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1991 J. Phys.: Condens. Matter 3 445

(http://iopscience.iop.org/0953-8984/3/4/008)

J. Phys.: Condens. Matter 3 (1991) 445–453. Printed in the UK

Rigorous determination of spontaneously dimerized ground states in 1D Heisenberg antiferromagnets

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Received 13 July 1990

Abstract. Starting from the exact result of Majumdar and Ghosh for the dimerized ground state of a Heisenberg $S = \frac{1}{2}$ antiferromagnet with competing next-nearest-neighbour interaction $J_2 = 1/2J_1$ on a linear chain, it is shown that this state is the ground state of the same kind of Hamiltonian, if couplings are extended up to $2n$-nearest-neighbours, and the relation $J_1 = 2n$, $J_2 = 2n-1, \cdots, J_{2n} = 1$ holds. Furthermore, it is proved rigorously that this state is the ground state when $n = 2$ and $J_1 - 2J_2 + J_3 = 0$, $J_3 = 2J_4$, in a finite interval of values of the parameter J_4. A rigorous lower limit for the extension of this interval is found to be $0 \leq J_4 \leq \frac{1}{4}J_1$. A comparison with ground-state configurations of the equivalent classical Heisenberg and Ising model is discussed.

1. Introduction

Since the discovery of high-T_c superconductors an ever-increasing interest has been focused on frustrated Heisenberg antiferromagnets, which are believed to describe the magnetic properties of these compounds. Many exact results have accumulated in the meantime, mainly on 1D models, or on higher-dimensional models often devised to yield a previously assigned ground state.

Frustration is most usually introduced in the form of competing exchange couplings extending beyond nearest neighbours; this kind of frustration is 'resolved' in classical spin models through the appearance of helical states [1], but evidence from spin-wave [2–4] and numerical [5] computations point to a possible disordering of the ground state in 2D as an effect of quantum fluctuations.

In one dimension the ground state of nearest-neighbour (NN) antiferromagnets with $S = 1/2$ is disordered, but antiferromagnetic next-nearest-neighbour (NNN) couplings induce a qualitative change of behaviour: at a critical value of $j_2 \equiv J_2/J_1$ a gap opens in the excitation spectrum [6,7] and ground-state correlations change from power-law to exponential decay. The ground state itself suffers a transition from the 'Bethe ansatz' to a 'dimer' phase, i.e. a state where short-range two-spin singlets dominate the wavefunction. This is known [8,9] to become the exact 1D resonating valence bond (RVB) state, where only NN singlets contribute, with equal weights, at $j_2 = 1/2$.

I have studied the effect of including further neighbours in the Hamiltonian, motivated by the fact that frustration induced by hole motion can be simulated via effective Heisenberg Hamiltonians with extended couplings [10]. Previous results have appeared in [11]. In this paper I will show that the RVB state is the exact ground

0953-8984/91/040445+09$03.50

state if any even number $2n$ of neighbours is included, provided the exchange integrals satisfy the chain of equalities $J_1 = 2n,\ J_2 = 2n-1, \cdots, J_{2n} = 1$. Taking $n = 2$, I will prove that this state is the ground state for $0 \leq J_4 \leq 1/4\ J_1$, if the following condition holds: $J_1 - 2J_2 + J_3 = 0$, $J_3 = 2J_4$. A comparison with the ground states of classical Heisenberg and Ising models shows that the RVB state appears in the helical phase of the former and exactly on the boundary between the Neél and antiphase-(2) of the latter, and corresponds to an infinitely degenerate state of the Ising model.

The plan of the paper is as follows. Section 2 is devoted to the investigation of the quantum ground state, section 3 to the classical Heisenberg, and section 4 to the Ising model. Section 5 is left for discussion and conclusions.

2. Quantum Heisenberg antiferromagnet

The Hamiltonian is the usual bilinear exchange, of the form

$$\mathcal{H} = \sum_{\alpha=1}^{n} \sum_{\delta_\alpha} J_\alpha \sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+\delta_\alpha} \tag{1}$$

