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1994 J. Phys. A: Math. Gen. 27 1139

(http://iopscience.iop.org/0305-4470/27/4/010)

J. Phys. A: Math. Gen. 27 (1994) 1139–1149. Printed in the UK

The spin-$\frac{1}{2}$ Heisenberg star with frustration: numerical versus exact results

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Received 9 August 1993

Abstract. We study a spin-$\frac{1}{2}$ Heisenberg model $H = J_1 \sum_{i=2}^{N} S_1 S_i + J_2 \sum_{i=2}^{N} S_i S_{i+1}$; $J_1, J_2 \geqslant 0$ (Heisenberg star) which may be considered either as an essential structure element of a lattice with frustration or, alternatively, as an antiferromagnetic linear chain with a perturbation. We discuss general relations for the energy eigenvalues, the eigenstates as well as the spin correlation of the system in dependence on J_2/J_1. The correlation function $\langle S_1 S_i \rangle$ scales with $1/Z$, where $Z = N - 1$ is the number of nearest neighbours i of the central spin 1. In the mean-field limit ($Z \rightsquigarrow \infty$) $\langle S_1 S_i \rangle$ goes to -0.25 for small J_2/J_1, but vanishes for strong frustration J_2/J_1. Adding exact numerical results for $N = 5, 7, \ldots, 23$ we discuss the ground-state phase diagram, in particular, the ground-state spin correlations versus J_2/J_1. Analysing the spin correlation of frustrated and non-frustrated stars we suggest an upper bound -0.25 for the ground-state correlator $\langle S_i S_j \rangle_0$ of two antiferromagnetically interacting spins i and j in a non-frustrated Heisenberg spin-$\frac{1}{2}$ antiferromagnet. We argue that any measured nearest-neighbour spin correlation $\langle S_i S_j \rangle_0$ larger than this bound indicates of frustration in quantum spin Heisenberg antiferromagnets.

1. Introduction

The ground state of quantum spin systems has attracted considerable interest over a long period. In connection with a possible magnetic mechanism for high-temperature superconductivity, in particular the low-dimensional quantum antiferromagnets have been widely discussed in recent times. However, the ground-state properties of low-dimensional quantum spin systems is a subject of considerable importance in its own right, in view of our poor knowledge of interacting many-body systems. One example is the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on the square lattice with nearest-neighbour interaction J_1 and frustrating next-nearest-neighbour interaction J_2. Though our knowledge of this model is more or less speculative, a rich physics is suggested including the possibility of a quantum spin liquid phase with exotic non-collinear ordering [1–3].

In this context solvable models can be quite useful in order to understand general aspects of magnetic ordering in quantum systems. For instance for quantum spin chains there are two known classes of solvable models: (i) models solvable by the Bethe ansatz [4–12] and (ii) models whose exact ground state can be expressed in terms of valence bonds [13–15]. For the latter, which can be realized also in higher dimensions [16], a special arrangement and magnitude of frustrating bonds play an important role. Another class of solvable models is connected with long-range interactions. In one dimension Haldane and Shastry [17, 18] found the spectrum and thermodynamics of the spin-$\frac{1}{2}$ Heisenberg chain with inverse-square exchange. Thirty years ago Lieb and Mattis [19] studied a model

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with long-range interaction of constant magnitude which has recently been used to discuss spontaneous symmetry breaking in spin systems [20–22]. This model can be also formulated with frustration [3].

In this paper we want to discuss a spin-$\frac{1}{2}$ Heisenberg Hamiltonian

$$H = J_1 \sum_{i=2}^{N} \boldsymbol{S}_1 \boldsymbol{S}_i + J_2 \sum_{i=2}^{N} \boldsymbol{S}_i \boldsymbol{S}_{i+1} \qquad J_1, J_2 > 0 \tag{1}$$

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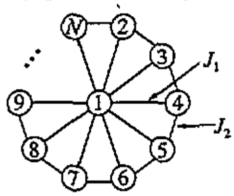


which we will refer to as the frustrated Heisenberg star in analogy with the Hubbard star discussed in [23]. We choose periodical boundary conditions, i.e. the spins $\boldsymbol{S}_2$ and $\boldsymbol{S}_{N+1}$ are identical. Both interactions J_1 and J_2 are antiferromagnetic, i.e. competing (frustrating). This model can be considered from different points of view: it represents an essential structure element of a lattice (namely a central site with $Z = N_{\mathrm{R}} = N - 1$ nearest neighbours which can be unconnected ($J_2 = 0$) or connected ($J_2 \neq 0$)). For large Z it approaches the molecular field situation and in this sense it resembles the Lieb–Mattis model. On the other hand in the limit of $J_2 \gg J_1$ the model describes the antiferromagnetic linear chain with a small frustration. To avoid additional frustration via boundary conditions we choose for the number of sites in the ring, $N_{\mathrm{R}} = N - 1$, even numbers only.

