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Finite cell calculations of an antiferromagnetic spin chain with long-range interactions

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Abstract. The ground state properties of the Heisenberg antiferromagnetic spin-$\frac{1}{2}$ chain with interactions varying as (distance)$^{-p}$ are investigated from finite cell calculations. The gap between the ground state and the first excited state as well as the end-to-end spin correlation function have been calculated for finite open chains up to 14 spins and 12 spins respectively. Aided by first-order perturbation calculations near $p=0$, we can extrapolate the gap in the thermodynamic limit, and we find that the gap vanishes for every $p \neq 0$. From the analysis of the spin correlation function we find that long-range order exists for $p<1$ and does not exist for $p>2$. The existence of long-range order in the range $1<p<2$ remains an open question.

1. Introduction

It is of interest to study the effect of varying the range of interactions on the ground state properties of a quantum system. It is expected, especially in low dimensions, that a Hamiltonian with short-range interactions behaves differently from the corresponding infinite-range Hamiltonian (which corresponds generally to mean field).

One of the most simple and non-trivial examples on which this effect has been studied is the one-dimensional spin-$\frac{1}{2}$ antiferromagnetic chain, where one can vary the index p of the power law decay of the interactions with distance (Rabin 1980a, b, Drell *et al* 1976a, b). This model is described by the Hamiltonian

$$H=\tfrac{1}{2}\sum_{\substack{i,j=1,\ldots,N\\ i\neq j}}(-1)^{i-j+1}\frac{1}{|i-j|^{p}}\boldsymbol{S}_i\boldsymbol{S}_j \tag{1}$$

where the spin components are the usual spin-$\frac{1}{2}$ Pauli matrices:

$$S^x=\frac{1}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\qquad S^y=\frac{1}{2}\begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix},\qquad S^z=\frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{2}$$

Such a kind of power law decay of the spin–spin interactions occurs often in model Hamiltonians for magnetism in solid state physics or in continuum field theories transcribed onto a lattice.

Before the recent study by Rabin (1980b) little was known on this model. The corresponding Ising model, where $\boldsymbol{S}_i\boldsymbol{S}_j$ is restricted to $S_i^zS_j^z$ in (1), has been investigated by Ruelle (1968) and Dyson (1969). They have proven that the model is disordered

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at all finite temperatures if $p>2$, while long-range order persists at $T\neq 0$ if $p<2$. Since, in all Ising models, long-range order occurs at $T=0$, this result implies that $T_c=0$ for $p>2$ while $T_c\neq 0$ for $p<2$. The sign factor $(-1)^{i-j+1}$ has no influence in the Ising case so that these results hold for both the ferromagnetic and the antiferromagnetic cases. Dyson (1969) conjectured that these properties must extend to the Heisenberg ferromagnet, i.e. for (1) where the sign factor is replaced by -1. Rabin (1980b) extended the conjecture to the antiferromagnetic case.

Rabin (1980b) has shown that the thermodynamic limit of (1) does not exist for $p<1$ (the ground state energy per site diverges). However, in this range, the gap between the ground state and the first excited state is well defined and non-infinite. For $p=0$, Rabin has also shown that the ground state corresponds to long-range antiferromagnetic order with an energy gap of 1. Then, applying in the general case $p\neq 0$ a real-space renormalisation group blocking procedure (Drell *et al* 1976a, b, Jullien 1981, Pfeuty *et al* 1982), he found that for $p\gtrsim 1.11$ the system becomes gapless while for $p\gtrsim 1.85$ long-range order vanishes. It is suggested that these approximate critical values of p correspond to effective transitions in the ground state at $p=1$ and $p=2$. These results imply a quite unusual behaviour for $1<p<2$ where long-range magnetic order persists together with a vanishing gap. Thus it appears to be useful to check these results by using a different approach.

