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Flux expulsion and greedy bosons: Frustrated magnets at large N

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Abstract. – We investigate the $Sp(N)$ mean-field theory for frustrated quantum magnets. First, we establish some general properties of its solutions; in particular, for small spin we propose simple rules for determining the saddle points of optimal energy. We then apply these insights to the pyrochlore lattice. For spins on a single tetrahedron, we demonstrate a continuous ground-state degeneracy for any value of the spin length. For the full pyrochlore lattice, this degeneracy translates to a large number of near-degenerate potential saddle points. Remarkably, it is impossible to construct a saddle point with the full symmetry of the Hamiltonian —at large N, the pyrochlore magnet *cannot* be a spin liquid. Nonetheless, for realistic finite values of N, tunnelling between the nearly degenerate saddle points could restore the full symmetry of the Hamiltonian.

Introduction. – The behavior of quantum magnets with strong frustration [1] is one of the central open questions in the study of modern magnetism. The most celebrated members of this class of problems are the nearest-neighbor Heisenberg antiferromagnets on the kagome and pyrochlore lattices and the challenge is to work out their phases at varying values of the spin S and temperature T. At large S, semiclassical computations become feasible if not straightforward [2]. Small spins have typically been treated by entirely separate methods, and for the case of the pyrochlore lattice these have involved starting from a symmetry-breaking decomposition of the lattice [3].

As a complement to this work, we employ a large-N method that can be applied over the full range of S and, particularly for the work described in this paper, allows us to keep all symmetries in the formalism at small S. Specifically, we consider the enlargement of the $SU(2) \equiv Sp(1)$ symmetry group of the Heisenberg model to $Sp(N)$. In the limit $N \to \infty$, the problem reduces to a mean-field theory for Schwinger bosons [4–6]. The mean-field theory can be improved by evaluating $1/N$ corrections. This method has been applied to the kagome

lattice [7] and found to predict a robust selection of a magnetically ordered state at large S melting into a disordered spin-liquid state at small S.

We first establish some general properties of mean-field ground states of $\mathrm{Sp}(N)$ magnets on regular lattices at small values of spin. The main variables of the mean-field theory are complex numbers Q_{ij} defined on links (ij) of the lattice and representing probability amplitudes of finding a valence-bond singlet. We derive a perturbative loop expansion, wherein spin length is used as a small parameter. To the lowest nontrivial order, valence bonds are found *exclusively* on links with largest exchange coupling. At higher orders, we find that a $U(1)$ flux, constructed from phases of the valence-bond amplitudes, tends to be expelled. These observations systematize previous results obtained for several quantum antiferromagnets in the large-N framework [7].

We then discuss the case of the pyrochlore antiferromagnet where we report three principal results: i) For a single tetrahedron, the two-parameter degeneracy of classical spins persists for *any* spin length despite the quantum effects encoded in the $\mathrm{Sp}(N)$ computation! ii) All of these solutions break a symmetry —spatial or time reversal— and exhibit bond or chiral order. iii) Embedding such states in the pyrochlore lattice results in a vast number of solutions whose energies are very close to one another at small spin. This behavior is fundamentally different from the triangular and kagome lattices, where the principle of flux expulsion alone was sufficient to fix the ground states. The import of ii) and iii) is that, if the pyrochlore lattice is indeed a spin liquid at $N = 1$, this will necessarily require tunnelling between saddle points. Such a scenario is not at all unlikely.

