Klein spin model ground states on general lattices

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We prove that in short range Klein spin models on general lattices, all ground states are of the dimer type—each fundamental plaquette must host at least one singlet. These ground states are known to rigorously exhibit high dimensional fractionalization. When combined with a recent theorem, this establishes that Klein spin models exhibit topological order on the pyrochlore and checkerboard lattices.

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INTRODUCTION

In this article, we illustrate that in general short range Klein type spin models, all ground states must be of the valence bond type. This will allow us to establish high dimensional fractionalization in these systems. We start with a concise definition of the Klein model Hamiltonian

\[ H = J \sum_{\square} P_{S_{\square}} = S_{\text{max}} \quad (J > 0), \]

Here, \( P_{S_{\square}} = S_{\text{max}} \) the projection operator onto the space with maximal spin. For instance, for a spin \( S = 1/2 \) system on a square lattice, \( \square \) is the elementary four site plaquette; here, we project onto the state of spin \( S_{\text{max}} = 4 \times 1/2 = 2 \). Explicit forms for Klein models for the hexagonal, square, decorated and general other lattices, extension of \( \square \) to \( S = \frac{1}{3} \), and a slightly comprehensive study of pyrochlore lattices are available. In it was first shown how the Klein spin model on the hexagonal lattice, two leg ladders, and on octagonal diamond lattices needed to be of superpositions of only dimer states of the form of Eq. (2). We now prove that this result is universal and holds on a far greater variety of lattices. This proof is the central result of this article.

THE SINGLE PLAQUETTE GROUND STATES

Henceforth, we focus on \( S = 1/2 \) spin systems. On any lattice, a single plaquette state is completely symmetric under all permutations if and only if it lies in the sector of total spin \( S_{\square} = S_{\text{max}} \). As each permutation can be expressed as a product of pair permutations, it follows that

\[ P_{S_{\square}} = S_{\text{max}} | \phi \rangle = 0 \quad (3) \]

iff \( | \phi \rangle \) can be written as a sum of plaquette state with at least one (antisymmetric) singlet state between two sites. Any wavefunction which is orthogonal to all plaquette wavefunctions having, at least, one singlet state must be completely symmetric in all of the spins and therefore lies entirely in \( S_{\square} = S_{\text{max}} \) sector. Far more demanding symmetry/antisymmetry restrictions of the wavefunction on the entire lattice formed the corner stone of the analysis of 2. We will now show that the above single plaquette result leads to the form of the ground state on the entire lattice.

GROUND STATES ON THE ENTIRE LATTICE

We now generalize the single plaquette result to the entire lattice. As (i) the projection operator on any pla-
quetté (□) is non-negative definite,

$$P^2_{\square} = s_{\text{max}} = P_{S} = s_{\text{max}},$$ \hspace{1cm} (4)

(ii) states with one dimer per plaquette have zero energy saturate consequent the low energy bound ($E = 0$) and are thus ground states (yet not obviously the sole ground states), and as (iii) the Hamiltonian is a sum over non-negative definite projection operators over each plaquette, we have that in any ground state $|\psi\rangle$

$$0 = \langle \psi | H | \psi \rangle \geq \langle \psi | P_{S;\square} = s_{\text{max}} | \psi \rangle. \hspace{1cm} (5)$$

Here, □$_i$ is any chosen plaquette $i$. As $\langle \psi | P_{S;\square} = s_{\text{max}} | \psi \rangle \geq 0$, this, of course, mandates that $\langle \psi | P_{S;\square} = s_{\text{max}} | \psi \rangle = 0$ for all plaquettes $i$. Now, by Eq. (4),

$$\langle \psi | P_{S;\square} = s_{\text{max}} | \psi \rangle = \langle \phi_i | \phi_i \rangle,$$

with $|\phi_i\rangle \equiv P_{S;\square} = s_{\text{max}} | \psi \rangle$. \hspace{1cm} (6)

If $\langle \psi | P_{S;\square} = s_{\text{max}} | \psi \rangle = 0$ then $|\phi_i\rangle = 0$. Thus, in the ground state we need to satisfy $|\phi_i\rangle = 0$ for all plaquettes $i$.