In this paper, we would like to make precise and complete the previous study of Rabin (1980b) by using the finite cell scaling method (Nightingale 1976, Sneddon 1978). In certain circumstances, it has been shown that the blocking method and the finite cell scaling could give different results, in particular when a line of fixed points or an essential singularity is present (this has been observed in the spin-1 chain with uniaxial anisotropy (Jullien and Pfeuty 1981) and in the Heisenberg–Ising chain (Spronken *et al* 1981)). It is therefore very useful to contrast both methods when applied to the same Hamiltonian. We have calculated the gap between the ground state and the first excited state of (1) for finite chains of N spins (up to $N=14$) as well as the end-to-end spin correlation function (up to $N=12$) in the ground state. Aided by the analytical result obtained by first-order perturbation for small p, one can extrapolate the gap more easily to the infinite chain and we find that the extrapolated gap vanishes for all $p\neq 0$. This result, different from the result of Rabin in the range $0<p<1$, can be understood when rendering the Hamiltonian asymptotically convergent in the thermodynamic limit. Concerning the asymptotic behaviour of the spin correlation functions, we confirm that long-range order exists for $p<1$ and does not exist for $p>2$. However no clear conclusion can be made in the range $1<p<2$. Finally we discuss the possibility of coexistence of long-range magnetic order together with a vanishing gap in the range $0<p<1$ (and perhaps in the range $1<p<2$).

2. Principles of the finite cell calculations

The principle of finite cell scaling is to calculate a given quantity for finite chains of N spins and then, by assuming a certain scaling hypothesis for the behaviour of this quantity with N, to extrapolate for $N\to\infty$. Here, we have computed the gap $G(N,p)$ between the ground state and the first excited state of (1), as well as the end-to-end spin correlation function at $T=0$ defined as

$$C(N,p)=-\langle \boldsymbol{S}_1\cdot\boldsymbol{S}_N\rangle=-3\langle S_1^z S_N^z\rangle \tag{3}$$

where the brackets refer to the expectation value in the ground state and where the minus sign ensures that $C(N, p)$ is a positive quantity for N even. We have restricted our calculations to even values of N. For $N=2$ and $N=4$ the calculations can be done analytically, and this provides a good check for the computations which have been performed by machine up to $N=14$.

The eigenstates of H can be classified according to the good quantum numbers which are the modulus of the total spin and the projection Σ^z of the total spin on the z axis:

$$\Sigma^z = \sum_{i=1}^{N} S_i^z. \tag{4}$$

We have observed that the ground state of the chain is always a singlet ($\Sigma^z = 0$), while the first excited state is a triplet containing the first excited state in the subspace $\Sigma^z = 0$ and the ground states of the subspaces $\Sigma^z = \pm 1$. It is thus sufficient to determine the two lowest eigenvalues of H in the subspace $\Sigma^z = 0$. Further symmetries are useful: the spin reverse (or time reverse) symmetry τ and the right–left symmetry along the chain direction σ. We have observed that when $N/2$ is even, the ground state is symmetric with respect to both transformations i.e. $\tau = \sigma = +1$, while the first excited state is antisymmetric, i.e. $\tau = \sigma = -1$. When $N/2$ is odd, the situation is reversed. It is thus sufficient to find the ground state in the two subspaces $\Sigma^z = 0$, $\sigma = \tau = 1$ and $\Sigma^z = 0$, $\sigma = \tau = -1$. To perform these calculations we have the Lanczös scheme (Whitehead and Watt 1978, Whitehead 1980).