$\mathrm{Sp}(N)$ *Hamiltonian.* – The Hamiltonian of an $\mathrm{Sp}(N)$ antiferromagnet may be written as [7]

$$H = -(1/2N) \sum_{\langle ij \rangle} J_{ij} \mathcal{A}_{ij}^{\dagger} \mathcal{A}_{ij}, \qquad \mathcal{A}_{ij} = \varepsilon_{\alpha\beta} b_{i\alpha} b_{j\beta}. \tag{1}$$

The antisymmetric tensor $\varepsilon_{\alpha\beta}$ is a block-diagonal $2N \times 2N$ matrix

$$\varepsilon = \begin{pmatrix} i\sigma_y & 0 & \cdots \\ 0 & i\sigma_y & \cdots \\ \vdots & \vdots & \end{pmatrix} \tag{2}$$

and σ_y is the 2×2 Pauli matrix. Here, $b_{i\alpha}$ is the annihilation operator of a boson of species α at site i. For $N = 1$, eq. (1) reduces to the $SU(2)$ Heisenberg Hamiltonian written in terms of Schwinger bosons, related to spin operators via $S_i^a = b_{i\alpha}^{\dagger} \sigma_{\alpha\beta}^a b_{i\beta}/2$ (a sum over doubly repeated flavor indices is implied); the number of bosons determines the spin length: $b_{i\alpha}^{\dagger} b_{i\alpha} = 2S$. In the large-$N$ generalization, the spin length is related to the number of bosons *per flavor* [7] $\kappa \equiv b_{i\alpha}^{\dagger} b_{i\alpha}/N$.

Mean-field approximation. – The $\mathrm{Sp}(N)$ mean-field equations [6], which become exact for $N \to \infty$, involve a decoupling of the quartic terms in eq. (1) with the aid of the link variables $\langle b_{i\alpha} b_{j\beta} \rangle = Q_{ij} \varepsilon_{\alpha\beta}/2$:

$$H_{\mathrm{MF}} = (J_{ij}/2) \sum_{\langle ij \rangle} \left(N|Q_{ij}|^2 - Q_{ij} \varepsilon_{\alpha\beta} b_{i\alpha}^{\dagger} b_{j\beta}^{\dagger} - Q_{ij}^* \varepsilon_{\alpha\beta} b_{i\alpha} b_{j\beta} \right) + \sum_i \lambda_i (b_{i\alpha}^{\dagger} b_{i\alpha} - \kappa N). \tag{3}$$

The chemical potential λ_i keeps the average number of bosons fixed at κN on every site. The mean-field equations are $\partial \langle H_{\mathrm{MF}} \rangle / \partial \lambda_i = 0$ (constraints on the boson numbers) and $\partial \langle H_{\mathrm{MF}} \rangle / \partial Q_{ij} = 0$ (minimization of energy).

The mean-field Hamiltonian (3) is a sum of N identical copies, each containing two flavors only (up and down in the Schwinger-boson language). The energy of each copy is $\mathcal{O}(1)$ in N. Therefore, two different vacua will have an energy difference $\mathcal{O}(N)$, *i.e.*, well separated in the limit $N \to \infty$ considered here. The low-lying excitations are $S = 1/2$ bosons (spinons) whose energy is $\mathcal{O}(1)$.

For a total of $\mathcal{N}$ sites, this Hamiltonian can, for each pair of flavors, be written in terms of $\mathcal{N}$-component row vectors $b_{i\uparrow}^\dagger$ and $b_{i\downarrow}$, column vectors $b_{i\uparrow}$ and $b_{i\downarrow}^\dagger$, and $\mathcal{N} \times \mathcal{N}$ matrices $P_{ij} = J_{ij}Q_{ij}/2$ and $\Lambda_{ij} = \lambda_i\delta_{ij}$. A Bogoliubov transformation diagonalizes the part quadratic in bosons and yields a diagonal matrix of eigenfrequencies Ω for the bosonic spinons giving the energy per flavor

$$\langle H_{\mathrm{MF}}\rangle/N = \mathrm{Tr}\left[PQ^\dagger/2 - (\kappa + 1)\Lambda + \Omega\right]. \tag{4}$$

Uniform λ. – In the remainder of this paper we consider the mean-field theory with two restrictions. Firstly, we have tacitly assumed the absence of a condensate of bosons, $\langle b_{i\alpha}\rangle \equiv 0$. (This translates into the lack of magnetic order, $\langle \boldsymbol{S}_i\rangle = 0$, for $SU(2)$ spins.) This regime, dominated by quantum fluctuations, always exists for small values of spin length κ [4,7]. In addition, we will only consider states with uniform chemical potential, so that $\Lambda = \lambda\mathbf{1}$, where $\mathbf{1}$ is the $\mathcal{N} \times \mathcal{N}$ unit matrix. This simplifies calculations as matrices Λ and P commute.

