The projective symmetry group method: An application to kagome-based frustrated quantum spin systems

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1 Introduction

In 1973 P.W. Anderson proposed a spin liquid state of matter [1]. He realised that the Néel ordered ground state is in principle not the only possible ground state of an Heisenberg antiferromagnet. Anderson reasoned that competing interactions might prevent ordering at low temperatures. On the example of the triangular lattice he proposed so-called resonating valence bond states. Those are super-positions of singlet-pair coverings of the lattice. Today it is believed that the triangular lattice ground state is Néel ordered. The spins manage to align in a 120° fashion [2, 3]. But Anderson started a long lasting search for spin liquids in other materials. After 40 years of research there is some evidence that spin liquid states might exist in other materials. One of the most promising candidates, experimentally, numerically and analytically, is the kagome lattice Heisenberg antiferromagnet [4, 5].

We can not solve the Heisenberg model Hamiltonian analytically. Exact solutions exist only for a few special cases. Therefore we don't know the actual ground state of most materials, which we suspect to behave liquid-like at low temperatures. It is for this reason that definitions of the term *spin liquid* are rather vague and differ from author to author. A spin liquid is a system of localised interacting spins with (some of) the following properties [6]:

- While the spins are highly entangled, they do not break any symmetries of the Hamiltonian. Their ground state is disordered.
- Fluctuations cause dynamical collective motion even at low temperatures. There is no freezing, spin liquids are not spin glass.
- A spin liquid has fractional excitations, called spinons. They change the total magnetisation by half an integer [7, p. 410].
- Although different spin liquid phases can not be distinguished by broken symmetries, they possess some kind of topological order [8, p. 393].

The last two characteristics are a more modern view of spin liquids. The concept of topological order, as proposed by X.G. Wen [9, 10], is connected with the idea of projective symmetry groups. Roughly speaking, projective symmetry groups are inequivalent ways in which a spin liquid can realise the symmetries of its Hamiltonian. X.G. Wen claims that the different projective symmetry groups of a lattice classify the spin liquid phases and allows to distinguish them, even though they all possess the same symmetries [8, p. 390].

Motivated by recent experimental results [4, 11], we will determine the projective symmetry groups of two lattices. The first lattice is the kagome lattice, drawn in figure 2. It is the ideal scenario of a frustrated spin system that might give rise to a spin liquid ground state. The second lattice can be found in a real world material. It is formed by the magnetic Cr_5^+-ions in the compound $Ca_{10}Cr_7C_{28}$ [12]. The projective symmetry groups (PSGs) of the kagome lattice have been determined before [13], but the precise calculation isn't published. I repeated the process and obtained a similar result. There are 30 different PSGs on the kagome lattice, only 20 of which can possibly describe a spin liquid state. The situation is quite different for the second lattice. We will find that its symmetry group gives rise to only four possible PSGs. A two of them require all bonds to vanish, they can not describe a spin liquid ground state. Therefore the symmetry group of the Cr_5^+-ion lattice, together with time reversal, can only implemented in two different ways.

2 A mean field theory for frustrated quantum spin systems

Notation: Let $\mathcal{H}$ be the Hilbert space of a single particle. I denote the Fock space of many such particles by

$$\Gamma_s(\mathcal{H}) = \bigoplus_{N=0}^{\infty} \Gamma_{s,N}(\mathcal{H}) \tag{2.1}$$

$s = -1$ in the fermionic case and $s = +1$ for bosons. $\Gamma_{s,N}(\mathcal{H}) = P_s(\mathcal{H}^{\otimes N})$ is the space of anti-symmetric (respectively symmetric) states in $\mathcal{H}^{\otimes N}$. P_s denotes the projection onto this space. $\Gamma_{-1,0}(\mathcal{H}) = \mathbb{C}^1$.

$|0_f\rangle \in \Gamma_{-1,0}(\mathcal{H})$ is an arbitrary normed vector and denotes the vacuum state. $n_\triangle = f^\dagger_\triangle f_\triangle$ is the number operator of a generic state $\triangle$.

$[\,\cdot\,,\cdot\,]_+$ is the anticommutator and $[\,\cdot\,,\cdot\,]_-$ the commutator. τ^μ, $\mu = 1,2,3$, are the three Pauli matrices. τ^0 is the identity matrix.

$$\tau^0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \tau^1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \tau^2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \tau^3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{2.2}$$

Inner products are antilinear in the first and linear in the second argument. $\mathbb{C}^2$ is always the two state system of a single spin 1/2. I will use the intuitive notation $\mathbb{C}^2 = \text{span}\{e_\uparrow, e_\downarrow\}$. **h.c.** in an expression denotes the hermitian conjugate of the previous term. S_X denotes the boundary of the unit sphere of the normed space X. $\hbar = 1$.

2.1 Heisenberg model and frustrated spin systems

Consider d atoms arranged periodical on a $2D$- or $3D$-grid (in other words, a solid). Assume there are electrons which can occupy the outermost orbit of each atom. Electrons have spin 1/2. According to the spin-statistics theorem, their many-particle wave function must be antisymmetric. The Hilbert space for the electrons in this simplified picture is given by

$$\mathcal{F} = \bigoplus_{N=0}^{2d} P_{-1} \left(\text{span}\{|i\sigma\rangle | i \in \text{lattice}, \sigma = \uparrow, \downarrow\} \right)^{\otimes N} \tag{2.3}$$

Time propagation is generated by the Hubbard model Hamiltonian [14, p. 197]

$$H : \mathcal{F} \to \mathcal{F}, \qquad H = H_{\text{kin}} + H_U = -\sum_{\langle ij\rangle,\sigma} t_{ij} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{2.4}$$

(Neglecting the chemical potential, since we consider only one orbit per atom). $\langle ij\rangle$ ranges over each bond in the lattice. $U, t_{ij} \in \mathbb{R}^+$. The first term of H corresponds to the kinetic energy of the system. t_{ij} are hopping amplitudes. I.e. t_{ij} is proportional to the probability of an electron on site i to tunnel to site j. Its magnitude depends on the spatial overlap of the atomic orbits. The second term describes the Coulomb interaction between electrons. A high amount of energy is required for tow electrons to share the same orbit. Coulomb interaction between electrons in distinct orbits is much smaller and can be neglected. We are interested in a special case: We want to find the ground state at half filling and for $t_{ij} \ll U$. I.e. we assume there is a small overlap between the orbits. Half filling means the total number of electrons in the system is the same as the total number of atoms. Since the kinetic term is much smaller than the Coulomb interaction, it is reasonable to treat H_{kin} as a perturbation of H_U. Suppose we turn H_{kin} completely off. Then in the ground state there is exactly one electron localised on each site, and there is no interaction between the electrons. It makes no difference for the total energy in which direction an electron spin points. Thus, the ground state space of H_U is 2^d degenerate. The spins can point in arbitrary direction. When we slowly turn on H_{kin}, we expect the electrons to remain localised. The energy cost U is too high to allow doubly occupied orbits. But the hopping term couples the spins to each other. Pushing one of them slightly does move the other ones. This causes collective magnetic behaviour and possibly a preferred order at ground state level. For example some antiferromagnets prefer anti-parallel alignment of their spins [15].

H_{kin} always maps singly occupied states to doubly occupied states. Therefore first order perturbation theory yields no correction of the ground state energy. Unfortunately, this means that the first order correction does not lift the degeneracy either. This makes a rigorous treatment of H_{kin} in second order perturbation theory complicated. I will only quote the result, a detailed derivation can be found here [14, p. 219]. The effective Hamiltonian, in second order perturbation theory, with $t \ll U$ and at half filling [8, p. 355], is the Heisenberg Hamiltonian

$$\tilde{H} : \left(\mathbb{C}^2\right)^{\otimes d} \to \left(\mathbb{C}^2\right)^{\otimes d}, \qquad \tilde{H} = \sum_{ij} J_{ij}\, \tilde{\boldsymbol{S}}_i \cdot \tilde{\boldsymbol{S}}_j \qquad \text{where} \qquad J_{ij} = -\frac{4t_{ij}^2}{U} \tag{2.5}$$

$\tilde{S}^\mu_i$ are the standard spin operators acting on the spin at site i. Note that the charge degree of freedom is frozen. The electrons remain localised. Their interaction is caused by second order exchange paths,

which can connect single occupied states. Each coefficient J_{ij} is negative. Such an interaction is called antiferromagnetic. In general spin pairs connected by an antiferromagnetic bond prefer to align anti-parallelly. In a two spin system the energy is minimised by the singlet $2^{-1/2}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. A Hamiltonian is frustrated if all of its interaction terms can not be minimised simultaneously. In the classical limit $\boldsymbol{S}_i$ are three-component vectors. Therefore a simple example of a classical frustrated system is a triangle with one electron sitting on each vertex. It is impossible to align the two spins of each bond anti-parallel at the same time. Such a system is called geometrically frustrated. We can not solve the Heisenberg Hamiltonian reliably. Geometrical frustration is the simplest indicator for actual frustration that we have. Unfortunately, the classical picture does not predict the quantum mechanical behaviour very well.

It is necessary to split the operators $\tilde{S}_i^+$ and $\tilde{S}_i^-$ to get a working mean field theory for liquids. Mean field theories that working with amplitudes $\langle \tilde{S}_i^\mu \rangle$ predict symmetry breaking and some kind of order at low temperatures. They fail to describe spin liquids, which are long-range disordered and do not break any symmetries. In a spin liquid fluctuations $\delta\tilde{S}_i^\mu = \tilde{S}_i^\mu - \langle \tilde{S}_i^\mu \rangle$ from a preferred direction can not be considered small, even below Néel temperature. The reason is simply that there is no preferred direction. A common way to deal with the Heisenberg Hamiltonian is a slave-boson approach [9, 16]. The spin operators are expressed in terms of pseudo fermions:

$$S_i^\mu = \frac{1}{2} \sum_{\alpha\beta} \tau_{\alpha\beta}^\mu f_{i\alpha}^\dagger f_{i\beta} \tag{2.6}$$

This is also the machinery behind the projective symmetry group method. $f_{i\sigma}$ are not real particles. Excitations by a single $f_{i\alpha}^\dagger$ do not have an interpretation in $(\mathbb{C}^2)^{\otimes d}$. Rather they are a mathematical trick to map the problem (2.5) to an easier one. $f_{i\alpha}$ act on a Fock space $\Gamma_{-1}(\mathcal{H})$ that is way bigger than the actual Hilbert space $(\mathbb{C}^2)^{\otimes d}$. We have to identify $(\mathbb{C}^2)^{\otimes d}$ with a subspace $\mathcal{H}_p \subset \Gamma_{-1}(\mathcal{H})$ via an isomorphism $\mathscr{K} : (\mathbb{C}^2)^{\otimes d} \to \mathcal{H}_p$. The slave-boson spin operators should extend $\mathscr{K}\tilde{S}_i^\mu\mathscr{K}^{-1}$. Figure 1 shows the construction schematically. In the rest of this chapter I will briefly review a widely used mean field theory for spin liquids [8] and its gauge structure [17].