2. General properties of the Heisenberg star

2.1. Definitions

We define the following quantities:
(i) the total spin of the system

$$\boldsymbol{S} = \sum_{i=1}^{N} \boldsymbol{S}_i \tag{2}$$

(ii) the total spin of the outer ring

$$\boldsymbol{S}_{\mathrm{R}} = \sum_{i=2}^{N} \boldsymbol{S}_i = \boldsymbol{S} - \boldsymbol{S}_1 \tag{3}$$

(iii) the Hamiltonian of the outer ring (Heisenberg model of the antiferromagnetic linear chain with periodical boundary conditions)

$$H_{\mathrm{R}} = \sum_{i=2}^{N} \boldsymbol{S}_i \boldsymbol{S}_{i+1} \,. \tag{4}$$

With these definitions the Hamiltonian (1) reads

$$H = J_1 \boldsymbol{S}_1 \boldsymbol{S}_{\mathrm{R}} + J_2 H_{\mathrm{R}} \,. \tag{5}$$

2.2. *Commutation rules*

The Hamiltonian fulfills the following commutation rules:

$$\begin{aligned} &[H, \boldsymbol{S}^2]_- = 0 \qquad [H, S_z]_- = 0 \qquad [\boldsymbol{S}^2, S_z]_- = 0 \\ &[H_{\rm R}, \boldsymbol{S}_{\rm R}^2]_- = 0 \qquad [H_{\rm R}, S_{R,z}]_- = 0 \qquad [\boldsymbol{S}_{\rm R}^2, S_{R,z}]_- = 0 \end{aligned} \tag{6}$$

which are standard for any Heisenberg Hamiltonian H or $H_{\rm R}$, and

$$\begin{aligned} &[H, H_{\rm R}]_- = 0 \qquad [H, \boldsymbol{S}_{\rm R}^2]_- = 0 \qquad [\boldsymbol{S}^2, \boldsymbol{S}_{\rm R}^2]_- = 0 \\ &[S_z, \boldsymbol{S}_{\rm R}^2]_- = 0 \qquad [H_{\rm R}, \boldsymbol{S}^2]_- = 0 \qquad [H_{\rm R}, S_z]_- = 0 \end{aligned} \tag{7}$$

which are specific for model (1). (Notice that H does not commute with the z-component of $\boldsymbol{S}_{\rm R}$).

2.3. *Eigenvalues*

The commutation rules allow us to classify the eigenstates by the quantum numbers E, s, m, r, which belong to $H, \boldsymbol{S}^2, S_z, \boldsymbol{S}_{\rm R}^2$, respectively. For s and r we have

$$s = r \pm \tfrac{1}{2}\,. \tag{8}$$

Using $\boldsymbol{S}_1\boldsymbol{S}_{\rm R} = \frac{1}{2}(\boldsymbol{S}^2 - \boldsymbol{S}_{\rm R}^2 - \boldsymbol{S}_1^2)$ we find for the energy

$$E = J_2 E_{\rm R} + \tfrac{1}{2} J_1 r \qquad \text{for} \quad r = s - 12 \quad r = 0, 1, 2, \ldots, (N-1)/2 \tag{9}$$

$$E = J_2 E_{\rm R} - \tfrac{1}{2} J_1 (r+1) \qquad \text{for} \quad r = s + \tfrac{1}{2} \quad r = 1, 2, \ldots, (N-1)/2\,. \tag{10}$$

For the energy of the ring $E_{\rm R}$ we have Lieb and Mattis' [19] general relations for the lowest eigenvalue in every subspace with fixed $\boldsymbol{S}_{\rm R}^2 = r(r+1)$

$$E_{\rm R}(r) < E_{\rm R}(r+1)\,. \tag{11}$$

Hence, for the ordering of the energy levels and, in particular, for the realization of the ground state we have a competition between the J_1 term and the J_2 term in the energy. For dominating J_1 we have a ground state with the maximum $r = (N-1)/2$ and with $s = r - \frac{1}{2}$. Increasing J_2, the term $J_2 E_{\rm R}$ in the energy becomes more important and states with lower quantum numbers r have lower energies. Finally, for dominating J_2, the state with $r = 0$ and $s = \frac{1}{2}$ is the ground state. Varying the ratio J_2/J_1 between the two limits of zero and infinity, the system undergoes a series of $(N-1)/2$ transitions between different ground states.

