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LETTER TO THE EDITOR

Two-dimensional spin models with resonating valence bond ground states

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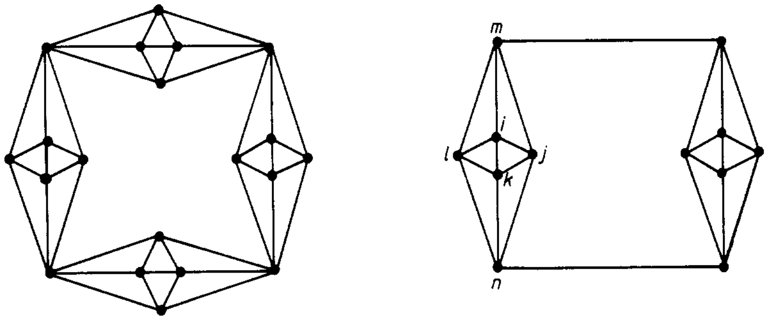
Abstract. Two spin models in two dimensions are constructed for which the exact ground states can be written down in a certain parameter regime of the Hamiltonian. The ground state of the first model is a local resonating valence bond (RVB) state in which not all the spins participate in resonance. The ground state is highly degenerate and there is a gap in the excitation spectrum. The second model is shown to have a ground state which is a quantum spin liquid with all the spins taking part in resonance. The ground state obtained is non-degenerate and there is no gap in the excitation spectrum.

Recently, Bose (1989) has suggested a quasi-one-dimensional spin model for which the local RVB state is the exact ground state in a certain parameter regime of the Hamiltonian. Several excited states can also be constructed exactly. The model consists of a chain of octahedra (instead of 'octahedron' a more correct description which will be used henceforth is a double pyramid with square or rhombic base (DPSB) for which the length of a side of the square base need not be equal to the height of the pyramid). Each DPSB has four basal spins and two vertex spins (see figure 1 for notation). The spins interact through the Hamiltonian

$$H = \sum_{\gamma} (J(S_i \cdot S_j + S_j \cdot S_k + S_k \cdot S_l + S_l \cdot S_i) + \alpha J(S_m + S_n) \cdot (S_i + S_j + S_k + S_l)) \qquad (1)$$

where $\alpha \leqslant 1$, $|S_i| = \frac{1}{2}$ and γ denotes the sum over $N/5$ DPSBs of spins, the number of spins, N, being an integral multiple of five. Also, a periodic boundary condition is assumed. For $\alpha \leqslant \frac{1}{2}$, the ground state spin configuration is as follows: in each basal plane the $S = 0$ spin state is resonating between two valence bond structures and the vertex spins are kept free. The ground state energy is given by $E_g = -2JN/5$. The ground state is called a local RVB state because resonance is confined to the squares. The ground state is highly degenerate, there being $2^{N/5}$ possible configurations. In the $\alpha = 1$ limit, the ground state is not exactly known and the ground state energy E_g satisfies the inequality $-3JN/5 \leqslant E_g \leqslant 2JN/5$. In this letter, we give an improved estimate of the upper bound of E_g and give more details on the chain eigenstates. Next, we generalise the model to two new models in 2D and write down the exact ground states. The ground states are of the RVB type. For $\alpha = 1$, the ground state energy of a single DPSB is $-3J$. The corresponding eigenfunction is a spin singlet which is formed out of two spin triplets, one corresponding to the basal spins and the other formed out of the vertex spins. The spin configuration is



A B

Figure 1. Unit cells for models A and B; i, j, k, l, m, n denote spin sites.

given by

$$\psi_1 = (\uparrow\uparrow\uparrow\downarrow - \uparrow\uparrow\downarrow\uparrow + \uparrow\downarrow\uparrow\uparrow - \downarrow\uparrow\uparrow\uparrow)\downarrow\downarrow + (\uparrow\downarrow\downarrow\downarrow - \downarrow\downarrow\downarrow\uparrow + \downarrow\downarrow\uparrow\downarrow - \downarrow\uparrow\downarrow\downarrow)\uparrow\uparrow + (\downarrow\uparrow\downarrow\uparrow - \uparrow\downarrow\uparrow\downarrow)(\uparrow\downarrow + \downarrow\uparrow). \tag{2}$$

