Exact ground state of a class of quantum spin systems

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We present some exact results for the ground-state wave function and the energy of disordered quantum-mechanical spin systems in any dimensions. The system contains all nearest- and some of the next-nearest-neighbor interactions. The solution is also available for some range of anisotropy. In all the cases the ground-state wave function is insensitive to the disorder.

A number of models of interest in statistical mechanics, field theory, and many-body problems are related to quantum spin systems. Among them, besides the well-known integrable models, a few examples of quantum spin systems in the thermodynamic limit have been discovered whose ground-state wave function and energy can be found exactly. The first class of these models,[1] called valence-bond states (VBS), was obtained for a lattice with coordination number z and where the spin per site is equal to $z/2$. The interactions are the projection on the highest possible total spin of two neighboring spins. The second class of an exactly solvable ground state is an elaboration based on the original observation of Majumdar and coworkers,[2] and extended by Shastry and Sutherland.[3,4] The Majumdar system consists of a linear spin-$\frac{1}{2}$ chain Heisenberg antiferromagnet, with all nearest-neighbor and next-nearest-neighbor interactions included. In the special case where the next-nearest-neighbor coupling is half as strong as the nearest-neighbor one, the Hamiltonian can be written in the following form:

$$H=\frac{J}{2}\sum_{i=1}^{2N}(S_i+S_{i+1}+S_{i+2})^2 , \tag{1}$$

where J is the strength of the nearest-neighbor interactions, $2N$ is the total number of spins and we assume periodic boundary conditions. One can verify that there are two linearly independent ground states given by

$$|\psi_1\rangle=[1,2][3,4]\cdots[2N-1,2N] ,$$

and

$$|\psi_2\rangle=[2N,1][2,3]\cdots[2N-2,2N-1] ,$$

where $[i,j]$ stands for a normalized singlet combination of spin i and j.

Our solution is inspired by the solution of Majumdar.[2] In this paper we extend these results to a random anisotropic quantum spin Heisenberg Hamiltonian, with some range of next-nearest-neighbor interactions in any dimensions. For clarity we concentrate mainly on the one-dimensional (1D) case.

The system we consider is a linear chain of $2N$ spins, described by the Hamiltonian

$$H=\sum_{1\le i\le N} h_{2i-1,2i}+h_{2i,2i+1}+h_{2i-1,2i+1} , \tag{2}$$

where periodic boundary conditions are imposed, so that $S_{2N+k}=S_k$. The two-spin Hamiltonian h_{ij} is

$$h_{ij}=J_{ij}^x S_i^x S_j^x+J_{ij}^y S_i^y S_j^y+J_{ij}^z S_i^z S_j^z , \tag{3}$$

where we take $J_{2i-1,2i}^{\alpha}=K^{\alpha}$ and $J_{2i,2i+1}^{\alpha}=J_{2i-1,2i+1}^{\alpha}$ for $i=1,2,\ldots,N$, $\alpha=x,y,z$ (see Fig. 1). This model describes a 1D chain with next-nearest-neighbor operators only between odd spins. The disorder in Eq. (2) is limited by the fact that $J_{2l,2l+1}^{\alpha}=J_{2l-1,2l+1}^{\alpha}$ for $\alpha=x,y,z$. Nevertheless, the model could exhibit frustration through the competition of nearest- and next-nearest-neighbor interactions. Unlike the case where all next-nearest-neighbor interactions are presented, the dilution of the next-nearest-neighbor interactions between even spins gives us the ability to find the ground-state wave function and the energy for some range of disorder and anisotropy.

Consider the state

$$|\psi\rangle=[1,2][3,4][5,6]\cdots[2N-1,2N] , \tag{4}$$

where $[i,j]$ stands for the normalized singlet combination of spins i and j and is given by

$$[i,j]=\frac{1}{\sqrt{2S+1}}\sum_{m=-S}^{S}(-1)^m|S,m\rangle\otimes|S,-m\rangle . \tag{5}$$

It is easy to see that $|\psi\rangle$ is an eigenstate of Eq. (2) by using the relation $(S_k^{\alpha}+S_l^{\alpha})[k,l]=0$ $(\alpha=x,y,z)$[3]. The eigenvalue E_0 is given by

$$E_0=-\frac{N}{3}S(S+1)(K^x+K^y+K^z) . \tag{6}$$

We next show that E_0 saturates a lower bound to Eq. (2), for some appropriate range of disorder, and hence $|\psi\rangle$ is the exact ground-state wave function. Following Refs. 2 and 3 we decompose $H=\sum H_{2i}$, where the sum is over N triangles (see Fig. 1). Each triangle consists of two nearest-neighbor interactions and one next-nearest-