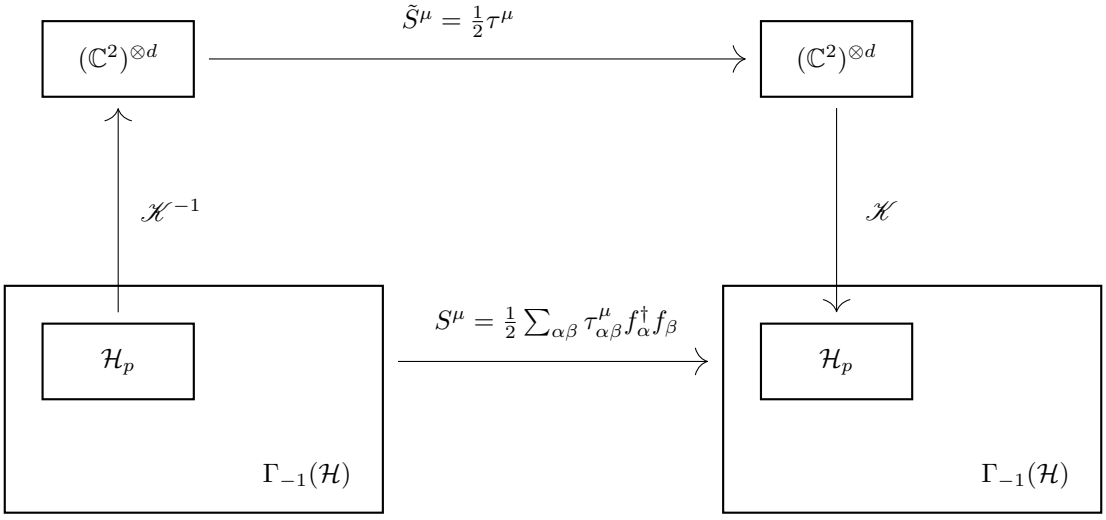

Figure 1: slave-boson representation of finite spin systems; $S_i^\mu|_{\mathcal{H}_p} = \mathscr{K}\tilde{S}_i^\mu\mathscr{K}^{-1}$

2.2 Hilbert space and spin operators

The aim of this section is to make figure 1 precise. This naturally involves a lot of definitions and new notation. We will construct the Fock space $\Gamma_{-1}(\mathcal{H})$, choose a subspace $\mathcal{H}_p$, and fix an isomorphism $\mathscr{K} : (\mathbb{C}^2)^{\otimes d} \to \mathcal{H}_p$. Lastly we will define spin operators S_i^μ acting on the full Fock space and check that their definition is consistent with the definition of $\mathscr{K}$.

A Fock space is generated by some single particle Hilbert space. Set $\mathcal{H} = \mathbb{C}^{2d}$ and let

$$\Gamma_{-1}(\mathcal{H}) = \bigoplus_{N=0}^{\infty} P_{-1}(\mathbb{C}^{2d})^{\otimes N} = \bigoplus_{N=0}^{2d} P_{-1}(\mathbb{C}^{2d})^{\otimes N} \tag{2.7}$$

The last equality holds because fermions obey the Pauli exclusion principle. Label an orthonormal basis of $\mathcal{H}$ by $\mathcal{B} = \{|\mu_{i\alpha}\rangle \,|\, i \in \text{lattice},\, \alpha = \uparrow, \downarrow\}$. For each state $|\mu_{i\alpha}\rangle \in \mathcal{B}$ define its creation operator $f^\dagger_{i\alpha}$ by

$$f^\dagger_{i\alpha} : \Gamma_{-1}(\mathcal{H}) \to \Gamma_{-1}(\mathcal{H}), \qquad \left(f^\dagger_{i\alpha}\,|\psi\rangle\right)_N = \sqrt{N}\, P_{-1}\left(|\mu_{i\alpha}\rangle \otimes |\psi\rangle_{N-1}\right), \qquad f^\dagger_{i\alpha}\,|0_f\rangle = |\mu_{i\alpha}\rangle \tag{2.8}$$

$|\psi\rangle_N$ is the part of $|\psi\rangle$ living in the subspace $\Gamma_{-1,N}(\mathcal{H}) = \mathcal{P}_{-1}\left(\mathcal{H}^{\otimes N}\right)$ of N particles. Based on the single particle states $\mathcal{B}$, one can define occupation number vectors. Let $\underline{n} \in \{0,1\}^{2d}$. I will create particles in the following order:

$$|\,\underline{n}_f\rangle = {f^\dagger_{1\uparrow}}^{n_{1\uparrow}} {f^\dagger_{1\downarrow}}^{n_{1\downarrow}} ... {f^\dagger_{d\downarrow}}^{n_{d\downarrow}}\,|0_f\rangle \tag{2.9}$$

The set of all occupation number vectors is an orthonormal basis of $\Gamma_{-1}(\mathcal{H})$ [18]. I promised to identify $(\mathbb{C}^2)^{\otimes d}$ with a subspace of $\Gamma_{-1}(\mathcal{H})$. First we have to choose a subspace. We call states $|\psi\rangle \in \Gamma_{-1}(\mathcal{H})$ *physical* or *single occupied* if they satisfy the constraint

$$\forall i \in \text{lattice}: \quad \langle\psi|f^\dagger_{i\uparrow}f_{i\uparrow} + f^\dagger_{i\downarrow}f_{i\downarrow}|\psi\rangle = 1 \tag{2.10}$$

I will denote the subspace of physical states by $\mathcal{H}_p$. Examples of states in $\mathcal{H}_p$ are:

$$|10,01,10,10,01,....\rangle\,,\ |01,01,10,10,01,...\rangle\,,\ |01,10,01,01,01...\rangle \tag{2.11}$$

Examples of states which are not in $\mathcal{H}_p$:

$$|11,10,01,10,01,...\rangle\,,\ |01,00,01,10,00,...\rangle\,,\ |01,01,01,00,01,...\rangle \tag{2.12}$$

The aim is to identify $\mathcal{H}_p$ with the actual Hilbert space of d localised spin-1/2 particles. This is possible if and only if $\mathcal{H}_p$ has the right dimension.

$$\dim\left(\mathcal{H}_p = \left\{|\psi\rangle \in \Gamma_{-1}(\mathcal{H}) \,\middle|\, \forall i : \langle\psi|\,\left(f^\dagger_{i\uparrow}f_{i\uparrow} + f^\dagger_{i\downarrow}f_{i\downarrow}\right)\,|\psi\rangle = 1\right\}\right) = 2^d = \dim\left((\mathbb{C}^2)^{\otimes d}\right) \tag{2.13}$$

$\mathcal{H}_p$ is spanned by a certain subset of occupation number basis vectors. It is a simple combinatorial exercise to count them. It follows immediately that $\mathcal{H}_p \cong (\mathbb{C}^2)^{\otimes d}$. The isomorphism which we will use throughout the text is

$$\mathscr{K}: \quad (\mathbb{C}^2)^{\otimes d} \to \mathcal{H}_p \tag{2.14}$$

It maps

$$e_\uparrow \otimes e_\downarrow \otimes ... \otimes e_\downarrow \otimes e_\downarrow \otimes e_\uparrow \mapsto |10,01,...,01,01,10\rangle \tag{2.15}$$

Similar for the other basis vectors and extended by linearity. $\mathscr{K}$ is bijective and linear by construction. Next, introduce spin-operators $\Gamma_{-1}(\mathcal{H})$. Define

$$S^\mu_i : \Gamma_{-1}(\mathcal{H}) \to \Gamma_{-1}(\mathcal{H}), \qquad S^\mu_i = \frac{1}{2}\sum_{\alpha\beta} \tau^\mu_{\alpha\beta} f^\dagger_{i\alpha} f_{i\beta} \tag{2.16}$$

Each index in the sum above ranges over $\{\uparrow,\downarrow\}$. The definition of S^μ_i is consistent with the choice of coordinates $\mathscr{K}$.

Proposition: *(S^μ_i act like spin operators on $\mathcal{H}_p$)*

(i) S^μ_i extend the physical spin operators. I.e. $S^\mu_i|_{\mathcal{H}_p} = \mathscr{K}\,\tilde{S}^\mu_i\,\mathscr{K}^{-1}$.

(ii) S^μ_i satisfy the spin operator commutation relation $[S^\mu_k, S^\nu_j]_- = i\,\epsilon_{\mu\nu\gamma}\,S^\gamma_k\,\delta_{kj}$ not only on $\mathcal{H}_p$ but on all of $\Gamma_{-1}(\mathcal{H})$.

(iii) $(\boldsymbol{S}_j)^2|_{\mathcal{H}_p} = S(S+1)\,id$ with $S = \frac{1}{2}$. This does not hold for $(\boldsymbol{S}_j)^2|_{\Gamma_{-1}(\mathcal{H})\setminus\mathcal{H}_p}$.

Proof: (i) Using definition (2.9) and canonical anticommutation relations one can derive how $f_{i\alpha}$ and $f_{i\alpha}^\dagger$ act on occupation number basis vectors [18].

$$f_{i\alpha}^\dagger: \quad \Gamma_{-1}(\mathcal{H}) \to \Gamma_{-1}(\mathcal{H}), \qquad f_{i\alpha}^\dagger \, |n_{1\uparrow}...n_{d\downarrow}\rangle = (-1)^{\left(\sum_{j\beta<i\alpha} n_{j\beta}\right)} \sqrt{1-n_{i\alpha}} \, |n_{1\uparrow}...(n_{i\alpha}+1)...n_{d\downarrow}\rangle$$

$$f_{i\alpha}: \quad \Gamma_{-1}(\mathcal{H}) \to \Gamma_{-1}(\mathcal{H}), \qquad f_{i\alpha} \, |n_{1\uparrow}...n_{d\downarrow}\rangle = (-1)^{\left(\sum_{j\beta<i\alpha} n_{j\beta}\right)} \sqrt{n_{i\alpha}} \, |n_{1\uparrow}...(n_{i\alpha}-1)...n_{d\downarrow}\rangle \quad (2.17)$$

extended by linearity. The operators $f_{i\alpha}^\dagger f_{i\beta}$ act on occupation number basic vectors in $\mathcal{H}_p$ as follows:

$$\begin{aligned}
&f_{i\uparrow}^\dagger f_{i\uparrow} \, |...(10)_i...\rangle = |...(10)_i...\rangle \,, && f_{i\uparrow}^\dagger f_{i\uparrow} \, |...(01)_i...\rangle = 0 \\
&f_{i\uparrow}^\dagger f_{i\downarrow} \, |...(10)_i...\rangle = 0, && f_{i\uparrow}^\dagger f_{i\downarrow} \, |...(01)_i...\rangle = |...(10)_i...\rangle \\
&f_{i\downarrow}^\dagger f_{i\uparrow} \, |...(10)_i...\rangle = |...(01)_i...\rangle \,, && f_{i\uparrow}^\dagger f_{i\downarrow} \, |...(01)_i...\rangle = 0 \\
&f_{i\downarrow}^\dagger f_{i\downarrow} \, |...(01)_i...\rangle = 0, && f_{i\downarrow}^\dagger f_{i\downarrow} \, |...(01)_i...\rangle = |...(01)_i...\rangle
\end{aligned} \quad (2.18)$$

I marked in the equations above which entries of $|\underline{n}_f\rangle$ are changed. The signs cancel each other out, no matter what numbers occur before the entries $n_{i\uparrow}n_{i\downarrow}$. $f_{i\alpha}^\dagger f_{i\beta}$ are used to express matrix multiplication with τ^μ in $\mathcal{H}_p$. With (2.18) and (2.15) it should be clear that $S_i^\mu|_{\mathcal{H}_p} = \mathscr{K}\tilde{S}_i^\mu\mathscr{K}^{-1}$.

