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Finite-size scaling in the spin-$\frac{1}{2}$ XY model on a square lattice

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Abstract. Energy eigenvalues and order parameters are calculated by exact diagonalization for the isotropic spin-$\frac{1}{2}$ XY model on square lattices of up to 6×6 sites. The finite-size scaling behaviour is in excellent agreement with the effective Lagrangian predictions of Hasenfratz and Niedermayer (Hasenfratz P and Niedermayer F 1993 *Z. Phys.* B **92** 91). Estimates are obtained for the bulk ground-state energy per site, the spontaneous magnetization, the spin-wave velocity and the spin-wave stiffness.

1. Introduction

Recent advances in computer technology have allowed the exact diagonalization of Ising-type quantum spin systems up to 36 sites in size. Schultz *et al* (1996), for example, studied the $J1$–$J2$ XXZ Heisenberg spin model on square lattices up to 6×6 sites. Our aim in this paper is to carry out an exact diagonalization study of the spin-$\frac{1}{2}$ isotropic XY model on the square lattice, in order to verify that its finite-size scaling behaviour agrees with the predictions of effective Lagrangian theory (Hasenfratz and Niedermayer 1993), and to estimate the spin-wave parameters of the model.

A review of the model was given by Betts and Miyashita (1990). The first finite-cell exact diagonalization studies were performed by Pearson (1977) and Oitmaa and Betts (1978), and further studies were carried out by Oitmaa *et al* (1980), and Betts and Kelland (1983). A renormalization-group analysis was made by Penson *et al* (1980), and a variational study by Suzuki and Miyashita (1978). Monte Carlo simulations were done by Loh, Scalapino and Grant (1985) and Okabe and Kikuchi (1988), which were followed by a very large and accurate simulation from Zhang and Runge (1992). More recently, Farnell *et al* (1997) have used a coupled-cluster method to treat the model.

Spin-wave theory was originally thought to be unsatisfactory for this model (Mattis 1981), but Gomez-Santos and Joannopoulos (1987) showed that by a judicious choice of the quantized spin axis one can obtain a good theoretical fit to the model. The spin-wave treatment was extended to second order by Hamer *et al* (1991), who also presented a series analysis based on an expansion about the Ising limit.

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These studies have shown beyond doubt that there is long-range order in the ground state of the isotropic model, as first predicted by Oitmaa and Betts (1978). The existence of long-range order has since been rigorously proven by Kennedy *et al* (1988), and Kubo and Kishi (1988). This implies that the O(2) rotational symmetry of the original Hamiltonian must be spontaneously broken in the ground state, giving rise to massless Goldstone bosons (the spin waves or 'magnons'), according to field theory. Hasenfratz and Niedermayer (1993) have presented an effective Lagrangian treatment of the Goldstone boson degrees of freedom which covers this situation, and predicts the long-range or finite-size scaling behaviour of the model, as well as its behaviour at low temperatures and small magnetic fields. The parameters of the effective Lagrangian in leading order are the spin-wave stiffness ρ_s, the spin-wave velocity v, and the spontaneous magnetization Σ.

In this paper we diagonalize the model exactly on square lattices up to 6×6 sites in size, using methods outlined in section 2. The results are presented in section 3, and turn out to match the predictions of effective Lagrangian theory very closely. Fitting the data to the predicted finite-size scaling forms, we obtain estimates of the bulk ground-state energy per site, and the parameters ρ_s, v and Σ. It would be interesting to see how well these results could be predicted by an extended spin-wave calculation.

2. Method

The isotropic spin-$\frac{1}{2}$ XY ferromagnet on the square lattice has the Hamiltonian

$$H = -\tfrac{1}{2}\sum_{\langle ij\rangle}(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y) \tag{2.1}$$

$$= -\sum_{\langle ij\rangle}(\sigma_i^+\sigma_j^- + \sigma_i^-\sigma_j^+) \tag{2.2}$$

where the sum $\langle ij\rangle$ runs over nearest-neighbour pairs on the lattice, and the σ matrices are the usual Pauli spin operators acting on a 2-state spin-variable at each site. We shall employ a representation in which the σ_i^z are diagonal. The total magnetization operator is

$$\boldsymbol{M} = \sum_i \boldsymbol{S}_i = \tfrac{1}{2}\sum_i \boldsymbol{\sigma}_i. \tag{2.3}$$

The ground state (for even N) lies in the sector with $M^z = 0$.