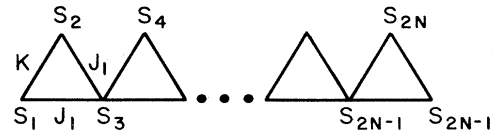

FIG. 1. A system, which is described by Eq. (2), where $\alpha=x,y,z$, S_i are Pauli matrices of spin S and we assume periodic boundary condition $S_{2N+1}=S_1$.

neighbor interaction. The Hamiltonian H_{2i} is of the form

$$H_{2i}=h_{2i-1,2i+1}+h_{2i-1,2i}+h_{2i,2i+1}\,, \tag{7}$$

where in a general case

$$\gamma_\alpha K^\alpha_{2i-1,2i}=J^\alpha_{2i,2i+1}=J^\alpha_{2i-1,2i+1}\,, \tag{8}$$

where $\alpha=x,y,z$, and γ_α is a constant depending on α. The Rayleigh-Ritz variational principle based on the observation that the expectation value of the Hamiltonian in any state is always greater than or equal to the ground-state energy. Modification of this variational principle implies[2,3]

$$E_{\rm GS}=\langle\psi_{\rm GS}|\sum_i H_{2i}|\psi_{\rm GS}\rangle\geq\sum E_{2i}\,,$$

where E_{2i} is the ground-state energy of H_{2i}. Therefore, $|\psi\rangle$ is the ground state provided $\gamma_{\min}(\alpha)\leq\gamma_\alpha\leq\gamma_{\max}(\alpha)$. The lower bound $\gamma_{\min}(\alpha)$ and the upper bound $\gamma_{\max}(\alpha)$ depend both on the special form of the anisotropy and on the value of the spin. Let us now concentrate on a few examples.

(a) *Isotropic case* ($J^\alpha=J$, $K^\alpha=K>0$, $\gamma_\alpha=\gamma$, $\alpha=x,y,z$). In such a case the Hamiltonian of each triangle can be written in the following form:

$$H_l=\frac{K}{2}[\gamma S_t^2+(1-\gamma)L^2-S^2_{2i-1}-S^2_{2i}-\gamma S^2_{2i+1}]\,, \tag{9}$$

where $S_t=S_{2i-1}+S_{2i}+S_{2i+1}$ and $L=S_{2i}+S_{2i+1}$. One can find that the lower and the upper bounds for γ as a function of S for $S\geq 1$ are given by

$$-1/S\leq\gamma(S)\leq 1/(S+1)\,, \tag{10}$$

and for $S=\frac{1}{2}$ by $-2\leq\gamma\leq 1$. One can verify these results from Eq. (9), using the observation that the closest energy level to the singlet level is $L=1$ and $S_t=|S-1|$ for $\gamma>0$, and $L=1$ and $S_t=S+1$ for $\gamma<0$.

This result indicates that the system is dimerized to a pair of singlets, even in the presence of ferromagnetic interactions. Moreover, for spin $\frac{1}{2}$, the strength of the ferromagnetic interactions could be twice as strong (in absolute value) as antiferromagnetic interactions. This is a result of the quantum nature of the system, where the energy of the singlet state is three times the energy of the triplet state. The allowed range of the ferromagnetic interactions is a decreasing function of S, which is a result of the fact that $E_{\rm singlet}(S)/E_{\rm triplet}(S)=1+1/S$.

(b) *Spin-$\frac{1}{2}$ anisotropic.* The problem is reduced to a 4×4 matrix which is solved numerically. Results for the case $\gamma_\alpha=\gamma$ and $K^z=K^x=\delta K^y$, for example, are presented in Fig. 2. The range of γ with a dimerized ground state of the form (4) is indicated by the hatched area. The lower bound for γ decreases linearly with δ for $-1<\delta<1$, where the upper bound for $\delta>0.5$ is independent of δ and equal to 1. For $\delta\rightarrow\infty$, one can verify that the lower bound for γ converges to -1.