(ii) We can check the commutation relation directly.

$$\begin{aligned}
[S_k^\mu, S_j^\nu]_- &= \frac{1}{4}\left(\sum_{\alpha\eta\varphi\beta} \tau_{\alpha\eta}^\mu \, \tau_{\varphi\beta}^\nu \, f_{j\alpha}^\dagger \, f_{j\eta} \, f_{k\varphi}^\dagger \, f_{k\beta}\right) - \frac{1}{4}\left(\sum_{\alpha\eta\varphi\beta} \tau_{\alpha\eta}^\nu \, \tau_{\varphi\beta}^\mu \, f_{k\alpha}^\dagger \, f_{k\eta} \, f_{j\varphi}^\dagger \, f_{j\beta} \, \tau_{\alpha\eta}^\nu \, \tau_{\varphi\beta}^\mu\right) \\
&= \frac{1}{4}\left(\sum_{\alpha\eta\varphi\beta} \tau_{\alpha\eta}^\mu \tau_{\varphi\beta}^\nu f_{j\alpha}^\dagger \left(\delta_{jk}\delta_{\eta\varphi} - f_{k\varphi}^\dagger f_{j\eta}\right) f_{k\beta}\right) - \frac{1}{4}\left(\sum_{\alpha\eta\varphi\beta} \tau_{\alpha\eta}^\nu \tau_{\varphi\beta}^\mu f_{k\alpha}^\dagger \left(\delta_{jk}\delta_{\eta\varphi} - f_{j\varphi}^\dagger \, f_{k\eta}\right) f_{j\beta}\right) \\
&= \delta_{jk} \sum_{\alpha\beta} \left(\frac{1}{4}\sum_\eta \tau_{\alpha\eta}^\mu \, \tau_{\eta\beta}^\nu - \tau_{\alpha\eta}^\nu \, \tau_{\eta\beta}^\mu\right) \, f_{j\alpha}^\dagger f_{j\beta} - \frac{1}{4}\left(\sum_{\alpha\eta\varphi\beta} \tau_{\alpha\eta}^\mu \, \tau_{\varphi\beta}^\nu \, f_{j\alpha}^\dagger \, f_{k\varphi}^\dagger \, f_{j\eta} \, f_{k\beta}\right) \\
&+ \frac{1}{4}\left(\sum_{\alpha\eta\varphi\beta} \tau_{\alpha\eta}^\nu \, \tau_{\varphi\beta}^\mu \, f_{k\alpha}^\dagger \, f_{j\varphi}^\dagger \, f_{k\eta} \, f_{j\beta}\right) = A - \frac{1}{4}B + \frac{1}{4}C
\end{aligned} \quad (2.19)$$

The Pauli matrices satisfy

$$\frac{1}{4}[\tau^\mu, \tau^\nu]_- = \frac{1}{2} \, i \, \epsilon_{\mu\nu\gamma}\tau^\gamma, \quad (2.20)$$

which immediately yields

$$A = \delta_{jk} \sum_{\alpha\beta} f_{j\alpha}^\dagger \left(\frac{1}{4}\sum_\eta \tau_{\alpha\eta}^\mu \, \tau_{\eta\beta}^\nu - \tau_{\alpha\eta}^\nu \, \tau_{\eta\beta}^\mu\right) f_{j\beta} = \delta_{jk} \sum_{\alpha\beta} f_{j\alpha}^\dagger \left(\frac{1}{2} \, i \, \epsilon_{\mu\nu\gamma}\tau^\gamma\right)_{\alpha\beta} f_{j\beta} = i \, \epsilon_{\mu\nu\gamma} \, \delta_{kj} \, S_j^\gamma \quad (2.21)$$

It remains to show that $B = C$. After relabelling summation indices in the sum B, this is the same as

$$\sum_{\alpha\eta\varphi\beta} \tau_{\alpha\eta}^\nu \, \tau_{\varphi\beta}^\mu \, f_{j\varphi}^\dagger \, f_{k\alpha}^\dagger \, f_{j\beta} \, f_{k\eta} = \sum_{\alpha\eta\varphi\beta} \tau_{\alpha\eta}^\nu \, \tau_{\varphi\beta}^\mu \, f_{k\alpha}^\dagger \, f_{j\varphi}^\dagger \, f_{k\eta} \, f_{j\beta} \quad (2.22)$$

For any labels $\square$ and $\triangle$ it holds that $f_\square \, f_\triangle = -f_\triangle \, f_\square$ and $f_\square^\dagger \, f_\triangle^\dagger = -f_\triangle^\dagger f_\square^\dagger$. It is enough to interchange the operators on the right hand side twice to see equality in equation (2.22).

(iii) This is a standard result for $\tilde{\boldsymbol{S}}_j$. Therefore it also holds in the subspace $\mathcal{H}_p$. There is no way to do this with $(\boldsymbol{S}_j \cdot \boldsymbol{S}_j)|_{\Gamma_{-1}(\mathcal{H})\setminus\mathcal{H}_p}$.The reason is that $(\boldsymbol{S}_j \cdot \boldsymbol{S}_j) \, |\psi\rangle = 0$ for some states $|\psi\rangle \in \Gamma_{-1}(\mathcal{H})\setminus\mathcal{H}_p$ and not for some others. $\square$

2.3 Mean field theory for spin liquids

The aim of this section is to develop a mean field theory which can in principle describe spin liquid states at low temperatures. This section closely follows [7, p. 416]. The Heisenberg Hamiltonian of localised spin-1/2 particles is

$$H = \sum_{\langle ij \rangle} J_{ij}\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{2.23}$$

In terms of annihilation and creation operators:

$$\boldsymbol{S}_i \cdot \boldsymbol{S}_j = \frac{1}{2}\left(f^\dagger_{i\uparrow} f_{i\downarrow} f^\dagger_{j\downarrow} f_{j\uparrow} + f^\dagger_{i\downarrow} f_{i\uparrow} f^\dagger_{j\uparrow} f_{j\downarrow}\right) + \frac{1}{4}\left(\hat{n}_{i\uparrow}\hat{n}_{j\uparrow} + \hat{n}_{i\downarrow}\hat{n}_{j\downarrow} - \hat{n}_{i\downarrow}\hat{n}_{j\uparrow} - \hat{n}_{i\uparrow}\hat{n}_{j\downarrow}\right). \tag{2.24}$$

The Hamiltonian is quartic in fermionic operators and in general hard to solve. To simplify the equation, we replace some of the operators with their ground state average. First I will show the decoupling, then I will explain the result. Define matrices

$$\Phi_i = \begin{bmatrix} f_{i\uparrow} & f_{i\downarrow} \\ f^\dagger_{i\downarrow} & -f^\dagger_{i\uparrow} \end{bmatrix} \qquad \text{and} \qquad \Phi^\dagger_i = \begin{bmatrix} f^\dagger_{i\uparrow} & f_{i\downarrow} \\ f^\dagger_{i\downarrow} & -f_{i\uparrow} \end{bmatrix} \tag{2.25}$$

Let $\left\langle \Phi_i \Phi^\dagger_j \right\rangle$ denote the entrywise expected value of the matrix $\Phi_i \Phi^\dagger_j$ in the ground state.

$$\delta\Phi_i \Phi^\dagger_j = \Phi_i \Phi^\dagger_j - \left\langle \Phi_i \Phi^\dagger_j \right\rangle \tag{2.26}$$

are *fluctuations* from the mean field. A long but straightforward calculation gives

$$\boldsymbol{S}_i \cdot \boldsymbol{S}_j = -\frac{1}{8}\operatorname{tr}\left(\Phi_i \Phi^\dagger_j \Phi_j \Phi^\dagger_i\right) \tag{2.27}$$

This can be verified by expanding expression (2.27), using fermionic anticommutation relations several times and collecting terms until finding (2.24). In consequence

$$\begin{aligned} H &= -\sum_{\langle ij \rangle} \frac{J_{ij}}{8}\operatorname{tr}\left(\Phi_i \Phi^\dagger_j \Phi_j \Phi^\dagger_i\right) = -\sum_{\langle ij \rangle} \frac{J_{ij}}{8}\operatorname{tr}\left(\left(\left\langle \Phi_i \Phi^\dagger_j \right\rangle + \delta\Phi_i \Phi^\dagger_j\right)\left(\left\langle \Phi_j \Phi^\dagger_i \right\rangle + \delta\Phi_j \Phi^\dagger_i\right)\right) \\ &\approx \sum_{\langle ij \rangle} \frac{J_{ij}}{8}\operatorname{tr}\left(\left\langle \Phi_i \Phi^\dagger_j \right\rangle \left\langle \Phi_j \Phi^\dagger_i \right\rangle\right) - \sum_{\langle ij \rangle} \frac{J_{ij}}{8}\operatorname{tr}\left(\Phi_i \Phi^\dagger_j \left\langle \Phi_j \Phi^\dagger_i \right\rangle\right) - \sum_{\langle ij \rangle} \frac{J_{ij}}{8}\operatorname{tr}\left(\left\langle \Phi_i \Phi^\dagger_j \right\rangle \Phi_j \Phi^\dagger_i\right), \end{aligned} \tag{2.28}$$

ignoring second order fluctuations $\delta\Phi_i \Phi^\dagger_j\, \delta\Phi_j \Phi^\dagger_i$. Note that

$$\Phi_i \Phi^\dagger_j = \begin{bmatrix} f_{i\uparrow} f^\dagger_{j\uparrow} + f_{i\downarrow} f^\dagger_{j\downarrow} & f_{i\uparrow} f_{j\downarrow} - f_{i\downarrow} f_{j\uparrow} \\ f^\dagger_{i\downarrow} f^\dagger_{j\uparrow} - f^\dagger_{i\uparrow} f^\dagger_{j\downarrow} & f^\dagger_{i\downarrow} f_{j\downarrow} + f^\dagger_{i\uparrow} f_{j\uparrow} \end{bmatrix} \tag{2.29}$$

satisfies

$$\left\langle \Phi_j \Phi^\dagger_i \right\rangle = \left\langle \Phi_i \Phi^\dagger_j \right\rangle^\dagger \tag{2.30}$$

A mean field Hamiltonian can be obtained by replacing the operators in (2.29) with their ground state expected value. For each bond ij choose complex numbers η_{ij} and χ_{ij}. Write

$$U_{ij} = \begin{bmatrix} \chi^*_{ij} & \eta_{ij} \\ \eta^*_{ij} & -\chi_{ij} \end{bmatrix} \tag{2.31}$$

A mean field Hamiltonian, derived from (2.23), takes the form

$$H^{\{U_{ij}\}}_{MF} = \sum_{\langle ij \rangle} 2\operatorname{tr}\left(\Phi^\dagger_i U_{ij} \Phi_j\right) + \sum_{\langle ij \rangle} 2\operatorname{tr}\left(\Phi^\dagger_j U^\dagger_{ij} \Phi_i\right) + \sum_{\langle ij \rangle} \frac{32}{J_{ij}}\operatorname{tr}\left(U_{ij} U^\dagger_{ij}\right) \tag{2.32}$$

The factor 2 is just for convenience and will vanish later. The new Hamiltonian is quadratic in fermionic operators and can be solved more easily. For each family of matrices $\{U_{ij} | \, ij \in \text{bonds}\}$ there is at least one ground state $\left|\psi_{MF}^{\{U_{ij}\}}\right\rangle$ of $H_{MF}^{\{U_{ij}\}}$. Comparing (2.32) with (2.28) gives rise to the self-consistency condition

$$U_{ij} = \frac{J_{ij}}{16} \left\langle \psi_{MF}^{\{U_{ij}\}} \middle| \Phi_i \Phi_j^\dagger \middle| \psi_{MF}^{\{U_{ij}\}} \right\rangle \tag{2.33}$$

A set of matrices $\{U_{ij} \,|\, ij \in \text{bonds}\}$ is called an ansatz if the corresponding ground state satisfies the self-consistency condition (2.33). The idea is to treat the numbers $\{U_{ij}\}$ as variables and to solve (2.32) in general. This yields a ground state in dependence of $2 \times |\text{bonds}|$ unknown variables. Those can be determined using (2.33). Of course, it is impossible to solve (2.32) and (2.33) with $2 \times |\text{bonds}|$ unknown. It is necessary to exploit the symmetries of $\{U_{ij}\}$ first.

