Simplex solid states of SU(N) quantum antiferromagnets

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I define a set of wave functions for SU(N) lattice antiferromagnets, analogous to the valence bond solid states of Affleck *et al.* [Phys. Rev. Lett. **59**, 799 (1987); Commun. Math. Phys. **115**, 477 (1988)], in which the singlets are extended over N-site simplixes. As with the valence bond solids, the new simplex solid (SS) states are extinguished by certain local projection operators, allowing one to construct Hamiltonians with local interactions which render the SS states exact ground states. Using a coherent state representation, I show that the quantum correlations in each SS state are calculable as the finite temperature correlations of an associated classical model with N-spin interactions on the same lattice. In three and higher dimensions, the SS states can spontaneously break SU(N) and exhibit N-sublattice long-ranged order as a function of a discrete parameter which fixes the local representation of SU(N). I analyze this transition using a classical mean field approach. For $N>2$, the ordered state is selected via an "order by disorder" mechanism. As in the Affleck-Kennedy-Lieb-Tasaki case, the bulk representations fractionalize at an edge, and the ground state entropy is proportional to the volume of the boundary.

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I. INTRODUCTION

At the classical level, the thermodynamic properties of ferromagnets and antiferromagnets are quite similar. Both states break certain internal symmetries, whether they be discrete or continuous, and often crystalline point group symmetries as well. Antiferromagnetism holds the interesting possibility of frustration, which can lead to complex behavior even at the classical level.

Quantum mechanics further distinguishes antiferromagnetism as the more interesting of the two phenomena. Quantum fluctuations compete with classical ordering, and many models of quantum antiferromagnetism remain disordered even in their ground states. The reason is that on the local level, quantum antiferromagnets prefer distinctly nonclassical correlations in that they form singlets, which are superpositions of classical states. For an $S=\frac{1}{2}$ Heisenberg antiferromagnet on a bipartite lattice, theorems by Marshall[2] and by Lieb and Mattis[3] rigorously prove that the ground state is a *total* spin singlet: $S_{\rm tot}=0$. Any total singlet can be expanded in a (nonorthogonal) basis of valence bonds, which are singlet pairs $(ij)\equiv 2^{-1/2}(|\uparrow_i\downarrow_j\rangle-|\downarrow_i\uparrow_j\rangle)$ extending between sites i and j. The most probable singlets are between nearest neighbors, which thereby take full advantage of the Heisenberg interaction $J\boldsymbol{S}_i\cdot\boldsymbol{S}_j$ and achieve a minimum possible energy $\varepsilon_0=-\frac{3}{4}J$ for that particular link. Taking linear combinations of such states lowers the energy, via delocalization, with respect to any fixed singlet configuration; this is the basic idea behind Anderson's celebrated resonating valence bond (RVB) picture.[4] If one allows the singlet bonds to be long ranged, such a state can even possess classical Néel order.[5]

Taking advantage of quantum singlets, one can construct correlated quantum-disordered wave functions which are eigenstates of local projection operators. This feature allows one to construct a many-body Hamiltonian which renders the parent wave function an exact ground state, typically with a gap to low-energy excitations. Perhaps the simplest example is the Majumdar-Ghosh (MG) model for an $S=\frac{1}{2}$ spin chain,[6] the parent state of which is given by alternating singlet bonds, viz.,

$$|\Psi\rangle = |\cdots \bullet\!\!-\!\!\bullet \quad \bullet\!\!-\!\!\bullet \quad \bullet\!\!-\!\!\bullet \cdots\rangle . \tag{1}$$

The key feature to $|\Psi\rangle$ is that any consecutive trio of sites $(n,n+1,n+2)$ can only be in a state of total spin $\mathcal{S}=\frac{1}{2}$; there is no $\mathcal{S}=\frac{3}{2}$ component. Thus, $|\Psi\rangle$ is an eigenstate of the projection operator

$$P_{3/2}(n,n+1,n+2)=-\frac{1}{4}+\frac{1}{3}(\boldsymbol{S}_n+\boldsymbol{S}_{n+1}+\boldsymbol{S}_{n+2})^2, \tag{2}$$

with zero eigenvalue, and an exact ground state for $\mathcal{H}=J\Sigma_n P_{3/2}(n,n+1,n+2)$. As $|\Psi\rangle$ breaks lattice translation symmetry, a second (degenerate) ground state follows by shifting $|\Psi\rangle$ by one lattice spacing. Extensions of the MG model to higher dimensions and to higher spin, where the ground state is again of the Kekulé form, i.e., a product of local valence bond singlets, were discussed by Klein.[7]

Another example is furnished by the valence bond solid (VBS) states of Affleck *et al.* [Affleck-Kennedy-Lieb-Tasaki (AKLT)].[1] The general AKLT state is compactly written in terms of Schwinger boson operators:[8]

$$|\Psi(\mathcal{L};M)\rangle=\prod_{\langle ij\rangle}(b_{i\uparrow}^\dagger b_{j\downarrow}^\dagger-b_{i\downarrow}^\dagger b_{j\uparrow}^\dagger)^M|0\rangle, \tag{3}$$

which assigns m singlet creation operators to each link of a lattice $\mathcal{L}$. The total boson occupancy on each site is zM, where z is the lattice coordination number; in the Schwinger representation, this corresponds to $2S$. Thus, a discrete family of AKLT states with $S=\frac{1}{2}zM$ is defined on each lattice, where M is any integer. The maximum total spin on any link is then $S_{ij}^{\rm max}=2S-M$, and any Hamiltonian constructed out of link projectors for total spin $\mathcal{S}\in[2S-M+1,2S]$, with positive coefficients, renders $|\Psi(\mathcal{L};M)\rangle$ an exact zero-energy ground state. The elementary excitations in these states were treated using a single mode approximation (SMA) in Ref. 8.

The ability of two spins to form a singlet state is a special property of the SU(2) group. Decomposing the product of two spin-S representations yields the well-known result

$$S \otimes S = 0 \oplus 1 \oplus 2 \oplus \cdots \oplus 2S, \tag{4}$$

and there is always a singlet available. If we replace SU(2) by SU(3), this is no longer the case. The representations of SU(N) are classified by $(N-1)$-row Young tableaux $(l_1, l_2, \ldots, l_{N-1})$ with l_j boxes in row j and with $l_1 \geq l_2 \geq \cdots \geq l_{N-1}$. The product of two fundamental (1,0) representations of SU(3) is

$$\underset{\mathbf{3}}{\square} \otimes \underset{\mathbf{3}}{\square} = \underset{\bar{\mathbf{3}}}{\begin{array}{|c|}\hline \\ \hline \\ \hline \end{array}} \oplus \underset{\mathbf{6}}{\square\!\square}, \tag{5}$$

which does not contain a singlet. One way to rescue the two-site singlet for general SU(N) is to take the product of the fundamental representation $\boldsymbol{N}$ with the antifundamental $\bar{\boldsymbol{N}}$. This yields a singlet plus the (N^2-1)-dimensional adjoint representation. In this manner, generalizations of the SU(2) antiferromagnet can be defined in such a manner that the two-site valence bond structure is preserved, but only on bipartite lattices.[9,10]

Another approach is to keep the same representation of SU(N) on each site but to create SU(N) singlets extending over multiple sites. When each site is in the fundamental representation, one creates N-site singlets,

$$\epsilon^{\alpha_1 \cdots \alpha_N} b^\dagger_{\alpha_1}(i_1) \cdots b^\dagger_{\alpha_N}(i_N)|0\rangle, \tag{6}$$

where $b^\dagger_\alpha(i)$ creates a Schwinger boson of flavor index α on site i. The SU(N) spin operators may be written in terms of the Schwinger bosons as

$$S^\alpha_\beta = b^\dagger_\alpha b_\beta - \frac{p}{N}\delta_{\alpha\beta}, \tag{7}$$

with $\mathrm{Tr}(S)=0$, for the general symmetric $(p,0)$ representation. These satisfy the SU(N) commutation relations

$$[S^\alpha_\beta, S^\mu_\nu] = \delta_{\beta\mu} S^\alpha_\nu - \delta_{\alpha\nu} S^\beta_\mu. \tag{8}$$

Extended valence bond solid (XVBS) states were first discussed by Affleck *et al.* in Ref. 11. In that work, SU($2N$) states where $N=mz$ were defined on lattices of coordination number z, with singlets extending over $z+1$ sites. Like the MG model, the XVBS states break lattice translation symmetry t and their ground states are doubly degenerate; they also break a charge conjugation symmetry $\mathcal{C}$, preserving the product $t\mathcal{C}$. In addition to SMA magnons, the XVBS states were found to exhibit soliton excitations interpolating between the degenerate vacuums. More recently, Greiter and Rachel[12] considered SU(N) valence bond spin chains in both the fundamental and other representations, constructing their corresponding Hamiltonians and discussing soliton excitations. Extensions of Klein models, with Kekulé ground states consisting of products of local SU(N) singlets, were discussed by Shen[13] and more recently by Nussinov and Ortiz.[14] An SU(4) model on a two-leg ladder with a doubly degenerate Majumdar-Ghosh-type ground state has been discussed by Chen *et al.*[15]

Shen also discussed a generalization of Anderson's RVB state to SU(N) spins as a prototype of a spin-orbit liquid state.[13] A more clearly defined and well-analyzed model was recently put forward by Pankov *et al.*,[16] who generalized the Rokhsar-Kivelson quantum dimer model[17] to a model of resonating singlet valence plaquettes. Their plaquettes are N-site SU(N) singlets ($N=3$ and $N=4$ models were considered), which resonate under the action of the SU(N) antiferromagnetic Heisenberg Hamiltonian, projected to the valence plaquette subspace. The models and states considered here do not exhibit this phenomenon of resonance. Rather, they are described by static "singlet valence simplex" configurations. Consequently, their physics is quite different and in fact simpler. For example, with resonating valence bonds or plaquettes, one can introduce vison excitations[18] which are $\mathbf{Z}_2$ vortex excitations, changing the sign of the bonds or plaquettes which are crossed by the vortex string.[19] For simplex (or plaquette) solids, there is no resonance, and the vison does not create a distinct quantum state. The absence of "topological quantum order" in the Klein and AKLT models has been addressed by Nussinov and Ortiz.[14]

Here, I shall explore further generalizations of the AKLT scheme, describing a family of "simplex solid" (SS) states on N-partite lattices. While the general AKLT state is written as a product over the links of a lattice $\mathcal{L}$, with M singlet creation operators applied to a given link, the SS states, *mutatis mutandis*, apply M SU(N) singlet operators on each N simplex. Each site then contains an SU(N) spin whose representation is determined by M and the lattice coordination. Furthermore, as is the case with the AKLT states, the SS states admit a simple coherent state description in terms of classical CP^{N-1} vectors. Their equal-time quantum correlations are then computable as the finite temperature correlations of an associated classical model on the same lattice. A classical ordering transition in this model corresponds to a zero-temperature quantum critical point as a function of M (which is, however, a discrete parameter). I argue that the ordered SS states select a particular ordered structure via an "order by disorder" mechanism. Finally, I discuss what happens to these states at an edge, where the bulk SU(N) representation is effectively fractionalized, and a residual entropy proportional to the volume of the boundary arises.