The four-spin configurations in brackets denote the basal spin configurations. One can check that ψ_1 is an exact eigenfunction for all values of α, the eigenvalue being $-J(1 + 2\alpha)$. For $\alpha \leqslant \frac{1}{2}$, the ground state energy of a single DPSB, as already mentioned, is $-2J$, the corresponding eigenstate (say, ψ_2) is also an exact eigenstate for all values of α with the same energy $-2J$. For this state, since the vertex spins are free, the state can be repeated for all the DPSBs in the spin chain whereas in the $\alpha = 1$ limit, the vertex spins are not free in the ground state configuration and one cannot repeat the configuration for the whole DPSB chain. For a single DPSB in the $\alpha = \frac{1}{2}$ limit, the eigenstates ψ_1 and ψ_2 become degenerate and a crossing of energy levels occurs. The eigenstate ψ_1 becomes the ground state for $\alpha > \frac{1}{2}$. In terms of valence bonds, ψ_1 has the structure $\psi_1 = \varphi_3 - \varphi_4 - \varphi_2$ where $\varphi_2 = [12][54][36]$, $\varphi_3 = [16][32][54]$ and $\varphi_4 = [14][56][32]$. The top and bottom vertex spins are 1 and 6 and the basal spins are 2, 3, 4, 5 in clockwise order. The notation $[lm]$ denotes, the singlet $(1/\sqrt{2})(\alpha(l)\beta(m) - \beta(l)\alpha(m))$ where α and β are spin-up and spin-down states, respectively. Now consider again the chain model. In the $\alpha = 1$ limit, the upper bound of the ground state energy as reported in Bose (1989) is $-2JN/5$. This bound can be improved. Consider the chain state which has alternate DPSBs in states ψ_1 and ψ_2 respectively ($N/5$ is even). This is an exact eigenstate with energy $-2.5JN/5$ and so the ground state energy obeys the inequality $-3JN/5 \leqslant E_g \leqslant -2.5JN/5$. An exact solution is yet to be obtained.

We now describe the 2D spin models: models A and B. Figure 1 shows the unit cells of the two models. Both the models obey periodic boundary conditions. Model A consists of DPSB chains in both horizontal (x) and vertical (y) directions on a square network. For $\alpha \leqslant \frac{1}{2}$, the ground state is again a local RVB state, the vertex spins being kept free. The ground state energy $E_g = -2J \times 2N/9$ where N is the total number of spins in the system, $2N/9$ is the total number of square bases and $N/9$ the number of vertex spins (N is a multiple of nine). The ground state is highly degenerate. Again, several excited states can be constructed exactly as in the chain model (Bose 1989). Model B is more interesting. It consists of DPSB chains aligned in the y direction and linear chains of vertex spins aligned in the x direction with the vertex spins interacting with each other through nearest-neighbour (NN) Heisenberg interactions of strength J.

The exact ground state has the following structure in the $\alpha \leqslant \frac{1}{2}$ limit: the square bases are in the resonating state ψ_2. The linear chains of vertex spins are the usual AFM Heisenberg spin chains for which the exact ground state is given by the Bethe *ansatz* (BA, see Majumdar 1985 for a review). The ground state structure cannot be written down explicitly. The ground state is, however, known to be disordered with no staggered magnetisation and power-law decay of the correlation function. The ground state can be expressed as a linear combination of valence bond states, the valence bonds being of all possible lengths. The ground state of model B in the $\alpha \leqslant \frac{1}{2}$ limit is thus a global RVB state with all the spins in the system participating in resonance. The ground state is a quantum spin liquid (QSL), i.e. disordered with power-law decay of the correlation function for the vertex spins and ultra-short range correlation for the spins in the square bases of the DPSBs. To the author's knowledge, model B is the first example of a spin model for which the exact ground state is known to be a QSL. The proof that this state is the ground state is similar to that given for the DPSB chain (Bose 1989). The Hamiltonian is written as a sum over DPSB chain Hamiltonians and linear vertex spin chain Hamiltonians for proceeding with the proof. The ground state energy $E_g = -2JN/5 - (\ln 2 - \frac{1}{4})JN/5$. The first term is contributed by the spins in the square bases. The total number of DPSBs in the system is $N/5$, so there are $N/5$ square bases in all; each of these has a ground state energy $-2J$. There are $N/5$ vertex spins in the system and the second term in E_g is the exact BA ground state energy corresponding to the chains formed by these spins. For a linear chain of spins, the BA ground state has momentum wave vector zero if $M/2$ is even and π if $M/2$ is odd, where M is the number of spins in the chain. We assume that in model B the number of DPSB chains is even so that the number of vertex spins in a linear chain is also even. The ground state thus has momentum wave vector (0, 0).

