IC/89/246

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

EXACT GROUND AND EXCITED STATES OF AN ANTIFERROMAGNETIC QUANTUM SPIN MODEL

Indrani Bose

INTERNATIONAL ATOMIC ENERGY AGENCY

UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

1989 MIRAMARE - TRIESTE

International Atomic Energy Agency
and
United Nations Educational Scientific and Cultural Organization
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

EXACT GROUND AND EXCITED STATES OF AN ANTIFERROMAGNETIC QUANTUM SPIN MODEL *

Indrani Bose **
International Centre for Theoretical Physics, Trieste. Italy.

ABSTRACT

A quasi–one–dimensional spin model which 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 RVB state for which resonance is confined to rings of spins. Some exact numerical results for an octahedron of spins have also been reported.

MIRAMARE – TRIESTE
August 1989

* Submitted for publication.

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

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-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 magnetization 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 can not be written down explicitly.Various simple spin models in dimensions $d \geq 1$ and for spins $S \geq 1/2$ have been suggested (Majumdar 1969 ,Majumdar and Ghosh 1969,Shastry and Sutherland 1981,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 dimerized 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 rigorously shown 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 exist (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 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 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 ,$\alpha \leq$ 1.The Hamiltonian is written as

$$H = \sum_{\gamma} (J(\vec{S}_i.\vec{S}_j + \vec{S}_j.\vec{S}_k + \vec{S}_k.\vec{S}_l + \vec{S}_l.\vec{S}_i) + \alpha J(\vec{S}_m + \vec{S}_n).(\vec{S}_i + \vec{S}_j + \vec{S}_k + \vec{S}_l)) \qquad (1)$$

where γ denotes sum over N/5 octahedra of spins ,N the number of spins being an integral multiple of five.Consider the classical limit $S \to \infty$ of the Hamiltonian (1).For$\alpha < 1/2$ the ground state is given by a Néel arrangement of spins in the A planes with the B spins being kept free.For $\alpha > 1/2$ the B spins are parallel to each other .The spins in the A planes are parallel to each other but antiparallel to the B spins.For $\alpha = 1/2$, any one of the above configurations is a ground state.Now consider the quantum case.For $\alpha \leq 1/2$, 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

$$\psi_A = 1/\sqrt{8}(\uparrow\uparrow\downarrow\downarrow + \downarrow\downarrow\uparrow\uparrow + \uparrow\downarrow\downarrow\uparrow + \downarrow\uparrow\uparrow\downarrow - 2\uparrow\downarrow\uparrow\downarrow - 2\downarrow\uparrow\downarrow\uparrow) \qquad (2)$$

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 $\vec{S}_m(\vec{S}_i + \vec{S}_j)[ij] = 0$ where [i j] describes the singlet $1/\sqrt{2}(\alpha(i)\beta(j) - \beta(i)\alpha(j))$. Using this relation one can easily verify that the above spin configurations are exact eigenstates of the Hamiltonian (1) with energy $E_{exact} = -2JN/5$. So the true ground state energy is $E_g \leq E_{exact}$.The Hamiltonian can be written as $\sum_{\gamma} H_\gamma$ 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 principle (Shastry and Sutherland 1981) suggests that $E_g \geq \sum_{\gamma} E_{\gamma'}$ where $E_{\gamma'}$ is the lowest energy of the octahedron of spins.Table 1 gives the lowest energy eigenvalues for values of the coupling strength α ranging from 0.0 to 1.0.For $\alpha \leq 1/2$, the lowest eigenvalue is given by -2J and one arrives at the inequality $-2JN/5 \leq E_g \leq -2JN/5$ 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 six-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 which can be in any one of the 64 possible eigen- functions 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 $\alpha \leq 1/2$. Appendix A 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 $\alpha > 1/2$. 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 which 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 $\leq E_g \leq$ -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.Forα=1 and for just an octahedron of spins the ground state is nondegenerate.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 odd integer.For the chain of octahedra,the total spin per unit cell is 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$\alpha \leq 1/2$, 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 :

$$
\begin{aligned}
&< \psi_A \mid S_1^z S_2^z \mid \psi_A > = < \psi_A \mid S_1^z S_4^z \mid \psi_A > = -1/4 \\
&< \psi_A \mid S_1^z S_3^z \mid \psi_A > = 1/8 \\
&< \psi_A \mid S_1^+ S_2^- \mid \psi_A > = < \psi_A \mid S_1^+ S_4^- \mid \psi_A > = -1 \\
&< \psi_A \mid S_1^+ S_3^- \mid \psi_A > = 1/2
\end{aligned}
\tag{3}
$$

The last three correlation funtions 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 nondegenerate and a singlet.For the six spin octahedron the ground state is nondegenerate 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 regime of the hamiltonian ($\alpha \leq 1/2$) 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 can orient themselves freely.Several exact excited states have also been constructed.Also, exact diagonalization of a six spin octahedron shows that in the$\alpha = 1$ limit the ground state is nondegenerate and a singlet.Analysis of the chain ground state in this limit is in progress and the results will be reported elsewhere.