One can extend this model in several ways: (i) anisotropic case where γ_α depends on α; (ii) anisotropy which varies from one triangle to another (in such a case the range of γ_α is a function of the index i); (iii) a quantum chain where $\mathbf{S}^2_{2i}=\mathbf{S}^2_{2i+1}=\mathbf{S}^2_q$, where $\mathbf{S}^2_q=q(q+1)$ is a random spin value which depends on the site index i; (iv)

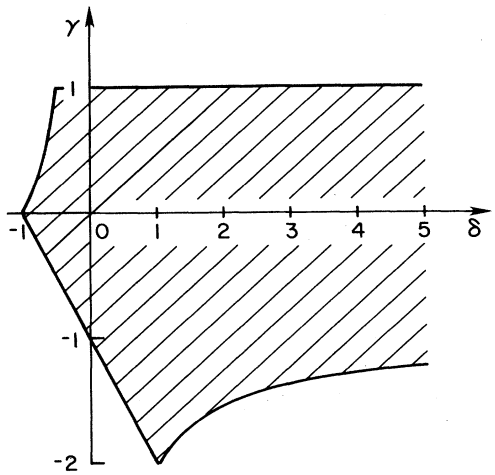

FIG. 2. Anisotropic case with $K^z=K^x=\delta K^y$. $\gamma_\alpha=\gamma$ is defined in Eq. (6). The hatched area indicates the range of dimerized ground state.

some particular cases, where parts of the chain contain only next-nearest-neighbor interactions between the odd spins and the rest of the chain contains all next-nearest-neighbor interactions. For all the above-mentioned cases, one can find lower and upper bounds for γ_α, under which the ground state is dimerized. These results are due to the fact that any triangle which consists of a strong enough antiferromagnetic bond with remaining two bonds equal, is dimerized in the ground state along the strongest bond. The third spin is free to be up or down, and will be fixed by the adjacent part of the system. Since the ground-state energy of a single triangle is proportional to the strongest bond, we can choose a rescaling of this bond so that the ground-state energy will agree with the rest of the system.

Generalization of the above-mentioned results to 2D systems is straightforward. For example, a square lattice with some equal additional diagonal interactions[3] of the form $K^\alpha_{2i,2j;2i+1,2j+1}$ and $K^\alpha_{2i+1,2j;2i+2,2j-1}$ where $\alpha=x,y,z$ (see Fig. 3). In this case each next-nearest-neighbor interaction with $2K^\alpha$ strength belongs to two

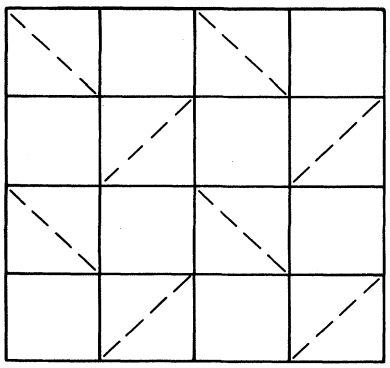

FIG. 3. A 2D square lattice, where the additional diagonal bonds (dashed bonds) indicates the dimerized bonds.

different triangles. On the other hand, each nearest-neighbor interaction belongs to only one triangle. Hence, one can decompose again the Hamiltonian as a sum of triangles, each one of them consists of two nearest-neighbor interactions and one diagonal bond equal to K^a. Therefore, the range of randomness under which the ground state is dimerized along the diagonal bonds is the same as for a 1D system with strongest antiferromagnetic bonds equal to K^a. Generalization of this picture to 3D systems is also straightforward. The simplest case is a bond *dilution* cubic lattice with some additional next-nearest-neighbor interactions. The lattice obeys the constraints that each nearest-neighbor interaction belongs to only one triangle, and each next-nearest-neighbor interaction belongs to two triangles. One can easily verify that there are many ways to construct such a system, and hence, the range of the randomness is the same as for the 2D system. One can generalize this picture again to include systems where the strength of a next-nearest-neighbor interaction belongs to l triangles is $K^a l$.

The results for the above-mentioned systems also show that the ground state is insensitive to the presence of up to a $\frac{2}{3}$ fraction of ferromagnetic interactions, but is sensitive to the presence of any small fraction of strong ferromagnetic interactions. Therefore, these results indicate that in general quantum spin systems the concentration of the ferromagnetic (antiferromagnetic) interactions cannot be rescaled by their strengths.[5]

In all the above-mentioned cases the Hamiltonian (2) does not have a translational invariance, and the ground state is not degenerated for any finite systems. There are some 1D cases where the existence of an energy gap has been proven in the thermodynamic limit. For example, the Majumdar model which has a translationally invariant Hamiltonian with a continuous symmetry but has a gap in the energy spectrum.[1] In this model, however, the ground state is degenerated and breaks the translational symmetry. The VBS solution is an example to a system with continuous symmetry, exponentially decaying correlation function, a unique ground state, and an energy gap.[1,6] On the other hand, the uniform spin-$\frac{1}{2}$ antiferromagnetic chain has been proven to be gapless. The general question of the existence of an energy gap in 1D quantum spin systems and the dependence of the energy gap on the randomness, the distribution of the weakest bonds, and the anisotropy in the system is still an open question.

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