2.4. *Structure of the eigenfunctions*

The basic structure of the eigenstates of (1) reads as follows:

$$|\Phi_{E,s,m,r}\rangle = a|\uparrow\rangle \left|\Phi^R_{E_{\rm R},r,m-\frac{1}{2}}\right\rangle + b|\downarrow\rangle \left|\Phi^R_{E_{\rm R},r,m+\frac{1}{2}}\right\rangle \tag{12}$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are the eigenfunctions of the z-component of the central spin $S_{1,z}$ and the $|\Phi^R_{E_{\rm R},r,m\pm\frac{1}{2}}\rangle$ are the eigenfunctions of $H_{\rm R}$, $\boldsymbol{S}_{\rm R}^2$, $S_{{\rm R},z}$ with the corresponding eigenvalues

E_R, $r(r+1)$, $m \pm \frac{1}{2}$. Of course, the wavefunction $|\Phi_{E,s,m,r}\rangle$ has to obey the equations $H|\Phi_{E,s,m,r}\rangle = E|\Phi_{E,s,m,r}\rangle$ and $\langle\Phi_{E,s,m,r}|\Phi_{E,s,m,r}\rangle = 1$. The first one yields a quadratic equation for the energy E with the two solutions given in (9), (10). With these expressions for E we obtain for a and b

$$a = \sqrt{\frac{r+m+\frac{1}{2}}{2r+1}} \qquad b = \sqrt{\frac{r-m+\frac{1}{2}}{2r+1}} \tag{13}$$

for $r = s - \frac{1}{2}$ and E from (9) and

$$a = -\sqrt{\frac{r-m+\frac{1}{2}}{2r+1}} \qquad b = \sqrt{\frac{r+m+\frac{1}{2}}{2r+1}} \tag{14}$$

for $r = s + \frac{1}{2}$ and E from (10). It is remarkable that the coefficients a and b, and therefore the wavefunction $|\Phi_{E,s,m,r}\rangle$ too, do not depend on J_1 and J_2. On the other hand, as discussed above, the energy of a certain state depends on J_1 and J_2, i.e. the thermodynamic properties determined by the spectrum vary with J_2/J_1.

2.5. Spin correlations

The spin correlation of the central spin with a spin of the ring determines the term proportional to J_1 in the energy E. From the expressions (9), (10) we get

$$\langle\Phi_{E,s,m,r}|S_1S_i|\Phi_{E,s,m,r}\rangle = \frac{r}{2(N-1)} \qquad \text{for} \quad r = s - \tfrac{1}{2} \tag{15}$$

$$\langle\Phi_{E,s,m,r}|S_1S_i|\Phi_{E,s,m,r}\rangle = \frac{-(r+1)}{2(N-1)} \qquad \text{for} \quad r = s + \tfrac{1}{2}. \tag{16}$$

For fixed r the correlation function decreases with $1/(N-1)$. We can discuss the correlation in the two limits of the model $J_2/J_1 \ll 1$ and $J_2/J_1 \gg 1$. In the first one we have a ground state with r close to its maximum value $r_{\max} = (N-1)/2$, i.e. $r = r_{\max} - p$ ($p = 0, 1, \ldots$) and

$$\langle\Phi_{E,s,m,r=r_{\max}-p}|S_1S_i|\Phi_{E,s,m,r=r_{\max}-p}\rangle = -\frac{1}{4} - \frac{1}{2}\frac{1-p}{N-1} \qquad i = 2, 3, \ldots, N \tag{17}$$

i.e. *in a weakly frustrated system the spin correlation of a central spin with its neighbours is* proportional to the inverse of the number of nearest neighbours $Z = N-1$ and reaches the molecular field value -0.25 for $Z \to \infty$. In the second case of strong frustration we have a ground state with small r *close to its minimum value* $r_{\min} = 0$. For $r = r_{\min}$ we have $\langle\Phi_{E,s,m,r}|S_1S_i|\Phi_{E,s,m,r}\rangle \equiv 0$, i.e. the strong frustration suppresses the antiferromagnetic correlation completely. If the frustrating J_2 is not strong enough to realize $r = 0$ but any small value $r \ll Z$, *we have a spin correlation going to zero with* $1/Z$.