We shall measure the long-range order of the system in terms of the quantity

$$f_{LRO} = 4\frac{\langle \boldsymbol{M}^2\rangle}{N^2} - \frac{2}{N} \tag{2.4}$$

following Fujiki and Betts (1986), where $\langle \boldsymbol{M}^2\rangle$ is the ground-state expectation value of $\boldsymbol{M}^2$, and $N = L^2$ is the total number of sites.

The isotropic system possesses a spontaneously broken O(2) rotational symmetry, so that according to effective Lagrangian theory (Hasenfratz and Niedermayer 1993) the ground-state energy per site for a finite system of size L with periodic boundary conditions should scale as

$$\epsilon_0(L) = \epsilon_0(\infty) - \frac{\alpha_1 v}{2L^3} + \mathrm{O}(L^{-5}) \tag{2.5}$$

where the geometrical 'shape coefficient' $\alpha_1 = 1.4377\ldots$ for the square lattice, and v is the spin-wave velocity. The mass gaps should scale as

$$E_j - E_0 = \frac{j^2 v^2}{2\rho_s L^2} + \mathrm{O}(L^{-4}, j^4) \tag{2.6}$$

for a state with spin $j = M^z$, where ρ_s is the spin-wave stiffness or helicity modulus.

Exact diagonalizations have been carried out for $L \times L$ lattices, $L = 1, \ldots, 6$. The methods employed are fairly standard, for the most part, and will not be described in detail here. First, a list of allowed basis states in the given sector was prepared, using the 'sub-lattice coding' technique of Lin (1990). This efficient technique produces a sorted list of states, requiring only one integer word of storage per state. Since only the zero-momentum ground state is considered here, the states were 'symmetrized': that is, all copies of a given state under translations, reflections and rotations were represented by a single state. Thus for the 6×6 lattice in the $M^z = 0$ sector, the total number of 'unsymmetrized' states is ${}^{36}C_{18} = 9 \times 10^9$, whereas under symmetrization this is reduced by a factor of approximately 288, down to 31 566 122.

Next, the Hamiltonian matrix elements are generated, by applying the spin–flip operators of equation (2.2) to each initial state, symmetrizing the resulting final state, and looking it up in the master file. The elements were grouped into blocks, each of which acts between small sub-sets of the initial and final state vectors, to avoid 'thrashing' during the matrix multiplications. Within each sub-set, the initial and final addresses can be fitted into a half-integer, so that the matrix elements occupied 5 Gbyte of storage over all.

Finally, the lowest eigenvalue and eigenvector of the Hamiltonian were found, using the conjugate gradient method. Nightingale *et al* (1993) showed that the conjugate gradient method converges faster than the Lanczos method for large problems such as this. Once the ground-state eigenvector is known, it is a simple extension to compute the long-range order expectation value f_{LRO}.

3. Results

Table 1 gives a list of the ground-state energies as a function of lattice size L and total magnetization $j = M^z$. This list agrees with a previous finite-cell calculation (Betts and Kelland 1983) for the case $L = 4$, $M^z = 0$. Note that we have not restricted ourselves here to the cases N even, or $M^z = 0$.

Figure 1 graphs the results as functions of j for fixed values of L. It can be seen that the behaviour is almost linear in j^2, showing that the leading behaviour (2.6) sets in very quickly. A polynomial fit in powers of j^2 to the ground-state energy per site:

$$\epsilon_0(L, j) = \sum_n a_n(L)(j^2)^n \tag{3.1}$$

using powers sufficient to fit all the available data exactly at each L, gives coefficients $a_0(L), a_1(L)$ as listed in table 2.

Figure 2 graphs the leading coefficient $a_0(L)$, i.e. the '$j = 0$ value', as a function of $1/L^3$. Again, the graph is almost linear, so that the leading behaviour (2.5) predicted by effective Lagrangian theory is very quickly established. The graph also appears quite smooth, even though only the even values of L correspond to actual physical eigenvalues. Closer examination shows that there is in fact a small alternation in the coefficients. A fit to the coefficients at higher L of the form

$$a_0(L) = b_0 + \frac{b_1}{L^3} + \frac{b_2}{L^5} + \frac{(-1)^L b_3}{L^6} \tag{3.2}$$

leads us to the estimates

$$b_0 = -1.0976(2) \tag{3.3}$$

$$b_1 = -1.64(7) \tag{3.4}$$

Table 1. Ground-state energy per site as a function of lattice size L and magnetization $j = M^z$.

