

Generalized Shastry-Sutherland models in three and higher dimensions

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We construct Heisenberg antiferromagnetic models in arbitrary dimensions that have isotropic valence-bond crystals (VBC's) as their exact ground states. The $d=2$ model is the Shastry-Sutherland model. In the three-dimensional case we show that it is possible to have a lattice structure, analogous to that of $\text{SrCu}_2(\text{BO}_3)_2$, where the stronger bonds are associated with shorter bond lengths. A dimer mean-field theory becomes exact at $d \rightarrow \infty$ and a systematic $1/d$ expansion can be developed about it. We study the Néel-VBC transition at large d and find that the transition is first order in even but second order in odd dimensions.

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Recently there has been a renewed interest in the two-dimensional (2D) Shastry-Sutherland model (SSM) (Ref. 1), owing to its physical realization in $\text{SrCu}_2(\text{BO}_3)_2$.^{2,3} The model has an exactly solvable ground state. There exists some generalized antiferromagnetic Hamiltonians with exact ground states.⁴⁻⁷

The SSM was initially constructed as a 2D generalization of the 1D Majumdar-Ghosh model.⁸ Both models have a valence-bond crystal (VBC) as the exact ground state. Other such models, including a three-dimensional one,⁹ have since been constructed.

All the above-mentioned models can be thought of as special cases of the class of models which we will define below and refer to as generalized Majumdar-Ghosh models (GMGM's) (see Fig. 1). Consider Hamiltonians of the form

$$H = \sum_n J_n h_n, \quad (1)$$

where the sum is over all possible triangles formed by the sites of the lattice, J_n 's are arbitrary positive semidefinite couplings, and h_n are given by

$$h_n = \mathbf{S}(\mathbf{r}_i) \cdot \mathbf{S}(\mathbf{r}_j) + \mathbf{S}(\mathbf{r}_j) \cdot \mathbf{S}(\mathbf{r}_k) + \mathbf{S}(\mathbf{r}_k) \cdot \mathbf{S}(\mathbf{r}_i). \quad (2)$$

Here $\mathbf{S}(\mathbf{r}_i)$, $\mathbf{S}(\mathbf{r}_j)$, and $\mathbf{S}(\mathbf{r}_k)$ are the spins at sites \mathbf{r}_i , \mathbf{r}_j , and \mathbf{r}_k , respectively, and n labels the triangle formed by them. A particular \mathbf{r}_i can be a part of more than one h_n .

It was noted in Ref. 1 that if, in the triangle corresponding to h_n , two of the spins are forming a singlet, then the state will be a ground state of h_n . It was also pointed out that h_n could be more general than given above. It could be spin anisotropic, the three terms could have different coefficients and the spin could be arbitrary. In suitable parameter ranges the dimer state will remain the ground state.^{1,10} Thus, if it is possible to cover the lattice with dimers in such a way that each of the triangles that appear in H with a nonzero coupling contains a dimer, then the state with singlets on all the dimers will be a simultaneous ground state of all h_n and hence that of H .

The problem of constructing GMGM's then reduces to the purely geometric one of assigning the nonzero couplings to the triangles such that a dimer covering of the above type is possible. We will now give a class of solutions to this prob-

lem which naturally generalizes the SSM to arbitrary dimensions (see Fig. 2). For simplicity, we will work with h_n as in Eq. (2) and with $s=1/2$.

We will first construct the 3D model and then generalize to arbitrary dimensions. We first set up the VBC and then build the Hamiltonian around it. We take a simple cubic lattice and choose the dimers to lie along the body diagonals. The body diagonals are assigned as follows. The sites are denoted by $\mathbf{x} = \sum_{\mu=1}^3 x_{\mu} \hat{\mathbf{e}}_{\mu}$. Here x_{μ} 's take integer values and $\hat{\mathbf{e}}_{\mu}$ are three orthogonal unit vectors. The spin $\mathbf{S}(\mathbf{x})$ is paired to the spin $\mathbf{S}(\mathbf{y}(\mathbf{x}))$ where

$$\mathbf{y}(\mathbf{x}) = \mathbf{x} + \mathbf{D}(\mathbf{x}), \quad (3)$$

$$\mathbf{D}(\mathbf{x}) = \sum_{\mu=1}^3 (-1)^{x_{\mu}+1} \hat{\mathbf{e}}_{\mu}, \quad (4)$$

where we define $x_{3+1} \equiv x_1$. Two such body diagonals are shown in Fig. 3.