Let us compare the spin correlation of the unfrustrated Heisenberg star for $Z = 4$, $Z = 6$, $Z = 8$ with the values given in the literature for the square lattice, the simple cubic lattice and the body-centred cubic lattice. We find for the square lattice $\langle\Phi_0|S_1S_i|\Phi_0\rangle \approx -0.335$, for the SC lattice $\langle\Phi_0|S_1S_i|\Phi_0\rangle \approx -0.30$ [25] and for the BCC lattice $\langle\Phi_0|S_1S_i|\Phi_0\rangle \approx -0.29$ [25]. These values are close to the values -0.375 ($Z = 4$), $-0.33\bar{3}$ ($Z = 6$) and -0.3125 ($Z = 8$) obtained for the unfrustrated star (17). On the other hand, for the triangular lattice the nearest-neighbour correlation function is $\langle\Phi_0|S_1S_i|\Phi_0\rangle \approx -0.18$ [26] indicating the effect of frustration. From (16) we find for the corresponding star ($Z = N-1 = 6$) a comparable value $-0.16\bar{6}$ for the quantum number $r = 1$. We argue, that any ground-state correlation $\langle\Phi_0|S_iS_j|\Phi_0\rangle > -0.25$ of two antiferromagnetically interacting spins S_i and S_j indicates frustration.

3. The limit of small J_2/J_1

In the case of $J_2/J_1 \ll 1$ the interaction of the central spin with its $Z = N - 1$ neighbours is weakly frustrated and the low-lying states have a large quantum number r close to its maximum value $(N-1)/2$. For $J_2 = 0$ the ground-state wavefunction belongs to $r = (N-1)/2$ and reads

$$|\Phi_{E,s=(N-2)/2,m=-s,r=(N-1)/2}\rangle = \frac{1}{\sqrt{N}}\left[\sqrt{N-1}\,|\uparrow\downarrow\ldots\downarrow\rangle - \sum_{i=2}^{N}|\downarrow\downarrow\ldots\uparrow_i\ldots\downarrow\rangle\right]. \tag{18}$$

Of course, this state is degenerate with

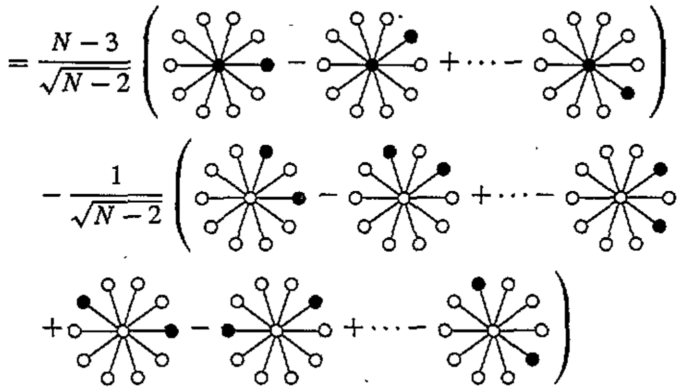
$$|\Phi_{E,s=(N-2)/2,m=-s+n,r=(N-1)/2}\rangle \sim (S^+)^n|\Phi_{E,s=(N-2)/2,m=-s,r=(N-1)/2}\rangle \qquad (n = 1,\ldots,N-2)\,.$$

The energy of these states is

$$E_{s=(N-2)/2,r=(N-1)/2} = -J_1\frac{(N+1)}{4} + J_2\frac{(N-1)}{4}\,. \tag{19}$$

Increasing J_2, the state with the next quantum number $r = (N-3)/2$ becomes the ground state at a critical ratio J_2/J_1. We can give the explicit expression for this wavefunction too:

$$|\Phi_{E,s=(N-4)/2,m=-s,r=(N-3)/2}\rangle = \frac{1}{\sqrt{N-2}}\left[(N-3)\sum_{i=2}^{N}(-1)^i|\uparrow\downarrow\ldots\uparrow_i\ldots\downarrow\rangle - \sum_{\substack{i,j=2\\|i-j|\ \text{even}}}^{N}(-1)^i|\downarrow\downarrow\ldots\uparrow_i\ldots\uparrow_j\ldots\downarrow\rangle\right] \tag{20}$$



● spin up ○ spin down.

The same Kramers degeneracy as for the state (18) holds, of course, for the state (20). The energy of (20) is

$$E_{s=(N-4)/2,r=(N-3)/2} = -J_1\frac{(N-1)}{4} + J_2\frac{(N-9)}{4}\,. \tag{21}$$

The explicit knowledge of the energies of the states with $r = r_{\max}$ and $r = r_{\max} - 1$, (19), (21) allows us to find an exact value for the critical ratio J_2/J_1 for the transition $r_{\max} \rightarrow r_{\max} - 1$. We find $J_2/J_1 = \frac{1}{4}$, i.e. independent of the system size N the state with the strongest antiferromagnetic correlation between the central spin and its neighbours remains the ground state up to a relatively strong frustration.