where δ_α is a vector joining site i to its αth neighbours on a linear chain. J_1 is assumed positive, while further coupling constants can have either signs. I will take a slightly unusual attitude, in rewriting this Hamiltonian by way of a graph-theoretic device, the adjacency matrix of the lattice [12], i.e. a matrix $\mathbf{A}$ whose element A_{ij} is 1 if sites i and j are nearest-neighbours on the lattice, and 0 otherwise. It is a property of the one-dimensional Euclidean lattice, but not in general of higher-dimensional ones, that sites which are at a certain distance in terms of Euclidean metric, are at the same distance in terms of chemical length, that is the minimum number of bonds joining them. Since the element $(A^n)_{ij}$ of the nth power of the adjacency matrix, is equal to the number of paths consisting of n bonds between sites i and j, it is possible to write the Hamiltonian in (1) as a polynomial in $\mathbf{A}$. To be specific, consider NN and NNN; then we can write

$$\mathcal{H} = \sum_{ij} \boldsymbol{S}_i \mathbf{P}_{ij} \boldsymbol{S}_j \tag{2}$$

with

$$\mathbf{P} = J_1 \mathbf{A} + J_2 \left(\mathbf{A}^2 - 2\mathbf{I}\right) \tag{3}$$

because

$$\left(\mathbf{A}^2\right)_{ij} = \delta_{j,i-2} + \delta_{j,i+2} + 2\delta_{ij} \tag{4}$$

(here δ_{ij} is the Kronecker delta).

As previously mentioned, it is known that for $J_1 = 2J_2$ there are two degenerate ground states for $S = 1/2$, the dimer states $|\Psi_{\mathrm{D}}^{\pm}\rangle$, defined as

$$|\Psi_{\mathrm{D}}^{\pm}\rangle \equiv |\psi_1\rangle \pm |\psi_2\rangle \tag{5}$$

where, in the thermodynamic limit,

$$|\psi_1\rangle = \cdots [1,2][3,4]\cdots[2N-1,2N]\cdots \tag{6}$$

$$|\psi_2\rangle = \cdots [2,3][4,5]\cdots[2N,2N+1]\cdots \tag{7}$$

with an almost universal notation for the two-spin singlet $[i,i+1] \equiv \frac{1}{\sqrt{2}}(\alpha(i)\beta(i+1) - \beta(i)\alpha(i+1))$, $\alpha(i) = (1,0)$, $\beta(i) = (0,1)$.

It is a simple identity to rewrite $\mathbf{P}$ as

$$\mathbf{P} = (J_1 - 2J_2)\mathbf{A} + J_2(\mathbf{A}+\mathbf{I})^2 - 3J_2\mathbf{I} \tag{8}$$

and therefore at $J_2 = 1/2J_1$ equation (2) becomes

$$\mathcal{H} = \sum_{ij} \boldsymbol{S}_i \left[\tfrac{1}{2}J_1(\mathbf{A}+\mathbf{I})^2 - \tfrac{3}{2}J_1\mathbf{I}\right]_{ij} \boldsymbol{S}_j. \tag{9}$$

It is not difficult to realize that this is exactly the Hamiltonian in equation (1) with $n = 1$ and $J_1 = 2J_2$. However, we can profit of equation (9) to write the Hamiltonian in the form

$$\mathcal{H} = J_1 \sum_i (\boldsymbol{S}_{i-1} + \boldsymbol{S}_i + \boldsymbol{S}_{i+1})^2 - \tfrac{9}{8}J_1 N. \tag{10}$$

In fact, leaving constants aside,

$$\begin{aligned}\mathcal{H} &= \sum_{ij} \boldsymbol{S}_i \left(\sum_k (\mathbf{A}+\mathbf{I})_{ik}(\mathbf{A}+\mathbf{I})_{kj}\right) \boldsymbol{S}_j \\ &= \sum_k \left(\sum_i \boldsymbol{S}_i(\delta_{i,k-1} + \delta_{i,k+1} + \delta_{i,k})\right)\left(\sum_j (\delta_{j,k-1} + \delta_{j,k+1} + \delta_{j,k})\boldsymbol{S}_j\right)\end{aligned} \tag{11}$$

from which equation (10) immediately follows.

It is now straightforward to show that $|\psi_1\rangle$ and $|\psi_2\rangle$ are eigenfunctions with minimum eigenvalue, by means of the property

$$\boldsymbol{S}_l \cdot (\boldsymbol{S}_i + \boldsymbol{S}_j)[i,j] = 0. \tag{12}$$

The advantage in the use of the adjacency matrix formulation is that it can be easily extended to further neighbours interactions.