In the Lanczös algorithm one starts from a trial normalised vector ψ_1 on which we apply H:

$$H\psi_1 = \alpha_1\psi_1 + \beta_1\psi_2. \tag{5}$$

α_1 and β_1 are determined unambiguously such that ψ_2 must be normalised and orthogonal to ψ_1. The procedure is repeated on ψ_2 etc up to step (n) where

$$H\psi_n = \ldots + \delta_{n-2}\psi_{n-2} + \gamma_{n-1}\psi_{n-1} + \alpha_n\psi_n + \beta_n\psi_{n+1}. \tag{6}$$

ψ_{n+1} is normalised and orthogonal to $\psi_1, \ldots, \psi_n$. The fact that H is symmetric implies many simplifications: in particular, all the coefficients in (6) are zero except the α, β, γ and furthermore $\beta_n \equiv \gamma_n$. Finally (6) reduces to

$$H\psi_n = \beta_{n-1}\psi_{n-1} + \alpha_n\psi_n + \beta_n\psi_{n+1}. \tag{7}$$

In the basis $\{\psi_n\}$, H is represented by a tridiagonal matrix. At each step the tridiagonal matrix is determined and diagonalised by standard subroutine.

One can observe that after about 15 to 20 Lanczös steps the ground state energy is obtained within 10^{-7} accuracy.

Here the two lowest eigenstates are determined by using the following trial starting vectors

$$\psi_1 = (|+-+\ldots+-\rangle + \tau|-+-+\ldots-+\rangle)/\sqrt{2} \tag{8}$$

where $\tau = +1$ corresponds to the ground state and $\tau = -1$ to the first excited state for $N/2$ even (and the opposite for $N/2$ odd). For the largest cell reached, $N=14$, the subspace is of dimensionality 3432, so that the Lanczös procedure replaces, in principle, the direct diagonalisation of a 3432×3432 matrix by a diagonalisation of a 20×20 tridiagonal matrix. The limitation then occurs when performing the scalar products of such large vectors.

The Lanczös algorithm is very well adapted for the determination of the eigenvalues. To compute the eigenvectors one needs much more computation time and space, so that for the end-to-end correlation function we have performed the calculations up to $N = 12$ only.

3. Results for the gap, comparison with first-order perturbation near $p = 0$

The results for the gap are given in figure 1 as a plot of $G(N, p)$ against p for different sizes up to $N = 14$. For $N = 2$, the gap is trivially equal to one, independent of p. For larger N, the gap starts from 1 for $p = 0$ and then decreases monotonically with increasing p. The problem is how to estimate the limiting curve $G^{\infty}(p)$ from these finite cell results. For large p values we recover that the gap tends to zero as N^{-1}, as is well known exactly for short-range interactions (des Cloizeaux and Pearson 1962). When looking at our results it is tempting to extend this conclusion for every $p > 1$. Our results can be very well fitted by polynomials in powers of N^{-1} for $p > 1$; however, these fits are not very well converging especially for $1 \leqslant p \leqslant 2$. More dramatically, for small p values it is very difficult to extrapolate our results, and either a vanishing or a non-vanishing gap can be obtained depending on the choice of N dependence adopted to fit the results. Fortunately, for small p values, a good approximation for the gap is given from the first-order perturbation calculation near $p = 0$, which provides good suggestions for fitting.

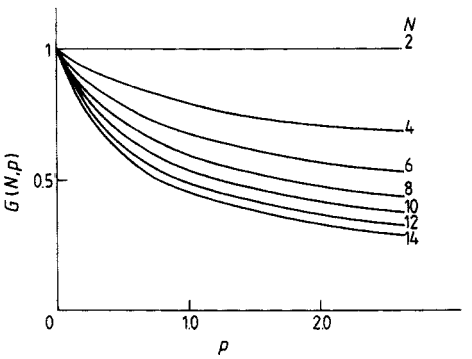

Figure 1. Plot of the gap $G(N, p)$ as a function of p for sizes up to $N = 14$.