For completeness we give the spin correlations. In the state (18) we have

$$\langle S_1 S_i \rangle = -\frac{1}{4} - \frac{1}{2(N-1)} \qquad \langle S_i S_j \rangle = \frac{1}{4} \qquad i, j = 2, 3, \ldots, N \tag{22}$$

and in the state (20)

$$\langle S_1 S_i \rangle = -\frac{1}{4} \qquad \langle S_i S_j \rangle = \frac{1}{4} - \frac{7}{4(N-2)} \qquad |i-j| \quad \text{odd)}$$
$$\langle S_i S_j \rangle = \tfrac{1}{4} \qquad |i-j| \quad \text{even} \quad i, j = 2, 3, \ldots, N\,. \tag{23}$$

4. The limit of large J_2/J_1

In this limit the interaction J_2 within the ring dominates the interaction J_1 of the central spin with its neighbours and the system can be considered as a one-dimensional ring with a small perturbation (frustration). If J_2/J_1 exceeds a critical value, the ground state belongs to the quantum numbers $r = 0$ and $s = \frac{1}{2}$. Using (12) and (13) the wavefunction reads

$$\left|\Phi_{E,s=\frac{1}{2},m=\frac{1}{2},r=0}\right\rangle = |\uparrow\rangle \left|\Phi^{R}_{E^0_R,r=0,m-\frac{1}{2}=0}\right\rangle \tag{24}$$

which is degenerate to $\left|\Phi_{E,s=\frac{1}{2},m=-\frac{1}{2},r=0}\right\rangle$. The wavefunction of the ring $\left|\Phi^{R}_{E^0_R,r=0,m-\frac{1}{2}=0}\right\rangle$ is then the Bethe ground state of the one-dimensional Heisenberg antiferromagnet [4]. In the limit $N_R = (N-1) \rightarrow \infty$ the ring energy E_R (which according to (9) is equal to the total energy of the system) is given by Hulthen's result [5]

$$E^0_R(N_R \rightarrow \infty) = N_R\left(\tfrac{1}{4} - \ln 2\right). \tag{25}$$

For finite systems the $1/N_R$ corrections are given by [27, 28]

$$E^0_R(N_R) = E^0_R(N_R \rightarrow \infty) - \frac{1}{N_R}\frac{\pi^2}{12}\left[1 + O\left(\frac{1}{\ln^3 N_R}\right)\right]. \tag{26}$$

The energy of the first triplet excitation for the ring reads [27, 28]

$$E^1_R(N_R) = E^0_R + \frac{1}{N_R}\frac{\pi^2}{4}\left[2 - \frac{1}{\ln N_R} + \frac{\ln(4/\pi)}{\ln^2 N_R} + O\left(\frac{1}{\ln^3 N_R}\right)\right]. \tag{27}$$

Hence, we find the critical ratio

$$\frac{J_1}{J_2} = \frac{1}{N_R}\frac{\pi^2}{4} \qquad \left[2 - \frac{1}{\ln N_R} + \frac{\ln(4/\pi)}{\ln^2 N_R}\right] \tag{28}$$

where Bethe's singlet ground state and the first triplet excitation of the ring become degenerate. Clearly, in the thermodynamic limit the gap between the singlet ($r = 0$) ground state and the triplet ($r = 1$) excitation closes and an infinitesimally small $J_1 \sim N_R^{-1} J_2$ is sufficient to destroy the singlet ground state of the ring.

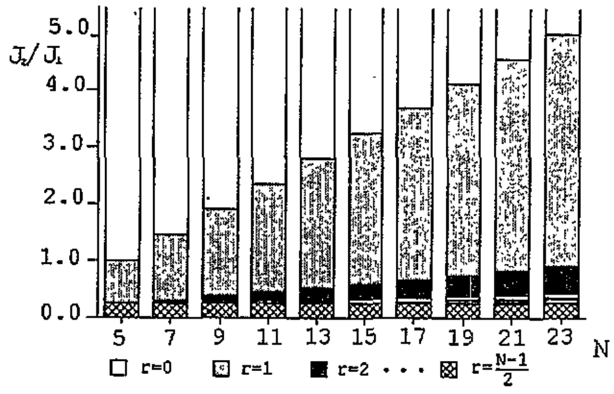


Figure 1. Ground-state transitions between states with different quantum numbers r versus J_2/J_1 for systems of several size N.

