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LETTER TO THE EDITOR

Construction of spin models with dimer ground states

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Abstract. A method to construct various $s = \frac{1}{2}$ isotropic spin models with exact dimer ground states is proposed. Constructed models are usually of much simpler forms than those produced by the method using Löwdin's projection operators. They include a series of one-dimensional Heisenberg models which consist of linearly decayed exchange interactions and are natural extensions of the Majumdar–Ghosh model. A two-dimensional spin model with four spin interactions is also constructed to have the same spatial symmetry as a simple square lattice.

Quantum spin systems with frustrated interactions have strong fluctuation and the fluctuation causes particular ground states in some cases. The Majumdar–Ghosh model is such a quantum system in one dimension known to have dimer ground states [1–3]. That is, the ground states are doubly degenerate and each of them is exactly a direct product of dimers or singlet pairs of nearest-neighbour spins. A dimer state is purely quantum mechanical and has no correspondent in classical states.

It can be seen that the dimer states are the ground states of the Majumdar–Ghosh model if the Hamiltonian is rewritten as a linear combination of projection operators with positive coefficients [4]. Each of the projection operators consists of three spin operators and projects a state of three spins to the subspace of total spin $\frac{3}{2}$. Each projection operator is positive semidefinite and the lowest eigenvalue is 0. When the Hamiltonian operates on the dimer states, the projection operators in it give the value 0, so that the eigenvalue of the Hamiltonian becomes the lowest.

Klein [4] introduced generalized projection operators to construct other Hamiltonians with dimer ground states. Following this method many Hamiltonians with 4-spin interactions are created and examined [4, 5]. There is also a similar formulation with Löwdin's projection operators [4, 6]. If we simply develop the method to use projection operators consisting of many spins, we have complicated Hamiltonians with many-spin interactions. It is difficult to consider physical meanings of interactions among more than four spins.

In the present work, I propose a new method to construct spin models with exact dimer ground states. This method is a generalization of the above method using Löwdin's projection operators and includes it as a special case. By this method various simple spin models including many Heisenberg models are constructed; in this paper a Heisenberg model means an isotropic spin model with no interactions among more than two spins. This method is independent of the spatial dimension of the lattice.

I present typical Heisenberg spin models in one and two dimensions using this method and show that they actually have dimer ground states; they have non-degenerate, finitely degenerate or infinitely degenerate dimer ground states depending on the choice of the models. Among them there are a series of one-dimensional models with linearly decayed exchange interactions. The ground states are doubly degenerate and the same as those of

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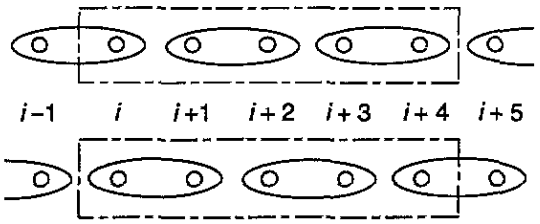


Figure 1. Degenerate dimer ground states for the spin model in (8). Lattice sites are represented by small circles and dimers (short singlet pairs) are by loops. The operation range of a Q_5^1 is also shown by a rectangle of dash-dotted lines.

the Majumdar–Ghosh model. I also present a spin model with 4-spin interactions, which has the complete symmetry of a simple square lattice and degenerate dimer ground states.

First we consider projection operators by examining the Majumdar–Ghosh model. For an N-site periodic chain, the Hamiltonian is written as

$$H = J\sum_{i=1}^{N}(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \tfrac{1}{2}\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2}) \tag{1}$$

where $J > 0$ and $\boldsymbol{S}_i$ is the spin operator at site i. The doubly degenerate dimer ground states are shown in figure 1. The Hamiltonian (1) is rewritten as

$$H = \tfrac{3}{4}J\sum_{i=1}^{N} P_3[i, i+1, i+2] + E_0 \tag{2}$$

with $E_0 = -\frac{3}{8}JN$ [4]. Here the projection operator of three spins at sites, $i, i+1$ and $i+2$, is defined as

$$P_3[i, i+1, i+2] = \tfrac{1}{3}\{(\boldsymbol{S}_i + \boldsymbol{S}_{i+1} + \boldsymbol{S}_{i+2})^2 - \tfrac{1}{2}(\tfrac{1}{2}+1)\} \tag{3}$$