With the said restrictions, the boson spectrum Ω_n can be obtained from the eigenvalues ν_n^2 of the matrix $PP^\dagger$:

$$\Omega_n = \sqrt{\lambda^2 - \nu_n^2}, \qquad \det\left(PP^\dagger - \nu_n^2\mathbf{1}\right) = 0. \tag{5}$$

The expectation value of the Hamiltonian is then

$$\langle H_{\mathrm{MF}}\rangle/N = \mathrm{Tr}\left[PQ^\dagger/2 + \sqrt{\lambda^2\mathbf{1} - PP^\dagger} - \lambda(1+\kappa)\mathbf{1}\right].$$

The boson-number constraint gives the condition

$$1 + \kappa = \mathrm{Tr}\left[(\mathbf{1} - PP^\dagger/\lambda^2)^{-1/2}\right]/\mathrm{Tr}\,\mathbf{1}. \tag{6}$$

A scaling transformation $Q_{ij} \to aQ_{ij}$, $\lambda \to a\lambda$ does not affect the constraint equation (6). Minimization of the energy determines the optimal scale a and yields

$$\frac{\langle H\rangle}{N} = -\frac{\left\{\mathrm{Tr}\left[\left(PP^\dagger/\lambda^2\right)\left(1 - PP^\dagger/\lambda^2\right)^{-1/2}\right]\right\}^2}{2\,\mathrm{Tr}\left(PQ^\dagger/\lambda^2\right)}. \tag{7}$$

Further minimization of the vacuum energy (7) is done by varying the relative strengths and phases of the link variables Q_{ij}, subject to constraint (6). Our *ad hoc* assumption of a uniform chemical potential restricts the choice of trial states in that all sites must be equivalent.

Loop expansion at small κ. – The structure of the mean-field equations (6) and (7) suggests a solution by expansion in powers of $PP^\dagger/\lambda^2$. Taking the trace makes it a loop expansion: a generic term of the Taylor-expanded right-hand side of eq. (6) has the form

$$\mathrm{Tr}\left(PP^\dagger\right)^n = \sum_{a\ldots z} P_{ab}(-P_{bc}^*)\ldots P_{yz}(-P_{za}^*) \equiv \Xi e^{i\Phi}, \tag{8}$$

where we have accounted for antisymmetry, $P_{cb} = -P_{bc}$. Expressions for κ and $E = \langle H\rangle$ involve sums over all possible closed loops $abc\ldots za$ of even length. The $U(1)$ flux Φ defined in eq. (8) will play an important role below [8].

Convergence is particularly good when spinons have a short correlation length, as is the case for small κ. In this limit, the physics is determined by the shortest loops. Formally, the loop expansion is a series in powers of κ. In the following paragraphs, we develop the loop expansion and demonstrate that it leads to simple organizing principles for the behavior of $\mathrm{Sp}(N)$ antiferromagnets in the quantum limit of small κ. A variant of this strategy at high temperatures has been described previously [9].