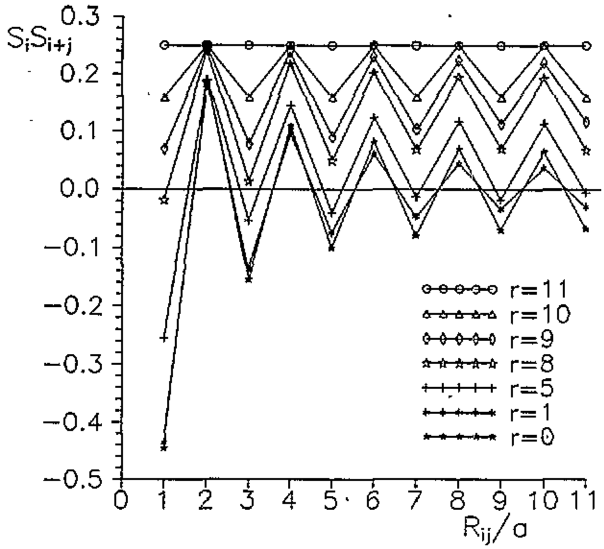


Figure 2. Spin–spin correlation $\langle\Phi_{E,s,m,r}|S_iS_{i+j}|\Phi_{E,s,m,r}\rangle$ of two spins in the outer ring for states with different quantum numbers r. The numerical data are presented for $N = 23$.

5. Numerical results

We have calculated the ground-state phase diagram for arbitrary J_2/J_1 for finite systems up to $N = 23$ sites by the Lanczos technique. The result is shown in figure 1. According to the general discussion in section 2 the ground state is a state with maximum quantum number r and strongest antiferromagnetic correlation $\langle \boldsymbol{S}_1\boldsymbol{S}_i\rangle$ for $J_2/J_1 < \alpha_{\text{crit}}$. We find $\alpha_{\text{crit}} = \frac{1}{4}$ as an exact and universal value independent of the size of the system. If J_2/J_1 exceeds α_{crit} it follows a series of transitions to ground states with decreasing r and weaker correlations $\langle \boldsymbol{S}_1\boldsymbol{S}_i\rangle$. With decreasing r the correlation $\langle \boldsymbol{S}_i\boldsymbol{S}_j\rangle$ ($i \neq j = 2, N$) (which is shown in figure 2 for $N = 23$) starts with a pure ferromagnetic correlation for $r = r_{\max}$ and then becomes more and more spatially modulated towards an antiferromagnetic correlation with a power-law decay for $r = 0$. The ground-state transitions between various quantum numbers r immediately following the first transition $r_{\max} \to (r_{\max} - 1)$ are very close to each other and build a quasicontinuum for stars with large N (see figure 3, where the numerical results are extrapolated to large N). However, for r going to its minimum value, $r = 0$, the transitions are well separated from each other (the leading term for the critical J_2/J_1 is proportional to N_{R}; see section 4). This is illustrated in figure 4, where the critical inverse

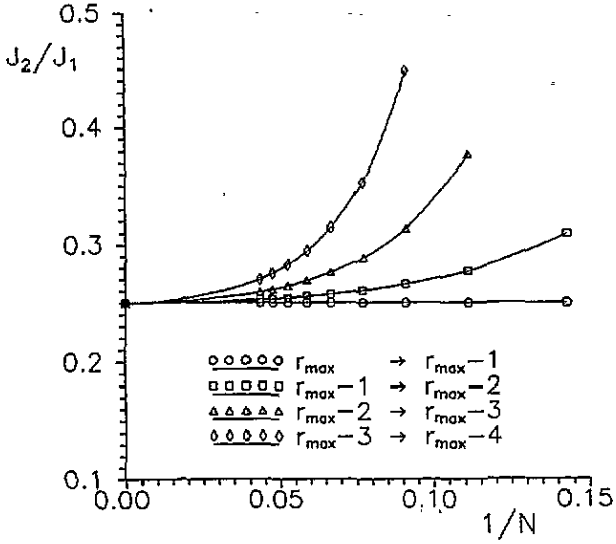


Figure 3. Critical ratio J_2/J_1 for transitions between states with different quantum numbers r close to $r_{max} = (N-1)/2$ versus $1/N$. The numerical data for $N = 5, 7, \ldots, 23$ are extrapolated to infinite N.