First of all, notice that NN dimers minimize the total spin of any odd number of consecutive spins; and since they are, as can be esplicitly checked, eigenstates of any Hamiltonian of the form

$$\mathcal{H} = \sum_i (\boldsymbol{S}_{i-n} + \boldsymbol{S}_{i-n+1} + \cdots \boldsymbol{S}_i + \cdots \boldsymbol{S}_{i+n})^2 \tag{13}$$

$|\Psi_{\mathrm{D}}^{\pm}\rangle$ are the ground states for such Hamiltonians. To see this, lay on the linear chain lattice one of the two NN dimer coverings, $|\psi_1\rangle$, say, and consider $2n+1$ consecutive spins. Then $|\psi_1\rangle$ is an eigenstate with eigenvalue $-\frac{3}{4}J_1$, since $2n$ spins are in a singlet state. The following term in the Hamiltonian is another block of $2n+1$ spins, shifted

by one site along the chain. Again $2n$ spins are in a singlet, and so on, proving that $|\psi_1\rangle$ (and therefore $|\psi_2\rangle$) is an eigenstate (actually the lowest-energy one) of the whole Hamiltonian in equation (13).

From a direct expansion of the squares in equation (13) one can see that NN couplings are counted $2n$ times, NNN $2n-1$ times, and so on up to $2n$th neighbours which are counted once. This allows the identification of this Hamiltonian with the one in equation (1), letting $J_1 = 2n$, $J_2 = 2n-1, \cdots, J_{2n} = 1$. If $n = 1$ this is the previously treated case, so now let $n = 2$. Equation (13), in terms of the adjacency matrix, is

$$\sum_i \left(S_{i-2} + S_{i-1} + S_i + S_{i+1} + S_{i+2}\right)^2 = \sum_{ij} S_i \left(\mathbf{A}^2 + \mathbf{A} - \mathbf{I}\right)^2_{ij} S_j. \tag{14}$$

This includes couplings up to fourth-NN (FNN), that is

$$J_3\left(\mathbf{A}^3 - 3\mathbf{A}\right) \qquad J_4\left(\mathbf{A}^4 - 4\mathbf{A}^2 + 2\mathbf{I}\right).$$

Since now the parameter space has enlarged, we ask whether $|\Psi_{\mathrm{D}}^{\pm}\rangle$ are eigenstates, possibly ground states, on a larger region than the single points given by the conditions $J_1 = 2$, $J_2 = 1$, $J_3 = J_4 = 0$ and $J_1 = 4$, $J_2 = 3$, $J_3 = 2$, $J_4 = 1$ seen above. We therefore start from the beginning, writing matrix $\mathbf{P}$ so as to include TNN and FNN interactions. After a little algebra, we get

$$\begin{aligned}\mathbf{P} = {} & (J_1 - 2J_2 - 3J_3 + 8J_4)\mathbf{A} + (J_2 - 3J_4)\left(\mathbf{A} + \mathbf{I}\right)^2 \\ & + (J_3 - 2J_4)\mathbf{A}^3 + J_4\left(\mathbf{A}^2 + \mathbf{A} - \mathbf{I}\right)^2 - (3J_2 - 4J_4)\mathbf{I}.\end{aligned} \tag{15}$$

Notice at this point that letting

$$J_1 - 2J_2 + J_3 = 0 \qquad 2J_4 = J_3 \tag{16}$$

we find a Hamiltonian that 'interpolates' between those given by equation (10) and equation (14) (that is equation (13) with either $n = 1$ or $n = 2$)

$$\mathbf{P} = \tfrac{1}{2}(J_1 - 4J_4)\left(\mathbf{A} + \mathbf{I}\right)^2 + J_4\left(\mathbf{A}^2 + \mathbf{A} - \mathbf{I}\right)^2 - \tfrac{1}{2}(3J_1 - 2J_4)\mathbf{I} \tag{17}$$

$$\begin{aligned}\mathcal{H} = {} & \tfrac{1}{2}(J_1 - 4J_4)\sum_i \left(S_{i-1} + S_i + S_{i+1}\right)^2 \\ & + J_4 \sum_i \left(S_{i-2} + S_{i-1} + S_i + S_{i+1} + S_{i+2}\right)^2 - \tfrac{3}{4}N\left(\tfrac{3}{2}J_1 - J_4\right).\end{aligned} \tag{18}$$