II. SIMPLEX SOLIDS

Consider an N-site simplex Γ and define the SU(N) singlet creation operator:

$$\mathcal{R}^\dagger_\Gamma = \epsilon^{\alpha_1 \cdots \alpha_N} b^\dagger_{\alpha_1}(\Gamma_1) \cdots b^\dagger_{\alpha_N}(\Gamma_N), \tag{9}$$

where $i=1,\ldots,N$ labels the sites Γ_i on the simplex. Any permutation μ of the labels has the trivial consequence of $\mathcal{R}^\dagger_\Gamma \to \mathrm{sgn}(\mu)\mathcal{R}^\dagger_\Gamma$. Next, partition a lattice $\mathcal{L}$ into N-site simplixes, i.e., into N sublattices, and define the state

$$|\Psi(\mathcal{L};M)\rangle = \prod_\Gamma (\mathcal{R}^\dagger_\Gamma)^M |0\rangle, \tag{10}$$

where M is an integer. Since each $\mathcal{R}^\dagger_\Gamma$ operator adds one Schwinger boson to every site in the simplex, the total boson

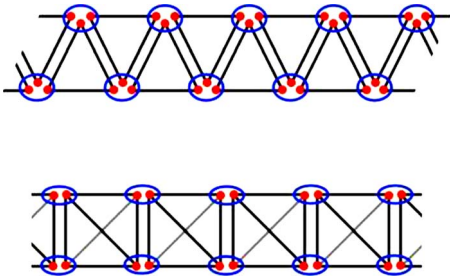
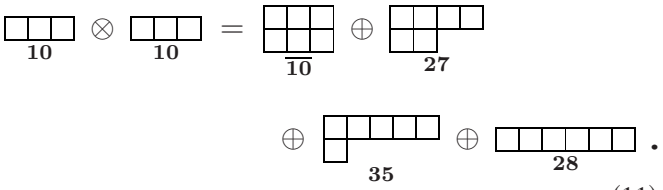


FIG. 1. (Color online) Top: SU(3) SS state on a two-leg zigzag chain. Each site is in the ten-dimensional totally symmetric representation with three boxes (the red dots). Bottom: SU(4) SS state on a two-leg ladder of tetrahedra. Each site is in the ten-dimensional totally symmetric representation with two boxes.

occupancy of any given site is $p=\zeta M$, where ζ is the number of simplixes associated with each site. For lattices such as the Kagomé and pyrochlore systems, where two neighboring simplixes share a single site, we have $\zeta=2$. For the tripartite triangular lattice, $\zeta=3$. Recall that each site is in the $(p,0)$ representation of SU(N), with one row of p boxes.

Two one-dimensional examples are depicted in Fig. 1. The first is defined on a two-leg zigzag chain. The chain is partitioned into triangles, as shown, with each site being a member of three triangles. Each triangle represents a simplex Γ and accommodates one power of the SU(3) singlet creation operator $\mathcal{R}_\Gamma^\dagger$. Thus, for this state, we have $N=3$ and $\zeta=3$. With $M=1$ then, the local SU(3) representation on each site is (3,0), i.e., $\square\square\square$, which is ten dimensional. The $M=1$ case is in fact a redrawn version of the state defined by Greiter and Rachel in Eq. (52) of Ref. 12. For this state, a given link may be in any of four representations of SU(3) or a linear combination thereof:



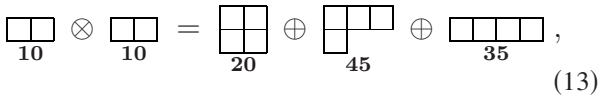
(11)

Thus, the zigzag chain SU(3) SS state is an exact zero-energy eigenstate of any Hamiltonian of the form

$$\mathcal{H}=\sum_{\substack{\langle ij\rangle\\ \text{sides}}} J_1\,\mathrm{P}_{\square\square\square\square\square\square}(ij) + \sum_{\substack{\langle ij\rangle\\ \text{zigzag}}} J_2\,\mathrm{P}_{\square\square\square\square\square\square}(ij) + J_3\,\mathrm{P}_{\begin{smallmatrix}\square\square\square\square\square\\ \square\end{smallmatrix}}(ij)\ , \tag{12}$$

with positive coefficients J_1, J_2, and J_3.

The SU(4) SS chain in Fig. 1 is topologically equivalent to a chain of tetrahedra, each joined to the next along an opposite side. Thus, $\zeta=2$ and for the $M=1$ parent state, each site is in the ten-dimensional $\square\square$ representation. From



(13)

we can construct a Hamiltonian,

$$\mathcal{H}=\sum_{\substack{\langle ij\rangle\\ \text{sides}}} J_1\,\mathrm{P}_{\square\square\square\square}(ij) + \sum_{\substack{\langle ij\rangle\\ \text{crosses}}} J_4\,\mathrm{P}_{\square\square\square\square}(ij) + \sum_{\substack{\langle ij\rangle\\ \text{rungs}}} J_2\,\mathrm{P}_{\square\square\square\square}(ij) + J_3\,\mathrm{P}_{\begin{smallmatrix}\square\square\square\square\\ \square\square\end{smallmatrix}}(ij)\ , \tag{14}$$

again with positive coefficients J_1, J_2, J_3, and J_4, which renders the wave function $|\Psi\rangle$ an exact zero-energy ground state. For both this and the previously discussed SU(3) chain, the ground state is nondegenerate.

A. SU(N) Casimirs

For a collection of K spins, each in the fundamental of SU(N), we write

$$\mathcal{S}_\beta^\alpha=\sum_{k=1}^{K} S_\beta^\alpha(k). \tag{15}$$

From the spin operators $\mathcal{S}_\beta^\alpha$, one can construct $N-1$ Casimirs, $C^{(n)}=\frac{1}{n!}\mathrm{Tr}(\mathcal{S}^n)$, with $n=2,\ldots,N$. The eigenvalues of $C^{(n)}$ for totally symmetric $(+)$ and totally antisymmetric $(-)$ representations of p boxes were obtained by Kobayashi:[20]

$$C^{(n)}(h;\pm)=\frac{h(N\mp 1)(N\pm p)}{n!N^n(N\pm p\mp 1)} \times\{(-1)^n p^{n-1}+[(N\mp 1)(N\pm p)]^{n-1}\}. \tag{16}$$

The Casimirs can be used to construct the projectors onto a given representation as a polynomial function of the spin operators. In order to do so, though, we will need the eigenvalues for all the representations which occur in a given product. Consider, for example, the case of three SU(3) objects, each in their fundamental representation. We then have

(17)

The eigenvalues of the quadratic and cubic Casimirs are found to be

$$C^{(2)}(\bullet)=0,\quad C^{(2)}\left(\begin{smallmatrix}\square\square\\ \square\square\end{smallmatrix}\right)=3,\quad C^{(2)}(\square\square\square)=6,$$

$$C^{(3)}(\bullet)=-4,\quad C^{(3)}\left(\begin{smallmatrix}\square\square\\ \square\square\end{smallmatrix}\right)=0,\quad C^{(3)}(\square\square\square)=8\ .$$

Therefore,

$$P_{\bullet}(ijk)=2-\tfrac{2}{3}C^{(2)}+\tfrac{1}{4}C^{(3)}, \tag{18}$$

$$P_{\begin{smallmatrix}\square\square\\ \square\square\end{smallmatrix}}(ijk)=-2+C^{(2)}-\tfrac{1}{2}C^{(3)}, \tag{19}$$

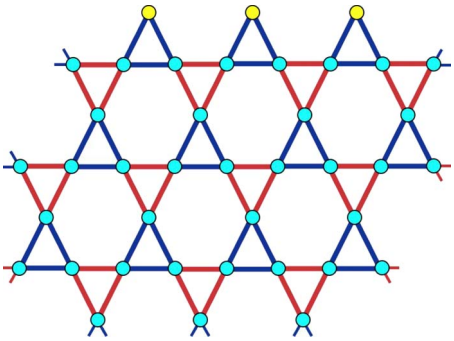


FIG. 2. (Color online) SU(3) simplex solid states on the Kagomé lattice. Applying the singlet operator $\mathcal{R}^\dagger_\Gamma$ to all the up (down) triangles generates the state $|\Psi_{\triangle(\triangledown)}\rangle$. Applying $\mathcal{R}^\dagger_\Gamma$ to *all* the triangular simplixes generates the state $|\Psi\rangle$ of Eq. (25). The twofold coordinated yellow sites at the top form a (10) edge (see Sec. VIII).

$$P_{\square\square\square}(ijk) = 1 - \frac{1}{3}C^{(2)} + \frac{1}{4}C^{(3)}. \tag{20}$$

Expressing the projector $P_{\square\square\square}(ijk)$ in terms of the local spin operators $S^\alpha_\beta(l)$, I find

$$\begin{aligned} P_{\square\square\square}(ijk) &= 1 - \frac{1}{6}\mathrm{Tr}(\mathcal{S}^2_{ijk}) + \frac{1}{24}\mathrm{Tr}(\mathcal{S}^3_{ijk}) \\ &= -\frac{1}{3}\mathrm{Tr}[S(i)S(j) + S(j)S(k) + S(k)S(i)] \\ &\quad + \frac{1}{8}\mathrm{Tr}[S(i)S(j)S(k) + S(k)S(j)S(i)] - \frac{2}{27}. \end{aligned} \tag{21}$$

The projector thus contains both bilinear and trilinear terms in the local spin operators. One could also write the projector in terms of the quadratic Casimir $C^{(2)}$ only as

$$P_{\square\square\square}(ijk) = \frac{1}{18}C^{(2)}(C^{(2)} - 3). \tag{22}$$

This, however, would result in interaction terms such as $\mathrm{Tr}[S(i)S(j)]\mathrm{Tr}[S(j)S(k)]$, which is apparently quadratic in $S(j)$. For the $\square$ representation, however, products such as $S^\alpha_\beta(i)S^\mu_\nu(i)$ can be reduced to linear combinations of the spin operators $S^\sigma_\tau(i)$, as is familiar in the case of SU(2). This simplification would then recover the expression in Eq. (21).