Shortest loops, greedy bosons. – The lowest order in $PP^\dagger/\lambda^2$ yields the energy per site, per flavor:

$$\frac{\langle H \rangle}{\mathcal{N}N} = -\kappa \, \frac{\mathrm{Tr}\left(PP^\dagger\right)}{\mathrm{Tr}\left(PQ^\dagger\right)} = -\frac{\kappa}{2} \, \frac{\sum_{\langle ij \rangle} J_{ij}^2 |Q_{ij}|^2}{\sum_{\langle ij \rangle} J_{ij} |Q_{ij}|^2}. \tag{9}$$

To leading order ("loops" of length 2), the energy depends on the absolute values, but not the phases of the link variables Q_{ij}. Minimization can be easily done if one interprets $J_{ij}|Q_{ij}|^2$ as a probability distribution. The energy is then simply the expectation value of $-\kappa J_{ij}/2$. An optimal probability distribution then will have zero probabilities $J_{ij}|Q_{ij}|^2$ for all links *except* those with the largest J_{ij}. For example, on a square lattice with first- and second-neighbor couplings $J_1, J_2 > 0$, the second-neighbor bonds will vanish, $Q_2 = 0$, if $J_1 > J_2$; similarly, $Q_1 = 0$ if $J_1 < J_2$ in this approximation. Hence

> THEOREM (greedy bosons): in the limit of small κ, bosons form bonds $Q_{ij} \neq 0$ on the links with the largest J_{ij} only.

For small but finite κ, there will be three phases: i) $Q_2 = 0$ for J_2/J_1 below a critical value $(J_2/J_1)_{c1} < 1$; ii) $Q_1 = 0$ for J_2/J_1 above another critical value $(J_2/J_1)_{c2} > 1$; and iii) coexisting $Q_1 \neq 0$ and $Q_2 \neq 0$ for intermediate values of J_2/J_1.

Longer loops, flux expulsion. – The terms of order $(PP^\dagger)^2$ represent loops containing up to 4 links. For a single (*e.g.*, nearest-neighbor) nonzero exchange constant J, $PQ^\dagger = 2PP^\dagger/J$ and the energy, to this order, is

$$\frac{\langle H \rangle}{\mathcal{N}N} = -\frac{\kappa J}{2} - \frac{\kappa^2 J}{4} \, \frac{\mathrm{Tr}\left[\left(PP^\dagger\right)^2\right] \mathrm{Tr}\, 1}{\left[\mathrm{Tr}\left(PP^\dagger\right)\right]^2}. \tag{10}$$

For a fixed "norm" $\mathrm{Tr}(PP^\dagger) = \sum_{\langle ij \rangle} J_{ij}^2 |Q_{ij}|^2$, lower energy means larger $\mathrm{Tr}(PP^\dagger PP^\dagger)$. This can be achieved by tuning the *phases* of link fields Q_{ij}, as the contributions to $\mathrm{Tr}(PP^\dagger PP^\dagger)$ from loop *abcda* and its reverse are $P_{ab}P_{bc}^* P_{cd} P_{da}^* + \mathrm{C.c.} = 2\Xi \cos\Phi$, cf. eq. (8). Clearly, for fixed magnitudes $|P_{ij}|$, the trace is maximized —and energy is minimized— when the flux Φ vanishes.

This establishes the principle of flux expulsion for the shortest nontrivial loops (length 4). As the loop expansion at small κ is organised by loop length, this principle provides the correct ground state as the (ideally, only) one in which all loops up to a certain length contain no flux. For example, it uniquely determines the $\mathrm{Sp}(N)$ ground states observed for the uniform triangular and kagome antiferromagnets [7].

More generally, we can formulate a conjecture on the behavior of longer loops. It provides *all* gauge-invariant information about the phases of link variables Q_{ij}.

> CONJECTURE (flux expulsion): in the ground state, the flux Φ is zero through all closed loops of even length, provided such a fluxless state is possible.
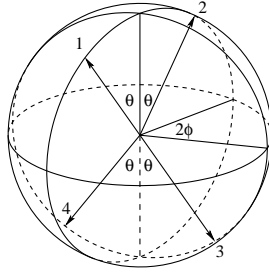
Fig. 1 – The two-parameter family of ground states of a single tetrahedron. The four spins combine to give zero total spin.