L	$2j$	E_0/N
2	0	−1.414 213 562 373
	2	−1.000 000 000 000
	4	0.000 000 000 000
3	1	−1.149 665 828 185
	3	−1.030 132 700 924
	5	−0.791 456 180 624
	7	−0.444 444 444 444
	9	0.000 000 000 000
4	0	−1.124 972 697 436
	2	−1.105 869 011 797
	4	−1.049 258 814 766
	6	−0.956 275 532 993
	8	−0.828 230 582 209
	10	−0.666 542 044 881
	12	−0.473 097 428 529
	14	−0.250 000 000 000
	16	0.000 000 000 000
5	1	−1.109 271 963 809
	3	−1.093 876 929 636
	5	−1.063 227 022 543
	7	−1.017 564 832 954
	9	−0.957 206 282 978
	11	−0.882 514 235 871
	13	−0.793 891 032 781
	15	−0.691 782 222 570
	17	−0.576 692 344 169
	19	−0.449 215 517 801
	21	−0.310 054 774 839
	23	−0.160 000 000 000
	25	0.000 000 000 000
6	0	−1.105 388 167 527
	2	−1.101 684 925 406

Table 2. Coefficients $a_0(L)$, $a_1(L)$ as functions of lattice size L.

L	$a_0(L)$	$a_1(L)$
1	−2.000 000 000 000	—
2	−1.414 213 562 373	0.434 433 619 6329
3	−1.164 535 184 209	0.059 429 621 3383
4	−1.124 972 697 436	0.019 184 299 7462
5	−1.111 199 939 587	0.007 713 569 3649
6	−1.105 388 167 527	[0.003 703 242 1210]

which from (2.5) correspond to

$$\epsilon_0(\infty) = -1.0976(2) \tag{3.5}$$

$$v = 2.28(10). \tag{3.6}$$

This result for the ground-state energy per site is compared with other estimates in table 3. It is compatible with the remarkably precise Monte Carlo estimate of Zhang and Runge (1992), but an order of magnitude less accurate. The spin-wave velocity v has not been estimated

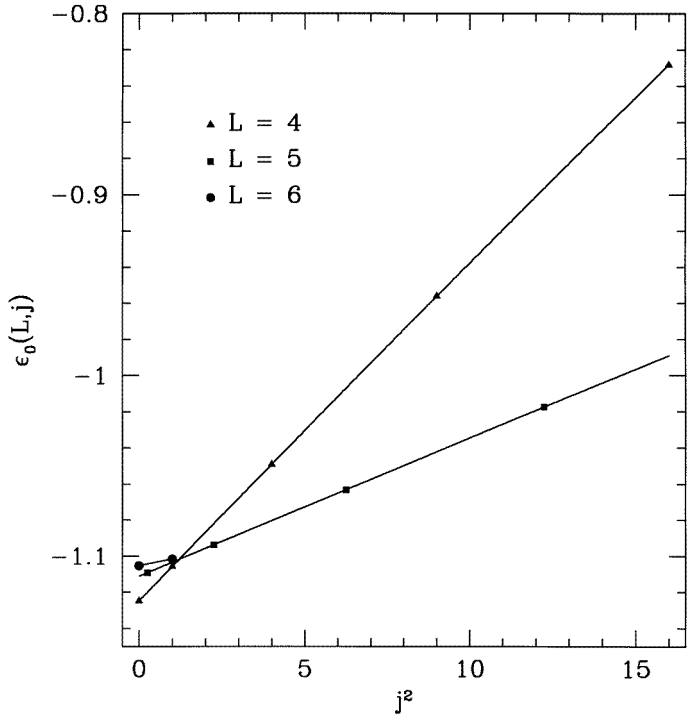

Figure 1. Graph of the ground-state energy per site $\epsilon_0(L, j)$ as a function of spin j^2 for lattice sizes $L = 4, 5, 6$.

before, as far as we are aware.

Table 3. Comparison of some numerical estimates for the ground-state energy per site $\epsilon_0(\infty)$ and the long-range order parameter Σ for the $S = \frac{1}{2}$ isotropic XY model on the square lattice.

$\epsilon_0(\infty)$	Σ	Method	Reference
−1.08(1)	0.47(1)	Finite-cell	Oitmaa and Betts (1978)
−1.086(4)	—	Monte Carlo	Loh *et al* (1985)
−1.074	0.48	Variational	Suzuki and Miyashita (1978)
−1.098(1)	—	Monte Carlo	Okabe and Kikuchi (1988)
−1.097 66(6)	0.435 48(3)	Series	Hamer *et al* (1991)
−1.0954	0.438	Spin-wave	Hamer *et al* (1991)
−1.097 66(2)	0.441(5)	Monte Carlo	Zhang and Runge (1992)
−1.097 84	0.435	Coupled-cluster	Farnell *et al* (1997)
−1.097 6(2)	0.44(1)	Finite-lattice	This work