It will be convenient to work with vectors instead of matrices. For each site introduce

$$\Psi_i = \begin{bmatrix} f_{i\uparrow} \\ f_{i\downarrow}^\dagger \end{bmatrix} \qquad \text{and} \qquad \Psi_i^\dagger = \begin{bmatrix} f_{i\uparrow}^\dagger & f_{i\downarrow} \end{bmatrix} \tag{2.34}$$

We can rewrite the Hamilton operator in equation (2.32):

$$H_{MF}^{\{U_{ij}\}} = \sum_{\langle ij \rangle} \left(\Psi_i^\dagger U_{ij} \Psi_j + \Psi_j^\dagger U_{ij}^\dagger \Psi_i \right) + \text{const.} \tag{2.35}$$

And we can express H_{MF} explicitly in terms of fermionic operators :

$$H_{MF}^{\{\chi_{ij}, \eta_{ij}\}} = \sum_{\langle ij \rangle} \left(\chi_{ij}^* f_{i\uparrow}^\dagger f_{j\uparrow} + \chi_{ij} f_{j\downarrow}^\dagger f_{i\downarrow} + \eta_{ij} f_{i\downarrow} f_{j\uparrow} + \eta_{ij}^* f_{i\uparrow}^\dagger f_{j\downarrow}^\dagger \right) + \text{h.c.} + \text{const.} \tag{2.36}$$

The slave-boson Heisenberg Hamiltonian H in (2.23) contains only physical excitations. Every term is either a number operator or causes a full spin-flip. H does not split excitations S_i^+: whenever $|\psi\rangle \in \mathcal{H}_p$ then also $H|\psi\rangle \in \mathcal{H}_p$. If we were able to solve the slave fermion Hamiltonian (2.23) exactly and restrict ourself to the eigenvectors in $\mathcal{H}_p$, this would be a correct solution of the original Hamiltonian $\tilde{H}$ without slave fermions. This is no longer the case for the mean field Hamiltonian. H_{MF} contains hopping and pairing terms of nonphysical excitations: it can create double-occupied or empty sites from one particle per site states. It does not even preserve the particle number due to pairing terms. Hence, in principle H_{MF} allows spin-charge separation and fractional excitation, which are proposed to be one of the defining characteristics of a quantum spin liquid. Spin rotation has the following form in slave-boson representation [7, p. 417]:

$$\Phi_i \xrightarrow{V} \Phi_i \, V \qquad \text{or} \qquad \Psi_i \xrightarrow{V} \Psi_i \, V \qquad V \in SU(2) \tag{2.37}$$

Hence, H_{MF} does not break spin rotation symmetry by construction. This is explicit in (2.28).

2.4 Local $SU(2)$ gauge structure

A transformation of fermionic operators is called *canonical* if the transformed operators remain adjoint to each other and if they satisfy canonical anticommutation relations (CARs). Operators which satisfy fermionic anticommutation relations naturally induce an orthonormal basis on their Hilbert space [18, 19](details in appendix B). A canonical transformation of the creation and annihilation operators therefore corresponds directly to a change of basis. I will introduce *local* $SU(2)$ transformations in this section. They are a canonical site-wise linear mixing of creation and annihilation operators. It will turn out later that there is a gauge freedom consisting exactly of those transformations.

A *local* $SU(2)$ transformation is a transformation W of the form

$$\begin{bmatrix} f_{i\uparrow} \\ f_{i\downarrow}^\dagger \end{bmatrix} = W(i) \begin{bmatrix} c_{i\uparrow} \\ c_{i\downarrow}^\dagger \end{bmatrix}, \qquad \begin{bmatrix} f_{i\uparrow}^\dagger \\ f_{i\downarrow} \end{bmatrix} = W(i)^* \begin{bmatrix} c_{i\uparrow}^\dagger \\ c_{i\downarrow} \end{bmatrix}, \qquad W(i) \in SU(2)\,. \tag{2.38}$$

It is clear from the definition that each $c_{i\alpha}$ is adjoint to $c^\dagger_{i\alpha}$. The transformation of $c^\dagger_{i\uparrow}$ and $c_{i\downarrow}$ can alternatively be written as

$$\begin{bmatrix} f_{i\downarrow} \\ -f^\dagger_{i\uparrow} \end{bmatrix} = W(i) \begin{bmatrix} c_{i\downarrow} \\ -c^\dagger_{i\uparrow} \end{bmatrix} \tag{2.39}$$

This holds because $SU(2)$ matrices take the form

$$W(i) = \begin{bmatrix} \alpha & -\beta^* \\ \beta & \alpha^* \end{bmatrix}, \qquad \alpha, \beta \in \mathbb{C}, \quad |\alpha|^2 + |\beta|^2 = 1\,. \tag{2.40}$$

A proof can be found in appendix B. The operators $c_{i\alpha}$ satisfy fermionic anticommutation relations. I omit a proof here since this is a special case of the more general non local transformation that I will need to introduce later. I denote local $SU(2)$ transformations shorthand by

$$\Phi_i \xrightarrow{W} W(i)\,\Phi_i \qquad \text{or} \qquad \Psi_i \xrightarrow{W} W(i)\Psi_i \tag{2.41}$$

The arrows should be understood as a replacing rule: Replace the left hand side by the right hand side in the current Hamiltonian to obtain the Hamiltonian in new coordinates. So (2.41) means the same as

$$U_{ij} \xrightarrow{W} W(i)^\dagger U_{ij} W(j) \tag{2.42}$$

It is immediately clear that all operators in the entries of $\Phi^\dagger_i\,\Phi_j$ are invariant under local $SU(2)$ transformations. We can express the spin-operators in terms of $\Phi^\dagger_i \Phi_i$. A rather long but straightforward calculation yields

$$S^\mu_i = \frac{1}{4}\,\mathrm{tr}\left(\Phi^\dagger_i \Phi_i (\tau^\mu)^t\right) \tag{2.43}$$

Thus, the spin operators are invariant under local $SU(2)$ transformations. It follows immediately that the physical system, as described by the Hamiltonian (2.23), is also invariant under local $SU(2)$ transformations. This is a first hint that those might be a gauge freedom of the mean field theory. From now one we will call them *gauge transformations*, even though this term isn't justified yet.

The mean field theory, which we derived in the previous chapter, has some flaws. The most obvious problem is that $\Gamma_{-1}(\mathcal{H})$ is much greater than $\mathcal{H}_p$. The eigenstates which we obtain from an ansatz $\{U_{ij}\}$ might not only be quantitatively wrong due to approximations. It is likely that they aren't even legal wave functions of the physical problem. At least we have to project onto $\mathcal{H}_p$. For each $|\psi\rangle \in \Gamma_{-1}(\mathcal{H})$ define a physical *spin wave function*

$$|\psi_{\mathrm{spin}}\rangle = \sum_{(\alpha_1,\ldots,\alpha_d)} \psi_{\mathrm{spin}}(\alpha_1,\ldots,\alpha_d)\;|\alpha_1,\ldots,\alpha_d\rangle \tag{2.44}$$

The tuples $(\alpha_1,\ldots,\alpha_d)$ range over $\{\uparrow,\downarrow\}^d$. $|\alpha_1,\ldots,\alpha_d\rangle$ are those occupation number basis vectors which span $\mathcal{H}_p$. E.g.

$$|\uparrow,\uparrow,\downarrow,\ldots,\uparrow\rangle = |10,10,01,\ldots,10\rangle \tag{2.45}$$

The spin wave function is the projection of $|\psi\rangle$ onto $\mathcal{H}_p$. The coefficients $\psi_{\mathrm{spin}}(\alpha_1,\ldots,\alpha_d)$ are given by [8, p. 377]

$$\psi_{\mathrm{spin}}(\alpha_1,\ldots,\alpha_d) = \left\langle 0_f \,\middle|\, \prod_{i=1}^{d} f_{i\alpha_i} \,\middle|\, \psi \right\rangle \tag{2.46}$$

The product above depends on the order. To get no unnecessary $-$ signs, apply the annihilation operators from lowest index first to highest last. The Hamiltonian in (2.23) is invariant under local $SU(2)$ transformations. Depending on the ansatz this is not necessarily true for H_{MF}. Gauge equivalent ansätze can give different eigenstates even though they should not, since the physical system is gauge invariant. But there is an easy fix. Mean field Hamiltonians obtained from gauge equivalent ansätze always have the same physical interpretation.

Proposition: *(Ansätze carry the same physical information iff they are gauge equivalent)*

Let $\{U_{ij}\}$ and $\{\tilde{U}_{ij}\}$ be two ansätze and let H and $\tilde{H}$ be their mean field Hamiltonians. Then H and $\tilde{H}$ share the same energy levels and their eigenstates project onto the same spin wave functions in $\mathcal{H}_p$ if and only if $\{U_{ij}\}$ and $\{\tilde{U}_{ij}\}$ differ by a local $SU(2)$ transformation.

Proof: Since the proof is lengthy and requires concepts which are not important for the rest of the text, it is given in appendix A. □

The ansätze $\{U_{ij}\}$ can be understood as labels for spin states and their energy levels. The above proposition shows that the labelling is not injective. Many ansätze, which might look different at first sight, carry the same physics. There is a gauge freedom which consists exactly of all local $SU(2)$ transformations. Any result is only relevant up to the choice of gauge. The intuitive way to deal with *up to ...* - situations are equivalence classes. And indeed, *up to the choice of gauge* defines an equivalence relation on the family of all ansätze. It is reflexive since *id* is a gauge transformation, symmetric since gauge transformations are invertible and transitive since the compositions of two gauge transformations is a gauge transformations.

3 The projective symmetry group

3.1 Motivation

A spatial symmetry is a bijective isometric mapping of lattice points. Let T : lattice $\to$ lattice be a symmetry. Consider a transformation of the physical Hamiltonian by T:

$$\sum_{\langle ij\rangle} J_{ij}\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j \quad \xrightarrow{T} \quad \sum_{\langle ij\rangle} J_{ij}\, \boldsymbol{S}_{T(i)} \cdot \boldsymbol{S}_{T(j)} \tag{3.1}$$

The lattice looks the same before and after the symmetry transformation. Therefore we expect that eigenstates and energies are invariant under T. In many systems this holds if and only if the Hamiltonian is invariant under T, i.e. $H = THT^{-1}$. In such a case one can impose additional constraints on the coefficients, which makes it easier to solve the problem. For example, we might be able to show that the physical spin Hamiltonian must satisfy

$$\forall ij: \quad J_{ij} = J_{T(i)T(j)} \tag{3.2}$$

The situation is different for the mean field Hamiltonian, though. Ansätze produce the same spin wave functions and energy levels if and only if they are gauge equivalent. Let $\{U_{ij}\}$ be an ansatz. Spin wave functions and energy levels should not change under T. But this does not imply that $\forall ij : U_{T(i)T(j)} = U_{ij}$. It only implies that $\{U_{T(i)T(j)}\}$ and $\{U_{ij}\}$ are in the same equivalence class of ansätze. It is hard to impose constraints on the matrices U_{ij} from such an abstract condition only. The right mathematical tool to implement symmetries into the mean field theory are projective symmetry groups. The main idea comes from this observation: $\{U_{T(i)T(j)}\}$ and $\{U_{ij}\}$ are in the same equivalence class if and only if there exists a gauge transformation G_T such that

$$U_{ij} \xrightarrow{G_T T} U_{ij} \tag{3.3}$$

3.2 Construction

This chapter explains what the projective symmetry group is mathematically. I will review the definition given by X.G. Wen in [9] and add some details which are taken for granted in the original paper. The projective symmetry group (PSG) is a property of an ansatz. I will write $PSG(\{U_{ij}\})$ (or $PSG(H)$ when H is a mean field Hamiltonian) whenever it is necessary to make the dependence explicit. Recall that

$$H = \sum_{\langle ij\rangle} \left(\Psi_i^\dagger U_{ij} \Psi_j + \Psi_j^\dagger U_{ij}^\dagger \Psi_i \right) + \text{const.} \tag{3.4}$$

where

$$\Psi_i = \begin{bmatrix} f_{i\uparrow} \\ f^\dagger_{i\downarrow} \end{bmatrix} \qquad \text{and} \qquad U_{ij} = U^\dagger_{ji} \in \mathrm{Mat}(2\times 2, \mathbb{C}) \tag{3.5}$$

A gauge transformation W consists of a matrix $W(i) \in \mathrm{SU}(2)$ for each lattice point i and acts on Ψ_i like

$$\begin{bmatrix} f_{i\uparrow} \\ f^\dagger_{i\downarrow} \end{bmatrix} = W(i) \begin{bmatrix} c_{i\uparrow} \\ c^\dagger_{i\downarrow} \end{bmatrix}, \qquad W(i) \in SU(2) \tag{3.6}$$