III. SS STATES IN $d \geqslant 2$ DIMENSIONS

A. Kagomé lattice

The Kagomé lattice, depicted in Fig. 2, is a two-dimensional network of corner-sharing triangles, with $\zeta=2$. It naturally accommodates a set of $N=3$ SS states. The simplest example consists of SU(3) objects in the fundamental representation at each site and places SU(3) singlets on all the upward-pointing triangles (see Fig. 2):

$$|\Psi_\triangle\rangle = \prod_\triangle \mathcal{R}^\dagger_\triangle |0\rangle. \tag{23}$$

The lattice inversion operator $\mathcal{I}$ then generates a degenerate mate, $|\Psi_\triangledown\rangle = \mathcal{I}|\Psi_\triangle\rangle$. Both states are exact zero-energy eigenstates of the Hamiltonian

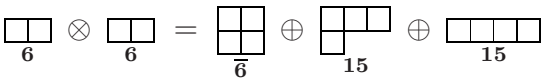
$$\mathcal{H} = \sum_{\langle ijk\rangle \in 120^\circ} P_{\square\square\square}(ijk), \tag{24}$$

where the sum is over all 120° trios (ijk); there are six such (ijk) trios for every hexagon. Since two of the three sites in each trio are antisymmetrized, the fully symmetric $\square\square\square$ representation is completely absent. This model bears obvious similarities to the MG model: its ground state is a product over independent local singlets; hence, there are no correlations beyond a single simplex, and it spontaneously breaks a discrete lattice symmetry (in this case $\mathcal{I}$).[21]

If we let the singlet creation operators act on both the up- and down-pointing triangles, we obtain a state which breaks no discrete lattice symmetries,

$$|\Psi\rangle = \prod_\triangle \mathcal{R}^\dagger_\triangle \prod_\triangledown \mathcal{R}^\dagger_\triangledown |0\rangle. \tag{25}$$

For this state, each site is in the six-dimensional $\square\square$ representation. On any given link, then, there are the following possibilities:



(26)

The fact that each link belongs to either an $\triangle$ or $\triangledown$ simplex and the fact that a singlet operator $\mathcal{R}^\dagger_{\triangle/\triangledown}$ is associated with each simplex mean that no link can be in the fully symmetric $\square\square\square\square$ representation. Thus, $|\Psi\rangle$ is an exact, zero-energy eigenstate of the Hamiltonian

$$\mathcal{H} = \sum_{\langle ij\rangle} P_{\square\square\square\square}(ij). \tag{27}$$

The states $|\Psi_\triangle\rangle$, $|\Psi_\triangledown\rangle$, and $|\Psi\rangle$ are depicted in Fig. 2.

The actions of the quadratic and cubic Casimirs on the possible representations for a given link are given in the following table:

Rep^{n}	$C^{(2)}$	$C^{(3)}$
$\square\square$	10/3	−80/27
$\square\square\square$	16/3	64/27
$\square\square\square\square$	28/3	352/27

Note that

$$C^{(2)} = \frac{8}{3}\left(C^{(2)} - \frac{320}{27}\right); \tag{28}$$

hence, the two Casimirs are not independent here. We can, however, write the desired projector,

$$P_{\square\square\square\square}(ij) = \frac{1}{24}\left(C^{(2)} - \frac{10}{3}\right)\left(C^{(2)} - \frac{16}{3}\right)$$
$$= \frac{1}{24}(\mathrm{Tr}[S(i)S(j)])^2 + \frac{7}{36}\mathrm{Tr}[S(i)S(j)] + \frac{5}{27}, \tag{29}$$

as a bilinear plus biquadratic interaction between neighboring spins. To derive this result, we write $C^{(2)} = \frac{1}{2}\mathrm{Tr}[S(i) + S(j)]^2$, where

$$C^{(2)} = \mathrm{Tr}[S(i)S(j)] + \mathrm{Tr}(S^2)$$
$$= \mathrm{Tr}[S(i)S(j)] + p(N + p - 1) - \frac{p^2}{N}. \tag{30}$$

Next, consider the pyrochlore lattice in Fig. 3. This lattice consists of corner-sharing tetrahedra, with $\zeta = 2$, and naturally accommodates an $N = 4$ SS state of the form

$$|\Psi\rangle = \prod_{\text{tetrahedra}} \mathcal{R}_\Gamma^\dagger |0\rangle. \tag{31}$$

Like the uniform SU(3) SS state on the Kagomé lattice, this SU(4) state describes a lattice of spins which are in the $\square\square$ representation on each site; in the SU(4) case, this representation is ten dimensional. From Eq. (13), we see that each link, the sites of which appear in some simplex singlet creation operator, cannot have any weight in the 35-dimensional totally symmetric $\square\square\square\square$ representation. Hence, once again, the desired Hamiltonian is that of Eq. (27). For SU(4),

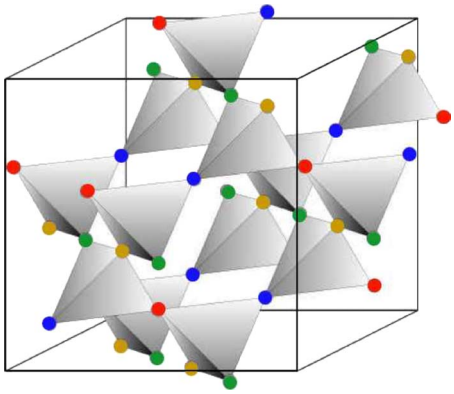


FIG. 3. (Color online) The pyrochlore lattice and its quadripartite structure.

$$C^{(2)}\left(\square\!\square\right) = 6, \quad C^{(2)}\left(\square\!\square\!\square\right) = 8, \quad C^{(2)}\left(\square\!\square\!\square\!\square\right) = 12,$$

and so

$$P_{\square\square\square\square}(ij) = \frac{1}{24}(C^{(2)} - 6)(C^{(2)} - 8)$$
$$= \frac{1}{24}(\mathrm{Tr}[S(i)S(j)])^2 + \frac{1}{6}\mathrm{Tr}[S(i)S(j)] + \frac{1}{8}. \tag{32}$$

Indeed, there is a rather direct correspondence between the possible SU(3) SS states on the Kagomé lattice and the SU(4) SS states on the pyrochlore lattice. For example, one can construct a model with a doubly degenerate ground state, similar to the MG model, by associating the simplex singlet operators $\mathcal{R}_\Gamma^\dagger$ with only the tetrahedra which point along the (111) lattice direction.

Finally, consider SU(4) states on the square lattice, again in the $\square\square$ representation on each site. We can once again identify the exact ground state of the $P_{\square\square\square\square}(ij)$ Hamiltonian of Eq. (27). In this case, the ground state is doubly degenerate and is described by the "planar pyrochlore" configuration shown in Fig. 4.

IV. MAPPING TO A CLASSICAL MODEL

The correlations in the SS states are calculable using the coherent state representation. From results derived in Appendix A, the coherent state SS wave function is given by

$$\Psi[\{\bar{z}(i)\}] = \mathcal{C}\prod_\Gamma [R_\Gamma(\bar{z}(\Gamma_1), \ldots, \bar{z}(\Gamma_N))]^M, \tag{33}$$

where $\mathcal{C}$ is a normalization constant, and

$$R_\Gamma \equiv \bar{z}(\Gamma_1) \wedge \bar{z}(\Gamma_2) \wedge \cdots \wedge \bar{z}(\Gamma_N)$$
$$= \epsilon^{\alpha_1 \cdots \alpha_N} \bar{z}_{\alpha_1}(\Gamma_1) \cdots \bar{z}_{\alpha_N}(\Gamma_N). \tag{34}$$

Here, I have labeled the N sites on each simplex Γ by an index i running from 1 to N.