Figure 3 graphs the coefficient $a_1(L)$ as a function of $1/L^4$, and again the behaviour is almost linear, as predicted by equation (2.6) (recall that by working with the energy per site we divide by a further factor of $N = L^2$). A fit to the coefficients at higher L of the form

$$a_1(L) = \frac{c_0}{L^4} + \frac{c_1}{L^6} + \frac{(-1)^L c_2}{L^6} \tag{3.7}$$

leads to the estimate

$$c_0 = 4.83(5). \tag{3.8}$$

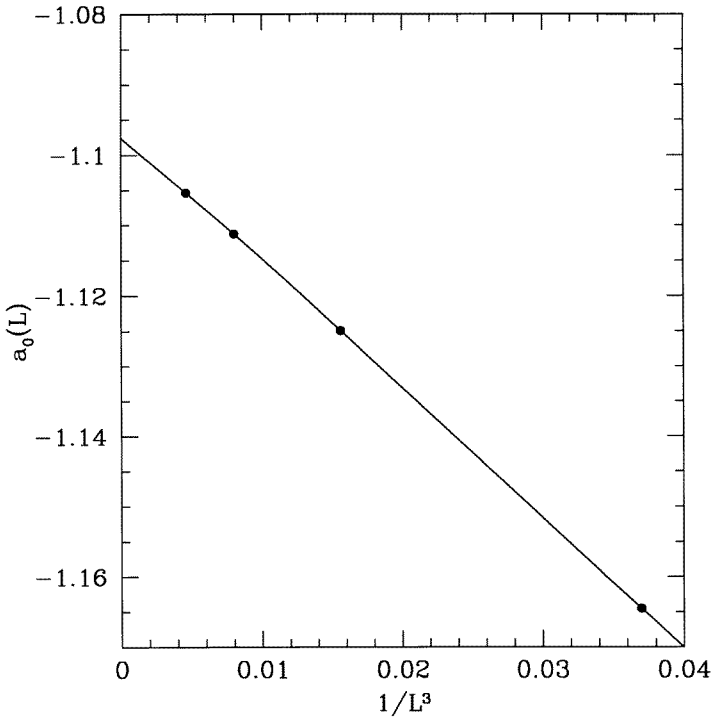

Figure 2. The coefficient $a_0(L)$ graphed against $1/L^3$, where L is the lattice size.

Note that $a_1(6)$ was not included in this fit, because its value is uncertain. Using (2.6) and (3.6), this corresponds to a spin-wave stiffness for this model

$$\rho_s = 0.54(3). \tag{3.9}$$

This also has not been estimated before, as far as we are aware.

Table 4. Ground-state expectation value f_{LRO} as a function of lattice size L.

L	f_{LRO}
2	0.957 106 781 1865
3	0.955 161 594 8951
4	0.937 531 451 8101
5	0.913 629 699 1358
6	0.893 603 736 9844

Table 4 lists the values calculated for the ground-state expectation value f_{LRO}. For even L, these are calculated for the $j = 0$ state. For odd L, we have listed values for

$$f_{LRO} = \left\langle \sum_{i,j} (S_i^x S_j^x + S_i^y S_j^y) \right\rangle = \tfrac{1}{2} \left\langle \sum_{i,j} (\sigma_i^+ \sigma_j^- + \sigma_i^- \sigma_j^+) \right\rangle \tag{3.10}$$

for the $j = \frac{1}{2}$ state. There is no strong justification for assuming that these values will vary smoothly with L; but in fact they appear to do so, as shown in figure 4. A fit of the form