For $p = 0$, Rabin has shown that the Hamiltonian can be conveniently written as

$$H = \tfrac{1}{2}\Sigma^2 - \Sigma_e^2 - \Sigma_o^2 + \tfrac{3}{8}N \tag{9}$$

where Σ is the sum of all the spins of the chain and where $\Sigma_e(\Sigma_o)$ is the sum over the even (odd) sites only. From that form it can be easily concluded that the $p = 0$ ground state ϕ_0 corresponds to $\Sigma = 0$ and to $\Sigma_o = \Sigma_e = \frac{1}{4}N$, while the $p = 0$ first excited state ϕ_1 corresponds to $\Sigma = 1$, $\Sigma_o = \Sigma_e = \frac{1}{4}N$. From these states one can calculate the approximate gap to first order defined as

$$G^0(N, p) = \langle \phi_1 | H | \phi_1 \rangle - \langle \phi_0 | H | \phi_0 \rangle. \tag{10}$$

In this approximate expression the dependence in p comes only from H and not from ϕ_0 and ϕ_1 which have been taken as for $p = 0$. We can generalise the calculation of

Rabin to evaluate $\langle\phi_0|H|\phi_0\rangle$ and $\langle\phi_1|H|\phi_1\rangle$. We get the following expression for $G^0(N,p)$:

$$G^0(N,p)=N^{-1}[F(N,p)-2^{-p}F(\tfrac{1}{2}N,p)] \tag{11}$$

where

$$F(N,p)=\zeta_{N-1}(p)-N^{-1}\zeta_{N-1}(p-1) \tag{12}$$

and $\zeta_N(p)$ is the truncated zeta function

$$\zeta_N(p)=1+2^{-p}+\ldots+N^{-p}. \tag{13}$$

When comparing with our numerical results, we find that $G^0(N,p)$ is a very good approximation for $G(N,p)$ in a large range of N and p values. Using the large N asymptotic expansion of $\zeta_N(p)$,

$$\begin{aligned}
&\zeta_N(p)\simeq\frac{1}{N^p}\left[\frac{N}{1-p}+\frac{1}{2}-\frac{p}{12N}+O\left(\frac{1}{N^3}\right)\right]+C(p) && \text{for } p<1,\\
&\zeta_N(p)\simeq\zeta(p)+\frac{1}{N^p}\left[\frac{N}{p-1}-\frac{1}{2}+\frac{p}{12N}+O\left(\frac{1}{N^3}\right)\right] && \text{for } p>1,
\end{aligned} \tag{14}$$

where $\zeta(p)$ is the Riemann zeta function and where $C(p)$ is a p-dependent positive numerical constant, one can derive the following asymptotic large-N expansion of $G^0(N,p)$:

$$\begin{aligned}
G^0(N,p)\simeq{}&\frac{C(p)}{N}\left(1-\frac{1}{2^p}\right)-\frac{C(p-1)}{N^2}\left(1-\frac{1}{2^{p-1}}\right)\\
&+\frac{1}{N^p}\left[\frac{1}{2(1-p)(2-p)}-\frac{1}{12N^2}+O\left(\frac{1}{N^4}\right)\right] && \text{for } p<1,\\
G^0(N,p)\simeq{}&\frac{\zeta(p)}{N}\left(1-\frac{1}{2^p}\right)-\frac{C(p-1)}{N^2}\left(1-\frac{1}{2^{p-1}}\right)\\
&+\frac{1}{N^p}\left[\frac{2p-3}{2(1-p)(2-p)}-\frac{2p-1}{12N^2}+O\left(\frac{1}{N^4}\right)\right] && \text{for } 1<p<2,\\
G^0(N,p)\sim{}&\frac{\zeta(p)}{N}\left(1-\frac{1}{2^p}\right)-\frac{\zeta(p-1)}{N^2}\left(1-\frac{1}{2^{p-1}}\right)\\
&+\frac{1}{N^p}\left[\frac{1}{2(1-p)(2-p)}+\frac{1}{12N^2}+O\left(\frac{1}{N^4}\right)\right] && \text{for } p>2.
\end{aligned} \tag{15}$$

Thus G^0 tends to zero as N^{-1} when $p>1$, while G^0 tends to zero as N^{-p} when $p<1$. For $p=1$ and $p=2$, logarithmic terms appear. For $p=1$, G^0 behaves as $(\ln N)/N$, and for $p=2$, G^0 behaves as N^{-1} with a leading term in $(\ln N)/N^2$. Even if the convergence is slower for $p<1$, $G^0(N,p)$ tends to zero everywhere for $p\neq 0$. Thus the asymptotic limit of the function $G^0(N,p)$ is discontinuous at $p=0$ since $G^0(N,0)=1$ for all N.