Note that the coherent state probability density is

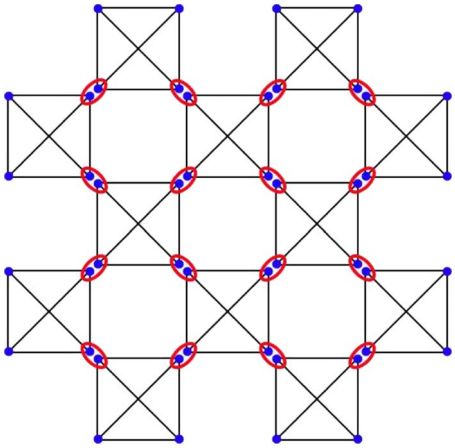


FIG. 4. (Color online) One of two doubly degenerate ground states for the Hamiltonian of Eq. (27) applied to the square lattice, where each site is in the (2,0,0) representation of SU(4). The squares with crosses (or, equivalently, tetrahedra) represent singlet operators $\epsilon^{\alpha\beta\gamma\delta} b^\dagger_\alpha(i) b^\dagger_\beta(j) b^\dagger_\gamma(k) b^\dagger_\delta(l)$ on the simplex $(ijkl)$. The resulting planar pyrochlore configuration is equivalent to a checkerboard lattice of tetrahedra.

$$|\Psi|^2 = |\mathcal{C}|^2 \prod_\Gamma |R_\Gamma|^{2M}, \tag{35}$$

and that

$$|R_\Gamma|^2 = \epsilon^{\alpha_1 \cdots \alpha_N} \epsilon^{\beta_1 \cdots \beta_N} Q_{\alpha_1\beta_1}(\Gamma_1) \cdots Q_{\alpha_N\beta_N}(\Gamma_N), \tag{36}$$

where $Q_{\alpha\beta}(i) = \bar{z}_\alpha(i) z_\beta(i)$. Writing $|\Psi|^2 \equiv e^{-H_{\rm cl}/T}$, we see that the probability density may be written as the classical Boltzmann weight for a system described by the classical Hamiltonian

$$H_{\rm cl} = -\sum_\Gamma \ln |R_\Gamma|^2 \tag{37}$$

at a temperature $T = 1/M$.[8,22] The classical interactions are N-body interaction, involving the matrices $Q_{\alpha\beta}(i)$ on all the sites of a given N-site simplex, summed over all distinct simplixes. For $N=2$, this results in a classical nearest-neighbor quantum antiferromagnet,[8] with

$$H_{\rm cl}^{\rm AKLT} = -\sum_{\langle ij \rangle} \ln\left(\frac{1 - \hat{\boldsymbol{n}}_i \cdot \hat{\boldsymbol{n}}_j}{2} \right), \tag{38}$$

with $\hat{\boldsymbol{n}} = z^\dagger \boldsymbol{\sigma} z$, where $\boldsymbol{\sigma}$ is the vector of Pauli matrices. This general feature of pair product wave functions of the Bijl-Feynman, Laughlin, and AKLT forms is thus valid for the SS states as well.

As shown in Appendix A, the matrix element $\langle \phi | \hat{T}_K | \psi \rangle$ of an operator

$$\hat{T}_K = \sum_{\boldsymbol{m},\boldsymbol{n}}{}' T_{\boldsymbol{k},\boldsymbol{l}} b_1^{k_1} \cdots b_N^{k_N} b_1^{\dagger l_1} \cdots b_N^{\dagger l_N} \tag{39}$$

may be computed as an integral with respect to the measure $d\mu$ (on each site) of the product $\bar{\phi}(z)\psi(\bar{z})$ of coherent state wave functions multiplied by the kernel

$$\hat{T}_K(\{b_\alpha\}, \{b^\dagger_\alpha\}) \to \frac{(N-1+p+K)!}{p!} \hat{T}_K(\{z_\alpha\}, \{\bar{z}_\alpha\}). \tag{40}$$

Thus, the *quantum mechanical* expectation values of Hermitian observables in the SS states are expressible as *thermal* averages over the corresponding classical Hamiltonian $H_{\rm cl}$ of Eq. (37). The SS and VBS states thus share the special property that their equal-time quantum correlations are equivalent to thermal correlations of an associated classical model on the same lattice, i.e., in the same number of dimensions.

In this paper, I will be content to merely elucidate the correspondence between quantum correlations in $|\Psi(\mathcal{L}; M)\rangle$ and classical correlations in $H_{\rm cl}$. An application of this correspondence to a Monte Carlo evaluation of the classical correlations will be deferred to a future publication.

V. SINGLE MODE APPROXIMATION FOR ADJOINT EXCITATIONS

Following the treatment in Ref. 8, I construct trial excited states at wave vector $\boldsymbol{k}$ in the following manner. First, define the operator

$$\phi_{\alpha\beta}(\boldsymbol{k}) = \sum_i \eta_i \phi_{i,\alpha\beta}(\boldsymbol{k}), \tag{41}$$

$$\phi_{i,\alpha\beta}(\boldsymbol{k}) = \mathcal{N}^{-1/2} \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} S^\alpha_\beta(\boldsymbol{R}, i), \tag{42}$$

where $\boldsymbol{R}$ is a Bravais lattice site and i labels the basis elements. Here, η_i is for the moment an arbitrary set of complex-valued parameters and $\mathcal{N}$ is the total number of unit cells in the lattice. The operators $\phi_{\alpha\beta}(\boldsymbol{k})$ transform according to the (N^2-1)-dimensional adjoint representation of SU(N). Next, construct the trial state

$$|\phi\rangle \equiv \phi_{\alpha\beta}(\boldsymbol{k}) |\Psi\rangle \tag{43}$$

and evaluate the expectation value of the Hamiltonian in this state:

$$E_{\rm SMA}(\boldsymbol{k}) = \frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle} = \frac{\eta_i^* f_{ij}(\boldsymbol{k}) \eta_j}{\eta_i^* s_{ij}(\boldsymbol{k}) \eta_j}. \tag{44}$$

Here, $f_{ij}(\boldsymbol{k})$ and $s_{ij}(\boldsymbol{k})$ are, respectively, the oscillator strength and structure factor given by

$$f_{ij}(\boldsymbol{k}) = \frac{1}{2} \langle \Psi | [\phi^\dagger_{i,\alpha\beta}(\boldsymbol{k}), [H, \phi_{j,\alpha\beta}(\boldsymbol{k})]] | \Psi \rangle, \tag{45}$$

$$s_{ij}(\boldsymbol{k}) = \langle \Psi | \phi^\dagger_{i,\alpha\beta}(\boldsymbol{k}) \phi_{j,\alpha\beta}(\boldsymbol{k}) | \Psi \rangle. \tag{46}$$

Here, I have assumed that H is a sum of local projectors and that $H|\Psi\rangle = 0$. Treating the η_i parameters variationally, one obtains the equation

$$f_{ij}(\boldsymbol{k}) \eta_j = E_{\rm SMA}(\boldsymbol{k}) s_{ij}(\boldsymbol{k}) \eta_j. \tag{47}$$

The lowest eigenvalue of this equation provides a rigorous upper bound to the lowest excitation energy at wave vector $\boldsymbol{k}$. The result is exact if all the oscillator strength is saturated by a single mode, hence the SMA label. When $|\Psi\rangle$ is quan-

tum disordered, the SMA spectrum is gapped. When $|\Psi\rangle$ develops long-ranged order (for sufficiently large M parameter and in $d>2$ dimensions), the SMA spectrum is gapless.

VI. MEAN FIELD TREATMENT OF QUANTUM PHASE TRANSITION

The classical Hamiltonian of Eq. (37) exhibits a global SU(N) symmetry, where $z_\sigma(i)\to U_{\sigma\sigma'}z_{\sigma'}(i)$ for every lattice site i. Since the interactions are short ranged, there can be no spontaneous breaking of this symmetry in dimensions $d\leqslant 2$. In higher dimensions, the classical model can order at finite temperature, corresponding to a quantum ordering at a finite value of m. For the AKLT states, where $N=2$, this phase transition was first discussed in Ref. 8. I first discuss the $N=2$ case and then generalize to arbitrary $N>2$.

A. $N=2$: valence bond solid states

Consider the $N=2$ case, which on a lattice of coordination number z yields a family of wave functions describing $S=\frac{1}{2}Mz$ objects with antiferromagnetic correlations. These are the AKLT VBS states. We have

$$z=\begin{pmatrix}\cos\left(\frac{\theta}{2}\right)\\ \sin\left(\frac{\theta}{2}\right)e^{i\phi}\end{pmatrix},\quad Q=\frac{1}{2}\begin{pmatrix}1+n^z & n^+\\ n^- & 1-n^z\end{pmatrix},\tag{48}$$

where $\boldsymbol{n}=z^\dagger\boldsymbol{\sigma}z$ is a real unit vector ($\boldsymbol{\sigma}$ are the Pauli matrices). Since

$$\epsilon^{\alpha_1\beta_1}\epsilon^{\alpha_2\beta_2}Q_{\alpha_1\beta_1}(\Gamma_A)Q_{\alpha_2\beta_2}(\Gamma_B)=\frac{1}{2}(1-\hat{\boldsymbol{n}}_A\cdot\hat{\boldsymbol{n}}_B),\tag{49}$$

the effective Hamiltonian is

$$H_{\rm cl}=-\sum_{\langle ij\rangle}\ln\left(\frac{1-\hat{\boldsymbol{n}}_i\cdot\hat{\boldsymbol{n}}_j}{2}\right).\tag{50}$$

The sum is over all links on the lattice. I assume that the lattice is bipartite, so each link connects sites on the A and B sublattices. I now make the mean field ansatz

$$\hat{\boldsymbol{n}}_A=\boldsymbol{m}+\delta\hat{\boldsymbol{n}}_A,\quad \hat{\boldsymbol{n}}_B=-\boldsymbol{m}+\delta\hat{\boldsymbol{n}}_B\tag{51}$$

and expand H in powers of $\delta\hat{\boldsymbol{n}}_i$. Expanding to lowest nontrivial order in the fluctuations $\delta\hat{\boldsymbol{n}}_i$, we obtain a mean field Hamiltonian

$$H^{\rm MF}=E_0-\boldsymbol{h}_A\sum_{i\in A}\hat{\boldsymbol{n}}_i-\boldsymbol{h}_B\sum_{j\in B}\hat{\boldsymbol{n}}_j,\tag{52}$$

where E_0 is a constant and

$$\boldsymbol{h}_A=-\boldsymbol{h}_B=\frac{z\boldsymbol{m}}{1+\boldsymbol{m}^2}\tag{53}$$

is the mean field. Here, z is the lattice coordination number. The self-consistency equation is then

$$\boldsymbol{m}=\langle\hat{\boldsymbol{n}}_A\rangle=\int d\hat{\boldsymbol{n}}\,\hat{\boldsymbol{n}}\,e^{\boldsymbol{h}_A\cdot\hat{\boldsymbol{n}}/T}\Big/\int d\hat{\boldsymbol{n}}\,e^{\boldsymbol{h}_A\cdot\hat{\boldsymbol{n}}/T},\tag{54}$$

which yields

$$m=\coth\lambda-\frac{1}{\lambda},\quad \lambda=\frac{z}{T}\frac{m}{1+m^2}.\tag{55}$$

The classical transition occurs at $T_c^{\rm MF}=\frac{1}{3}z$, so the VBS state exhibits a quantum phase transition at $M_c^{\rm MF}=3z^{-1}$. For $M>M_c$, the VBS exhibits long-ranged two-sublattice Néel order. On the cubic lattice, the mean field value $M_c^{\rm MF}=\frac{1}{2}$ suggests that all the square lattice VBS states, for which the minimal spin is $S=3$ (with $M=1$), are Néel ordered. Since the mean field treatment overestimates T_c due to its neglect of fluctuations, I conclude that the true M_c is somewhat greater than $3z^{-1}$, which leaves open the possibility that the minimal $M=1$ VBS state on the cubic lattice is a quantum-disordered state. Whether this is in fact the case could be addressed by a classical Monte Carlo simulation.