The new operators $c_{i\alpha}$ satisfy fermionic anti-commutation relations. A short form to denote the transformation is

$$\Psi_i \xrightarrow{W} W(i)\Psi_i \tag{3.7}$$

The arrow means: Replace the left hand side by the right hand side in the current Hamiltonian to obtain the Hamiltonian in new coordinates. So equation (3.7) is the same as

$$U_{ij} \xrightarrow{W} W(i)^\dagger U_{ij} W(j) \tag{3.8}$$

Let T : lattice $\to$ lattice be a bijective function. I define the symmetry transformation associated with T by

$$\Psi_i \xrightarrow{T} \Psi_{T(i)} \tag{3.9}$$

Let (G_T, T) be a pair consisting of a symmetry transformation T and a gauge transformation G_T. (G_T, T) is in the projective symmetry group of an ansatz iff the corresponding Hamilton operator is invariant under the combined transformation $G_T T$. This defines the projective symmetry group. $G_T T$ acts on Ψ_i as follows

$$\Psi_i \xrightarrow{T} \Psi_{T(i)} \xrightarrow{G_T} G(T(i))\Psi_{T(i)} \tag{3.10}$$

Thus, $(G_T, T) \in PSG(\{U_{ij}\})$ is equivalent to

$$\forall ij : G_T(T(i))^\dagger U_{ij} G_T(T(j)) = U_{T(i)T(j)} \qquad \Leftrightarrow \qquad \forall ij : U_{ij} = G_T(T(i)) U_{T(i)T(j)} G_T(T(j))^\dagger \tag{3.11}$$

Proposition: *(group operation and inverse elements)*

PSG is a group. The group operation is given by

$$\cdot : PSG \times PSG \to PSG, \quad (G_T, T)\cdot(G_S, S) = (G_T T G_S T^{-1}, TS) \tag{3.12}$$

Proof: Let $(G_T, T), (G_S, S) \in PSG$. T and S are symmetries, so TS is also a symmetry. $G_T T G_S T^{-1}$ is a gauge transformation:

$$\Psi_i \xrightarrow{T^{-1}} \Psi_{T^{-1}(i)} \xrightarrow{G_S} G_S(T^{-1}(i))\Psi_{T^{-1}(i)} \xrightarrow{T} G_S(T^{-1}(i))\Psi_i \xrightarrow{G_T} G_S(T^{-1}(i)) G_T(i)\Psi_i \tag{3.13}$$

and $G_S(T^{-1}(i))G_T(i) \in SU(2)$. The Hamilton operator is invariant under $G_T T G_S T^{-1} TS = G_T T G_S S$. Thus, $(G_T T G_S T^{-1}, TS) \in PSG$. $G_S S, G_T T$ were arbitrary. The group operation is well defined. The identity is (id, id). Let $(G_T, T) \in PSG$. An inverse is given by

$$(G_T, T)^{-1} = (T^{-1} G_T^{-1} T, T^{-1}) \tag{3.14}$$

Clearly

$$(G_T, T)\cdot(T^{-1}G_T^{-1}T, T^{-1}) = (T^{-1}G_T^{-1}T, T^{-1})\cdot(G_T, T) = (id, id)\,, \tag{3.15}$$

but it is not obvious at all that $(T^{-1}G_T^{-1}T, T^{-1}) \in PSG$. $T^{-1}G_T^{-1}$ transforms Ψ_i like

$$\Psi_i \xrightarrow{G_T^{-1}} G_T(i)^\dagger \Psi_i \xrightarrow{T^{-1}} G_T(i)^\dagger \Psi_{T^{-1}(i)}\,, \tag{3.16}$$

which is the same as

$$\Psi_i^\dagger U_{ij}\Psi_j \xrightarrow{T^{-1}G_T^{-1}} \Psi^\dagger_{T^{-1}(i)} G_T(i) U_{ij} G_T(j)^\dagger \Psi_{T^{-1}(j)}\,. \tag{3.17}$$

This means that the Hamilton operator is invariant under $T^{-1}G_T^{-1}$ if and only if

$$\forall ij : U_{T^{-1}(i)T^{-1}(j)} = G_T(i)U_{ij}G_T(j)^\dagger \qquad \Leftrightarrow \qquad \forall ij : U_{ij} = G_T(T(i))U_{T(i)T(j)}G_T(T(j))^\dagger \tag{3.18}$$

This is exactly the condition (3.11) for $(G_T, T) \in PSG$. Hence, H is invariant under $T^{-1}G_T^{-1} = T^{-1}G_T^{-1}TT^{-1}$. (G_T, T) was arbitrary. Inverse elements exist. The group operation is associative. □

Each projective symmetry group has special subgroup called invariant gauge group (IGG). It consists of all gauge transformations associated with the identity symmetry.

$$IGG = \{(W, id)\,|\,(W, id) \in PSG\} \tag{3.19}$$

Definition: An ansatz $\{U_{ij}\}$ has symmetry S iff there exists G_S such that $(G_S, S) \in PSG(\{U_{ij}\})$. The group of all symmetries of an ansatz will be called its symmetry group (SG).

Lemma: *(the invariant gauge group factors the projective symmetry group)*

Let $(G_T, T) \in PSG$ be any transformation corresponding to the symmetry T. Then all other transformations in the PSG corresponding to the same symmetry must be of the form

$$(W, id) \cdot (G_T, T), \qquad (W, id) \in IGG \tag{3.20}$$

Proof: Let $(G_T, T) \in PSG$ be fixed. If $(G_T, T) \in PSG$ and $(W, id) \in PSG$, then also $(W, id)\cdot(G_T, T) = (WG_T, T) \in PSG$. This holds because PSG is closed under its group operation. Conversely, assume there is a second $(A, T) \in PSG$. $(A, T) = (AG_T^{-1}, id) \cdot (G_T, T)$. Therefore it is sufficient to show that $(AG_T^{-1}, id) \in IGG$. Note that

$$(AG_T^{-1}, id) = (ATT^{-1}G_T^{-1}TT^{-1}, TT^{-1}) = (A, T) \cdot (G_T, T)^{-1} \tag{3.21}$$

Thus, $(AG_T^{-1}, id) \in PSG$ and by the definition of IGG we have that $(AG_T^{-1}, id) \in IGG$. □

The symmetry group is therefore a quotient of the projective symmetry group.

$$SG \cong PSG/IGG := PSG/_\sim \tag{3.22}$$

where $(G_T, T) \sim (G_S, S)$ iff there exists (W, id) s.t. $(G_T, T) = (W, id) \cdot (G_S, S)$.

The projective symmetry group seems to be a property of an ansatz rather than a property of its equivalence class. As we have shown before, anything we do can only be relevant up to the choice of gauge. Fortunately, we find that projective symmetry groups of gauge equivalent ansätze are isomorphic. Suppose

$$H = \sum_{\langle ij\rangle} \Big(\Psi_i^\dagger U_{ij}\Psi_j + \text{h.c.}\Big) + \text{const.} \tag{3.23}$$

is invariant under the transformation $G_T T$. Switch to a different gauge W. The new Hamilton operator is

$$\tilde{H} = \sum_{\langle ij\rangle} \Big((W(i)\Psi_i)^\dagger U_{ij} W(j)\Psi_j + (W(j)\Psi_j)^\dagger U_{ij}^\dagger W(j)\Psi_j\Big) + \text{const.} \tag{3.24}$$

There is an element $(\tilde{G}_T, T)$ in the PSG of $\tilde{H}$ which corresponds to (G_T, T). $(G_T, T) \mapsto (\tilde{G}_T, T)$ is a group isomorphism.

Proposition: *(the projective symmetry group is a property of equivalence classes)*

$PSG(H) \cong PSG(\tilde{H})$. More explicitly

$$\begin{aligned} &\mathscr{G} : PSG(H) \to PSG(\tilde{H}), \quad (G, T) \mapsto (WGTW^{-1}T^{-1}, T) \\ &\mathscr{G}^{-1} : PSG(\tilde{H}) \to PSG(H), \quad (G, T) \mapsto (W^{-1}GTWT^{-1}, T) \end{aligned} \tag{3.25}$$

defines a group isomorphism.

Proof: First observe that $\mathscr{G}$ is well-defined. If $(G,T) \in PSG(H)$, then $WGTW^{-1}$ acts on $\tilde{H}$ like this:

$$\tilde{H} \xrightarrow{W^{-1}} H \xrightarrow{GT} H \xrightarrow{W} \tilde{H} \tag{3.26}$$

Thus, $(WGTW^{-1}T^{-1},T) \in PSG(\tilde{H})$. Take any $(G,T) \in PSG(H)$.

$$\mathscr{G}^{-1}\mathscr{G}(G,T) = \mathscr{G}^{-1}(WGTW^{-1}T^{-1},T) = (W^{-1}WGTW^{-1}T^{-1}TWT^{-1},T) = (G,T) \tag{3.27}$$

In the same way for $\mathscr{G}\mathscr{G}^{-1}(G,T)$. Hence, $\mathscr{G}$ and $\mathscr{G}^{-1}$ are indeed inverse to each other. It remains to show that $\mathscr{G}$ preserves the group structure.

$$\mathscr{G}(id,id) = (W id\, id\, W^{-1} id^{-1}, id) = (id,id) \tag{3.28}$$

Take any two elements $(G_T,T),(G_S,S) \in PSG(H)$.

$$\begin{aligned}
&\mathscr{G}((G_T,T)\cdot(G_S,S)) = \mathscr{G}(G_TTG_ST^{-1},TS) = (WG_TTG_ST^{-1}TSW^{-1}S^{-1}T^{-1},TS)\\
&= (WG_TTW^{-1}T^{-1}TWG_SSW^{-1}S^{-1}T^{-1},TS) = (WG_TTW^{-1}T^{-1},T)\cdot(WG_SSW^{-1}S^{-1},S)\\
&= \mathscr{G}(G_T,T)\cdot\mathscr{G}(G_S,S)
\end{aligned} \tag{3.29}$$

That $\mathscr{G}^{-1}$ preserves group structure follows automatically from the fact that $\mathscr{G}$ does. □

This means the projective symmetry group really is a property of the equivalence classes. When we try to determine the PSG of an ansatz, we are allowed to switch gauge as often as we like. The $SU(2)$-matrices $\tilde{G}_T(i)$ in a new gauge W are given by

$$\tilde{G}(i) = WG_TTW^{-1}T^{-1}(i) = W(T^{-1}(i))^\dagger G_T(i)W(i) \tag{3.30}$$

To see this, examine how $\tilde{G}_T = WG_TTW^{-1}T^{-1}$ acts on Ψ_i:

$$\Psi_i \xrightarrow{T^{-1}} \Psi_{T^{-1}(i)} \xrightarrow{W^{-1}} W(T^{-1}(i))^\dagger\Psi_{T^{-1}(i)} \xrightarrow{T} W(T^{-1}(i))^\dagger\Psi_i \xrightarrow{WG_T} W(T^{-1}(i))^\dagger G_T(i)W(i)\Psi_i \tag{3.31}$$

4 Symmetry group of kagome-based spin liquids

It is time to introduce the two lattices on which we want apply the projective symmetry group method. The first one is the kagome lattice, shown in figure 2. It is one of the most promising candidates of a geometrically frustrated spin system that might give rise to a spin liquid like ground state. A lot of theoretical work has be done searching for such a state. An example is this paper [5] by Yan Siment et al., where the authors assume isotropic antiferromagnetic next-neighbour coupling. Such an ideal scenario proves difficult to realise experimentally. Real world Hamiltonians have additional terms, such as ferromagnetic interactions or second-neighbour coupling, which can cause symmetry breaking at low temperatures and thus prevent spin liquid behaviour. There are few examples of spin liquids observed in the real world. One is the mineral Herbertsmithite, which has recently been verified to have a spin liquid like ground state [4], including fractional excitations. It is an example of an ideal kagome lattice. Another promising candidate is the Heisenberg magnet $Ca_{10}Cr_7C_{28}$ [11]. The crystal has a magnetic sublattice comparable to the kagome lattice [12]. It has the same translation symmetries, but less rotation and no projection symmetry. The Cr_5^+-sublattice of $Ca_{10}Cr_7C_{28}$ is the second lattice we want to examine. Before we can start to classify the projective symmetry groups of both lattices, we have to determine their symmetry groups. This is the objective of the chapter.

4.1 Symmetry group of the kagome lattice

The symmetry group of an object in (a subset of) $\mathbb{R}^n$ consists of all isometric bijective functions from the object to itself. Figure 2 shows the kagome lattice and its basis vectors $\hat{x}$ and $\hat{y}$. There are three atoms per unit cell.