We next write the state $|\psi\rangle$ in a general form in the complete orthonormal $\otimes_{r \in \Lambda} \sigma_r^z$ eigenbasis of the entire lattice (Λ)

$$|\psi\rangle = \sum_{\sigma_j^z \not\in \square_i, j} \otimes_{j} |\sigma_j^z\rangle \sum_{\sigma_i^z \in \square_i} \chi(\sigma_j^z; \sigma_i^z) \otimes |\sigma_i^z\rangle. \hspace{1cm} (7)$$

We now write the conditions which we found before

$$0 = P_{S;\square} = s_{\text{max}} |\psi\rangle = \sum_{\sigma_j^z \not\in \square_i, j} \otimes_{j} |\sigma_j^z\rangle \sum_{\sigma_i^z \in \square_i} P_{S;\square} = s_{\text{max}} \chi(\sigma_j^z; \sigma_i^z) \otimes |\sigma_i^z\rangle. \hspace{1cm} (8)$$

Next, let us define

$$|\psi_{\square};\sigma_j^z \not\in \square_i\rangle = \sum_{\sigma_i^z \in \square_i} \chi(\sigma_j^z; \sigma_i^z) \otimes |\sigma_i^z\rangle. \hspace{1cm} (9)$$

If $P_{S;\square} = s_{\text{max}} |\psi;\sigma_j^z \not\in \square_i\rangle = 0$ then, according to our earlier proof of the last section (following Eq. (9)) concerning the single plaquette wavefunctions, $|\psi_{\square};\sigma_j^z \not\in \square_i\rangle$ must be a superposition of states each of which has, at least, one singlet. As this holds for all plaquettes $\square_i$, we must have

$$|\psi_{\square};\sigma_j^z \not\in \square_i\rangle = \sum_{\alpha \beta \in \square_i} c_{\alpha \beta}^{\sigma_j^z \not\in \square_i} \omega_{\alpha \beta} |\sigma_j^z \not\in \square_i\rangle \hspace{1cm} (10)$$

where $\mathcal{P}_{\square}^{\alpha \beta} |\omega_{\alpha \beta} \sigma_j^z \not\in \square_i\rangle = -|\omega_{\alpha \beta} \sigma_j^z \not\in \square_i\rangle$, $\alpha, \beta \in \square_i$. \hspace{1cm} (10)

Here, $\mathcal{P}_{\square}^{\alpha \beta}$ is the operator permuting the two sites $\alpha, \beta \in \square_i$. Every plaquette (□) must therefore have at least one intra-plaquette singlet dimer (or superpositions of states thereof). This concludes our proof.

FIG. 1: (Color online.) From [6]. Highly regular ground states on the checkerboard and pyrochlore lattices. The ovals denote singlet dimer states. The arrows denote the representations of these dimer states within the six–vertex model (see Fig. (4)) wherein on each plaquette (tetrahedron or crossed square) a dimer connects the bases of the two arrows going to the center of the plaquette on which the dimer is found.

On general lattices, all ground states are superpositions of states of the form of Eq. (2). All ground states are superpositions of states which have, at least, one singlet on every plaquette. For $S = 1/2$ Klein models on the square, pyrochlore, or checkerboard lattices endowed with periodic boundary conditions, the most general states satisfying this requirement are of the form

$$|\psi\rangle = \sum_{\alpha \beta \in \square_i} w_{\alpha \beta} \otimes \frac{1}{\sqrt{2}} \left[ |\uparrow_\alpha \downarrow_\beta\rangle - |\downarrow_\alpha \uparrow_\beta\rangle \right]. \hspace{1cm} (11)$$

Here, each lattice site appears in a singlet. An example of one such ground state is shown in Fig. 1.

Key steps in the above proof are (i) the basis states $\otimes_r |\sigma_r^z\rangle$ are linearly independent; this allowed us to impose the condition $|\phi_i\rangle = P_{S;\square} = s_{\text{max}} |\psi\rangle;\sigma_j^z \not\in \square_i\rangle = 0$ for any $\{\sigma_j^z \not\in \square_i\}$, (ii) The projection operator squared is equal to itself, Eq. (4); this led to the condition $|\phi_i\rangle = 0$ for all plaquettes $i$.

A decoration procedure readily allows for a demonstration of a gap between the ground and excited states. \hspace{1cm} (4)

Work in progress reaffirms this result for all lattices.

TOPOLOGICAL ORDER ON THE PYROCHLOR AND CHECKERBOARD LATTICES

To explicitly flesh out some of the more abstract concepts discussed hitherto, we examine the Klein model on the pyrochlore lattice. The Klein Hamiltonian on the pyrochlore and checkerboard lattices is a sum of nearest neighbor interactions augmented by ring exchange terms.
Here, the Hamiltonian is of the form

$$H = J_1 \sum_{\langle ij \rangle, \alpha} \vec{S}_i^\alpha \cdot \vec{S}_j^\alpha + J_2 \sum_\alpha [\vec{S}_i^\alpha \cdot \vec{S}_j^\alpha](\vec{S}_k^\alpha \cdot \vec{S}_l^\alpha) + (\vec{S}_i^\alpha \cdot \vec{S}_l^\alpha)(\vec{S}_j^\alpha \cdot \vec{S}_k^\alpha) + (\vec{S}_i^\alpha \cdot \vec{S}_k^\alpha)(\vec{S}_j^\alpha \cdot \vec{S}_l^\alpha),$$