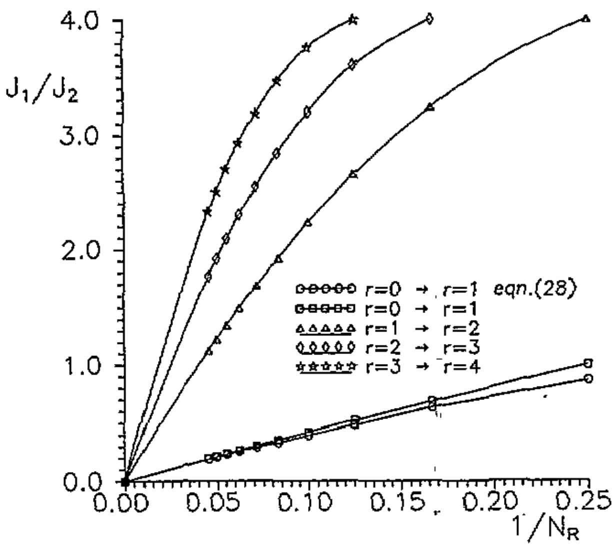


Figure 4. Inverse critical ratio J_1/J_2 for transitions between states with different quantum numbers r close to $r_{min} = 0$ versus $1/N_R$ ($N_R = N-1$). The numerical data for $N_R = 4, 6, \ldots, 22$ are extrapolated to infinite N_R.

ratio J_1/J_2 and its extrapolation to large N_R is shown for several transitions.

We illustrate the above general discussion of transitions for $N = 23$ in figure 5 by presenting *the correlation of the central spin with a neighbouring spin* $\langle S_1 S_i \rangle$, *the correlation* of nearest neighbours in the ring $\langle S_i S_{i+1} \rangle$ and the square of sublattice magnetization of the ring

$$M_s^2 = \left\langle \frac{1}{N_R^2} \sum_{i,j=2}^{N} (-1)^{i+j} S_i S_j \right\rangle \tag{29}$$

with dependence on J_2/J_1. For finite N_R the latter one is a measure of the overall antiferromagnetic correlation and goes to zero for $N_R \to \infty$. Clearly, we see the *quasicontinuous series of transitions if* J_2/J_1 slightly exceeds α_{crit} and the well separated

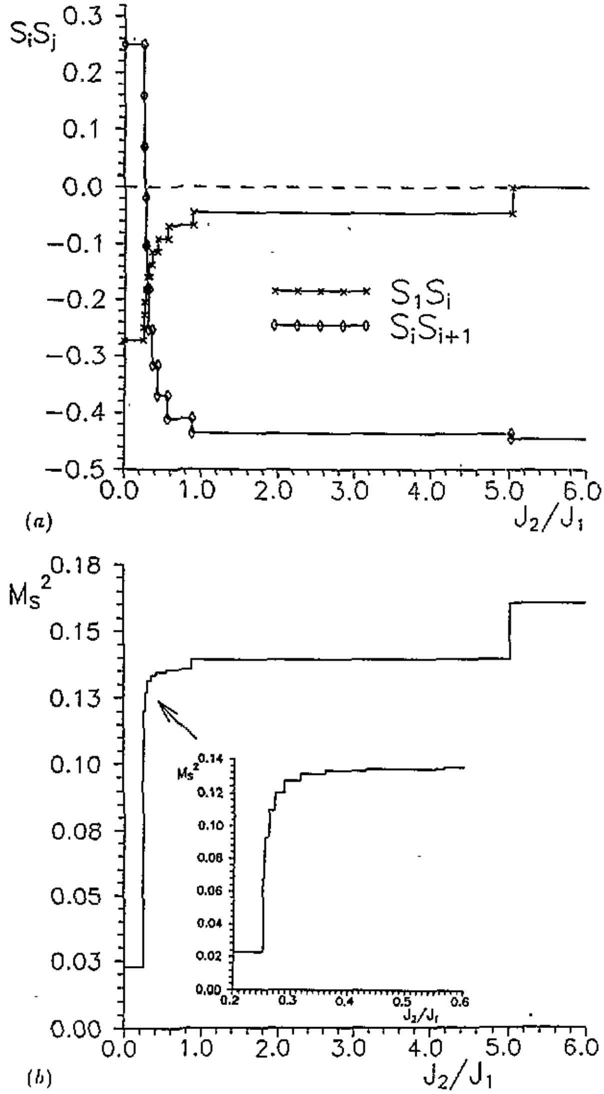


Figure 5. (*a*) Numerical data for the ground-state spin–spin correlation $\langle S_1 S_i \rangle_0$ between the central spin 1 and a neighbouring spin i as well as $\langle S_i S_{i+1} \rangle_0$ between two neighbouring spins in the ring versus J_2/J_1 for $N = 23$. (*b*) Numerical data for the square of sublattice magnetization M_s^2 (see (29)) of the ring versus J_2/J_1 for $N = 23$.

transitions for larger J_2/J_1. The change from strong antiferromagnetic correlations of the central spin with its neighbours (accompanied by ferromagnetic correlations in the ring) to a well pronounced antiferromagnetic correlation in the ring (accompanied by a drastic weakening of the correlation of the central spin) takes place in a small region above the first transition $J_2/J_1 = \alpha_{\rm crit}$.