We can immediately check that letting either $J_3 = J_4 = 0$, $J_1 = 2$, $J_2 = 1$, or $J_1 = 4$, $J_2 = 3$, $J_3 = 2$, $J_4 = 1$, we obtain equation (13) with $n = 1$ or $n = 2$, respectively. It is equally straightforward to realize that the two spin-dependent terms are positive, as long as

$$0 \le J_4 \le \tfrac{1}{4}J_1 \tag{19}$$

and $|\Psi_{\mathrm{D}}^{\pm}\rangle$ are then the ground-state wavefunctions in this range, since they minimize each term in a sum of positive addenda. What happens outside the interval in equation (19)? As long as we remain on the line defined by equation (16) above,

$J_4 = 0$ means $J_1 = 2J_2$. At this point it has been shown by Affleck *et al* [9] that no other state exists degenerate with $|\Psi_D^{\pm}\rangle$, so that this must be the ground state even for small negative values of J_4. Exact diagonalization of finite chains ($N \leq 12$) gives the following approximate bounds on the interval where $|\Psi_D^{\pm}\rangle$ are ground states [11]

$$\begin{aligned} -0.25 \leq j_4 \leq 0.25 \qquad & N = 6 \\ -0.5 \leq j_4 \leq 0.3 \qquad & N = 8 \\ -0.3 \leq j_4 \leq 0.3 \qquad & N = 12 \end{aligned}$$

showing that the interval seems to extend outside the rigorous lower bound given by equation (19).

We now turn to a brief examination of the ground-state configurations of the classical vector spin model.

3. Classical Heisenberg antiferromagnet at $T = 0$

We show in figures 1 and 2 sections at constant J_4 of the $T = 0$ phase diagram, as a function of J_2 and J_3. We consider explicitly only the ground-state energy on the line given by equation (16), that is

$$E(Q) = \tfrac{1}{2}J_1 N S^2 \left[(1 - 4j_4)(1 + 2\cos Q)^2 + j_4(4\cos^2 Q + 2\cos Q - 1)^2 - (3 - 2j_4)\right] \tag{20}$$

where we defined $j_4 \equiv J_4/J_1$. For $j_4 \leq -0.7825$, determined numerically, the ground state is ferromagnetic ($Q = 0$), and modulated for j_4 larger than this value. The transition is first order. Although it is not possible to give an analytical expression for the modulation wavevector along the whole line parametrized by j_4, it is easy to see that at $j_4 = 0$ $Q = \pm\frac{2}{3}\pi$, while at $j_4 = \frac{1}{4}$ two helices coexist, whose pitches are $Q_1 = \pm\frac{3}{5}\pi$ and $Q_2 = \pm\frac{4}{5}\pi$. Spin-wave excitations can considerably change the picture. Consider for simplicity only NN and NNN interactions (it means we are considering parameters along the $j_3 = 0$ line in figure 1); in this case the ground state changes from antiferromagnetic to helical at $j_2 = \frac{1}{4}$, but since zero-point fluctuations are the larger the more collinear the configuration, we espect that the antiferromagnet–helix boundary shifts towards the helical phase, enlarging the stability region of the Neél state.

Since it is not possible to compute the zero-point energy of a certain phase in the region of parameter space where this phase is unstable in the classical approximation, I have resorted to a perturbative approach devised by Harris and Rastelli [13] to investigate the effects of quantum fluctuations on the ferromagnetic–helical phase boundary. Spin operators are realized in terms of Dyson–Maleev bosonic operators, and the expectation value of the resulting Hamiltonian on the ferromagnetic ground state, which is classically stable where the ferro–helix transition is continuous, is expanded in powers of Q. This is meaningful since on the considered line $Q = 0$, so that Q is a valid perturbative parameter. The coefficients of this power series contain all orders in $1/S$, S being the quantum spin number, and it is fortunately possible to sum up all these contributions for the first coefficients, up to Q^4, thus evaluating them to all orders in $1/S$ [14]. In the present case the expansion is made around $Q - \pi$, but the