where subscript 3 of P_3 means that it consists of three spin operators. The eigenvalue of P_3 is 0 if $S = \frac{1}{2}$ and 1 if $S = \frac{3}{2}$, where S is the magnitude of the total spin of the three sites. It is easily seen that the operation of each P_3 in (2) on a dimer state gives the lowest value 0 and the ground-state energy is E_0. It has also been proved, by using the form of (2), that there is no ground state except for the dimer states and there is a finite excitation gap in the limit of infinite volume [7]. A variational calculation has been carried out for the first excited state with $S = 1$ [8], although the exact wavefunction has not been found. The variational state gives $\frac{1}{4}J$ for the spin gap and the value is close to $0.236J$ by numerical diagonalization [9, 10].

The projection operator P_3 is extended to Löwdin's projection operators [6]:

$$P_n[i_1, i_2, \ldots, i_n] = \prod_{S=S_{\min}}^{S_{\max}-1} \frac{(\boldsymbol{S}_{i_1} + \boldsymbol{S}_{i_2} + \cdots + \boldsymbol{S}_{i_n})^2 - S(S+1)}{S_{\max}(S_{\max}+1) - S(S+1)} \tag{4}$$

where $S_{\max}$ and $S_{\min}$ are the largest and the smallest values of the total spin S of n sites, $i_1, i_2, \ldots, i_n$. $S_{\min}$ takes value 0 for even n and $\frac{1}{2}$ for odd n. The eigenvalue of P_n is 1 on the eigenstates with $S = S_{\max}$ and 0 otherwise, so that P_n is also positive semidefinite. Hence

we can use P_n with arbitrary n instead of P_3 to construct spin models with dimer ground states. By making linear combinations of P_n's with various positive coefficients, numerous Hamiltonians can be created. Some of them actually have dimer ground states each of which is a direct product of dimers [4]. P_n with $n > 3$ generates many-spin interactions; e.g. $P_5(P_7)$ gives 4-(6-) spin interactions.

In the above extension, only the positive semidefiniteness is effective among properties of the projection operator (4). Therefore it is possible to generalize the method to use various but appropriate positive semidefinite operators instead of (4). The present method is based on the following operator:

$$Q_n^m[i_1, i_2, \ldots, i_n] = \prod_{l=1}^{m} \{(S_{i_1} + S_{i_2} + \cdots + S_{i_n})^2 - (S_{\min} + l - 1)(S_{\min} + l)\} \tag{5}$$

where m is an arbitrary integer in the range of $1 \leqslant m \leqslant S_{\max} - S_{\min}$, and $i_1, i_2, \ldots, i_n$ are arbitrary n sites. This operator Q_n^m is clearly positive semidefinite. When m is chosen as $m = S_{\max} - S_{\min}$, Q_n^m is the same as the projection operator (4) except for a numerical factor. Q_n^m with m less than $S_{\max} - S_{\min}$, however, is not a projection operator; it has more than two eigenvalues. If we use Q_n^m only with small m we can obtain simple spin models.

We now explain the new method by constructing a one-dimensional Heisenberg model, which may be the simplest extension of the Majumdar–Ghosh model. The Hamiltonian we consider here is

$$H = \frac{J}{8} \sum_{i=1}^{N} Q_5^1[i, i+1, i+2, i+3, i+4] + E_0 \tag{6}$$

where $J > 0$ and $E_0 = -\frac{3}{8}JN$. If we find a state that gives 0 by the operation of $Q_5^1[i, \ldots, i+4]$ with any i, the state is the very ground state with the ground-state energy E_0 because of the positive semidefiniteness of Q_5^1. When $Q_5^1[i, \ldots, i+4]$ is operated on each of two dimer states in figure 1, it works only spins on sites i to $i+4$ which are enclosed by a rectangle of dash-dotted lines. Since the five sites include two dimers, the total spin of the five sites takes the lowest value $S_{\min} = \frac{1}{2}$ so that the operation of Q_5^1 gives 0. Thus it is shown that the dimer states in figure 1 are actually the ground states. When Q_5^1 is expanded, equation (6) reduces to

$$H = J \sum_{i=1}^{N} (S_i \cdot S_{i+1} + \tfrac{3}{4} S_i \cdot S_{i+2} + \tfrac{1}{2} S_i \cdot S_{i+3} + \tfrac{1}{4} S_i \cdot S_{i+4}) \tag{7}$$

