Exact ground and excited states of an antiferromagnetic quantum spin model

1989 J. Phys.: Condens. Matter 1 9267

(http://iopscience.iop.org/0953-8984/1/46/018)

J. Phys.: Condens. Matter 1 (1989) 9267–9271. Printed in the UK

LETTER TO THE EDITOR

Exact ground and excited states of an antiferromagnetic quantum spin model

Indrani Bose†
International Centre for Theoretical Physics, Trieste, Italy

Received 29 August 1989

Abstract. A quasi-one-dimensional spin model that consists of a chain of octahedra of spins has been suggested, for which in a certain parameter regime of the Hamiltonian the ground state can be written down exactly. The ground state is highly degenerate and can be other than a singlet. Also, several excited states can be constructed exactly. The ground state is a local resonating valence band state for which resonance is confined to rings of spins. Some exact numerical results for an octahedron of spins have also been reported.

Antiferromagnetic (AFM) quantum spin models for which exact solutions exist are few in number. The ground state energy and excitation spectrum of the AFM Heisenberg spin-$\frac{1}{2}$ chain can be obtained exactly by using the Bethe *ansatz* (see Majumdar 1985 for a review). The ground state, a singlet, is disordered, i.e., has no sublattice magnetisation, and the two-spin correlation function has a power law decay. Also, the excitation spectrum is gapless. The ground state can be described as a resonating valence bond (RVB) state because the state resonates between various singlet or valence bond coverings of the chain with all possible lengths for the valence bonds. The ground state structure is, however, complicated and cannot be written down explicitly. Various simple spin models in dimensions $d \geqslant 1$ and for spins $S \geqslant \frac{1}{2}$ have been suggested (Majumdar 1969, Majumdar and Ghosh 1969, Shastry and Sutherland 1981a, b, Affleck *et al* 1987, Bose *et al* 1984, Bose 1988, Kanter 1989, Doucot and Kanter 1989) for which the ground state structure is simple and can be written down explicitly. Most of the models suggested have dimerised or valence-bond (VB) ground states for which the ground state is given by valence bond coverings. The valence bonds are short-ranged, i.e., confined to nearest neighbours or next-nearest neighbours. Such ground states are different from the RVB state, for which energy lowering is achieved through resonance between various valence bond configurations. In the VB ground states translational symmetry may or may not be broken (Majumdar 1969, Affleck *et al* 1987). In some cases it can be shown rigorously that the excitation spectrum has a gap and the two-spin correlation function has an exponential or faster decay. Neither the RVB state nor the VB state has long-range order (LRO) in the two-spin correlation function. A class of quantum Hamiltonians exists (Bose *et al* 1984, Bose 1988) for which Néel states ($d = 1$) and Néel-like states ($d = 3$) are exact ground states. The ground state has perfect long-range Néel order, a quadratic dispersion for the spin-wave spectrum and no gap in the excitation spectrum. Issues like the

† Permanent address: Department of Physics, Bose Institute, 93/1, A.P.C. Road, Calcutta-700009, India.

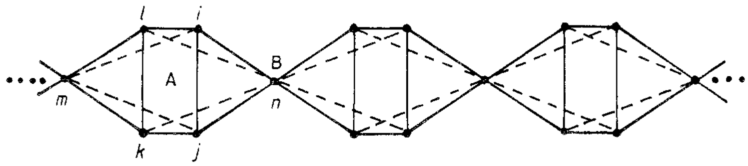

Figure 1. Chain of octahedra of spins. The central plane A in each octahedron is perpendicular to the plane of the paper; i, j, k, l, m, n denote spin sites.