In order to verify if these conclusions hold for our calculated gap, especially for small p values, we have reported the difference $G-G^0$ divided by p^2 as a function of $1/N$ in figure 2 for several small values of p. All the curves exhibit a maximum near $N\sim 12$ and are very well fitted by a polynomial in N^{-1} without a constant term.

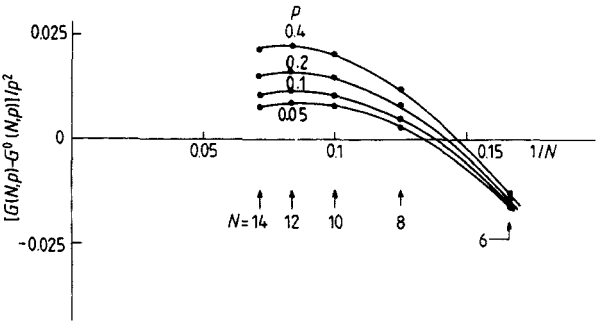

Figure 2. Plot of the difference $G(N, p) - G^0(N, p)$ divided by p^2, where $G^0(N, p)$ is the analytical expression given in the text, as a function of $1/N$ for several values of p: $p = 0.05, 0.1, 0.2, 0.4$.

We conclude that for small p, G has the same asymptotic form in N^{-p} as G^0, only the leading term in N^{-1} is changed by corrections of order or smaller than p^2 for small p. In particular, G exhibits the same discontinuity at $p = 0$.

The analytical study of $G^0(N, p)$ provides some ideas for the asymptotic behaviour of the real gap. In table 1 we have presented the results of some fits which show that taking into account terms in N^{-p} in the expansion of $G(N, p)$ gives better results than considering integer powers of N^{-1} alone. We have considered four successive sizes and, assuming an expansion of $G(N, p)$ containing a constant term G^∞ and other terms in integer powers of N^{-1}, with or without a term in N^{-p}, we have reported in each case the result for G^∞. When increasing the set of N values chosen for the fit,

Table 1.

p	Form of the fit	Range of N values	G^∞
0.6	$G^\infty + \frac{A}{N} + \frac{B}{N^2} + \frac{C}{N^3}$	4 to 10	0.247
		6 to 12	0.206
		8 to 14	0.180
	$G^\infty + \frac{A}{N^{0.6}} + \frac{B}{N} + \frac{C}{N^2}$	4 to 10	−0.112
		6 to 12	−0.070
		8 to 14	−0.044
1.4	$G^\infty + \frac{A}{N} + \frac{B}{N^2} + \frac{C}{N^3}$	4 to 10	0.126
		6 to 12	0.087
		8 to 14	0.063
	$G^\infty + \frac{A}{N} + \frac{B}{N^{1.4}} + \frac{C}{N^2}$	4 to 10	0.064
		6 to 12	0.027
		8 to 14	0.011
2.4	$G^\infty + \frac{A}{N} + \frac{B}{N^2} + \frac{C}{N^3}$	4 to 10	0.059
		6 to 12	0.046
		8 to 14	0.035
	$G^\infty + \frac{A}{N} + \frac{B}{N^2} + \frac{C}{N^{2.4}}$	4 to 10	0.052
		6 to 12	0.041
		8 to 14	0.030

one can observe that G^{∞} tends more quickly to zero for the fits which include the term in N^{-p}.