Note that $\mathbf{D}(\mathbf{y}) = -\mathbf{D}(\mathbf{x})$ as it should be, since if $\mathbf{S}(\mathbf{x})$ is paired with $\mathbf{S}(\mathbf{y})$, then $\mathbf{S}(\mathbf{y})$ should be paired with $\mathbf{S}(\mathbf{x})$. All four body diagonal directions occur in equal numbers and the VBC has cubic rotational symmetry. It is not parity invariant, the other parity choice being given by replacing $(-1)^{x_{\mu}+1}$ by $(-1)^{x_{\mu}-1}$ in Eq. (4).

We now choose the triangles with nonzero couplings as follows. Equation (4) uniquely associates a body diagonal and hence a unit cube with every dimer, (\mathbf{x}, \mathbf{y}) . We give nonzero couplings to the six triangles formed by these two sites and each of the other six sites that belong to the cube as illustrated in Fig. 4. Thus every such triangle has one edge, one face diagonal, and the body diagonal containing the dimer. This construction ensures that every triangle has one

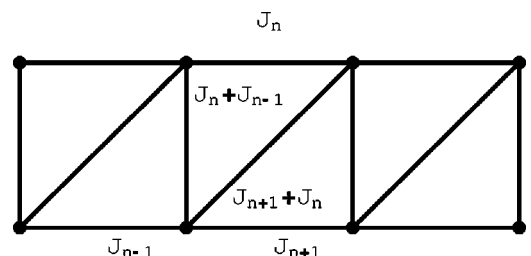


FIG. 1. A generalized Majumdar-Ghosh chain.

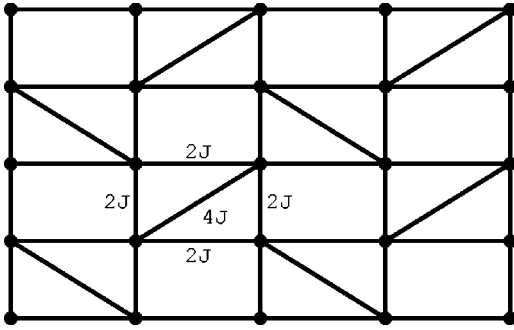


FIG. 2. Shastry-Sutherland model.

dimer (along the body diagonal) and hence is the exact ground state of Hamiltonians of the form given in Eq. (1). The Hamiltonian can be explicitly written as

$$H = \sum_{\mathbf{x}} \sum_{\mu=1}^3 J(\mathbf{x}, \mu) h(\mathbf{x}, \mu), \quad (5)$$

where

$$h(\mathbf{x}, \mu) = \mathbf{S}(\mathbf{x}) \cdot \mathbf{S}(\mathbf{z}(\mathbf{x}, \mu)) + \mathbf{S}(\mathbf{z}(\mathbf{x}, \mu)) \cdot \mathbf{S}(\mathbf{y}) + \mathbf{S}(\mathbf{y}) \cdot \mathbf{S}(\mathbf{x}), \quad (6)$$

$$\mathbf{z}(\mathbf{x}, \mu) = \mathbf{x} + (-1)^{x_{\mu}+1} \hat{\mathbf{e}}_{\mu}. \quad (7)$$

Here $\mathbf{z}(\mathbf{x}, \mu)$ and \mathbf{x} form the three edges emanating from \mathbf{x} in the direction of the body diagonal $\mathbf{D}(\mathbf{x})$ and \mathbf{y} is given by Eq. (3). Here $J(\mathbf{x}, \mu)$ is the coupling associated with the triangle formed by \mathbf{x} , $\mathbf{y}(\mathbf{x})$, and $\mathbf{z}(\mathbf{x}, \mu)$.