Finally, let us consider in figure 6 the correlation of the central spin with a neighbouring spin $\langle S_1 S_i \rangle$ versus the frustration parameter J_2/J_1 for stars with $Z = N_{\rm R} = N - 1 = 4, 6, 8, 12$ which correspond to some standard two- and three-dimensional lattices, e.g. for $Z = 6$ and $J_2 = J_1$ the star corresponds to an elementary cluster of the triangular lattice and, as dicussed already in section 2.5, the correlation fits quit well to the infinite triangular lattice. The critical ratio J_2/J_1, where the correlation of the central spin with its neighbours is completely suppressed by frustration, is of the order of unity ($J_2/J_1 = 1.0$ for $Z = 4$, $J_2/J_1 = 1.46$ for $Z = 6$, $J_2/J_1 = 1.91$ for $Z = 8$, $J_2/J_1 = 2.81$ for $Z = 12$).

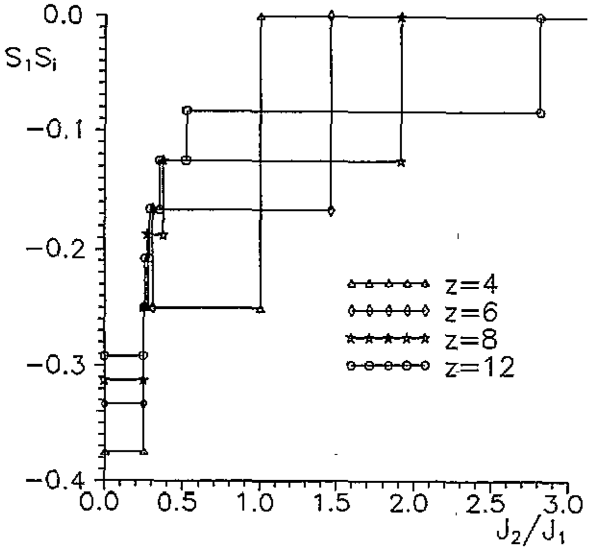


Figure 6. Numerical data for the ground-state spin–spin correlation $\langle S_1 S_i \rangle_0$ between the central spin 1 and a neighbouring spin i versus J_2/J_1 for clusters with different numbers of neighbours Z ($Z = N - 1$).

6. Summary

In this paper we discuss the spin-$\frac{1}{2}$ Heisenberg model for a cluster of a central spin interacting with Z nearest-neighbour spins via antiferromagnetic exchange coupling J_1 (Heisenberg star). Additionally, every neighbouring spin may interact antiferromagnetically via J_2 with two other neighbours, forming an outer antiferromagnetic ring around the central spin (frustrated Heisenberg star). In the two limits of the model, $J_1 \gg J_2$ and $J_1 \ll J_2$, the cluster can be considered as an essential structure element of a lattice with frustration or as an antiferromagnetic linear chain with a perturbation. General considerations for the energy, the eigenfunctions and the spin–spin correlation and their dependence on $\alpha = J_2/J_1$ give hints for the ground-state phase diagram. For $J_2/J_1 < \alpha_{\text{crit}}$ the ground state of the system is the state with strongest antiferromagnetic correlation

$$\langle S_1 S_i \rangle = -\frac{1}{4} - \frac{1}{2}\frac{1}{Z} .$$

If J_2/J_1 exceeds α_{crit}, it follows a series of transitions to states with successively weaker correlations $\langle S_1 S_i \rangle$ ending with $\langle S_1 S_i \rangle = 0$ for dominating J_2. For α_{crit} we find exactly $\frac{1}{4}$, independent of the size of the system. For larger N this weakening of antiferromagnetic correlation of the central spin takes place very rapidly when changing J_2/J_1 in a small region above the first transition.

The extrapolation $Z \to \infty$ (mean-field limit) yields for $J_2/J_1 < \alpha_{\text{crit}}$ the correlator $\langle S_1 S_i \rangle = -0.25$ which can be considered as an upper limit for the ground-state correlation $\langle S_i S_j \rangle_0$ of antiferromagnetically interacting spins i and j in a spin-$\frac{1}{2}$ Heisenberg antiferromagnet without frustration. Any ground-state spin correlation $\langle S_i S_j \rangle_0$ larger than -0.25 is an effect of frustration. If the frustration is strong enough the correlation $\langle S_i S_j \rangle_0$ goes to zero with $1/Z$ in the mean-field limit $Z \to \infty$.

Acknowledgments

We would like to thank C Gros for helpful discussions. This work was supported by the Deutsche Forschungsgemeinschaft (project Ri 615/1-1).

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