B. $N>2$: simplex solid states

For general N, I write

$$Q_{\alpha\beta}(i)=\langle Q_{\alpha\beta}(i)\rangle+\delta Q_{\alpha\beta}(i),\tag{56}$$

where the average is taken with respect to $|\Psi|^2=e^{-H_{\rm cl}/T}$. To maximize $|\Psi|^2$, i.e., to minimize $H_{\rm cl}$, choose a set $\{\mathrm{P}^\sigma_{\alpha\beta}\}$ of N mutually orthogonal projectors, with $\sigma=1,\ldots,N$. The projectors satisfy the relations

$$P^\sigma P^{\sigma'}=\delta_{\sigma\sigma'}P^\sigma\tag{57}$$

and can each be written as

$$P^\sigma_{\alpha\beta}=\bar{\omega}^\sigma_\alpha\omega^\sigma_\beta,\tag{58}$$

where $\{\omega^\sigma\}$ is a set of N mutually orthogonal CP^{N-1} vectors. Then, if $z(\Gamma_\sigma)=\omega^\sigma$ for each site Γ_σ in the simplex, we have $R_\Gamma=e^{i\eta}$, where η is an arbitrary phase, and $|R_\Gamma|^2=1$. One then writes

$$\mathcal{Q}^\sigma_{\alpha\beta}\equiv\langle Q_{\alpha\beta}(\Gamma_\sigma)\rangle=\frac{1}{N}\delta_{\alpha\beta}+m\left(P^\sigma_{\alpha\beta}-\frac{1}{N}\delta_{\alpha\beta}\right).\tag{59}$$

Here, $m\in[0,1]$ is the order parameter, analogous to the magnetization. When $m=0$, no special subspace is selected, and the correlations are isotropic. When $m=1$, the Q matrix is a projector onto the one-dimensional subspace defined by ω^σ. Note that $\langle\mathrm{Tr}Q(\Gamma_\sigma)\rangle=1$, as it must be.

At this point, there remains a freedom in assigning the vectors $\{\omega^\sigma\}$ to the sites $\{\Gamma_\sigma\}$ of each simplex. Consider, for example, the $N=3$ case on the Kagomé or triangular lattice. The lattice is tripartite, so every A sublattice site has two (Kagomé) or three (triangular) nearest neighbors on each of the B and C sublattices. However, as is well known, the individual sublattices may have lower translational symmetry than the underlying triangular Bravais lattice. Indeed, the sublattices may be translationally disordered. I shall return to this point below. For the moment, it is convenient to think in terms of N sublattices, each of which has the same discrete symmetries as the underlying Bravais lattice.

Expanding $H_{\rm cl}$ to lowest order in the fluctuations $\delta Q_{\alpha\beta}(i)$ on each site and dropping terms of order $(\delta Q)^2$ and higher, I obtain the mean field Hamiltonian

$$H_{\rm MF} = E_0 - \zeta \sum_i h_{\alpha\beta}(i) Q_{\alpha\beta}(i), \tag{60}$$

where E_0 is a constant. The mean field $h_{\alpha\beta}(i)$ is site dependent. On a Γ_N site, we have

$$h^{(N)}_{\alpha_N\beta_N} = \frac{\epsilon^{\alpha_1\alpha_2\cdots\alpha_N}\epsilon^{\beta_1\beta_2\cdots\beta_N}\mathcal{Q}^{(1)}_{\alpha_1\beta_1}\cdots\mathcal{Q}^{(N-1)}_{\alpha_{N-1}\beta_{N-1}}}{\epsilon^{\mu_1\cdots\mu_N}\epsilon^{\nu_1\cdots\nu_N}\mathcal{Q}^{(1)}_{\mu_1\nu_1}\cdots\mathcal{Q}^{(N)}_{\mu_N\nu_N}}. \tag{61}$$

In Appendix B, I show that

$$h^{\sigma}_{\alpha\beta} = \left[A_N(m)\delta_{\alpha\beta} + B_N(m)P^{\sigma}_{\beta\alpha}\right]/R_N(m), \tag{62}$$

where

$$A_N(m) = (N-2)!\sum_{j=0}^{N-2}\frac{N-j-1}{j!}m^j\left(\frac{1-m}{N}\right)^{N-j-1}, \tag{63}$$

$$B_N(m) = (N-2)!\sum_{j=0}^{N-2}\frac{m^{j+1}}{j!}\left(\frac{1-m}{N}\right)^{N-j-2}, \tag{64}$$

$$R_N(m) = N!\sum_{j=0}^{N}\frac{m^j}{j!}\left(\frac{1-m}{N}\right)^{N-j}. \tag{65}$$

Note that $B_N(0)=0$, $B_N(1)=1$, and $R(1)=1$.

The mean field Hamiltonian is then

$$H_{\rm MF} = -\sum_i {\rm Tr}(h^{\rm t}(i)Q(i)) = -\zeta B_N(m)\sum_i |\omega^\dagger(i)z(i)|^2, \tag{66}$$

where $h_{\alpha\beta}(i)=h^{\sigma(i)}_{\alpha\beta}$, where $\sigma(i)$ labels the projector associated with site i. The self-consistency relation is obtained by evaluating the thermal average of $Q_{\alpha\beta}(i)$. With $x_\alpha \equiv |z_\alpha|^2$, I obtain

$$\frac{1}{N} + \frac{N-1}{N}m = \frac{\int_0^1 dx\, x\,(1-x)^{N-2}\exp(\zeta b_N(m)x/T)}{\int_0^1 dx\,(1-x)^{N-2}\exp(\zeta b_N(m)x/T)}, \tag{67}$$

where $b_N(m)=B_N(m)/R_N(m)$. It is simple to see that $m=0$ is a solution to this mean field equation. To find the critical temperature T_c, expand the right hand side in powers of m for small m. To lowest order, one finds

$$b_N(m) = \frac{N}{N-1}m + \mathcal{O}(m^2). \tag{68}$$

The value of $T_c^{\rm MF}$ is determined by equating the coefficients of m on either side of the equation. I find

$$M_c^{\rm MF}(N,\zeta) = \frac{1}{T_c^{\rm MF}(N,\zeta)} = \frac{N^2-1}{\zeta}. \tag{69}$$

This agrees with our previous result $M_c^{\rm MF}=\frac{1}{2}$ for the $N=2$ state on the cubic lattice, for which $\zeta=6$. The $N=3$ SS on the Kagomé lattice cannot develop long-ranged order which spontaneously breaks SU(N) owing to the Mermin-Wagner theorem. For the $N=4$ SS on the pyrochlore lattice, our mean field theory analysis suggests that the SS states are quantum disordered up to $M \approx \frac{15}{2}$. Note that the expression for $M_c^{\rm MF}$ reflects a competition between fluctuation effects, which favor disorder, and the coordination number, which favors order. The numerator, N^2-1, is essentially the number of directions in which Q can fluctuate about its average $\mathcal{Q}$; this is the dimension of the Lie algebra SU(N).

VII. ORDER BY DISORDER

At zero temperature, the classical model of Eq. (37) is solved by maximizing $|R_\Gamma|^2$ for each simplex Γ. This is accomplished by partitioning the lattice $\mathcal{L}$ into N sublattices, such that no neighboring sites are elements of the same sublattice. One then chooses any set of N mutually orthogonal vectors $\omega_\sigma \in {\rm CP}^{N-1}$ and set $z_i=\omega_{\sigma(i)}$. On every N-site simplex, then, each of the ω_σ vectors will occur exactly once, resulting in $|R_\Gamma|^2=1$, which is the largest possible value. Thus, the model is unfrustrated, in the sense that every simplex Γ is fully satisfied by the z_i assignments, and the energy is the minimum possible value: $E_0=0$.

For $N=2$, there are two equivalent ways of partitioning a bipartite lattice into two sublattices. For $N>2$, there are, in general, an infinite number of inequivalent partitions, all of which have the same ground state energy $E_0=0$. At finite temperature, though, the free energy of these different orderings will, in general, differ due to the differences in their respective excitation spectra. A particular partition may then be selected by entropic effects. This phenomenon is known as order by disorder.[23–25]

To see how entropic effects might select a particular partitioning, I derive a nonlinear σ model by expanding $H_{\rm cl}$ about a particular zero-temperature ordered state. Start with

$$z(i) = \omega_{\sigma(i)}(1-\pi_i^\dagger\pi_i)^{1/2} + \pi_i, \tag{70}$$

where $\pi_i^\dagger\omega_{\sigma(i)}=0$. We may now expand

$$\begin{aligned}|R_\Gamma|^2 &= |\epsilon^{\alpha_1\cdots\alpha_N}z_{\alpha_1}(\Gamma_1)\cdots z_{\alpha_N}(\Gamma_N)|^2 \\ &= 1 - \frac{1}{2}\sum_{i,j}|\pi_i^\dagger\omega_{\sigma(j)} + \omega_{\sigma(i)}^\dagger\pi_j|^2 + \cdots.\end{aligned} \tag{71}$$

Thus, the "low temperature" classical Hamiltonian is

$$H_{\rm LT} = \sum_{\langle ij\rangle}|\pi_i^\dagger\omega_{\sigma(j)} + \omega_{\sigma(i)}^\dagger\pi_j|^2 + \cdots, \tag{72}$$

where the sum is over all nearest-neighbor pairs on the lattice. The full SU(N) symmetry of the model is of course not apparent in Eq. (72) since it is realized nonlinearly on the π_i vectors.