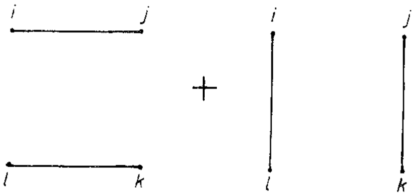

Figure 2. Resonating valence bond (RVB) state of four spins. This is the ground state configuration for the A-plane spins when α is $\leqslant \frac{1}{2}$.

presence or absence of LRO in the ground state of AFMs and the nature of the excitation spectrum are of special relevance in the context of high-T_c superconductors (Anderson 1988). A proper understanding of such issues is, however, still lacking for low-dimensional spin systems. In this Letter we construct a quasi-one-dimensional spin model for which the ground state in a certain parameter regime can be written down exactly. Also, several excited states can be determined exactly.

The spin model to be considered consists of a chain of octahedra of spins (figure 1). The spins have magnitude $\frac{1}{2}$ and periodic boundary condition is assumed. Each octahedron of six spins consists of a central plane A of four spins and two vertex spins denoted by B. The central spins interact with a coupling strength J and the vertex spins interact with the central spins with a strength αJ, $\alpha \leqslant 1$. The Hamiltonian is written as

$$H = \sum_{\gamma} (J(\boldsymbol{S}_i \cdot \boldsymbol{S}_j + \boldsymbol{S}_j \cdot \boldsymbol{S}_k + \boldsymbol{S}_k \cdot \boldsymbol{S}_l + \boldsymbol{S}_l \cdot \boldsymbol{S}_i) + \alpha J(\boldsymbol{S}_m + \boldsymbol{S}_n) \cdot (\boldsymbol{S}_i + \boldsymbol{S}_j + \boldsymbol{S}_k + \boldsymbol{S}_l)) \tag{1}$$

where γ denotes a sum over $N/5$ octahedra of spins, N the number of spins being an integral multiple of five. For $\alpha \leqslant \frac{1}{2}$, the ground state spin configuration is as follows: in each A plane the $S = 0$ spin state is resonating between the two valence bond structures shown in figure 2, the corresponding eigenfunction being given by

$$\psi_A = (1/\sqrt{12})\,(\uparrow\uparrow\downarrow\downarrow + \downarrow\downarrow\uparrow\uparrow + \uparrow\downarrow\downarrow\uparrow + \downarrow\uparrow\uparrow\downarrow - 2\uparrow\downarrow\uparrow\downarrow - 2\downarrow\uparrow\downarrow\uparrow). \tag{2}$$

The B spins are kept free. The ground state energy is given by $E_g = -2JN/5$. The ground state is a local RVB state and highly degenerate, there being $2^{N/5}$ possible ground state configurations. Let us now prove that the above spin eigenfunctions describe the ground state. For this, one makes use of the familiar spin identity $\boldsymbol{S}_m \cdot (\boldsymbol{S}_i + \boldsymbol{S}_j)[ij] = 0$ where $[ij]$ describes the singlet $(1/\sqrt{2})\{\alpha(i)\beta(j) - \beta(i)\alpha(j)\}$. Using this relation one can easily verify that the above configurations are exact eigenstates of the Hamiltonian (1) with energy $E_{\mathrm{exact}} = -2JN/5$. So the true ground state energy is $E_g \leqslant E_{\mathrm{exact}}$. The Hamiltonian can be written as $\Sigma_\gamma H_\gamma$ where H_γ is the Hamiltonian for an octahedron of spins. The sum over γ is the sum over all octahedra. Modification of the Rayleigh–Ritz variational

Table 1. Lowest energy eigenvalues E_g (in units of J) of the six-spin octahedron for various values of the coupling constant α. The figure in bracket denotes the degeneracy of the level.

α	E_g
0.0	−2.0 (4)
0.1	−2.0 (4)
0.2	−2.0 (4)
0.3	−2.0 (4)
0.4	−2.0 (4)
0.5	−2.0 (4)
0.6	−2.2
0.7	−2.4
0.8	−2.6
0.9	−2.8
1.0	−3.0