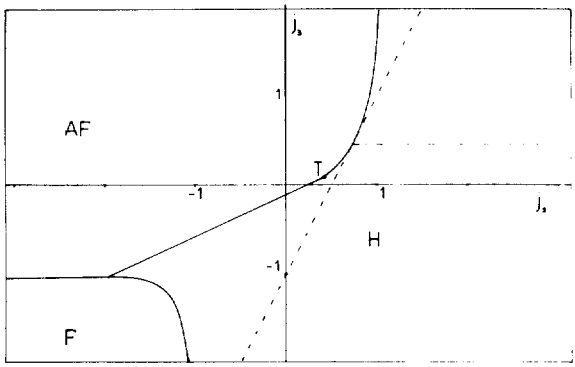

Figure 1. Section a $j_4 = 0$ of the zero-temperature phase diagram of the classical Heisenberg linear antiferromagnet with competition up to fourth-nearest-neighbours. AF marks the Neél phase, F the ferromagnetic and H the helical one. The broken line has the equation $1 - 2j_2 + j_3 = 0$ (see text). The chain line is the locus of an infinitely degenerate phase where the spin chain is decoupled in two independent sublattices antiferromagnetically ordered ($Q = \pi/2a$). T is a tricritical point where the first-order AF–H transition line (to the right of T) merges into the continuous AF–H border (to the left of T).

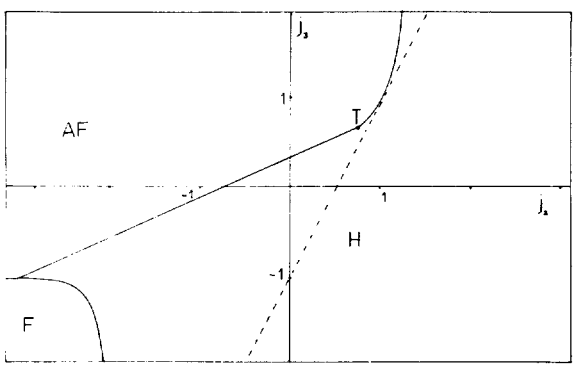

Figure 2. Same as figure 1 but for $j - 4 = \frac{1}{4}$. Notice that the infinitely degenerate phase mentioned before is not present at this value of j_4.

situation is not as fortunate as with the ferromagnet; in fact the first coefficients can be evaluated, but only to *first order* in $1/S$. In this way we find that the antiferro–helix transition occurs at $j_2 = \frac{3}{4}$ when quantum effects are accounted for [15], a result that seems to overestimate the real extension of the Neél-like phase, since numerical results on finite chains [16] point to a transition at $j_2 = \frac{1}{2}$. It should also be noted that more sophisticated perturbative calculations [17], also accounting for dimerized phases, seem to indicate a Neél–dimer transition near the classical instability point $j_2 = \frac{1}{4}$. These two findings are not at variance, since even in the dimer state one has ground-state correlations with a $Q = \pi$ modulation; at $j_2 = \frac{1}{2}$, for instance, the Fourier transform of the correlation function is $S(k) = \frac{1}{4}(1 - \cos k)$, and is therefore peaked at $k = \pi$, while the ground state is obviously dimerized.

We turn now to the investigation of another classical model, the Ising model, which can also be seen as an extremely anisotropic limit of Hamiltonian (18).

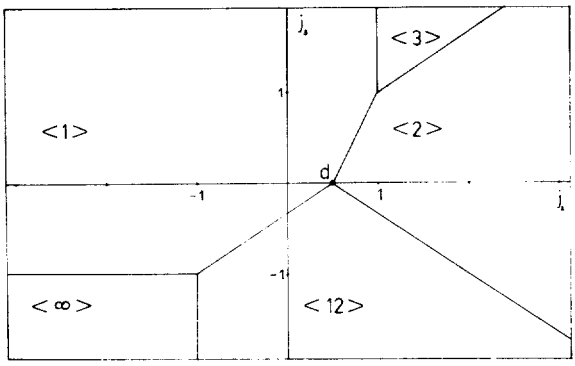

Figure 3. Section at $j_4 = 0$ of the zero-temperature phase diagram of the linear chain Ising antiferromagnet. The symbol $\langle n \rangle$ marks a phase where spins alternate with periodicity n (e.g. $n = 2$ means two spins up followed by two spins down and so on; $\langle 12 \rangle$ means one up, two down $\langle \infty \rangle$ is the ferromagnetic ordering). The location of the completely dimerized state in the quantum antiferromagnet is signalled by a full dot marked d.

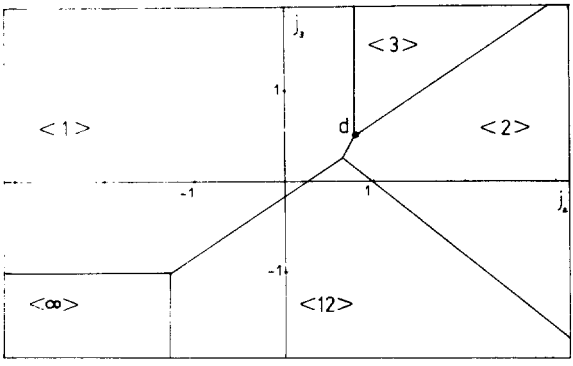

Figure 4. Same as figure 3 but for $j_4 = \frac{1}{4}$.