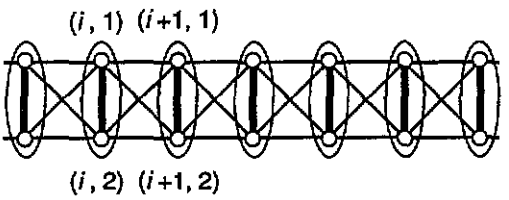
where constant terms have been cancelled out. Thus we have constructed a new spin model of a simple form with the exact dimer ground states. Note that the exchange interaction decays linearly and becomes 0 at the fifth neighbour site.

A similar argument stands if we use $Q_n^1[i, \ldots, i+n-1]$ with an arbitrary odd integer n instead of $Q_5^1[i, \ldots, i+4]$ in (6). Then the Hamiltonian is written and expanded as

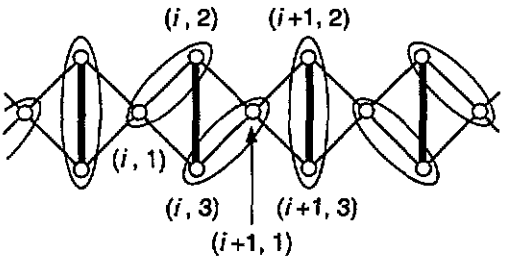
$$H^{(n)} = \frac{J}{2(n-1)} \sum_{i=1}^{N} Q_n^1[i, i+1, \ldots, i+n-1] + E_0 \tag{8a}$$

$$= \sum_{i=1}^{N} \sum_{k=1}^{n-1} J_k^{(n)} S_i \cdot S_{i+k} \tag{8b}$$

with $J_k^{(n)} = J(n-k)/(n-1)$. The exchange energy is $J_1^{(n)} = J$ for a nearest-neighbour spin ($k = 1$), decays linearly with increasing distance and vanishes for $k \geqslant n$ (the lattice constant is unity). This model reduces to the Majumdar–Ghosh model for $n = 3$ and to the model in (7) for $n = 5$. The ground states are the same dimer states (figure 1) as those of the Majumdar–Ghosh model again. It is noticed that the ground-state energy, $E_0 = -\frac{3}{8}JN$, is independent of n.



(a)



(b)

Figure 2. Lattices for one-dimensional decorated Hamiltonians consisting of operators Q_3^1's and dimers in their ground states. A bold (normal) solid line represents an exchange interaction of strength $2J$ (J), and a loop represents a dimer.

In general $Q_n^1[i_1, i_2, \ldots, i_n]$'s generate only two-spin interactions and then create Heisenberg Hamiltonians. Note that $i_1, i_2, \ldots, i_n$, need not be successive sites and can be chosen arbitrarily. I present two examples of Hamiltonians consisting of Q_3^1's in one-dimensional decorated lattices. Although Q_3^1 is equal to $3P_3$ and can also be treated in the old scheme using projection operators, it is instructive to examine the following examples. The first example is a Heisenberg model on a ladder lattice, in which the first and the second chains are connected by exchange interactions, as shown in figure 2(*a*). The exchange energy between spins connected by a bold solid line is $2J$ and that by a normal solid line is J. In terms of Q_3^1's the Hamiltonian is rewritten as

$$H = \frac{J}{4}\sum_{i=1}^{N}\sum_{\alpha=1}^{2}\{Q_3^1[(i,1),(i,2),(i+1,\alpha)] + Q_3^1[(i,1),(i,2),(i-1,\alpha)]\} + E_0 \qquad (9)$$

where $J > 0$ and $E_0 = -(J/4)2S_{\min}(S_{\min}+1)4N = -\frac{3}{2}JN$ for the $2N$-site (N-unit cell) system. Note that each Q_3^1 corresponds to a triangle of three sites in the lattice; e.g.

