)$
1	-0.6208
$\frac{4}{5}$	-0.6155
$\frac{3}{4}$	-0.6124
$\frac{2}{3}$	-0.6035
$\frac{1}{2}$	-0.5675
$\frac{1}{3}$	-0.4716

We now proceed to show, using $\alpha(\rho^2)$, one can replace the calculation of the integral giving the leading spin wave correction to $\mathcal{S}$ by the calculation of a corresponding lattice momentum sum. For L_1 and L_2 both even, Anderson has found over 30 years ago:[12]

$$\mathcal{S}=\tfrac{1}{2}-\Delta_\infty \ . \tag{82}$$

Δ_∞ is the $L \to \infty$ limit of Δ_L with

$$1+2\Delta_L=\frac{1}{L_1L_2}\sum_{i_1=0}^{L_1-1}\sum_{\substack{i_2=0\\(i_1,i_2)\neq(0,0)\\(i_1,i_2)\neq(L_1/2,L_2/2)}}(1-\{\tfrac{1}{2}(\cos[(2\pi/L_1)i_1]+\cos[(1\pi/L_2)i_2)]\}^2)^{-1/2} \ . \tag{83}$$

The above sum will approach its infinite-volume limit with a correction going like $1/\sqrt{L_1L_2}$. The factor in front of this leading correction is different from $\alpha(\rho^2)$ by a factor $2\sqrt{2}$. The factor of 2 reflects the fact that now we have two singularities in $f(k)$ instead of one. The factor of $\sqrt{2}$ comes about because the integrand at infinite volume goes as $\sqrt{2}/|k|$ as $k\to 0$ and as $\sqrt{2}/|k-T|$ as $k \to T$. Note that the sum is invariant under $(i_1,i_2)\to(i_1,i_2)+\frac{1}{2}(L_1,L_2)$ and thus all our previous analysis applies. We therefore obtain

$$\begin{aligned}1+2\Delta_L&=\int_{0\le k_\mu \le 2\pi}\frac{d^2k}{(2\pi)^2}\frac{1}{[1-\frac{1}{4}(\cos k_1+\cos k_2)^2]^{1/2}}\\&\quad+\frac{2\sqrt{2}\alpha(\rho^2)}{(L_1L_2)^{1/2}}+\cdots\\&\approx 1.393+\frac{2\sqrt{2}\alpha(\rho^2)}{(L_1L_2)^{1/2}}+\cdots \ .\end{aligned} \tag{84}$$

To get a feeling for how good finite volumes are on the numerical level, we evaluate the sum giving $1+2\Delta_L$ exactly for various small boxes and compare the result to the expression on the last line in Eq. (84)

L_1 L_2	$1+2\Delta_L$	$1+2\Delta_L-\dfrac{2\sqrt{2}\alpha(\rho^2)}{(L_1L_2)^{1/2}}$
2 2	0.5000	1.378
2 4	0.8274	1.393
4 4	0.9524	1.391
4 5	1.002	1.391
4 6	1.044	1.393

We see that the inclusion of the leading correction works surprisingly well for the smallest systems imaginable. If this property holds beyond the spin wave approximation we have very good chances to extract the parameters we are interested in from the results of exact diagonalization methods. The numerics works similarly for skewed periodic boundary conditions.

The calculation of $\beta(\rho^2)$ proceeds on similar lines. Starting from the identity

$$f=(4\pi)^{-1/2}\int_0^\infty \frac{d\tau}{\tau^2}[1-\exp(-\tau^2 f^2)] \ , \tag{85}$$

one obtains the following expression:

$$\begin{aligned}\beta(\rho^2)=\frac{-2}{3}-\sum_{\mathbf{m}\neq 0}&\left[\left[\frac{1}{2\pi R^2(\mathbf{m})}-2\pi R^2(\mathbf{m})\right]\right.\\&\left.\times\frac{Q(\sqrt{2\pi}R(\mathbf{m}))}{R(\mathbf{m})}\right]\\&+\sum_{\mathbf{m}\neq 0}\left[e^{-\pi R^2(\mathbf{m})}\left[1+\frac{1}{2\pi R^2(\mathbf{m})}\right]\right] \ .\end{aligned} \tag{86}$$

The numerical values are

ρ^2	$\beta(\rho^2)$
1	-0.7186
$\frac{4}{5}$	-0.7362
$\frac{3}{4}$	-0.7482
$\frac{2}{3}$	-0.7790
$\frac{1}{2}$	-0.9113
$\frac{1}{3}$	-1.296

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