Each π_i vector is subject to a nonholonomic constraint, $\pi_i^\dagger\pi_i \leqslant 1$. To solve for the thermodynamics of $H_{\rm LT}$, I will adopt a simplifying approximation, in which there is just one nonholonomic constraint, $\Sigma_i\pi_i^\dagger\pi_i \leqslant \mathcal{N}$, where $\mathcal{N}$ is the number of sites in the lattice. I fix the constraint by introducing an auxiliary variable χ and demanding

$$\mathcal{N}|\chi|^2 + \sum_i \pi_i^\dagger \pi_i = \mathcal{N}, \tag{73}$$

which I enforce with a Lagrange multiplier λ. The resulting model is

$$H_{\mathrm{LT}} = \sum_{\langle ij\rangle} |\pi_i^\dagger \omega_{\sigma(j)} + \omega_{\sigma(i)}^\dagger \pi_j|^2 + \lambda\left(\mathcal{N}|\chi|^2 + \sum_i \pi_i^\dagger \pi_i - \mathcal{N}\right). \tag{74}$$

The local constraints $\pi_i^\dagger \omega_{\sigma(i)} = 0$ are retained.

It is convenient to rotate to a basis where $\omega_\alpha^\sigma = \delta_{\alpha,\sigma}$, in which case $\omega_{\sigma(i)}^\dagger \pi_j = \pi_{j,\sigma(i)}$, i.e., the $\sigma(i)$ component of the vector π_i. As long as $\sigma(i) \neq \sigma(j)$ for nearest neighbors i and j, the local constraints have no effect on the Hamiltonian. We are then left with a Gaussian theory in the π_i vectors. Leaving the constraint term aside for the moment, we can solve for the spectrum of the first part of H_{LT}. From this spectrum, we compute the density of states per site, $g(\varepsilon)$. The free energy per site is then

$$\frac{F}{\mathcal{N}} = -\lambda + \lambda|\chi|^2 + T\int_0^\infty d\varepsilon g(\varepsilon) \ln\left(\frac{\varepsilon+\lambda}{T}\right). \tag{75}$$

Since $\mathcal{N}$ is thermodynamically large, we can extremize with respect to λ to find the saddle point, yielding

$$1 = |\chi|^2 + T\int_0^\infty d\varepsilon \frac{g(\varepsilon)}{\varepsilon+\lambda}. \tag{76}$$

Setting $\lambda = \chi = 0$, I obtain an equation for T_c,

$$T_c = \left[\int_0^\infty d\varepsilon \frac{g(\varepsilon)}{\varepsilon}\right]^{-1}. \tag{77}$$

For $T < T_c$, there is Bose condensation, and $|\chi|^2 > 0$. For $T > T_c$, the system is disordered. I stress that the disordered phase, described in this way, does not reflect the SU(N) symmetry which must be present owing to the truncation in Eq. (72).

A natural setting to investigate the order by disorder mechanism would be the SU(4) SS model on the pyrochlore lattice. I defer this analysis, together with a companion Monte Carlo simulation, to a later publication. Here, I will provide a simpler analysis of the SU(3) Kagomé SS. Since the Mermin-Wagner theorem precludes spontaneous breaking of SU(3) in two dimensions, this analysis at best will reveal which correlations should dominate at the *local* level. The two structures I wish to compare are the $\boldsymbol{Q}=0$ structure, depicted in Fig. 5, and the $\sqrt{3}\times\sqrt{3}$ structure, depicted in Fig. 6. Here, the A, B, and C sites correspond to CP^2 vectors,

$$\omega_A = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \omega_B = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \omega_C = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{78}$$

Both the $\boldsymbol{Q}=0$ and $\sqrt{3}\times\sqrt{3}$ structures are unfrustrated, in the sense that the interactions are fully satisfied on every simplex; $|R_\Gamma|^2 = 1$ for all Γ. Entropic effects, however, should favor one of the two configurations.

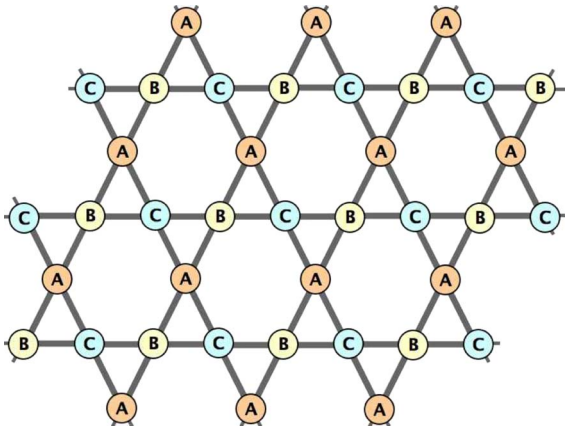


FIG. 5. (Color online) The $\boldsymbol{Q}=0$ structure on the Kagomé lattice.

The $\boldsymbol{Q}=0$ structure may be regarded as a triangular Bravais lattice with a three element basis (e.g., a triangular lattice of up triangles). Each triangular simplex contains three π vectors, each of which has two independent components (neglecting for the moment the global constraint). By solving for the spectrum in the absence of the constraint, one finds six branches:

$$\varepsilon_{l,\pm}(\boldsymbol{k}) = 2 \pm 2\cos\left(\frac{1}{2}\boldsymbol{k}\cdot\boldsymbol{a}_l\right), \tag{79}$$

where $\boldsymbol{k}$ is a vector in the Brillouin zone, and the direct lattice vectors are

$$\boldsymbol{a}_1 = a(1,0), \quad \boldsymbol{a}_2 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right), \tag{80}$$

with $\boldsymbol{a}_3 = \boldsymbol{a}_2 - \boldsymbol{a}_1$. This results in a free energy per site of

$$f(T) = -\lambda(T) + \frac{T}{\pi}\int_0^\infty d\alpha \ln\left(\frac{\lambda(T) + 2 + 2\cos\alpha}{T}\right), \tag{81}$$

with

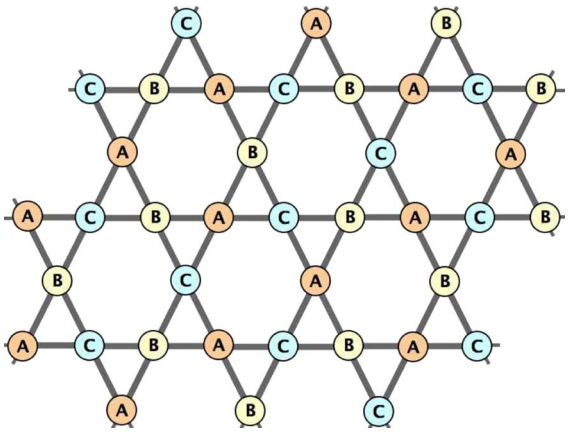


FIG. 6. (Color online) The $\sqrt{3}\times\sqrt{3}$ structure on the Kagomé lattice.

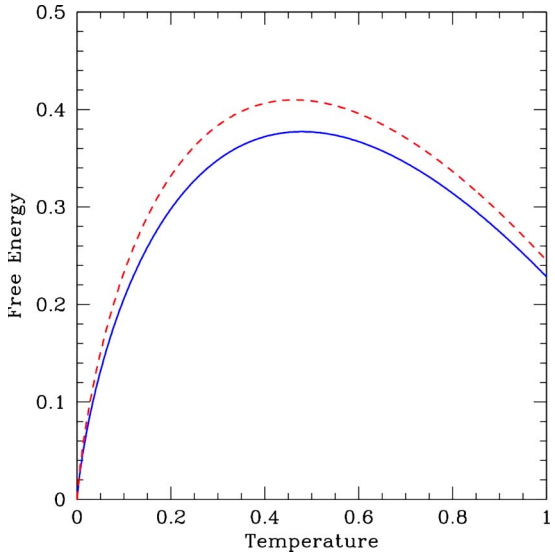


FIG. 7. (Color online) Free energy for SU(3) simplex solid states on the Kagomé lattice. Dashed (red): $\boldsymbol{Q}=0$ structure. Solid (blue): $\sqrt{3}\times\sqrt{3}$ structure.

$$\lambda(T) = \sqrt{4+T^2} - 2. \tag{82}$$

For the $\sqrt{3}\times\sqrt{3}$ structure, the underlying lattice is again triangular but now with a nine element basis (see Fig. 6). The Hamiltonian $H_{\rm LT}$ is then purely local, and there is no dispersion. The density of states per site is found to be

$$g(\varepsilon) = \frac{1}{6}\delta(\varepsilon) + \frac{1}{3}\delta(\varepsilon-1) + \frac{1}{3}\delta(\varepsilon-3) + \frac{1}{6}\delta(\varepsilon-4). \tag{83}$$

The free energy per site is

$$f(T) = 2 - u(T) + \frac{1}{6}T\ln\left(\frac{[u^2(T)-4][u^2(T)-1]^2}{T^6}\right), \tag{84}$$

with $u(T)\equiv\lambda(T)+2$, satisfying

$$\frac{1}{T} = \frac{u(u^2-3)}{(u^2-1)(u^2-4)}. \tag{85}$$

Our results are plotted in Fig. 7. One finds at all temperatures $T>0$ that

$$f_{\sqrt{3}\times\sqrt{3}}(T) < f_{\boldsymbol{Q}=0}(T), \tag{86}$$

suggesting that the local correlations should be better described by the $\sqrt{3}\times\sqrt{3}$ structure.

VIII. AT THE EDGE

With periodic boundary conditions applied, the translationally invariant AKLT states are nondegenerate. On systems with a boundary, the AKLT models exhibit completely free edge states, described by a local spin S_e on each edge site which is smaller than the bulk spin S. The energy is independent of the edge spin configuration; hence, there is a ground state entropy $(2S_e+1)k_B\ln N_e$, where N_e is the number of edge sites. As one moves away from the AKLT point in the space of Hamiltonians, the degeneracy is lifted and the edge spins interact.