principle (Shastry and Sutherland 1981a, b) suggests that $E_g \geqslant \Sigma_\gamma E_{\gamma'}$ where $E_{\gamma'}$ is the lowest energy of the octahedron of spins. Table 1 gives the lowest energy eigenvalues of the coupling strength α ranging from 0.0 to 1.0. For $\alpha \leqslant \frac{1}{2}$, the lowest eigenvalue is given by $-2J$ and one arrives at the inequality $-2JN/5 \leqslant E_g \leqslant -2JN/5$ from which it is proved that $E_g = -2JN/5$. Several excited states can also be written down immediately. For any value of α, the energy eigenvalues of the size-spin octahedron can be determined exactly. The number of such eigenvalues is 64. To construct an excited state let alternate A planes have the RVB spin configuration of figure 2. Such A planes are separated by $N/10$ octahedra of spins that can be in any one of the 64 possible eigenfunctions of an octahedron. Any such state is an exact eigenstate with the appropriate energy eigenvalue. Following the above prescription, the total number of exact eigenstates for any value of α is $64^{N/10}$, which also include the highly degenerate ground state configurations for $\alpha \leqslant \frac{1}{2}$. The appendix lists some of the exact eigenstates and energy eigenvalues of the spin octahedron. It has not been possible as yet to write down the ground states exactly for $\alpha > \frac{1}{2}$, The $\alpha = 1$ limit is of particular interest. An exact determination of the energy eigenvalues and eigenfunctions of the spin octahedron for $\alpha = 1$ shows the ground state energy of the octahedron to be $-3J$. The corresponding eigenfunction is a spin singlet that is formed out of two spin triplets, one corresponding to the A spins and the other formed out of the B spins of the octahedron. For $\alpha = 1$ the ground state energy E_g satisfies the inequality $-3JN/5 \leqslant E_g \leqslant -2JN/5$. Regarding the excitation spectrum, for $\alpha \neq 1$, all the excited states that have been constructed exactly are separated from the ground state by an energy gap, and this is possibly true for the whole excitation spectrum. For $\alpha = 1$ and for just an octahedron of spins the ground state is non-degenerate. The ground state for the whole chain of octahedra is not known in this limit. If it is unique then the Lieb–Schultz–Mattis (LSM) theorem (1961) can be applied to the chain. This is because, as pointed out by Affleck (1988), for half-integer spins on an arbitrary Bravais lattice the LSM theorem works whenever the total spin per unit cell is half an odd integer. For the chain of octahedra, the total spin per unit cell is $\frac{5}{2}$. Thus a unique ground state would mean a gapless excitation spectrum.

One can also calculate the various correlation functions in the ground state. For $\alpha \leqslant \frac{1}{2}$, any two B spins or one A spin and one B spin or any two A spins belonging to different rings are totally uncorrelated. For A spins in the same ring, the correlation functions can be written as

$$
\begin{aligned}
&\langle\psi_{\mathrm{A}}|S_1^z S_2^z|\psi_{\mathrm{A}}\rangle = \langle\psi_{\mathrm{A}}|S_1^z S_4^z|\psi_{\mathrm{A}}\rangle = -\tfrac{1}{6} \\
&\langle\psi_{\mathrm{A}}|S_1^z S_3^z|\psi_{\mathrm{A}}\rangle = \tfrac{1}{12} \\
&\langle\psi_{\mathrm{A}}|S_1^+ S_2^-|\psi_{\mathrm{A}}\rangle = \langle\psi_{\mathrm{A}}|S_1^+ S_4^-|\psi_{\mathrm{A}}\rangle = -\tfrac{2}{3} \\
&\langle\psi_{\mathrm{A}}|S_1^+ S_3^-|\psi_{\mathrm{A}}\rangle = \tfrac{1}{3}.
\end{aligned}
\tag{3}
$$