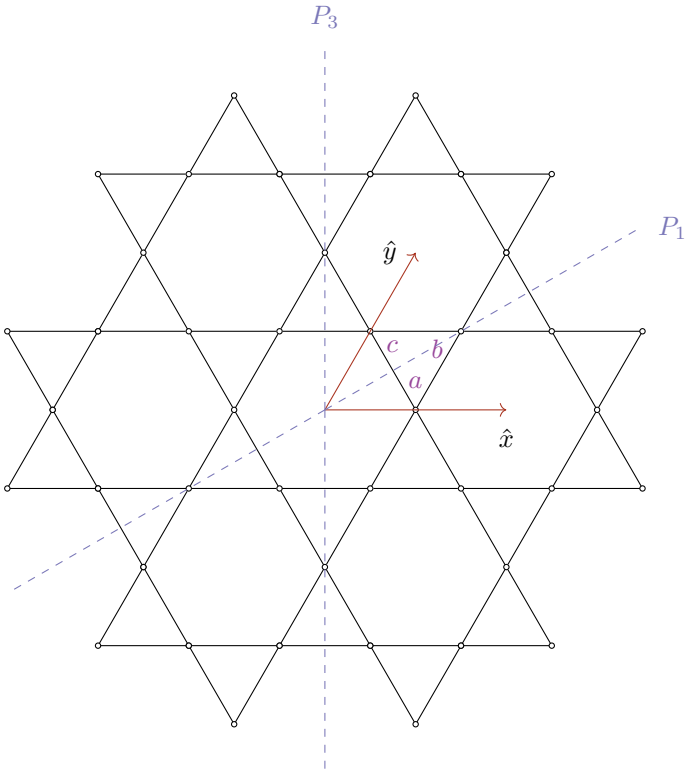

Figure 2: Kagome lattice

I will label the points in the kagome lattice by

$$\text{lattice} = \mathbb{Z} \times \mathbb{Z} \times \{a, b, c\} \tag{4.1}$$

For example, the first lattice point in the zeroth unit cell, marked with the purple letter a in figure 2, has the label $(0, 0, a)$. We will use polar coordinates as well to make the definition of rotation and reflection symmetries clearer. E.g. the lattice point $(0, 0, c)$ corresponds to $(0.5, \pi/3)$ in polar coordinates. Define the following symmetry operations:

$$\begin{aligned} T_x &: \text{lattice} \to \text{lattice}, \quad i \mapsto i - \hat{x} \\ T_y &: \text{lattice} \to \text{lattice}, \quad i \mapsto i - \hat{y} \end{aligned} \tag{4.2}$$

Using polar coordinates, define

$$\begin{aligned} P_0 &: \mathbb{R}^+ \times [0, 2\pi) \to \mathbb{R}^+ \times [0, 2\pi), \quad (r, \varphi) \mapsto (r, -\varphi) \\ D &: \mathbb{R}^+ \times [0, 2\pi) \to \mathbb{R}^+ \times [0, 2\pi), \quad (r, \varphi) \mapsto (r, \varphi - \frac{\pi}{3}) \end{aligned} \tag{4.3}$$

These four symmetry operations generate the symmetry group of the kagome lattice [13]. Not all bijective functions can be symmetries, only those which preserve distances and angles. Let S be any such function. Assume we know how three lattice points are transformed by S. If these points are not on a line, then S is completely determined. Thus, any symmetry transformation is either a translation, a projection, a rotation or a finite combination of those. Clearly, all translation symmetries of the kagome lattice are generated by T_x and T_y. Let P be any reflection symmetry. The reflection axis of P must go through the centre of each honeycomb cell it touches, otherwise P will never map lattice points to lattice points. Since we can move the reflection axis around with T_x and T_y, it is enough to consider reflections whose axis intersects the point of origin. Two of them are drawn in figure 2. Overall there are six possible symmetry axes through the point of origin. We will call them $P_0, ..., P_5$. P_0 is the one we defined above. The reflection axis of P_1 is drawn in figure 2. $P_1, ..., P_5$ are combinations of P_0 and D. To see this, let D_θ denote the transformation $(r, \varphi) \mapsto (r, \varphi - \theta)$. Then $P_1 = D^{-1}_{\pi/6} P_0 D_{\pi/6}$. In consequence

$$P_1(r, \varphi) = D^{-1}_{\pi/6} P_0 D_{\pi/6}(r, \varphi) = \left(r, -\left(\varphi - \frac{\pi}{6}\right) + \frac{\pi}{6}\right) = \left(r, -\left(\varphi - \frac{\pi}{3}\right)\right) = P_0 D(r, \varphi) \tag{4.4}$$

Thus, $P_1 = P_0 D$. In the same way one finds that $P_k = P_0 D^k$ for each $k = 0, ..., 5$. Hence, all reflections are generated by P_0, D, T_x and T_y. It remains to consider rotations. A $2D$ rotation is uniquely determined through a rotation centre and an angle. Because we can translate the centre using T_x and T_y, it is enough to consider rotations around points in the zeroth unit cell. Possible rotations are those with an angle of $k\frac{\pi}{3}$ around the point of origin, $k = 1, ..., 5$. Those are D^k, $k = 1, ..., 5$. Further possible rotations are those with an angle of π around the lattice points $(0, 0, a), (0, 0, b)$ and $(0, 0, c)$. They can be expressed as a combination of D, T_x and T_y. The rotation of angle π around the point $(0, 0, a)$ is $T_x^{-1} D^3$. The rotation of angle π around $(0, 0, b)$ is $T_x^{-1} T_y^{-1} D^3$. The rotation around $(0, 0, c)$ is $T_y^{-1} D^3$. The last two points in the first unit cell which we need to look at are $(\sqrt{3}/3, \pi/6)$ and $(2\sqrt{3}/3, \pi/6)$ (in polar coordinates with $\|\hat{x}\| = 1$). They are the midpoints of the two small triangles in the zeroth unit cell. Around both points rotations of angle $k2\pi/3$ are possible, $k = 1, 2$. Again, they can be expressed as a combination of D, T_x and T_y. The rotation of angle $2\pi/3$ around $(\sqrt{3}/3, \pi/6)$ is $T_y^{-1} D^2$. The rotation of angle $2\pi/3$ around $(2\sqrt{3}/3, \pi/6)$ is $T_y^{-1} T_y^{-1} D^2$.

4.2 Distorted kagome lattice

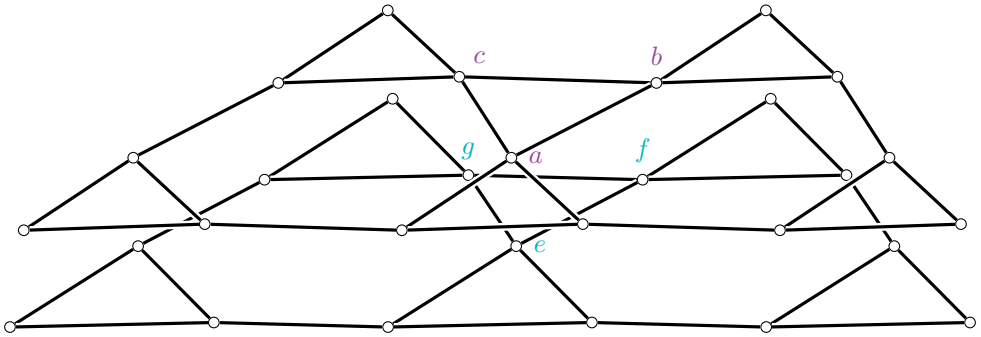

Figure 3: Cr_5^+-ion double layer kagome lattice

As mentioned before, the second lattice is realised as a substructure of the $Ca_{10}Cr_7C_{28}$ compound. The Cr_5^+-ions in each unit cell are responsible for the magnetic behaviour of the crystal. Cr_5^+-ions carry an effective total spin of $\frac{1}{2}$. They form a distorted double layer kagome lattice [12, 11], drawn in figure 3. $Ca_{10}Cr_7C_{28}$ has recently been shown to possess features expected of a quantum spin liquid [11]. Especially, $Ca_{10}Cr_7C_{28}$ undergoes no phase transition to a long-range ordered magnetic state down to temperatures of $0.3K$ [11, p. 2]. For this reason it is worth to search analytically for a possible spin liquid states on the lattice.

I will use the following notation to label the lattice points of the double layer Cr_5^+- lattice:

$$\text{lattice} := \mathbb{Z} \times \mathbb{Z} \times \{a, b, c, e, f, g\} \tag{4.5}$$

$\{a, b, c\}$ are the atoms in the upper layer and $\{e, f, g\}$ the atoms in the second layer. Both layers consist of two equilateral triangles of different side lengths repeated in the plane. The distorted lattice has fewer symmetries than the kagome lattice. Still present are the two translation symmetries, rotations of angle $2\pi/3$ around the centre of each honeycomb cell and rotations of angle $2\pi/3$ around the centres of the small triangles. The two layers are inequivalent, so there is no projection symmetry between them. It is not easy see the symmetries in the 3D plot. A more technical plot of the upper layer can be found in figure 4. It was made with the coordinates from table 1.

$\hat{x}$	2.0000, 0.0000	$\hat{y}$	1.0000, 1.7321
a	0.9580 , -0.0304	e	0.9692, 0.0417
b	1.5494 , 0.8488	f	1.4818 , 0.8224
c	0.4923 , 0.9213	g	0.5493 , 0.8760

Table 1: Cr_5^+-ion lattice, positions of the atoms

The black points in figure 4 mark the upper layer atoms, the green points mark the lower layer atoms. The red markers indicate the centres of the triangles and the honeycomb cell in the upper layer. The

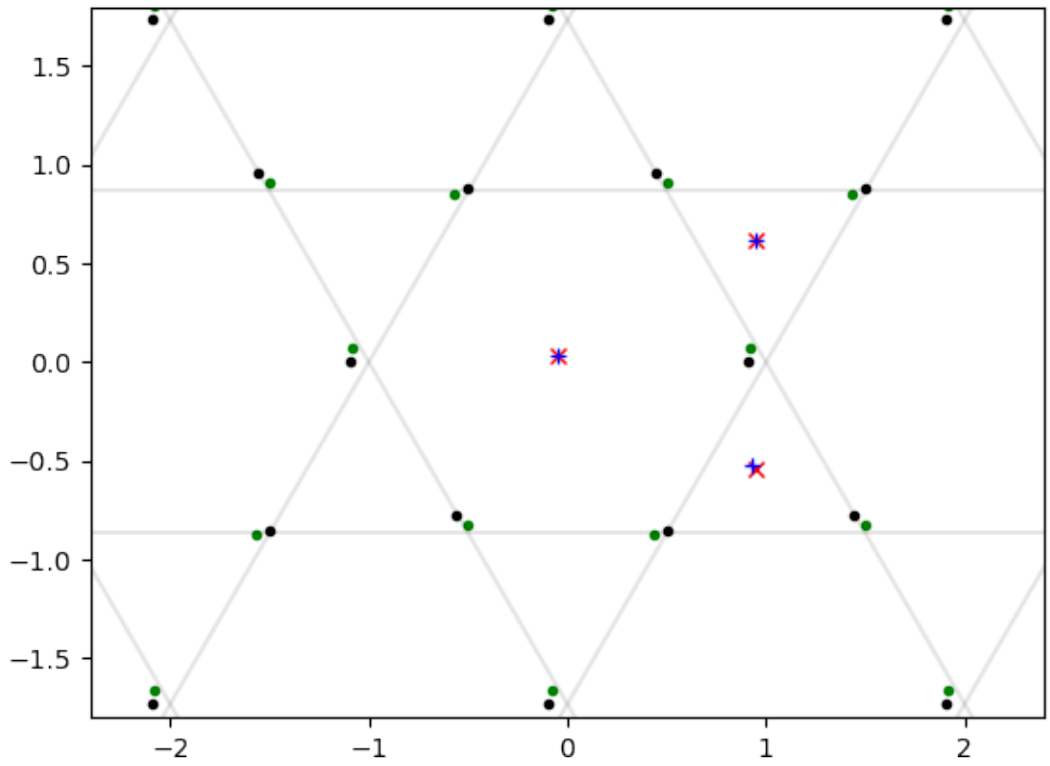

Figure 4: distorted kagome lattice

blue markers indicate the centres in the lower layer. It is crucial that the centres of upper and lower layer lie directly above each other. Otherwise there is no rotation symmetry. This is the case, at least within the accuracy of table 1. It should be clear from figure 4 that the projection symmetry P no longer exists. Thus, the spatial symmetry group is generated by three symmetries T_x, T_y and R. $R = D^2$ is the clockwise rotation of angle $2\pi/3$ around the centre of the zeroth honeycomb cell. Note that the rotations around the centres of the small triangles are generated by R, T_x and T_y. The clockwise rotation of angle $2\pi/3$ around the centre of the upper triangle is $T_y^{-1}R$. The clockwise rotation of angle $2\pi/3$ around the centre of the lower triangle is $T_x^{-1}R$.