Appendix A. Some exact energy eigenvalues and eigenstates of the six spin octahedron :

$E_1 = 0$

$\psi_1 = a_1\phi_2 + a_2\phi_{13} + a_3\phi_{15} + a_4\phi_{10} + a_5\phi_{20}$

$-a_6\phi_{10} - a_7\phi_{14} - a_8\phi_{16}$

$a_1 + a_2 + a_5 = a_7, a_3 + a_4 = a_6 + a_8, a_1 + a_3 + a_5 = a_8$

$a_1 + a_2 + a_4 = a_8, a_2 + a_4 = a_6 + a_7, a_3 + a_5 = a_6 + a_7$

$E_2 = 0$

$\psi_2 = a_1\phi_2 + a_2\phi_{10} + a_3\phi_{14} + a_4\phi_{10} + a_5\phi_{20}$

$-a_6\phi_{13} - a_7\phi_{15} - a_8\phi_{16}$

$a_1 + a_3 + a_5 = a_6, a_2 + a_4 = a_7 + a_8, a_1 + a_5 = a_7 + a_8$

$a_1 + a_4 = a_6 + a_8, a_2 + a_3 + a_4 = a_6, a_2 + a_3 + a_5 = a_7$

$E_3 = 0$

$\psi_3 = a_1\phi_{14} + a_2\phi_{16} + a_3\phi_{19} + a_4\phi_{20}$

$-a_5\phi_2 - a_6\phi_{10} - a_7\phi_{13} - a_8\phi_{15}$

$a_1 + a_4 = a_5 + a_7, a_2 + a_3 = a_6 + a_8, a_1 + a_3 = a_6 + a_7$

$a_1 + a_4 = a_6 + a_8, a_2 + a_4 = a_5 + a_8, a_2 + a_3 = a_5 + a_7$

$E_4 = 0$

$\psi_4 = a_1\phi_{10} + a_2\phi_{13} + a_3\phi_{16} + a_4\phi_{20}$

$-a_5\phi_2 - a_6\phi_{14} - a_7\phi_{15} - a_8\phi_{19}$

$a_1 + a_3 = a_7 + a_8, a_2 + a_4 = a_5 + a_6, a_1 + a_2 = a_6 + a_8$

$a_1 + a_4 = a_6 + a_7, a_2 + a_3 = a_5 + a_8, a_3 + a_4 = a_5 + a_7$

$E_5 = 1.0$

$\psi_5 = a_1(\phi_2 + \phi_{14} + \phi_{13} + \phi_{20} + \phi_{17} + \phi_{12}$

$-\phi_{16} - \phi_{10} - \phi_{19} - \phi_{15} - \phi_{11} - \phi_{18})$

$E_6 = -1.0$

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

The spin configurations are :

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

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

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

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

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

Acknowledgments

The author would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste, where this work was carried out.

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 in Frontiers and borderlines in many particle physics , Varenna Summer School ,Varenna ,Italy (North Holland)

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

Bose I 1988 J.Phys.C :Solid State Physics 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. (N.Y.) 16 407

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

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

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

Shastry B S and Sutherland B 1981 Phys.Rev.Lett. 47 964; Physica B 108 1069

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

Table 1

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	-2.17149
0.7	-2.37755
0.8	-2.58441
0.9	-2.79192
1.0	-3.0

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 degeneracy of the level.

Figure captions

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 $\leq 1/2$.

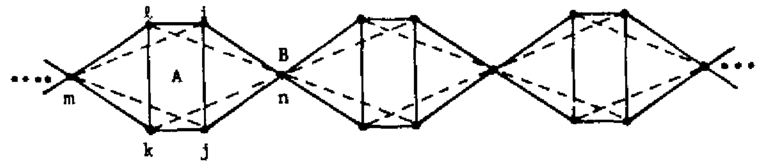

Fig. 1

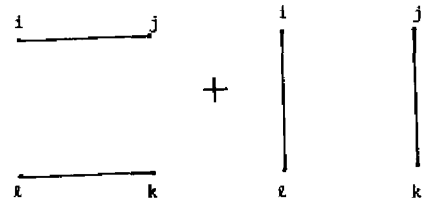

Fig. 2

Stampato in proprio nella tipografia
del Centro Internazionale di Fisica Teorica

INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

IN REPLY PLEASE REFER TO

ERRATA

IC/89/246
2 November 1989

Exact ground and excited states of an antiferromagnetic quantum spin model

Indrani Bose

Page 3 - lines 18 - 23 starting from *Consider the classical* ..... ending at *Now consider the quantum case.* should be omitted.

Page 4 - Eq.(2) Should read: $\psi_A = 1/\sqrt{12}$ .....

Page 6 - Eq.(3) Should read

$$
\begin{aligned}
&< \psi_A|S_1^z S_2^z|\psi_A > = < \psi_A|S_1^z S_4^z|\psi_A > = -1/6 \\
&< \psi_A|S_1^z S_3^z|\psi_A > = 1/12 \\
&< \psi_A|S_1^+ S_2^-|\psi_A > = < \psi_A|S_1^+ S_4^-|\psi_A > = -2/3 \\
&< \psi_A|S_1^+ S_3^-|\psi_A > = 1/3
\end{aligned}
\quad (3)
$$

Page 10 - Table 1 Should read:

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(5)
0.6	−2.2
0.7	−2.4
0.8	−2.6
0.9	−2.8
1.0	−3.0