The last three correlation functions are variants of the Thouless order parameter (Thouless 1967). The correlation decays as one moves away from a spin. The sign of the short range order indicates that on an average an up spin is surrounded by down spins and vice versa. The ground state in short is a quantum-spin liquid state with ultra-short-range order confined to rings of four spins. The rings are in $S = 0$ state but because the vertex spins can orient themselves freely, the ground state is highly degenerate and the ground state can be other than a singlet. On the other hand, for bipartite lattices and for rather general AFM Hamiltonians the Lieb–Mattis theorem (1962) tells us that the ground state is non-degenerate and a singlet. For the six-spin octahedron the ground state is non-degenerate and a singlet only in the $\alpha = 1$ limit. To sum up, we have studied a quasi-one-dimensional spin model, namely, a chain of spin octahedra, for which in a certain parameter régime of the Hamiltonian ($\alpha \leqslant \frac{1}{2}$) the ground state can be written down exactly. The ground state, which is highly degenerate, can be called a local RVB state because resonance is confined to rings of spins, the other spins being able to orient themselves freely. Several exact excited states have also been constructed. Also, exact diagonalisation of a six-spin octahedron shows that in the $\alpha = 1$ limit the ground state is non-degenerate and a singlet. Analysis of the chain ground state in this limit is in progress and the results will be reported elsewhere.

The author gratefully acknowledges the hospitality provided by the International Centre for Theoretical Physics, Trieste, Italy where this work was carried out.

Appendix

Some exact energy eigenvalues and eigenstates of the six-spin octahedron:

$E_1 = 0$

$$\psi_1 = a_1\phi_2 + a_2\phi_{13} + a_3\phi_{15} + a_4\phi_{19} + a_5\phi_{20} - a_6\phi_{10} - a_7\phi_{14} - a_8\phi_{16}$$

$$a_1 + a_2 + a_5 = a_7 \qquad a_3 + a_4 = a_6 + a_8 \qquad a_1 + a_3 + a_5 = a_8$$

$$a_1 + a_2 + a_4 = a_8 \qquad a_2 + a_4 = a_6 + a_7 \qquad a_3 + a_5 = a_6 + a_7$$

$E_2 = 0$

$$\psi_2 = a_1\phi_2 + a_2\phi_{10} + a_3\phi_{14} + a_4\phi_{19} + a_5\phi_{20} - a_6\phi_{13} - a_7\phi_{15} - a_8\phi_{16}$$

$$a_1 + a_3 + a_5 = a_6 \qquad a_2 + a_4 = a_7 + a_8 \qquad a_1 + a_5 = a_7 + a_8$$

$$a_1 + a_4 = a_6 + a_8 \qquad a_2 + a_3 + a_4 = a_6 \qquad a_2 + a_3 + a_5 = a_7$$

$E_3 = 0$

$$\psi_3 = a_1\phi_{14} + a_2\phi_{16} + a_3\phi_{19} + a_4\phi_{20} - a_5\phi_2 - a_6\phi_{10} - a_7\phi_{13} - a_8\phi_{15}$$

$$a_1 + a_4 = a_5 + a_7 \qquad a_2 + a_3 = a_6 + a_8 \qquad a_1 + a_3 = a_6 + a_7$$

$$a_1 + a_4 = a_6 + a_8 \qquad a_2 + a_4 = a_5 + a_8 \qquad a_2 + a_3 = a_5 + a_7$$

$$E_4 = 0$$

$$\psi_4 = a_1\phi_{10} + a_2\phi_{13} + a_3\phi_{16} + a_4\phi_{20} - a_5\phi_2 - a_6\phi_{14} - a_7\phi_{15} - a_8\phi_{19}$$

$$a_1 + a_3 = a_7 + a_8 \qquad a_2 + a_4 = a_5 + a_6 \qquad a_1 + a_2 = a_6 + a_8$$

$$a_1 + a_4 = a_6 + a_7 \qquad a_2 + a_3 = a_5 + a_8 \qquad a_3 + a_4 = a_5 + a_7$$

$$E_5 = 1.0$$

$$\psi_5 = a_1(\phi_2 + \phi_{14} + \phi_{13} + \phi_{20} + \phi_{17} + \phi_{12} - \phi_{16} - \phi_{10} - \phi_{19} - \phi_{15} - \phi_{11} - \phi_{18})$$

$$E_6 = -1.0$$

$$\psi_6 = a_1(\phi_{18} - \phi_{11} - \phi_{12} + \phi_{17})$$

The spin configurations are:

$\phi_1 = |\uparrow\uparrow\,\uparrow\downarrow\,\downarrow\downarrow\rangle$ $\phi_2 = |\uparrow\uparrow\,\downarrow\downarrow\,\downarrow\uparrow\rangle$ $\phi_3 = |\uparrow\downarrow\,\downarrow\downarrow\,\uparrow\uparrow\rangle$ $\phi_4 = |\downarrow\downarrow\,\downarrow\uparrow\,\uparrow\uparrow\rangle$

$\phi_5 = |\uparrow\uparrow\,\downarrow\uparrow\,\downarrow\downarrow\rangle$ $\phi_6 = |\uparrow\downarrow\,\uparrow\uparrow\,\downarrow\downarrow\rangle$ $\phi_7 = |\downarrow\uparrow\,\uparrow\uparrow\,\downarrow\downarrow\rangle$ $\phi_8 = |\downarrow\downarrow\,\uparrow\downarrow\,\uparrow\uparrow\rangle$

$\phi_9 = |\downarrow\uparrow\,\downarrow\downarrow\,\uparrow\uparrow\rangle$ $\phi_{10} = |\downarrow\downarrow\,\uparrow\uparrow\,\uparrow\downarrow\rangle$ $\phi_{11} = |\uparrow\downarrow\,\uparrow\downarrow\,\uparrow\downarrow\rangle$ $\phi_{12} = |\downarrow\uparrow\,\downarrow\uparrow\,\downarrow\uparrow\rangle$

$\phi_{13} = |\uparrow\downarrow\,\downarrow\uparrow\,\downarrow\uparrow\rangle$ $\phi_{14} = |\downarrow\downarrow\,\uparrow\uparrow\,\downarrow\uparrow\rangle$ $\phi_{15} = |\downarrow\uparrow\,\uparrow\downarrow\,\uparrow\downarrow\rangle$ $\phi_{16} = |\uparrow\uparrow\,\downarrow\downarrow\,\uparrow\downarrow\rangle$

$\phi_{17} = |\uparrow\downarrow\,\uparrow\downarrow\,\downarrow\uparrow\rangle$ $\phi_{18} = |\downarrow\uparrow\,\downarrow\uparrow\,\uparrow\downarrow\rangle$ $\phi_{19} = |\uparrow\downarrow\,\downarrow\uparrow\,\uparrow\downarrow\rangle$ $\phi_{20} = |\downarrow\uparrow\,\uparrow\downarrow\,\downarrow\uparrow\rangle$

References

Affleck I 1988 *Phys. Rev.* B **37** 5186

Affleck I, Kennedy T, Lieb E H and Tasaki H 1987 *Phys. Rev. Lett.* **59** 799

Anderson P W D 1988 *Frontiers and Borderlines in Many-particle Physics, Varenna Summer School, Varenna, Italy* (Amsterdam: North-Holland)

Bose I, Chatterjee S and Majumdar C K 1984 *Phys. Rev.* B **29** 2741

Bose I 1988 *J. Phys. C: Solid State Phys* **21** L841

Doucot B and Kanter I 1989 *Phys. Rev.* B **39** 12399

Kanter I 1989 *Phys. Rev.* B **39** 7270

Lieb E H and Mattis D C 1962 *J. Math. Phys.* **3** 749

Lieb E, Schultz T and Mattis D 1961 *Ann. Phys., NY* **16** 407

Majumdar C K 1969 *J. Phys. C: Solid State Phys.* **3** 911

Majumdar C K and Ghosh D K 1969 *J. Math. Phys.* **10** 1388; 1399

Majumdar C K 1985 *Exactly Solvable Problems in Condensed Matter and Relativistic Field Theory* ed. B S Shastry, S S Jha and V Singh (Berlin: Springer) p 142

Shastry B S and Sutherland B 1981a *Phys. Rev. Lett.* **47** 964

—— 1981b Physica B **108** 1069

Thouless D J 1967 *Proc. Phys. Soc.* **90** 243