4.3 Time reversal symmetry

Time reversal in quantum mechanics behaves differently than spatial symmetries. I have to start with some general remarks. My argumentation closely follows a philosophy paper by R. Bryan [20]. For a more pragmatic approach to time reversal see Sakurai's *Modern Quantum Mechanics* [21]. In the end, the definition of time reversal is convention. Some systems break time reversal symmetry, some don't. Let X be a Hilbert space and let H be the Hamiltonian that generates time propagation. Assume H is time reversal symmetric. Naively this means there exists a bijective map $T : X \to X$ which produces states that propagate backwards in time under the action of H. More precisely: Whenever function $\varphi(\cdot) : \mathbb{R} \to X$, $t \mapsto \varphi(t)$ satisfies the time dependent Schrödinger equation then so does $t \mapsto T\varphi(-t)$. We want to know whether such a mapping can exist, and if it can, how it acts on states in X. For simplicity assume H is time independent. Then $t \mapsto \varphi(t)$ satisfies $i\partial_t \varphi(t) = H\varphi(t)$ if and only if it is of the form

$$\varphi(t) = e^{-itH}\varphi_0 \tag{4.6}$$

for some $\varphi_0 \in X$. Note that

$$T\varphi(-t) = Te^{itH}\varphi_0 \qquad \text{and} \qquad T\varphi(0) = T\varphi_0 \tag{4.7}$$

The solution of the time dependent Schrödinger equation is unique for fixed boundary conditions. We want $t \mapsto T\varphi(-t)$ to satisfy the time dependent Schrödinger equation. Thus,

$$\forall\varphi_0 \forall t: \qquad Te^{itH}\varphi_0 = e^{-itH}T\varphi_0 \tag{4.8}$$

Since this holds for all $\varphi_0 \in X$, it follows that

$$\forall t: \qquad e^{-itH} = Te^{itH}T^{-1} = e^{TitHT^{-1}} \tag{4.9}$$

The exponential map of bounded operators is not injective. But a weaker result is sufficient: if $\forall t : e^{tA} = e^{tB}$, then $A = B$. To prove this rigorously one needs the concept of generalised derivatives of functions between normed spaces [22, p. 126] and the fact that exponentials of operators are invertible:

$$\forall t:\ e^{tA} = e^{tB} \quad \Rightarrow \quad \forall t:\ \partial_t e^{tA} = \partial_t e^{tB} \quad \Rightarrow \quad \forall t:\ Ae^{tA}e^{-tA} = Be^{tB}e^{-tA} \quad \Rightarrow \quad A = B \tag{4.10}$$

In consequence, $-iH = TiHT^{-1}$. Suppose T is linear. Then $-H = THT^{-1}$. In this case, whenever $H\varphi_n = E_n\varphi_n$, then $HT\varphi_n = -E_nT\varphi_n$. This can not hold for Hamiltonians with a semi-positive spectrum. An example are free Hamiltonians, and certainly we want to be able to time reverse those. Hence, time reversal, if it exists, can not be linear. In contrast, all spatial symmetries defined before are linear. They transform one set of fermionic operators into another which is, as shown in the appendix A, a change of orthonormal basis.

In general a symmetry is something which does not change the physical content of a system, only the mathematics with which we describe it. All experimental observations can be expressed by transition probabilities $|\langle\psi|\varphi\rangle|$ between normed vectors in X. Therefore the vectors in X do not correspond 1-to-1 to states of the physical system. Instead physical states are equivalence classes of unit vectors, called rays. It makes sense to define quantum symmetries as bijective maps on ray space that preserve all transition probabilities. Such a mapping is called Wigner symmetry. Every unitary and antiunitary operator acting on X naturally induces a Wigner symmetry on ray space [23]. Wigner himself famously showed the other direction. Any Wigner symmetry on ray space can be lifted into either an unitary or antiunitary operator acting on the underlying Hilbert space [23, 24].

Hence, time reversal symmetry, if it exists, has to be antiunitary. This does not yet determine uniquely how T transforms angular momentum $\boldsymbol{J}$. It turns out that we need additionally assumptions. The most fundamental definition of angular momentum in quantum mechanics is in terms of the Lie group $SO(3)$. Angular momentum operators J^μ can be defined as generators of rotation in X [21, p. 161]. A rotation of angle θ around $\hat{n}$ is represented by

$$R(\hat{n},\theta) : X \to X, \qquad \psi \mapsto e^{-i\theta\hat{n}\cdot\boldsymbol{J}}\,\psi \qquad \text{where} \qquad \theta \in [0, 2\pi), \quad \hat{n} \in S_{\mathbb{R}^3} \tag{4.11}$$

It is a reasonable assumption that time reversal should not change the spatial coordinate system. Especially, it should make no difference if one applies time reversal first and than rotates the system or the other way around. Thus, T should commute with all rotation operators.

$$\forall\hat{n}, \forall\theta: \qquad e^{-i\theta\hat{n}\cdot\boldsymbol{J}} = Te^{-i\theta\hat{n}\cdot\boldsymbol{J}}T^{-1} = e^{T(-i\theta\hat{n}\cdot\boldsymbol{J})T^{-1}} = e^{i\theta T(\hat{n}\cdot\boldsymbol{J})T^{-1}} \tag{4.12}$$

The derivative-inverse argument again gives

$$\forall\hat{n} \in S_{\mathbb{R}_3}: \quad T\,(\hat{n}\cdot\boldsymbol{J})\,T^{-1} = -\hat{n}\cdot\boldsymbol{J} \tag{4.13}$$

as the classical picture would suggest. Consider now the case that $X = \mathbb{C}^2$ is the Hilbert space of a single spin 1/2 particle. Requirement (4.13) and T antiunitary are enough to determine T up to a phase. If the action of T on a basis is known, then T is uniquely defined through its antilinearity property. This implies that T can always be decomposed into $T = UK$, where U is linear and K is a basis-dependent complex conjugate operator. T is antiunitary iff U is unitary. Fix the basis $\{|\uparrow\rangle, |\downarrow\rangle\}$. From the form of the Pauli-matrices, which represent S^μ in S_z-basis, follows that $KS^yK^{-1} = -S^y$, $KS^xK^{-1} = S^x$ and $KS^zK^{-1} = S_z$. On the other hand, T must satisfy (4.13). Hence (in matrix form and with an additional factor i):

$$U\,i\tau^1\,U^\dagger = -i\tau^1, \qquad U\,i\tau^2U^\dagger = i\tau^2, \qquad Ui\tau^3U^\dagger = -i\tau^3 \tag{4.14}$$

If $\det(U) = -1$, multiply U by a phase $e^{i\pi/2}$. This will not change the induced Wigner transformation on ray space, but it will switch the sign of the determinant. Without loss of generality $U \in SU(2)$. Now I can use results form appendix B. U has no τ^0- component, since it anticommutes with $i\tau^1$ and $i\tau^3$ (proposition 5, appendix B). U has to point in τ^2-direction, since it commutes with $i\tau^2$. Thus, $U = \pm i\tau^2$. Up to a phase $U = -i\tau^2$ and in consequence $T = -i\,2S^yK$. Finally: $T|\uparrow\rangle = |\downarrow\rangle$ and $T|\downarrow\rangle = -|\uparrow\rangle$ extended by antilinearity.

The single particle expression motivates the standard implementation of time reversal in the Fock space $\Gamma_{-1}(\mathcal{H})$. The rule to obtain $TH_{MF}T^{-1}$ from H_{MF} is: Replace

$$\begin{bmatrix} f_{i\uparrow} \\ f_{i\downarrow} \end{bmatrix} \xrightarrow{T} \begin{bmatrix} f_{i\downarrow} \\ -f_{i\uparrow} \end{bmatrix} \qquad \text{or} \qquad \begin{bmatrix} f_{i\uparrow} \\ f^\dagger_{i\downarrow} \end{bmatrix} \xrightarrow{T} \begin{bmatrix} f_{i\downarrow} \\ -f^\dagger_{i\uparrow} \end{bmatrix} \tag{4.15}$$

and complex conjugate every scalar in H_{MF} [25, 8, p. 392]. (4.15) is the same as

$$\Psi_i \xrightarrow{T} \left(\left(-i\tau^2\Psi_i\right)^\dagger\right)^t =: \left(-i\tau^2\Psi_i\right)^* \tag{4.16}$$

Since we are allowed to switch gauge as often as we like, we can simplify (4.16) if we declare that we always apply $\Psi_i \to i\tau^2\Psi_i$ after time reversal. Define a new transformation T being time reversal + the above gauge transformation. The transforming rule for H_{MF} becomes:

$$U_{ij} \xrightarrow{T} U^*_{ij} \qquad \text{and} \qquad \Psi_i \xrightarrow{T} \Psi^*_i \tag{4.17}$$

Recall that $H^{\{U_{ij}\}}_{MF}$ of an ansatz $\{U_{ij}\}$ takes the from

$$H^{\{U_{ij}\}}_{MF} = \sum_{\langle ij\rangle} \left(\Psi^\dagger_i U_{ij}\Psi_j + \Psi^\dagger_j U^\dagger_{ij}\Psi_i\right) + \text{const.} \tag{4.18}$$

Under time reversal T:

$$\begin{aligned} \Psi^\dagger_i U_{ij}\Psi_j + \Psi^\dagger_j U^\dagger_{ij}\Psi_i \xrightarrow{T} \left(\Psi^*_i\right)^\dagger U^*_{ij}\Psi^*_j + \left(\Psi^*_j\right)^\dagger \left(U^*_{ij}\right)^\dagger \Psi^*_i &= \left(\Psi^\dagger_j U_{ij}\Psi_i\right)^t + \left(\Psi^\dagger_i U^\dagger_{ij}\Psi_i\right)^t \\ &= \Psi^\dagger_j U_{ij}\Psi_i + \Psi^\dagger_i U^\dagger_{ij}\Psi_i = \Psi^\dagger_i\left(-U_{ij}\right) + \Psi^\dagger_j(-U_{ij})^\dagger\Psi_i \end{aligned} \tag{4.19}$$

The last line holds because of fermionic anticommutation relations. Hence, we can write time reversal as

$$U_{ij} \xrightarrow{T} -U_{ij} \tag{4.20}$$

5 Classification of kagome-based $\mathbb{Z}_2$ projective symmetry groups

The classification of the $\mathbb{Z}_2$ projective symmetry groups on the kagome lattice has been worked out before [13], but the precise calculation is not published. I have repeated the calculation. A detailed step-by-step derivation can be found in appendix C. There are 30 different projective symmetry groups, up to gauge transformations. For 10 of them all bonds vanish and the Hamiltonian is constant. Thus, only 20 different PSGs can possibly describe a $\mathbb{Z}_2$ spin liquid state on the kagome lattice. I will only present the result here, so that I can compare them it with the distorted Cr^+_5-lattice.