Consider the simplest case when all the couplings are equal: i.e., $J(\mathbf{x}, \mu) = J$. The triangle corresponding to $h(\mathbf{x}, \mu)$ contributes a strength J to the edge it contains. Each edge is contained in exactly one triangle. Thus all edges have bond strengths J . Each triangle contributes a strength J to the face diagonal that it contains. Half the face diagonals are con-

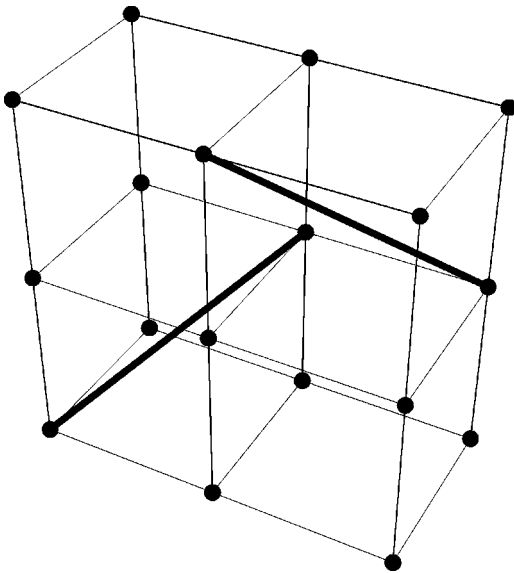


FIG. 3. The 3D lattice containing 18 sites, depicting the diagonals along which dimers are formed.

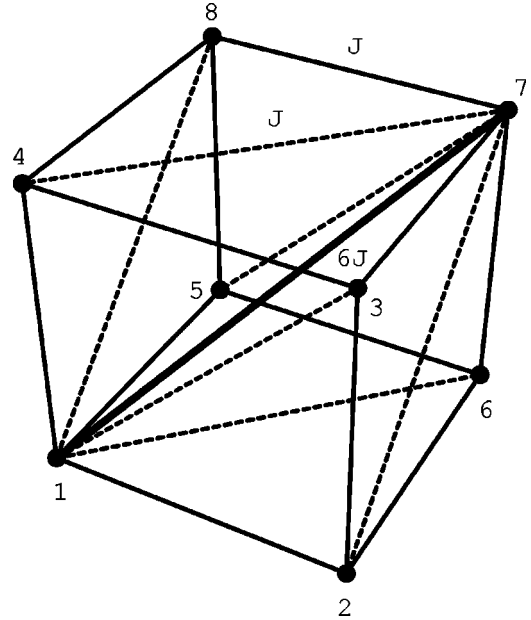


FIG. 4. A cube containing diagonal bond. All bonds are shown.

tained in exactly one triangle each, and the other half are not contained in any triangle. Thus half the face diagonals have bond strength J and the others have no bonds. Figure 4 illustrates the situation. Finally, each triangle contributes J to the body diagonal. Half the body diagonals are contained in six triangles each and hence have bond strengths $6J$ and the other half have no bonds. See Fig. 3.

The generalization to higher dimensions, $d=4,5, \dots$, is straightforward. Simply replace 3 by d in all formulas from Eq. (3) to Eq. (7). All the 2^{d-1} body diagonal directions occur in equal numbers in the d -dimensional VBC. The model is a simple hypercubic lattice with bonds of strength J along all the edges and along one of the face diagonals of each $(d-1)$ -dimensional face. There are also bonds of strength $2dJ$ along one of the body diagonals of half the hypercubes. The construction ensures that the VBC is the exact ground state of the model.

It can be seen that the model reduces to the SSM at $d=2$, shown in Fig. 2. The diagonals are given by Eq. (3). The strength of the bonds along the diagonals is $4J$. Here $d=2$ is a special case in that the $(d-1)$ -dimensional face diagonals are also the edges. Thus the strength along the edges is $2J$; i.e., the strength of edge bonds is half that of the diagonal ones. Thus we have recovered the 2D SSM.