4. Ising antiferromagnet at $T = 0$

The ground state of a frustrated Ising chain has been extensively treated in literature [18–21]. In figures 3 and 4 sections at constant j_4 of the phase space are shown, for the same parameters as before. A full dot signals the location of the dimer state in the corresponding quantum model. Notice that the dots fall on the border between Neél ($\langle 1 \rangle$) and antiphase-2 ($\langle 2 \rangle$); in fact, this line has equation $1 - 2j_2 + j_3 = 0$. To understand the relationship between these happenings, we proceed in this way: take a pair of adjacent antiparallel spins in phase $\langle 2 \rangle$; the energy *per spin* in this phase is $e_{\langle 2 \rangle} = -2j_2 + 2j_4$. If we overturn the pair we pay an energy cost $\Delta e_{\langle 2 \rangle} = -2(1 - 2j_2 + 2j_4)$. In the Neél phase the same operation has an energy cost $\Delta e_{\langle 1 \rangle} = 2(1 - 2j_2 + 2j_3 - 2j_4)$. We then come out with the result that, if $\Delta e_{\langle 1 \rangle} = \Delta e_{\langle 2 \rangle} = 0$, that is equation (16), we can flip pairs of spins inside both phases at zero energy cost; or, in a 'quantum' language, pairs of antiparallel spins are free to resonate between 'up–down' and 'down–up'. It is not so surprising, therefore, that dimer states are the ground states of the $S = \frac{1}{2}$ quantum model at the point given by equation (16). Notice that at the classical level the dimer state has as a counterpart an infinitely degenerate

state; this is interesting since one can devise infinitely degenerate ground states even for 2D frustrated Ising [22] and classical Heisenberg [23] models.

Let us finish this section by noting that this infinitely degenerate state is the ground state of the present Ising model for $0 \leq j_4 \leq \frac{1}{4}$ (always on the line defined by equation (16)), and is superseded by a $\langle 21 \rangle$ ('two-up-one-down') phase for $-\frac{3}{4} \leq j_4 \leq \frac{1}{4}$ and by phase $\langle 3 \rangle$ for $j_4 \geq \frac{1}{4}$. At $j_4 = -\frac{3}{4}$ the ground state becomes ferromagnetic.

5. Discussion and conclusions

We can see that some features of quantum $S = \frac{1}{2}$ frustrated 1D antiferromagnet are better approximated by the related Ising model than classical Heisenberg; I refer in particular to the persistence of Neél-like correlations in the ground state up to $j_2 = \frac{1}{2}$ (and $j_3 = j_4 = 0$, figure 3), and the presence of dimerized states at the same points in parameter space. For Heisenberg spins, the topology of the order parameter space (see [24] for terminology) is different in the collinear and in the helical phase: in a collinear phase the order parameter space is homeomorphic to $SO(3)/SO(2) = S_2$, the 2D sphere, while in the helical phase (as well as in the '120°' phase of a triangular antiferromagnet) it is SO(3), since one needs two orthogonal versors to fix the plane in which the helix [25] lies. The two possible choices of the helicity (chirality) introduce an Ising-like Z_2 structure, which corresponds to stable point defects (mathematically one would say that the first homotopy group is non-trivial, $\Pi_1(SO(3)) = Z_2$). This should lead to the appearance of a finite-temperature Ising behaviour [17] in the ground state of quantum models in $1 + 1$ dimensions, mapping classical thermal fluctuations on quantum ones, which is in agreement with our results.

In conclusion, we have rigorously proved that the NN dimer covering of a 1D lattice is the ground state of a frustrated, $S = \frac{1}{2}$, Heisenberg antiferromagnet, for particular values of competing couplings beyond nearest-neighbours, generalizing the result of Majumdar and Ghosh. At present we are studying numerically the behaviour of the ground-state and of triplet excitations for the case of interactions up to fourth-nearest-neighbours, and these results will be reported elsewhere.

Acknowledgments

I wish to thank B Carazza for providing me the computer code for treating finite-spin chains. I am also grateful to E Rastelli, A Tassi and C Destri for useful discussions and a critical reading of the manuscript.

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