Let us now consider the excited states. A set of exact excited states can be constructed in the following manner: in the ground state ($\alpha \leqslant \frac{1}{2}$) each square base contributes an energy $-2J$. Exact excited states can be obtained if the spin configuration is

$$\varphi = \tfrac{1}{2}(\uparrow\uparrow\downarrow\downarrow + \downarrow\downarrow\uparrow\uparrow - \uparrow\downarrow\downarrow\uparrow - \downarrow\uparrow\uparrow\downarrow) \qquad (3)$$

in any one (or more) of the square bases of the model. The spin configuration (3) can be written as a linear superposition of nearest-neighbour valence bond configurations, so the interaction terms denoting interaction between the vertex and basal spins give zero when acting on φ. The energy corresponding to φ is zero and the excited state energies for the whole model are given by $E_n = -2J(N/5 - n)$, where n is the number of square bases having spin configuration φ. The excited states are separated from the ground state by a finite amount of energy. In all the excited states, the linear chains of vertex spins are in their ground state. Another set of exact excited states can be constructed by keeping the basal spins in their ground state configuration and assuming one (or more) linear chain of vertex spins to be in an exact excited state. For the NN Heisenberg spin chain, the excitation spectrum is given by the des Cloizeaux and Pearson (DCP, 1962) spectrum, the dispersion relation for which is given by

$$\varepsilon = \pi J |\sin q_x| \qquad (4)$$

where q_x is the momentum wave vector of the excitation with respect to that of the ground state and ε denotes the excitation energy. Consider any one of the linear chains to be in an excited state. If there are L linear chains, any one of the chains may be in the DCP state. By taking a linear combination of such states, one can obtain an excited state of momentum wave vector $(\boldsymbol{q}_x, \boldsymbol{q}_y)$. As is evident from (4), there is no gap in the excitation spectrum at the line (π, q_y) in momentum space. One may construct other exact excited states by considering more than one linear chain to be in an excited state. The 'gaplessness' of the exact excitation spectrum holds for any $L \times M$ lattice provided M is very large (L is the number of linear chains in model B and M the number of spins in a linear chain, i.e. $5LM = N$, the total number of spins in the system). There is no restriction on L as far as the gaplessness of the spectrum is concerned. The ground state of model B ($\alpha \leq \frac{1}{2}$) is non-degenerate and the number of spins per unit cell is five. The Lieb, Schultz and Mattis (LSM, 1961) theorem is then applicable (see also Affleck 1988) and the spectrum should be gapless. However, the construction of the proof of the LSM theorem in 2D assumes that L is odd and also $L \ll M$. We have given an example of an exactly solvable model where the above restriction need not be obeyed. For model A the ground state is degenerate and the LSM theorem is inapplicable.

A possible realisation of the DPSB chain is as follows: in the parent compound La_2CuO_4 of lanthanum-based high-temperature superconductors, consider a particular CuO_2 plane of AFM spins. The next plane of spins is the dual of the first, i.e. the Cu spins in the second plane are located above the centres of the underlying square plaquettes in the first plane. Choose any one of the square plaquettes of four spins in a CuO_2 plane. The plaquette serves as the base of a double pyramid; the vertices of this pyramid are located above and below the centre of the square base. A DPSB chain can be isolated by replacing the surrounding Cu spins by non-magnetic impurity atoms. Similarly one can isolate an array of spins in La_2CuO_4 having the same structure as that in model B. To conclude, we have constructed 2D spin models for which exact ground states and some excited states are known. Model A has a ground state in which not all the spins are participating in resonance. The ground state of model B is a quantum spin liquid and there is no gap in the excitation spectrum. The RVB model of Anderson (1987) and similar other models suggest that high-temperature superconductivity is superconductivity of a spin liquid. The Heisenberg AFM in 2D has LRO in the ground state but the order is fragile and can be destroyed by the introduction of dopants or by inclusion of further-neighbour interactions. In such situations, the ground state is expected to be a QSL. Model B is an example of a spin system for which the exact ground state is a QSL. Models A and B can be generalised to higher dimensions. In fact, one can construct other spin models for which the ground state consists of clusters of spins joined to each other by isolated spins. The isolated spins are free if they do not interact with each other or assume fixed configurations if they form interacting arrays as in model B. The model systems can further be used to study problems like the dynamics of holes in spin systems, such studies being of relevance in the context of high-temperature superconductivity.

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