Now we come back to the $d=3$ case. As it stands, it is not very physically realistic since the stronger bonds are between spins further apart. The same is true in the case of the 2D model. However, the structure of magnetic ions in $\text{SrCu}_2(\text{BO}_3)_2$ can be obtained from the original theoretical lattice by moving the sites along the diagonals that have bonds. The squares containing the diagonals deform to rhombi and the body diagonal containing the dimer becomes shorter than the edges. As we will see, the procedure generalizes to 3D and we can obtain an analogous structure where the stronger bonds have shorter bond lengths.

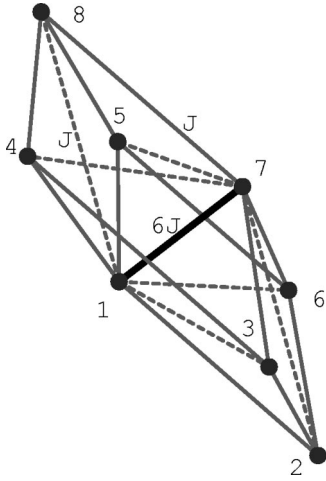


FIG. 5. A deformed cube. Now the strongest bond is between nearest-neighbor sites.

We move all sites along the body diagonals with nonzero bond strengths. The new sites are then

$$\mathbf{R}(\mathbf{x}) = \mathbf{x} + \frac{s}{2}\mathbf{D}(\mathbf{x}), \quad (8)$$

where s is a parameter and $\mathbf{D}(\mathbf{x})$ is given by Eq. (4). The cube shown in Fig. 4 deforms to the rhombohedron shown in Fig. 5. Before the deformation the sites formed a simple cubic lattice. The Hamiltonian was, however, only symmetric under translations by two units. After deformation, the lattice periodicity is also halved. It remains a cubic lattice but with eight sites in a unit cell.

The lengths of the edges, face diagonals, and body diagonals can be computed and are plotted as functions of s in Fig. 6. As we can see, for s more than around 0.7 or so, the edges and face diagonal, with bonds become almost equal in length, are longer than the body diagonal with the bond and shorter than the other face diagonals and body diagonals. When $s=1$ the body diagonal becomes of zero length. The

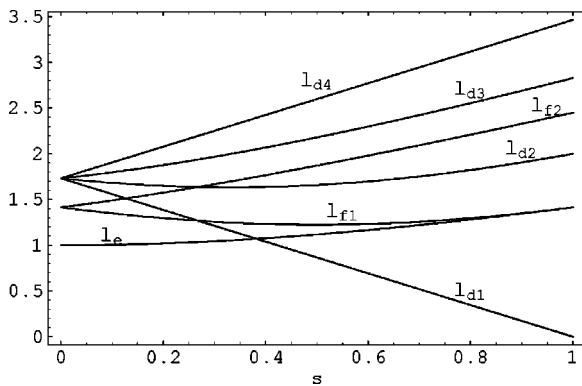


FIG. 6. The various bond lengths as functions of s . Here l_e is the length of the edges, l_{f1} that of the face diagonals containing bond, and l_{f2} corresponds to face diagonals without bonds. l_{d1} is the length of the diagonals along which dimers are formed, and l_{d2} , l_{d3} and l_{d4} correspond to body diagonals without bonds.

rhombohedron is then squashed into a hexagon lying in the plane orthogonal to the body diagonal.

We will now examine the models away from the exact ground-state point at $d \rightarrow \infty$. We put the bond strengths along the body diagonals equal to $dJ_D/2$, along edges equal to $J_E/2$, and along the face diagonals to $J_F/2$. Actually, the VBC is an exact eigenstate when $J_E = J_F = J'$ for all J_D .¹ As we have shown, it is the ground state when $J' \leq 0.5J_D$. However, the ground state is Néel ordered for $J_F = 0 = J_D$. So there will be a phase transition somewhere. The location and nature of the transition at $d=2$ have been topics of much activity.^{3,11-15}

Since the VBC is the exact ground state in some parameter range for all d , it is clear that mean-field theory in terms of the spin variables fails even as $d \rightarrow \infty$. This is because one of the bond strengths grows as d and so the interactions cannot be approximated by an average field. However, if we take the dimers—i.e. the two-spin systems—on the body diagonals to be the basic units, then each dimer interacts with $\sim d$ of the dimers around it with bonds of strength ~ 1 . Thus the mean-field theory in terms of the dimer variables is exact at $d \rightarrow \infty$ in this class of models. Perturbation theory around the mean-field Hamiltonian then yields a systematic $1/d$ expansion for the fluctuations. We will now use this mean-field theory to explore the physics at large d .