In conclusion of this analysis, one can say that the gap tends to zero as N^{-1} for all p values greater than one, suggesting that the ground state is the bottom of a continuum of states with a dynamical exponent z equal to one (the dynamical exponent being defined as $G \sim N^{-z}$ when $N \to \infty$). Considering the classical 2D equivalent model of this quantum system, this model would be 'critical' for all $p > 1$. In the case $p < 1$, we must be more careful since the Hamiltonian has no thermodynamic limit. In that case, the energy per site diverges as N^{1-p}. It is thus more convenient to consider a modified Hamiltonian

$$H' = H/N^{1-p} \tag{16}$$

which has a well defined thermodynamic limit (in the special case $p = 1$, one must consider $H' = H/\ln N$).

Since G tends to zero as N^{-p} for $p < 1$, the corresponding gap G' for H' tends to zero as N^{-1}. Thus one can conclude that the general result $z = 1$ is valid for every value of p, but when $p < 1$, H must be replaced by the more realistic Hamiltonian H' which has a well defined thermodynamic limit, and which could accept a two-dimensional classical equivalent (note that the discontinuity at $p = 0$ becomes meaningless when considering H').

4. Results for the end-to-end correlation function

The numerical results for the end-to-end correlation function in the ground state are given in figure 3 where we have plotted $C = -3\langle S_1^z S_N^z \rangle$ for $N = 4, 6, \ldots, 12$ as a function of p. For $N = 2$, C is trivially equal to $\frac{3}{4}$, independent of p. For $p = 0$, we have precisely recovered the exact result of Rabin:

$$C(N, 0) = -3\langle S_1^z S_N^z \rangle = \tfrac{1}{4} + 1/N. \tag{17}$$

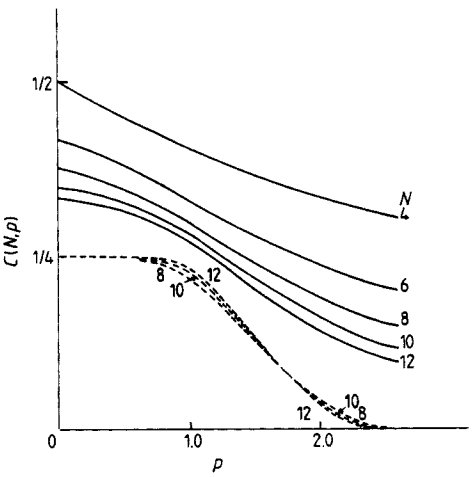

Figure 3. Plot of the end-to-end correlation function $C(N, p) = -3\langle S_1^z S_N^z \rangle$ as a function of p for sizes up to $N = 12$. The extrapolations to $N = \infty$ obtained by fitting by a polynomial in N^{-1} the curves up to size N, $C_N^{\infty}(p)$, are given by the broken lines for $N = 8$, 10, 12.

When p increases, $C(N, p)$ decreases monotonically. Here also the problem is how to estimate the limiting curve when $N \to \infty$. For $p \to \infty$ one must recover the exact result, which is that C tends to zero as N^{-1}. It is thus tempting to fit C by polynomials in N^{-1} in the whole range of p values, since this procedure gives the correct results in the limiting cases $p = 0$ and $p = \infty$. Here, we have applied a procedure already adopted in another case (Spronken *et al* 1981) which consists in comparing all the results from size 2 up to size N by fitting with a polynomial of degree $N/2 - 1$ in N^{-1}:

$$C(N, p) = C_N^{\infty}(p) + A_1/N + \ldots + A_{N/2-1}/N^{N/2-1}. \tag{18}$$

This method gives the following estimation for $C_N^{\infty}(p)$:

$$C_N^{\infty}(p) = \sum_{M=1}^{N/2} Q_M^N C(2M, p) \tag{19}$$

with

$$Q_M^N = \prod_{\substack{M'=1,\ldots,N/2 \\ M' \neq M}} \frac{M}{M - M'}. \tag{20}$$

The curves giving the numerical results for $C_N^{\infty}(p)$, $N = 8$, 10, 12 are given by the broken curves of figure 3. Obviously for $p = 0$ the exact result $\frac{1}{4}$ is recovered exactly. The procedure converges very well in the whole range $p < 1$, suggesting strongly that the result $\frac{1}{4}$ remains valid up to $p = 1$. Also for $p > 2$ the procedure converges very well and suggests that the correlation functions tend to zero, i.e. that there is no long-range order.