Keep in mind that the *tendency to expel* flux does not always guarantee the actual *absence* of flux. If the lattice is not bipartite, fluxes may be frustrated and will not be expelled from every loop. This happens already for the triangular and kagome cases and for the latter this makes the selection more delicate than believed previously [10]. It happens with a vengeance on the pyrochlore lattice.

Pyrochlore I: the single tetrahedron. – The shortest loop (of even length) on the pyrochlore lattice contains four links and is confined to a single tetrahedron. There are, in fact, three such loops on every tetrahedron and it can be verified that the sum of their fluxes equals π (unless some link amplitudes vanish). The fluxes are thus frustrated and cannot be expelled from all three loops. Unlike in all previously studied systems, the principle of flux expulsion does not point to a unique ground state.

In fact, for the single tetrahedron, we find a two-parameter family of ground states, all with exactly the same mean-field energy $E/(JN\mathcal{N}) = -\kappa(\kappa+1)/2$. These have link variables

$$
\begin{aligned}
Q_{12} = Q_{34} &= \sqrt{\kappa(\kappa+1)}\sin\theta, \\
Q_{13} = Q_{24} &= \sqrt{\kappa(\kappa+1)}(\cos\phi - i\cos\theta\sin\phi), \\
Q_{14} = Q_{23} &= \sqrt{\kappa(\kappa+1)}(\cos\theta\cos\phi - i\sin\phi).
\end{aligned}
\tag{11}
$$

This is quite remarkable as one of the charms of $\mathrm{Sp}(N)$ is its capacity to yield *unique* quantum disordered states at small κ —indeed, this is the first counterexample! Remarkably, there is a mapping between these ground states and those of *classical* Heisenberg spins on a tetrahedron, which can be constructed by a) parametrizing the ground states as shown in fig. 1, b) representing the spins $\boldsymbol{S}_i$ by two-component spinors $\psi_{i\alpha}$ and c) translating the spinors into link variables $Q_{ij} \propto \varepsilon_{\alpha\beta}\psi_{i\alpha}\psi_{j\beta}$.

Possible orders. – All of these mean-field ground states violate a symmetry of the Hamiltonian (1): a point-group symmetry, time reversal, or both. These symmetry breakings are best illustrated by the sets of states which break only a single symmetry.

First, breaking the symmetry group of the tetrahedron T_d, are three *bond-ordered* states with maximally inhomogeneous bond amplitudes, *e.g.* $Q_{12} = Q_{34} = 0$ and $Q_{13} = Q_{24} = Q_{14} = Q_{23} \neq 0$. These we call the "collinear" states, as their classical counterparts have collinear spins (fig. 2(a)). The flux through loop 13241 vanishes; the other two fluxes are ill-defined. The valence-bond order parameter characterizing the broken symmetry is described in refs. [11] and [12].

Second, are states which leave the spatial symmetry intact but break the time-reversal symmtery. These have $\theta = \frac{1}{2}\arccos(-1/3)$, $\phi = \pm\pi/4$. They distribute the flux π equally
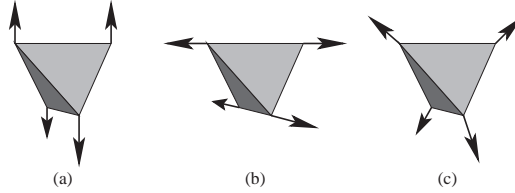
Fig. 2 – Trial ground states of the single tetrahedron: (a) collinear, (b) coplanar, (c) anticollinear.

between the three loops, each receiving either $+\pi/3$ or $-\pi/3$. The classical analogs of the two states have spins pointing at equal angles of $\arccos(-1/3) \approx 109°$ to each other (fig. 2(c)). The order parameter is spin *chirality* $\chi = \langle \boldsymbol{S}_a \cdot (\boldsymbol{S}_b \times \boldsymbol{S}_c) \rangle$, where abc is an oriented face of the tetrahedron [12, 13].