We label the spins as $\mathbf{S}_{I\alpha}$, where I labels the positions of the centers of the dimers and $\alpha = 1, 2$ label the two spins that form the dimer. The Hamiltonian can be written as

$$H = \sum_I \frac{dJ_D}{4} (\mathbf{S}_{I1} + \mathbf{S}_{I2})^2 + \frac{1}{2} \sum_{I\alpha, J\beta} J_{I\alpha, J\beta} \mathbf{S}_{I\alpha} \cdot \mathbf{S}_{J\beta}, \quad (9)$$

where $J_{I\alpha, J\beta}$ denote the edge and face diagonal bonds. The mean-field Hamiltonian is

$$H_{MF} = \sum_I \frac{dJ_D}{4} (\mathbf{S}_{I1} + \mathbf{S}_{I2})^2 + \sum_{I\alpha, J\beta} J_{I\alpha, J\beta} \mathbf{b}_{I\alpha} \cdot \mathbf{S}_{J\beta} - \frac{1}{2} \sum_{I\alpha, J\beta} J_{I\alpha, J\beta} \mathbf{b}_{I\alpha} \cdot \mathbf{b}_{J\beta}. \quad (10)$$

The self consistency equations are then

$$\mathbf{b}_{I\alpha} = \langle \mathbf{S}_{I\alpha} \rangle. \quad (11)$$

In different parameter regimes, the VBC as well as a variety of other phases is possible. The $1/d$ expansion, which is valid in all phases, can be used to analyze the phase diagram. In this paper we study the Néel-VBC transition at large d . There is a qualitative difference between odd and even dimensions and we treat them separately.

In even dimensions, the dimer lattice is bipartite and both the sites of a dimer have the same parity. The parity of a dimer is defined to be same as that of its sites. The Néel state is described by the ansatz $\mathbf{b}_{I\alpha} = P_I b \hat{z}$, where P_I is $+1$ on one sublattice and -1 on the other. Then the mean-field Hamiltonian is

$$H_{MF}^{even} = \sum_I \left(\frac{dJ_D}{4} (\mathbf{S}_{I1} + \mathbf{S}_{I2})^2 + P_I 2dJ' b (S_{I1}^z + S_{I2}^z) + 2db^2 J' \right), \quad (12)$$

where $J' \equiv (J_E + J_F)/2$. For all values of $\alpha \equiv J'/J_D$, all the dimers forming singlets—i.e., the VBC—is a mean-field solution with $b=0$. The state has energy 0. When $\alpha > 1/2$, the Néel state is a solution with $b=1/2$ and has energy

$$E^{N\acute{e}el} = \frac{NJ_D}{4} (1 - \alpha), \quad (13)$$

where N is the number of sites. However, this solution has lower energy than the VBC only when $\alpha > 1$. Thus we get a first-order transition at $\alpha=1$ at $d=\infty$.

We have also computed the leading-order correction to the ground-state energy in the Néel phase by treating ($H - H_{MF}$) as a perturbation. We get

$$E^{N\acute{e}el} = \frac{NJ_D}{4} \left[d(1 - \alpha) - \frac{\alpha}{4} \left(\frac{2\alpha}{4\alpha - 1} + \frac{1}{2} \right) \right]. \quad (14)$$

At $d=2$, the transition now occurs at $\alpha \approx 0.8$. More sophisticated calculations at $d=2$ (Refs. 3 and 12) put this number at 0.69. There are indications that the transition may be second order¹¹ or that there may be an intermediate phase.^{13–15}