In the range $1 < p < 2$ we cannot conclude so clearly. When looking at the broken curves of figure 3, one could conclude a non-zero correlation function varying smoothly from $\frac{1}{4}$ to 0 when p is varying from 1 to 2. However one could have tried other fits, in particular by forcing $C^{\infty} = 0$ and a power law decay $N^{-\alpha}$; then we would get a continuously varying exponent from $\alpha = 0$ for $p = 1$ to $\alpha = 1$ for $p = 2$. However we were not able to find such fits converging better than those presented in figure 3. Note that we have here no help from any approximate analytical expression for C: the first-order perturbation near $p = 0$ gives no more than expression (17) which becomes completely wrong for $p > 1$.

From this study, we conclude that long-range order exists for $p < 1$ and vanishes for $p > 2$. In the range $1 < p < 2$ our analysis suggests that the long-range order persists with a continuous decrease of the magnetisation up to $p = 2$; however, it cannot be excluded that instead the long-range order does not exist, and that we have here a 'line of fixed points' with a continuously varying exponent for the power law decay of the correlation functions. In this last hypothesis the conclusion of Rabin concerning the disappearance of long-range order at $p = 2$ could be wrong and the transition at $p = 2$ would be more subtle (perhaps an essential singularity terminating a line of fixed points).

5. Conclusion

Our calculations confirm the previous conjecture of Rabin which predicted a change in the long-range properties at $p = 2$. However some differences with his study must be noticed. First, we found that the gap vanishes everywhere and not only for $p > 1$.

When replacing H by $H' = N^{p-1}H$ for $p < 1$, we find that the dynamical exponent is equal to one for every value of p. Moreover, we are not completely sure that long-range order exists in the range $1 < p < 2$, and further studies are needed to know if there is rather a line of fixed points in that range. The existence of long-range order while there is no gap in the range $0 < p < 1$, and perhaps up to $p = 2$, is a quite unusual situation which requires some further discussion of our results. It is very difficult to prove that there is really no gap. In the thermodynamic limit, the system could have a ground state with a finite degeneracy well separated from the continuum of excited levels by a finite gap, and we may have picked up only two components of this multiplet by our method. In fact, it is practically impossible to rule out this hypothesis completely: it would have been necessary to perform the same study for all the excited levels. However, some arguments are in favour of a gapless continuum near the ground state. First, in the limit $p = 0$ the Hamiltonian $H' = H/N$ has a continuum of states corresponding to all possible values of Σ, Σ_o, Σ_e near $\Sigma = 0$, $\Sigma_o = \Sigma_e = N/4$. Second, the gap vanishes as N^{-1} and not exponentially as generally in the case of a finite asymptotic degeneracy.

This apparent anomalous situation must be explained by the presence of long-range interactions. Let us imagine a two-dimensional equivalent classical model. This model would be highly anisotropic with long-range interactions varying as (distance)$^{-p}$ in the original direction (space direction) and with regular short-range next-neighbour interactions in the perpendicular direction (time direction). The gap of the quantum model corresponds to the inverse of the coherence length in the time direction. For sufficiently long-range interactions one can imagine that the long-range order is induced in the space direction, while the spins remain uncorrelated at long distance in the time direction, as traduced by the vanishing gap.

To conclude, we would say that our calculations confirm some points and complete the previous study by Rabin, but demand some further investigations and especially exact analytical results, to make precise the nature of the ground state for $1 < p < 2$. Moreover, this study shows that finite cell methods can be very limited in presence of long-range interactions. If there is no support coming from an analytical study the extrapolation to the infinite system can become very hard.

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