Pyrochlore II: the full lattice. – The pyrochlore lattice is a network of corner-sharing tetrahedra. In the loop expansion up to $\mathcal{O}(\kappa^2)$, the system behaves as if it were made up of disjoint simplices: the energy is minimized as long as each tetrahedron is in any of its ground states (11). This extremely large degeneracy will be lifted, at least partially, at $\mathcal{O}(\kappa^3)$, which includes loops enclosing the hexagons of the pyrochlore lattice. In the spirit of degenerate perturbation theory, we must minimize the terms $\mathcal{O}(\kappa^3)$ among all such possible states. This is a problem of considerable complexity [14].

On a first approach we have minimized the energy over a restricted set of trial states in which all tetrahedra are in the same state (11). Evaluation of the energy for a finite cluster shows that, in accordance with our earlier conjecture, the energy reaches a minimum when the hexagons enclose zero flux; this choice is similar to Sachdev's $Q_1 = -Q_2$ state on the kagome [7].

We obtain the following energies per site for the ground states derived from classical spin states shown in fig. 2:

$$\frac{E}{JN\mathcal{N}} = -\frac{\kappa}{2} - \frac{\kappa^2}{2} - \begin{cases} 0.18750\kappa^3, & \text{fig. 2(a)}, \\ 0.19922\kappa^3, & \text{fig. 2(b)}, \\ 0.20139\kappa^3, & \text{fig. 2(c)}. \end{cases} \qquad (12)$$

The energy is lowest in the state with equal link amplitudes that is related to the classical state with equal angles between the spins (fig. 2(c)). We have evaluated the energy difference between the states (a) and (c) analytically and found that $(E_{(a)} - E_{(c)})/(JN\mathcal{N}) = \kappa^3/72$. Note that the splitting is rather small: for the nominal equivalent of spin $1/2$ ($\kappa = 1$), the energies per spin differ by about one percent of the exchange constant. The order-from-disorder effect is extremely weak.

Unfortunately, we have been unable to prove that the state described above is indeed the state of lowest energy, for we have discovered another state with the same energy at $\mathcal{O}(\kappa^3)$. Without going into details, we note that the other state has a larger unit cell and contains tetrahedra with "coplanar" spins (fig. 2(b)).

Outlook. – We have learned that finding *the* ground state of the $\mathrm{Sp}(N)$ pyrochlore antiferromagnet is a hard problem. For all previously studied systems, our method yields unique ground states in agreement with numerical minimizations at lowest non-trivial order in κ. In contrast, simplices of the pyrochlore have continuously degenerate ground states. Apart from flux expulsion, there is no simple principle that can guide the search for the ground state in this case.

At the same time, our study has produced some useful insights. First and foremost, we find that there is no ground state retaining the full symmetry of the Hamiltonian; such a state is already ruled out at the level of a single tetrahedron, in a controlled fashion at small κ. *In* $\mathrm{Sp}(N)$, *there is no spin liquid on the pyrochlore lattice at zero temperature.* Furthermore, there is a huge number of nearly degenerate saddle points, which are not related by a symmetry, with a splitting $\mathcal{O}(\kappa^3)$. These small splittings suggest that determining the precise nature of the symmetry breaking is going to be very hard and, for experimental systems, exquisitely sensitive to small additional terms in the Hamiltonian.

In the large-N treatment, tiny energy differences between saddle points are made infinite as they come with a large prefactor $N \to \infty$. In practice, $N = 1$, and therefore local tunneling events will probably play a role. Whereas individual saddle points do break symmetries, tunneling can lead to symmetry restoration. At the end of our investigation, we therefore have to declare ourselves agnostic as to the eventual fate of the quantum pyrochlore magnet at zero temperature. Whatever order may be present there will likely melt rapidly at finite temperature.

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