In odd dimensions the two sites of a dimer are not of the same parity. By convention, we assign $\alpha=1$ for the odd site and $\alpha=2$ for the even site. Then the Néel ansatz is $\mathbf{b}_{I\alpha} = (-1)^{\alpha} b \hat{z}$. The mean-field Hamiltonian is then given by

$$H_{MF}^{odd} = \sum_I \left(\frac{dJ_D}{4} (\mathbf{S}_{I1} + \mathbf{S}_{I2})^2 + 2db\Delta J (S_{I1}^z - S_{I2}^z) + 2db^2\Delta J \right), \quad (15)$$

where $\Delta J \equiv (J_E - J_F)/2$. In the ground state the dimer wave function is given by

$$|\Psi\rangle = \cos \frac{\theta}{2} |0,0\rangle + \sin \frac{\theta}{2} |1,0\rangle, \quad (16)$$

where, in $|l,m\rangle$, l is the total spin and m the z component and $\sin \theta = 2\Delta J |\mathbf{b}| / [\sqrt{J_D^2 + (8\Delta J |\mathbf{b}|)^2}]$. The self-consistency equation (11) reduces to

$$\frac{4\Delta J}{\sqrt{J_D^2 + (8\Delta J |\mathbf{b}|)^2}} = 1. \quad (17)$$

Thus the transition occurs at $J_D = 4\Delta J$. The sublattice magnetization $|\mathbf{b}|$ goes continuously to zero at the transition as $\sim [1 - (J_D/4\Delta J)]^{1/2}$. The interesting thing is that unlike in even dimensions, the transition point depends on the difference of J_E and J_F , so the VBC can occur at relatively low values of J_D .

The different physics in the even and odd dimensions arises from the fact that the two spins on a dimer belong to

the same sublattice in former and on opposite ones in the latter. Consequently, the dimer wave function in the VBC and in the Néel state have the same value of $S^z (=0)$ in odd dimensions whereas in even dimension $S^z=0$ in the VBC but $S^z = \pm 1$ (on odd and even sublattices) in the Néel state. Since the S^z symmetry is unbroken in both the phases, the mean-field Hamiltonian always conserves it. Thus in even dimensions the VBC state cannot smoothly transit to the Néel state and we get a first-order transition whereas in odd dimensions it can and we get a second-order transition.

A remark about the scaling of the diagonal bond is in order here. For the dimer mean-field theory to be valid in both the phases, the diagonal bond has to scale as d , so that d scales out of H_{MF} of Eqs. (12) and (15). But numerically, the critical value of the diagonal bond could be small. For example, in odd dimensions the critical value of diagonal bond is proportional to $\Delta J \equiv [(J_E - J_F)/2]$ and can be made arbitrarily small by suitable choice of J_E and J_F .

The mean-field equations can be solved in the presence of an external magnetic field \mathbf{B} . The mean-field Hamiltonian in the presence of $\mathbf{B} = B\hat{z}$ is given by

$$H_{MF} = \sum_I \frac{dJ_D}{4} (\mathbf{S}_{I1} + \mathbf{S}_{I2})^2 + \sum_{I\alpha, J\beta} J_{I\alpha, J\beta} \mathbf{b}_{I\alpha} \cdot \mathbf{S}_{J\beta} - B \sum_{I\alpha} S_{I\alpha}^z - \frac{1}{2} \sum_{I\alpha, J\beta} J_{I\alpha, J\beta} \mathbf{b}_{I\alpha} \cdot \mathbf{b}_{J\beta}. \quad (18)$$

We concentrate on the regime where the VBC is the ground state, in the absence of \mathbf{B} . A state in which one of the dimers is excited to a triplet with $S^z=1$ and the rest are all in singlets is a self-consistent solution of the mean-field Hamiltonian of Eq. (18), with $\mathbf{b}_{I\alpha}=0$ for those dimers in singlets and $\mathbf{b}_{I\alpha} = \frac{1}{2}\hat{z}$ for the one in triplets. The energy of this state is $dJ_D/2 - B$. Thus as we increase the strength of the magnetic field, when $B > dJ_D/2$, it is energetically favorable to excite as many dimers as possible into triplets pointing along \mathbf{B} , but no two of them being connected by a bond.