$Q_3^1[(i,1),(i,2),(i+1,1)]$ represents a triangle where sites $(i,1)$, $(i,2)$ and $(i+1,1)$ are three apices. A bold solid line and a normal solid line in figure 2(a) belong to four and two triangles, respectively, so that the exchange energy of the former is twice as large as that of the latter. Dimers in the ground state are shown by loops in figure 2(a). Each triangle includes one dimer in the dimer configuration so that the corresponding Q_3^1 gives value 0 and the ground-state energy becomes E_0. Since there is no dimer configuration equivalent to that in figure 2(a), the ground state may be unique.

The second example of a decorated one-dimensional model is defined on the lattice shown in figure 2(b). The exchange energy between spins connected by a bold solid line is $2J$ and that by a normal solid line is J. In terms of Q_3^1's, the Hamiltonian is rewritten as

$$H = \frac{J}{2}\sum_{i=1}^{N}[Q_3^1[(i,1),(i,2),(i,3)] + Q_3^1[(i+1,1),(i,2),(i,3)]] + E_0 \quad (10)$$

where $J > 0$ and $E_0 = -(J/2)2S_{\min}(S_{\min}+1)2N = -\frac{3}{2}JN$ for the $3N$-site (N-unit cell) system. Dimers in a ground state are shown by loops in figure 2(b). Like the previous model in (9), each triangle corresponding to Q_3^1 includes one dimer so that Q_3^1's give eigenvalue 0 and H gives the ground-state energy E_0. Unlike the previous model, there are many equivalent dimer configurations in this case. In fact we have another ground state if we replace two dimers, $(i,1)-(i,2)$ and $(i,3)-(i+1,1)$, in figure 2(b) by $(i,1)-(i,3)$ and $(i,2)-(i+1,1)$. Thus the number of degeneracy of the ground states is $2\times 2^{N/2}$ under the periodic boundary condition.

In two dimensions, the method works essentially in the same way. I present an example in which a Heisenberg Hamiltonian written in terms of Q_5^1 has degenerate ground states. On an $N\times N$ lattice (N: an even integer) with the periodic boundary condition, the Hamiltonian is given as

$$H = \frac{J}{2}\sum_{i=1}^{N/2}\sum_{j=1}^{N/2}\sum_{k} Q_5^1[(2i,2j),(2i+1,2j),(2i,2j+1),(2i+1,2j+1),k] + E_0 \quad (11)$$

where $J > 0$ and $E_0 = -4S_{\min}(S_{\min}+1)N^2J = -3JN^2$. k is summed over $(2j-1,2)$, $(2i,2j-1)$, $(2i+1,2j-1)$, $(2i+2,2j)$, $(2i+2,2j+1)$, $(2i+1,2j+2)$, $(2i,2j+2)$ and $(2i-1,2j+1)$.

The lattice is shown in figure 3, where the dash-dotted loop encloses a set of spins contributing a typical Q_5^1. After Q_5^1's are expanded and constant terms are cancelled out, the Hamiltonian appears in the form of $H = \sum_{ij} J_{ij}S_i\cdot S_j$. Non-zero exchange interactions are shown in figure 3; they are $8J$ for a bold solid line, $2J$ for a normal solid line and J for a dashed line. A ground state is obtained if we place two dimers on each unit of four sites connected by bold solid lines. As shown in the bottom of figure 3, there are two ways to place dimers (loops in the figure) for each unit so that we have $2^{N^2/4}$-fold degeneracy.

Here we refer to two-dimensional spin models which can be written in terms of Q_3^1's and have already been found. One of them has been introduced by Shastry and Sutherland [11]. The Hamiltonian defines a square lattice with partially selected next-nearest-neighbour exchange interactions as well as all nearest-neighbour exchange interactions. The ground state consists of dimers on the next-nearest-neighbour bonds and may be unique since there is no other equivalent dimer configuration. Another model has been introduced by Bose and Mitra [12]. The Hamiltonian is invariant under a translation of double lattice spacings and has a non-degenerate dimer ground state. This Hamiltonian is given in a linear combination of operators, $(S_i+S_j+S_k)^2$'s, which are essentially the same as Q_3^1's.