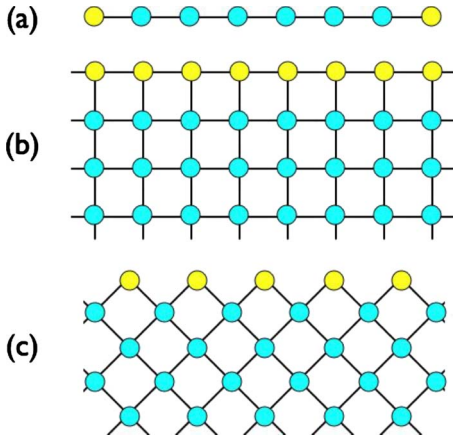


FIG. 8. (Color online) (a) Edge states for the linear chain. (b) (10) edge sites for the square lattice. (c) (11) edge sites for the square lattice. For the AKLT states, there is an effective free spin of length $S_e=\frac{1}{2}M(z-z_e)$ on the edge sites (see text).

The existence of weakly interacting $S=\frac{1}{2}$ degrees of freedom at the ends of finite $S=1$ Heisenberg chains was first discussed by Kennedy,[26] who found numerically an isolated quartet of low-energy states for a one-parameter family of $S=1$ antiferromagnetic chains. These four states are arranged into a singlet and a triplet, corresponding to the interaction of two $S=\frac{1}{2}$ objects. The spin quantum number of the ground state alternates with chain length L: singlet for even L and triplet for odd L. The singlet-triplet splitting was found to decay exponentially in L as $\exp(-L/\xi)$, where ξ is the spin-spin correlation length. Thus, for long chains, the $S=\frac{1}{2}$ objects at the ends are independent. Experimental evidence for this picture was adduced from electron spin resonance (ESR) studies of the compound NENP [Ni(C2H8N2)2NO2ClO4].[27]

The situation for the linear chain and for the (10) and (11) edges on the square lattice is depicted in Fig. 8. Recall that each link in the AKLT model supplies one Schwinger boson to each of its termini. The spin on any site is given by half the total Schwinger boson occupation: $S=\frac{1}{2}(b_\uparrow^\dagger b_\uparrow + b_\downarrow^\dagger b_\downarrow)$. Consider first the $M=1$ AKLT state of Eq. (3) on the linear chain. The bulk sites have total boson occupancy $n=2$ (hence, $S=1$), while the end sites have $n=1$ (hence, $S=\frac{1}{2}$). If the end sites are also to have $S=1$, they must each receive an extra Schwinger boson of either spin ($\uparrow$ or $\downarrow$). Thus, the end sites are described by an effective $S=\frac{1}{2}$ degree of freedom. Each of these four states is an exact ground state for the AKLT Hamiltonian, written as a sum over projection operators for total bond spin $S_{n,n+1}=2^1$.

Consider next the square lattice with $M=1$, for which the bulk spin is $S=2$. For a (10) edge, the edge sites are threefold coordinated, and each is "missing" one Schwinger boson. The freedom in supplying the last Schwinger boson corresponds once again to an $S=\frac{1}{2}$ object at each edge site. Along the (11) edge, the sites are twofold coordinated and must each accommodate two extra bosons, corresponding to $S=1$.

The general result for the edge spin S_e is clearly

$$S_e = \frac{1}{2}M(z - z_e), \tag{87}$$

where z and z_e are the bulk and edge coordination numbers. I stress that the edge spin configurations are completely degenerate at the AKLT point, since all the internal links are satisfied, i.e., annihilated by the local projector(s) in the corresponding AKLT Hamiltonian. Moving off of the AKLT point, in the direction of the Heisenberg model, the edge spins will interact. Based in part on Kennedy's results, I conclude that the $S=\frac{1}{2}$ chain along the (10) edge is antiferromagnetic, while the $S=1$ chain along the (11) edge is ferromagnetic (since consecutive edge sites are connected through an odd number of bulk sites).

By deriving and analyzing lattice effects in the spin path integral for the Heisenberg model, i.e., tunneling processes which have no continuum limit and which do not appear in the effective nonlinear sigma model, Haldane[28] argued that Heisenberg antiferromagnets with $2S=0$ mod 4 on the square lattice should have nondegenerate bulk ground states. This result was generalized by Read and Sachdev,[29] who, building on an earlier large-N Schwinger boson theory,[30] extended Haldane's analysis to SU(N) for $(N,\bar{N})$ models on bipartite lattices. This established a connection to the AKLT states, which are nondegenerate in the bulk and which exist only for $S=2M$ on the square lattice.

For the simplex solids, a corresponding result holds. Recall the $N=3$, $M=1$ model on the Kagomé lattice, where each site is in the fully symmetric, six-dimensional $\square\square$ representation, whose wave function $|\Psi\rangle$ is given in Eq. (25). Along a (10) edge, as in Fig. 2, the edge sites each belong to a single simplex. Hence, they are each deficient by one Schwinger boson. The freedom to supply this missing boson on each edge site is equivalent to having a free edge spin in the fundamental representation at every site. Thus, as in the SU(2) AKLT case, the bulk SU(N) representation is "fractionalized" at the edge. The $\square$ objects along the edge are of course noninteracting and degenerate for the SS projection operator Hamiltonian. For general SU(N) models which are in some sense close to the SS model, these objects will interact.

The determination of the interacting boundary Hamiltonian is somewhat tedious. First, one should fix a model which is parametrically close to the SS projection operator Hamiltonian. A natural choice is

$$H = H_0^{\mathrm{SS}} + \lambda \sum_{\langle ij \rangle} \mathrm{Tr}[S(i)S(j)], \tag{88}$$

where H_{SS}^0 is the projection operator Hamiltonian which annihilates the bulk SS state along with its associated manifold of edge states and where the sum is over nearest-neighbor pairs. Since there is a bulk excitation gap for H_{SS}^0, we consider a restricted basis consisting of the degenerate edge states $|\psi_\alpha\rangle$ of the unperturbed SS Hamiltonian. By writing $H=H_0^{\mathrm{SS}}+\lambda H_1$, the energy levels in this restricted basis are obtained by solving

$$\det(\lambda \langle \psi_\alpha | H_1 | \psi_\beta \rangle - E \langle \psi_\alpha | \psi_\beta \rangle) = 0. \tag{89}$$

For the (10) edge of the $S=2$ VBS model on the square lattice, the low-lying edge states are described in terms of an $S=\frac{1}{2}$ object on each edge site. Choosing basis states which are eigenstates of S^z, we can label the edge states by the locations of the $S^z=+\frac{1}{2}$ spins, i.e., in the state $|n_1,n_2,\ldots,n_K\rangle$, the boundary spins with $S^z=+\frac{1}{2}$ are located at n_1, n_2, etc., and all other boundary spins have $S^z=-\frac{1}{2}$. The difficulty lies in the fact that this basis, while complete for the degenerate ground states of H_{VBS}^0, is not orthogonal. There will be a finite overlap between any two such states with the same value of S_{total}^z. To be sure, overlaps such as $\langle n_1,n_2,n_3|n_1',n_2',n_3'\rangle$ can be written as sums of terms which each decay exponentially with the distances $|n_i-n_j'|$. Still, the boundary Hamiltonian will formally involve multisite interactions and any reduction to a nearest-neighbor Heisenberg-type model will entail several approximations.

IX. CONCLUSIONS

I have described here a natural generalization of the AKLT valence bond solid states for SU(2) quantum antiferromagnets. The new simplex solid states $|\Psi(\mathcal{L};M)\rangle$ are defined by the application of N-site SU(N) singlet creation operators $\mathcal{R}_\Gamma^\dagger$ to N-site simplixes Γ of a particular lattice. For each lattice, a hierarchy of SS states is defined, parametrized by an integer M, which is the number of singlet operators per simplex. The SS states admit a coherent state description in terms of CP^{N-1} variables, and using the coherent states, one finds that the equal-time correlations in $|\Psi(\mathcal{L};M)\rangle$ are equivalent to the finite temperature correlations of an associated classical CP^{N-1} spin Hamiltonian H_{cl} and on the same lattice. The fictitious temperature is $T=1/M$, and a classical ordering at T_c corresponds to a quantum phase transition as a function of the parameter M. This transition was investigated using a simple mean field approach. I further argued that for $N>2$, the ordered structure is selected by an order by disorder mechanism, which, in the classical model, amounts to an entropic favoring of one among many degenerate $T=0$ structures. I hope to report on classical Monte Carlo study of H_{cl} on Kagomé ($N=3$) and pyrochlore ($N=4$) lattices in a future publication; there, the coherent state formalism derived here will be more extensively utilized. Finally, a kind of fractionalization of the bulk SU(N) representation at the edge was discussed.

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APPENDIX A: PROPERTIES OF SU(N) COHERENT STATES

1. Definition of SU(N) coherent states

Consider the fully symmetric representation of SU(N) with p boxes in a single row (I call the p representation) of dimension $\binom{N+p-1}{p}$. Define the state

$$|z;p\rangle = \frac{1}{\sqrt{p!}}(z_1 b_1^\dagger + \cdots + z_N b_N^\dagger)^p |0\rangle, \tag{A1}$$

where $z \in \mathrm{CP}^{N-1}$ is a complex unit vector, with $z^\dagger z = 1$. In order to establish some useful properties regarding the SU(N) coherent states, it is convenient to consider the unnormalized coherent states

$$|z,\xi) = \exp(\xi z_\mu b_\mu^\dagger)|0\rangle = \sum_{p=0}^{\infty} \frac{\xi^p}{\sqrt{p!}}|z;p\rangle. \tag{A2}$$

Clearly, $|z,\xi)$ is a product of N (un-normalized) coherent states for the N Schwinger bosons. One then has

$$(z,\xi|z',\xi') = \exp(\bar{\xi}\xi' z^\dagger z') = \sum_{p=0}^{\infty} \frac{(\bar{\xi}\xi)^p}{p!}\langle z;p|z';p\rangle. \tag{A3}$$

Equating the coefficients of $(\bar{\xi}\xi)^p$, one obtains the coherent state overlap

$$\langle z;p|z';p\rangle = (z^\dagger z')^p. \tag{A4}$$

2. Resolution of identity

Define the measure

$$d\mu = \prod_{j=1}^{N} \frac{d\,\mathrm{Re}(z_j)\, d\,\mathrm{Im}(z_j)}{\pi}\delta(z^\dagger z - 1). \tag{A5}$$