$$f_{LRO}(L) = \sum_n \frac{d_n}{L^n} \tag{3.11}$$

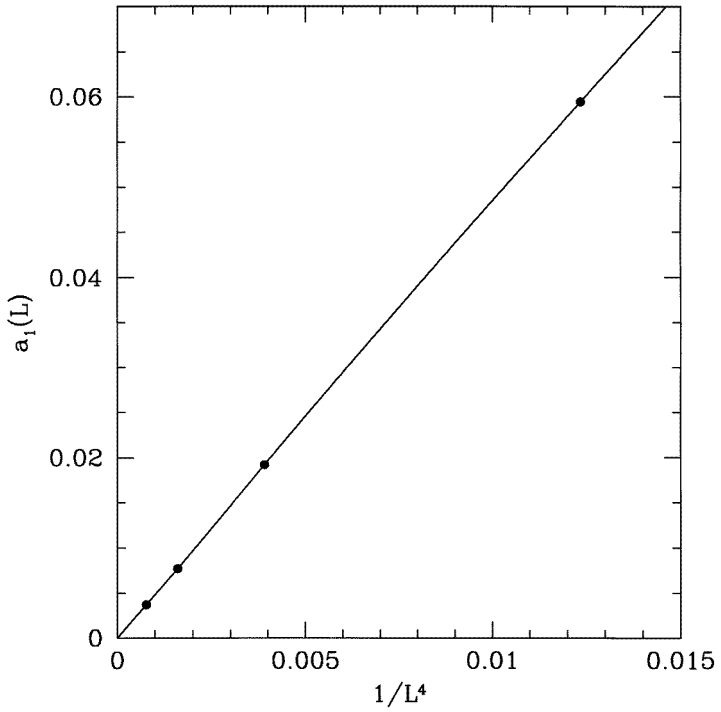

Figure 3. The coefficient $a_1(L)$ graphed against $1/L^4$.

gives an estimate for the bulk limit

$$f_{LRO}(\infty) = d_0 = 0.77(3). \tag{3.12}$$

Quite a large extrapolation is involved with this estimate, as seen in figure 4, and it depends heavily on the assumption of the functional form (3.11) (Betts and Miyashita 1990). Fortuitously perhaps, the result agrees very well with the Monte Carlo estimate of Zhang and Runge (1992)—see table 3, where $f_{LRO} = (2\Sigma)^2$.

4. Conclusions

We have calculated the energy eigenvalues and long-range order parameter by exact diagonalization for square lattices with periodic boundary conditions up to size 6×6. The major limitation on such calculations nowadays is data storage: fast disk access to 5 Gbyte of data was required in this case.

The finite-size scaling behaviour of the energy eigenvalues agrees extremely well with the effective field theory predictions of Hasenfratz and Niedermayer (1993). Extrapolating to the bulk limit, estimates were obtained for the bulk ground-state energy per site and the effective Lagrangian parameters, consisting of the spin-wave velocity v, the spin-wave stiffness ρ_s and the spontaneous magnetization Σ. The parameters v and ρ_s have not previously been estimated, as far as we know.

Our results for $\epsilon_0(\infty)$ and Σ are in excellent agreement with series and spin-wave estimates (Hamer *et al* 1991), and are more accurate than previous finite-cell estimates. They are not able to rival the Monte Carlo estimates of Zhang and Runge (1992) in precision, however. The

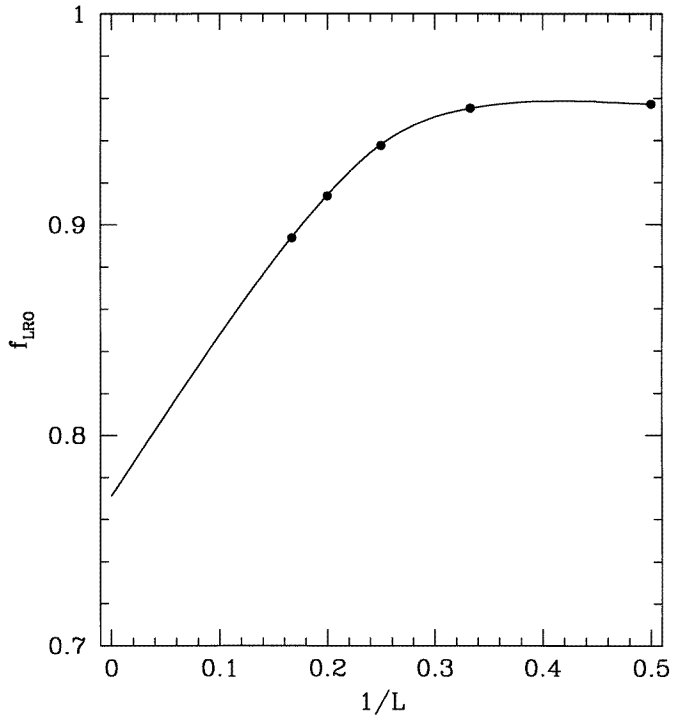

Figure 4. The long-range order parameter f_{LRO} graphed against $1/L$.

sequence of finite-lattice estimates, including both odd and even lattices, is not quite smooth enough to allow a really precise extrapolation to the bulk limit in this instance.

The 'spin deviation' or renormalization of the long-range order due to quantum fluctuations is even smaller in this model than in the XXZ Heisenberg antiferromagnet, and so one expects that spin-wave theory should converge even more quickly. It might well be worthwhile to extend the spin-wave calculations (Hamer *et al* 1991) to higher order, and use both spin-wave and series techniques to estimate ρ_s and v for this model. We hope to address these questions in future work.

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