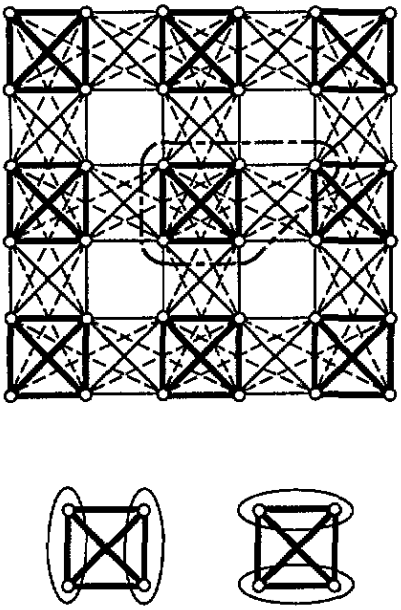


Figure 3. A two-dimensional lattice for Hamiltonians in terms of operators Q_5^1's. A bold solid line corresponds to $8J$, a normal solid line to $2J$ and a dashed line to J. In the bottom, two dimer configurations in a unit of the lattice is shown, where dimers are represented by loops. A ground state is given by placing any one of two configurations for each unit.

It is interesting to construct a two-dimensional spin model that has dimer ground states and holds the full symmetry of a simple square lattice. As far as I have examined, any Heisenberg model that has a dimer ground state is not invariant under a translation of a single lattice spacing and a rotation of $\pi/2$. However, if we take 4-spin interactions into account we can construct a model with the full symmetry. The model is written as

$$H = J\sum_{i=1}^{N}\sum_{j=1}^{N} Q_9^2[\{(i+\rho, j+\lambda)|\rho = 0, 1, 2; \lambda = 0, 1, 2\}] \tag{12a}$$

$$Q_9^2[\ldots] = \{S^2(i,j) - \tfrac{1}{2}(\tfrac{1}{2}+1)\}\{S^2(i,j) - \tfrac{3}{2}(\tfrac{3}{2}+1)\} \tag{12b}$$

$$S(i,j) = \sum_{\rho=0}^{2}\sum_{\lambda=0}^{2} S_{(i+\rho, j+\lambda)}. \tag{12c}$$

where $J > 0$. Each of operators Q_9^2's consists of nine spin operators in a 3×3 regime of the lattice. This Hamiltonian has eight degenerate dimer ground states in the infinite volume limit, as shown in figure 4. It is easily confirmed that every 3×3 regime includes three dimers in any of the dimer ground states and Q_9^2's give the eigenvalue 0.

We have discussed only the case that the spin magnitude is $\frac{1}{2}$ and demonstrated the new construction of spin models with dimer ground states. The construction is also applicable to isotropic spin models of spin magnitude 1 and of larger magnitudes, if we decompose each spin into spins of magnitude $\frac{1}{2}$ and apply the present method to the $\frac{1}{2}$-spins. Affleck *et al* [7, 13] first performed this decomposition and used projection operators like (3) to

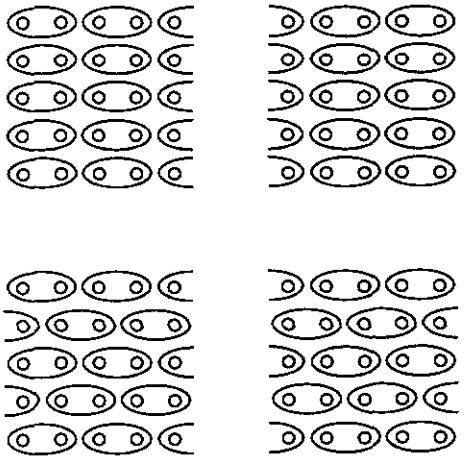


Figure 4. Four of the eight ground states of (12). The figures of the other four ground states are given by rotating them by $\pi/2$.

explain the Haldane gap [14] of the one-dimensional spin-1 Heisenberg system. In the present method we can replace their projection operators by positive semidefinite operators like (5) again. The method of Affleck *et al* is also extended differently to include anisotropy [15, 16]. According to the anisotropy, the ground states are deviated from the simple dimer (valence-bond-solid) state, but they are found exactly and systematically. Here positive semidefinite operators different from (5) are used.

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