Next, consider the expression

$$\mathcal{P}(\xi,\bar{\xi}) = \int d\mu\, |z,\xi)(z,\xi| = \sum_{n_1\cdots n_N} \frac{(\bar{\xi}\xi)^{\Sigma_j n_j}}{\prod_j n_j!} I^N_{n_1\cdots n_N} |\boldsymbol{n}\rangle\langle\boldsymbol{n}|$$

$$= \sum_{p=0}^{\infty} \frac{(\bar{\xi}\xi)^p}{p!} \int d\mu\, |z;p\rangle\langle z;p|, \tag{A6}$$

where $|\boldsymbol{n}\rangle = |n_1,\ldots,n_N\rangle$ and

$$I^N_{n_1\cdots n_N} \equiv \int_0^1 dx_1 \cdots \int_0^1 dx_N\, \delta\left(\sum_{j=1}^{N} x_j - 1\right)\prod_{j=1}^{N} x_j^{n_j}. \tag{A7}$$

Here, $x_j = |z_j|^2$. If we define $x_j = (1-x_N)y_j$ for $j = 1,\ldots,N-1$, then by integrating over x_N, one obtains the result

$$I^N_{n_1\cdots n_N} = I^{N-1}_{n_1\cdots n_{N-1}} \int_0^1 dx_N\, x_N^{n_N}(1-x_N)^{N-2+\Sigma_{j=1}^{N-1} n_j}$$

$$= \frac{n_N!\left(N-2+\sum_{j=1}^{N-1} n_j\right)!}{\left(N-1+\sum_{j=1}^{N-1} n_j\right)!} I^{N-1}_{n_1\cdots n_{N-1}}$$

$$= \frac{n_1!\cdots n_N!}{(N-1+n_1+\cdots+n_N)!}. \tag{A8}$$

Thus, equating the coefficient of $(\bar{\xi}\xi)^p$ in Eq. (A6), one arrives at the result

$$\mathbb{1}_p = \frac{(N-1+p)!}{p!}\int d\mu\, |z;p\rangle\langle z;p|, \tag{A9}$$

where the projector onto the p representation is

$$\mathbb{1}_p \equiv \sum_{n_1\cdots n_N} \delta_{p,\Sigma_j n_j} |\boldsymbol{n}\rangle\langle\boldsymbol{n}|. \tag{A10}$$

3. Continuous representation of a state $|\psi\rangle$

Let us define the state

$$|\psi\rangle \equiv \frac{1}{\sqrt{p!}}\psi(b_1^\dagger,\ldots,b_N^\dagger)|0\rangle = \frac{1}{\sqrt{p!}}{\sum_{\boldsymbol{n}}}'\, \psi_{\boldsymbol{n}}\, b_1^{\dagger n_1}\cdots b_N^{\dagger n_N}|0\rangle, \tag{A11}$$

where $\boldsymbol{n} = \{n_1,\ldots,n_N\}$ and where the prime on the sum reflects the constraint $\Sigma_{j=1}^N n_j = p$. The overlap of $|\psi\rangle$ with the coherent state $|z;p\rangle$ is

$$\langle z;p|\psi\rangle = {\sum_{\boldsymbol{n}}}'\, \psi_{\boldsymbol{n}}\, \bar{z}_1^{n_1}\cdots\bar{z}_N^{n_N} \tag{A12}$$

$$= \psi(\bar{z}_1,\ldots,\bar{z}_N). \tag{A13}$$

4. Matrix elements of representation-preserving operators

Next, consider matrix elements of the general representation-preserving operator,

$$\hat{T}_K = {\sum_{\boldsymbol{m},\boldsymbol{n}}}'\, T_{\boldsymbol{k},\boldsymbol{l}}\, b_1^{k_1}\cdots b_N^{k_N} b_1^{\dagger l_1}\cdots b_N^{\dagger l_N}. \tag{A14}$$

Here, the prime on the sum indicates the constraint $\Sigma_{j=1}^N k_j = \Sigma_{j=1}^N l_j = K$. Then,

$$\langle\phi|\hat{T}_K|\psi\rangle = \frac{1}{p!}{\sum_{\substack{\boldsymbol{m},\boldsymbol{n}\\ \boldsymbol{k},\boldsymbol{l}}}}''\, T_{\boldsymbol{k},\boldsymbol{l}}\,\phi^*_{\boldsymbol{m}}\psi_{\boldsymbol{n}}\prod_{j=1}^{N}[(m_j+k_j)!\,\delta_{m_j+k_j,n_j+l_j}], \tag{A15}$$

where the double prime on the sum indicates constraints on each of the sums for $\boldsymbol{m}$, $\boldsymbol{n}$, $\boldsymbol{k}$, and $\boldsymbol{l}$. This may also be computed as an integral over coherent state wave functions:

$$\int d\mu \bar{\phi}(z) T_K(z,\bar{z}) \psi(\bar{z}) = \sum_{\substack{m,n \\ k,l}} \bar{\phi}_m T_{k,l} \psi_n \prod_{j=1}^{N} z_j^{m_j+k_j} \bar{z}_j^{n_j+l_j}$$

$$= \sum_{\substack{m,n \\ k,l}}{}'' I^N_{m+k} \bar{\phi}_m T_{k,l} \psi_n \prod_{j=1}^{N} \delta_{m_j+k_j,n_q+l_n}$$

$$= \frac{p!}{(N-1+p+K)!} \langle \phi | \hat{T}_K | \psi \rangle. \quad \text{(A16)}$$

Thus, the general matrix element may be written as

$$\langle \phi | \hat{T}_K | \psi \rangle = \frac{(N-1+p+K)!}{p!} \int d\mu \bar{\phi}(z) T_K(z,\bar{z}) \psi(\bar{z}), \quad \text{(A17)}$$

where $T_K(z,\bar{z})$ is obtained from Eq. (A14) by the substitutions $b_j \to z_j$ and $b_j^\dagger \to \bar{z}_j$.

APPENDIX B: THE LOCAL MEAN FIELD

With the definition of Eq. (59), I first compute

$$R_N(m) \equiv \mathcal{Q}^{(1)} \wedge \cdots \wedge \mathcal{Q}^{(N)}$$

$$= \epsilon^{\alpha_1 \cdots \alpha_N} \epsilon^{\beta_1 \cdots \beta_N} \left(\frac{1-m}{N} \delta_{\alpha_1 \beta_1} + m P^1_{\alpha_1 \beta_1} \right)$$

$$\cdots \left(\frac{1-m}{N} \delta_{\alpha_N \beta_N} + m P^N_{\alpha_N \beta_N} \right), \quad \text{(B1)}$$

where

$$P^\sigma_{\alpha\beta} = \omega^\sigma_\beta \bar{\omega}^\sigma_\alpha \quad \text{(B2)}$$

is the projector onto subspace spanned by ω^σ. I now systematically expand in powers of the projectors and contract over all free indices. The result is

$$R_N(m) = N! \sum_{j=0}^{N} \frac{m^l}{j!} \left(\frac{1-m}{N} \right)^{N-j}.$$

The local mean field on a $j=1$ site is given by the expression in Eq. (61). Expanding the numerator,

$$R_N(m) h^N_{\alpha_N \beta_N} = \epsilon^{\alpha_1 \alpha_2 \cdots \alpha_N} \epsilon^{\beta_1 \beta_2 \cdots \beta_N} \mathcal{Q}^{(1)}_{\alpha_1 \beta_1} \cdots \mathcal{Q}^{(N-1)}_{\alpha_{N-1} \beta_{N-1}}, \quad \text{(B3)}$$

in powers of the projectors, the term of order j is

$$(N-j-1)! \left(\frac{1-m}{N} \right)^{N-j-1} m^j \epsilon^{\alpha_1 \alpha_2 \cdots \alpha_N}$$

$$\times \epsilon^{\beta_1 \beta_2 \cdots \beta_N} \sum_{k_1 < \cdots < k_j < N} P^{k_1}_{\alpha_1 \beta_1} P^{k_2}_{\alpha_2 \beta_2} \cdots P^{k_{N-1}}_{\alpha_{N-1} \beta_{N-1}}. \quad \text{(B4)}$$

Writing

$$\epsilon^{\alpha_1 \alpha_2 \cdots \alpha_N} \epsilon^{\beta_1 \beta_2 \cdots \beta_N} = \sum_{\sigma \in \mathcal{S}_N} \mathrm{sgn}(\sigma) \delta_{\alpha_1 \beta_{\sigma(1)}} \cdots \delta_{\alpha_N \beta_{\sigma(N)}}, \quad \text{(B5)}$$

we see that once this is inserted into Eq. (B4), the only surviving permutations are the identity and the $(N-1)$ two cycles which include index N. All other permutations result in contractions of indices among orthogonal projectors, and hence yield zero. Furthermore, using completeness, we have

$$\sum_{i=1}^{N-1} P^i_{\beta_N \alpha_N} = \delta_{\beta_N \alpha_N} - P^{(N}_{\beta_N \alpha_N}. \quad \text{(B6)}$$

Thus,

$$\epsilon^{\alpha_1 \alpha_2 \cdots \alpha_N} \epsilon^{\beta_1 \beta_2 \cdots \beta_N} \sum_{k_1 < \cdots < k_j < N} P^{k_1}_{\alpha_1 \beta_1} P^{k_2}_{\alpha_2 \beta_2} \cdots P^{k_{N-1}}_{\alpha_{N-1} \beta_{N-1}}$$

$$= \binom{N-1}{j} \delta_{\beta_N \alpha_N} - \sum_{k_1 < \cdots < k_j < N} \sum_{l=1}^{j} P^{k_l}_{\beta_N \alpha_N}$$

$$= \binom{N-1}{j} \delta_{\beta_N \alpha_N} - \binom{N-2}{j-1} (\delta_{\beta_N \alpha_N} - P^N_{\beta_N \alpha_N})$$

$$= \binom{N-2}{j} \delta_{\beta_N \alpha_N} + \binom{N-2}{j-1} P^N_{\beta_N \alpha_N}. \quad \text{(B7)}$$

From this expression, I obtain the results of Eqs. (62)–(65).

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