where \(\langle ij \rangle\) denotes all pairs of sites in the tetrahedron \(\alpha = ijk4\). The Klein model is realized when \(J_2 = 4J_1/5\). On the checkerboard lattice, \(\alpha\) denotes each tetrahedral unit of the pyrochlore lattice or crossed plaquette of the checkerboard lattice with cross-coupling interactions. The first term is equivalent to both nearest- and next-neighbor Heisenberg interactions of strength \(J_1\). The Heisenberg interaction on the tetrahedral units (crossed plaquettes of the checkerboard lattice). A detailed study (wherein fractionalization and criticality were established) of the Klein model that results and fluctuations about it was undertaken in [6]. Some highlights of this study are shown in Figs. [1,2]. As highlighted in Fig. [3], each dimer configuration corresponds to a system of continuous lines in the six-vertex representation. [4, 11, 12]

An operational definition of zero temperature Topological Quantum Order (TQO) [3] in degenerate systems goes as follows: Given a set of \(N\) orthonormal ground states \(\{\phi_\alpha\}_{\alpha=1,...,N}\), TQO exists iff for any bounded operator \(V\) with compact support (i.e. any quasi-local operator),

$$\langle g_\alpha | V | g_\beta \rangle = v \delta_{\alpha \beta} + c,$$

where \(v\) is a constant and \(c\) is a correction that is either zero or vanishes exponentially in the thermodynamic limit. [8, 9] [Thus, in such systems, only non-local “topological” quantities can become items of interest.] Relying on our demonstration that the Klein model only allows for singlet covering ground states (and superstitions thereof) and that a finite spectral gap appears, topological order on Klein spin systems on the pyrochlore and checkerboard lattices follows. To see this, we note that, e.g., on a checkerboard lattice in the sector of a fixed number of lines, imposed by boundary conditions, all states may be linked to each other by a sequence of local symmetry operations. Such a local symmetry operation is shown in Fig. [4]. This emergent local \((d = 0)\) gauge-like symmetry operation in a system with a gap mandates topological quantum order as proved in [3]: Glancing at Eq. (12), we note that as no local symmetry can be broken (Elitzur’s theorem), [10, 15] all diagonal elements of a non-gauge invariant observables \(V\) vanish while all gauge invariant observable \(V\) are the same regardless of the state \(\alpha\); the presence of the gap mandates that the off-diagonal terms of Eq. (12) vanish. Even though, in principle, local observables such \(V = \langle \vec{S}_i^\alpha \cdot \vec{S}_j^\alpha \rangle\) depend on whether or not a dimer exists between sites \(i\) and \(j\) in a given pure dimer state, e.g. \(\langle \phi | \vec{S}_i^\alpha \cdot \vec{S}_j^\alpha | \phi \rangle = -1/4\) in a state \(|\phi\rangle\) having a singlet dimer between sites \(i\) and \(j\), such an operator unfortunately cannot attain a non-zero value once infinitesimal symmetry restoring perturbations are introduced. This is similar to what occurs in a \(Z_2\) gauge theory given by the action \(S = -K \sum_{ijkl} U_{ij} U_{jk} U_{kl} U_{il}\) with the product of gauge fields \(U_{ij} = \pm 1\) taken around the sides of a
plaquette. (The gauge field \( \{ U_{ij} \} \) resides on the link between sites \( i \) and \( j \).) Here, \( U_{ij} \) is different for different \( Z_2 \) gauge configurations. However, by Elitzur’s theorem \( \langle U_{ij} \rangle = 0 \). Similarly, in our case, \( \langle V \rangle = 0 \) just as local observables vanish in gauge theory due to a generalized Elitzur’s theorem applied to the non (local) symmetry invariant quantity \( V \). An intuitive understanding may be gained by mapping Klein model ground states onto \( Z_2 \) gauge theory (\( K < 0 \)) ground states; this (non-invertible) mapping proceeds by replacing a singlet dimer between sites \( i \) and \( j \) within the Klein model to a link with \( U_{ij} = -1 \) in a \( Z_2 \) gauge theory. A complete treatment entails the presence of a transverse like field connecting the different dimer states (similar to a transverse field in \( Z_2 \) gauge theories, e.g. \[14\]). The result generally follows from symmetry considerations. \[9\], \[11\] The line number of the six vertex representation is a conserved topological charge in these systems.

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