In even dimensions, using the fact that the lattice formed by the dimers is bipartite, we shall now show that the maximum fraction of dimers that can be excited without any two of them being connected by a bond is 1/2.

Let us start with isolated dimers with no bonds connecting them. Now we add edge bonds such that every dimer is connected to one and only one other dimer. This can be done as follows. As mentioned before, both the sites of a dimer have the same parity. Each coordinate of the two sites will be differing by $+1$ or -1 . Choose an even dimer and pick out the site with odd x_1 coordinate. Put the edge bond from this site in the positive x_1 direction. This way every even dimer can be uniquely connected to one and only one odd dimer. Suppose these were the only bonds present. Then the configuration that maximizes the number of triplets without two of them being connected is where in every pair of connected dimers one is put in a singlet and the other in a triplet. Now the original model can be obtained by adding the remaining bonds. But in the presence of additional bonds also, each of the pairs that were initially connected can at the most have

one triplet. Thus the maximum fraction of dimers that can be excited without any two of them being connected by a bond is $1/2$. This upper bound can be satisfied by putting triplets on one of the sublattices and singlets on the other. This state is a mean-field solution with $\mathbf{b}_{I\alpha}=0$ for those dimers in singlets and $\mathbf{b}_{I\alpha}=\frac{1}{2}\hat{z}$ for those in triplets.

The state with the remaining singlets also being excited into triplets is also a mean-field solution and has energy $(N/2)(dJ_D/2+dJ'-B)$ above the half-magnetized state. Thus when $B>dJ_D/2+dJ'$ all the remaining dimers are excited into triplets and the system becomes fully magnetized.

When d is odd, the dimer lattice is not bipartite. We still assign parity to dimers as follows. In every dimer one site will be odd and the other even. The parity of the dimer is defined as the parity of the x_1 coordinate of the even site. It can be seen that out of the $4d$ dimers that are connected to a particular dimer only four are of the same parity. Since the critical B , at which it is energetically favorable to have isolated singlets, scales as d , this difference between odd and even dimensions is insignificant at large d .

For both the cases, there is a plateau at $1/2$ magnetization for $dJ_D/2<B<dJ_D/2+dJ'$. At stronger fields, the system is fully magnetized. The $1/2$ plateau corresponds to all the dimers on even sites in the triplet and the ones on the odd sites in the singlet state. At $d=\infty$, the dimers have only nearest-neighbor interactions. Previous work^{3,11,16} indicates

that the other fractions are due to longer-range interactions induced by fluctuations. Thus it is reasonable that only the $1/2$ plateau occurs at $d=\infty$.

To summarize, we have constructed d -dimensional models, $d\geq 2$, which are natural generalizations of the Shastry-Sutherland model. These are Heisenberg antiferromagnets on hypercubic lattices with bonds of strength $dJ_D/2$ along half the body diagonals, $J_E/2$ along all the edges, and $J_F/2$ along half the $(d-1)$ -dimensional face diagonals. They have isotropic VBC's as their exact ground states at $J_D\geq 2J_E=2J_F$. A dimer mean-field theory is exact in the $d\rightarrow\infty$ limit and a $1/d$ expansion can be developed about it. In this limit, the Néel-VBC transition is first order in even dimensions and occurs at $\alpha=1$. When leading-order ($1/d$) corrections are included, the transition shifts to $\alpha=0.8$ at $d=2$. In odd dimensions the transition is second order and occurs at $J_D=4\Delta J$. In the presence of an external magnetic field \mathbf{B} , in both even and odd dimensions, the system has a $1/2$ plateau from $B=dJ_D/2$ to $dJ_D/2+dJ'$ and becomes fully magnetized at higher fields.

At $d=3$, we have shown that it is possible to have a crystal structure where the stronger bonds have shorter bond lengths. Moreover, the mean-field theory indicates that the transition to the VBC phase occurs at relatively small values of J_D . Thus a physical realization of such a system seems feasible.

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