This is a good place to explain briefly how the classification works (for any lattice) and what the results mean. I will repeat some facts from the third and second chapter. Suppose $\{U_{ij}\}$ is an ansatz for a mean field spin liquid on the kagome lattice. That is, assume that the set of matrices $\{U_{ij}\}$ satisfies the self-consistency condition and that for each symmetry S of the lattice there exists a gauge transformation G_S such that $U_{ij} \xrightarrow{G_S S} U_{ij}$. The pairs $G_S S$ form the PSG of $\{U_{ij}\}$. The PSG has a special subgroup IGG. IGG is at least $\mathbb{Z}_2$. This follows directly from (3.18). IGG consists at most of all local $SU(2)$ transformations (i.e. is at most the gauge group). Every subgroup of the gauge group is a possible invariant gauge group of $\{U_{ij}\}$. I will assume $IGG = \mathbb{Z}_2$. There is no good reason why this should be true. E.g. there are many examples of $U(1)$ spin liquids. Since the mean field theory is a projective

construction and since we can not solve the Heisenberg Hamiltonian analytically, we can not tell for sure of any of the mean field liquids that it describes the actual ground state correctly. The only chance is to examine all possible mean field liquids carefully case by case to find what experimental data they would predict. We need experiments tell which one of them, if any, is realised. $IGG = \mathbb{Z}_2$ is the easiest option, so it is a good starting point. Mean field theory ignores second order fluctuations in hopping and pairing amplitudes. A spin liquid state can only be realised in a real material, if it is stable against fluctuations. The invariant gauge group starts to be important when dynamics are introduced into the mean field theory. E.g. mean-field $\mathbb{Z}_2$ liquids on the square lattice are all gapped [8, p. 382] and spin correlations are short-ranged [7, p. 427]. Let's go back to the ansatz $\{U_{ij}\}$. No matter which spin state it describes, we are allowed to gauge transform the ansatz as often as we like without changing its physical content. Every time we switch gauge, the PSG of the ansatz changes to a different but isomorphic group. The result of the classification (performed in appendix C) is that, no matter which ansatz $\{U_{ij}\}$ we picked, there always exists a gauge equivalent ansatz $\{\tilde{U}_{ij}\}$ for which five of the PSG elements take the simple form

$$\begin{aligned} &G_y(x,y,z) = \tau^0, && G_x(x,y,z) = \eta_x^y \tau^0, && G_T(x,y,z) = g_T, \\ &G_P(x,y,z) = \eta_x^{xy} g_{Pz}, && G_D(x,y,z) = \eta_x^{h_z(x,y)} g_{Dz} \end{aligned} \tag{5.1}$$

$h_a(x,y) = h_c(x,y) = x + y + xy + \frac{1}{2}(y^2 + y)$ and $h_b(x,y) = x + y + xy + \frac{1}{2}(y^2 - y)$. η_x is either $+1$ or -1. The matrices g_{Sz} are given by one of the options in table 2.

g_T	g_{Pa}	g_{Pb}	g_{Pc}	g_{Da}	g_{Db}	g_{Dc}	$\eta_T, \eta_P, \eta_{PD}, \eta_{Pt}, \eta_{Dt}, \eta_x\eta_D$
τ^0	τ^0	τ^0	τ^0	τ^0	τ^0	τ^0	$+,+,+,+,+,+$
τ^0	τ^0	τ^0	τ^0	$i\tau^3$	$-\tau^0$	τ^0	$+,+,-,+,+,+$
τ^0	$i\tau^3$	$i\tau^3$	$i\tau^3$	τ^0	τ^0	τ^0	$+,-,+,+,+,+$
τ^0	$i\tau^3$	$i\tau^3$	$i\tau^3$	$i\tau^1$	τ^0	τ^0	$+,-,+,+,+,-$
τ^0	$i\tau^3$	$i\tau^3$	$i\tau^3$	$i\tau^3$	τ^0	$-\tau^0$	$+,-,-,+,+,-$
$i\tau^3$	τ^0	τ^0	τ^0	τ^0	τ^0	τ^0	$-,+,+,+,+,+$
$i\tau^3$	τ^0	τ^0	τ^0	$i\tau^3$	τ^0	$-\tau^0$	$-,+,-,+,+,-$
$i\tau^3$	τ^0	τ^0	τ^0	$i\tau^1$	$i\tau^1$	$i\tau^1$	$-,+,-,+,-,-$
$i\tau^3$	τ^0	$i\tau^3$	$-\tau^0$	$i\tau^3$	τ^0	$i\tau^3$	$-,-,+,+,+,+$
$i\tau^3$	τ^0	$i\tau^3$	$-\tau^0$	$i\tau^1$	$i\tau^1$	$i\tau^2$	$-,-,+,+,-,-$
$i\tau^3$	$i\tau^1$	$i\tau^1$	$i\tau^1$	τ^0	τ^0	τ^0	$-,-,+,-,+,+$
$i\tau^3$	$i\tau^2$	$i\tau^1$	$i\tau^2$	τ^0	τ^0	$i\tau^3$	$-,-,+,-,+,-$
$i\tau^3$	$i\tau^1$	$i\tau^1$	$i\tau^1$	$i\tau^2$	$i\tau^1$	$-i\tau^1$	$-,-,+,-,-,-$
$i\tau^3$	$i\tau^1$	$i\tau^1$	$i\tau^1$	$i\tau^1$	$i\tau^1$	$i\tau^1$	$-,-,-,-,-,-$
$i\tau^3$	τ^0	$i\tau^3$	$-\tau^0$	τ^0	$-i\tau^3$	τ^0	$-,-,-,+,+,-$

Table 2: gauge-inequivalent choices for g_T, g_{Pz}, g_{Dz}

This holds as long as the invariant gauge group of the ansatz was indeed $\mathbb{Z}_2$. G_x, G_y, G_T, G_P and G_D are gauge transformations that belong to the symmetries T_x, T_y, T, P and D. Note that (5.1) together with $IGG = \mathbb{Z}_2$ determines the projective symmetry group of the ansatz completely. This is because $PSG \cong IGG \cdot SG$ and because every symmetry S in the symmetry group of the lattice can be generated by a finite combination of T_x, T_y, D, P and T. This classification is a strong result. The form of the projective symmetry group puts harsh constraints on its ansatz via equation (3.18). For example, if we limit ourself to next neighbour bonds on the kagome lattice, then it is enough to fix a projective symmetry group and one matrix U for a bond $i_0 j_0$. All other amplitudes U_{ij} are determined by the PSG elements and (3.18). Thus, we do not have to analyse infinitely many different ansätze to find one which might explain experimental observations. It is sufficient to analyse the 30 PSGs above (i.e. corresponding ansätze) case by case. Every other ansatz will be gauge equivalent to one of the 30 and give the same physical results in $\mathcal{H}_p$.

We can immediately rule out ten of the projective symmetry groups. $G_T T$ is in the PSG of a mean field Hamiltonian H if and only if H invariant under the combined transformation $G_T T$. The time reversal

symmetry transforms H like this:

$$\sum_{\langle ij\rangle}(\Psi_i^\dagger U_{ij}\Psi_j + \text{h.c.}) + \text{const.} \quad \xrightarrow{T} \quad -\sum_{\langle ij\rangle}(\Psi_i^\dagger U_{ij}\Psi_j + \text{h.c.}) + \text{const.} \tag{5.2}$$

So G_T must satisfy

$$\forall ij: \quad G_T(i)^\dagger U_{ij} G_T(j) = -U_{ij} \tag{5.3}$$

If $G_T(i) = \tau^0$ for all i, then (5.3) becomes

$$\forall ij: \quad U_{ij} = -U_{ij} \tag{5.4}$$

Thus, $\eta_T = 1$ implies that the mean field amplitude U_{ij} vanishes for every bond. But an ansatz which vanishes everywhere can only satisfy the self-consistency condition if $J_{ij} = 0$ for all ij. This means there is no interaction between the particles at all, which does not describe the physical system correctly.

30 is a small number of PSGs compared to other lattices. For example the symmetry group of the square lattice (together with time reversal) gives rise to 272 inequivalent $\mathbb{Z}_2$ projective symmetry groups [9, p. 15]. The result is even more drastic for the distorted double layer kagome lattice (see chapter 4.2). I find that every $\mathbb{Z}_2$ projective symmetry group takes the form

$$\begin{aligned} G_T(x,y,z) &= g_T, & G_y(x,y,z) &= \tau^0, \\ G_x(x,y,z) &= \eta_x^y\,\tau^0, & G_R(x,y,z) &= \eta_x^{\frac{1}{2}x(x-1)+xy}\,\tau^0 \end{aligned} \tag{5.5}$$

in some gauge. $\eta_x = \pm 1$ and $g_T = \tau^0, i\tau^3$. A detailed step-by-step derivation can be found in appendix D. Together with the free choice of $\eta_x = \pm 1$ there are only $2 \times 2 = 4$ different $\mathbb{Z}_2$ PSGs on the distorted kagome lattice. Again, two of them can be ruled out immediately: if $g_T = \tau^0$ then all mean field amplitudes must vanish.

Finding the projective symmetry groups is only the first step. The inequivalent PSGs need to be analysed case by case to see whether they can describe a stable spin liquid phase. We already ruled out two of the four PSGs on the Cr_5^+-ion lattice. Only two relevant PSGs remain. I will show next-neighbour coupling ansätze for both of them. They can be used for further analysis of the Cr_5^+-ion lattice.

It is convenient to switch to a gauge in which $g_T = i\tau^1$. This can be done without changing any of the other PSG elements. Let ij be any bond. In general, the coefficient matrix U_{ij} is of the form

$$U_{ij} = \begin{bmatrix} \chi_{ij}^* & \eta_{ij} \\ \eta_{ij}^* & -\chi_{ij} \end{bmatrix} \tag{5.6}$$

Time reversal symmetry implies

$$-U_{ij} = (i\tau^1)^\dagger\, U_{ij}\, i\tau^1 \tag{5.7}$$

This can only hold if $\text{Im}(\chi_{ij}) = 0$ and $\text{Re}(\eta_{ij}) = 0$. Thus, every coefficient matrix U_{ij} can be written as

$$U_{ij} = \chi_{ij}\tau^3 + \eta_{ij}\tau^2, \qquad \chi_{ij}, \eta_{ij} \in \mathbb{R} \tag{5.8}$$

We have to choose amplitudes for only one of bond in each of the two inequivalent triangles. All other bonds in the plane are determined by rotation and translation symmetries. Set $D_1 = T_y^{-1}R$ and $D_2 = T_x^{-1}R$. Refer to (7.166) or to chapter 4 for a definition of R, T_x and T_y. D_1 rotates the first triangle $(0,0,a)$ - $(0,0,b)$ - $(0,0,c)$ clockwise by an angle of $2\pi/3$. D_2 rotates the second triangle $(0,-1,b)$ - $(0,0,a)$ - $(1,-1,c)$ clockwise by an angle of $2\pi/3$. Using the law of composition from chapter 3 one finds that

$$G_{D_1}(x,y,z) = \eta_x^{\frac{1}{2}x(x+1)+xy}\tau^0 \qquad \text{and} \qquad G_{D_2}(x,y,z) = \eta_x^{\frac{1}{2}x(x+1)+xy+1}\tau^0 \tag{5.9}$$

This can be used together with (3.11) to determine the matrices in the first and second triangle. I find that

$$U_{(0,0,a),(0,0,c)} = U_{(0,0,c),(0,0,b)} = U_{(0,0,b),(0,0,a)} \tag{5.10}$$

and

$$U_{(0,-1,b),(0,0,a)} = U_{(0,0,a),(1,-1,c)} = U_{(1,-1,c),(0,-1,b)} \tag{5.11}$$

A similar result holds at the lower layer. The sign structure in the plane is ruled by (G_x, T_x) and (G_y, T_y):

$$U_{i-\hat{y},j-\hat{y}} = U_{ij} \qquad \text{and} \qquad U_{i-\hat{x},j-\hat{x}} = \eta_x^{i_y+j_y} U_{ij} \tag{5.12}$$

The bonds in-between the two layers are all equal to each other. Figure 5 shows the two ansätze on the distorted lattice schematically. Two bonds are marked in the same colour if their hopping and pairing amplitudes are equal. If $\eta_x = 1$, then blue = green. If $\eta_x = -1$, then blue = −green.

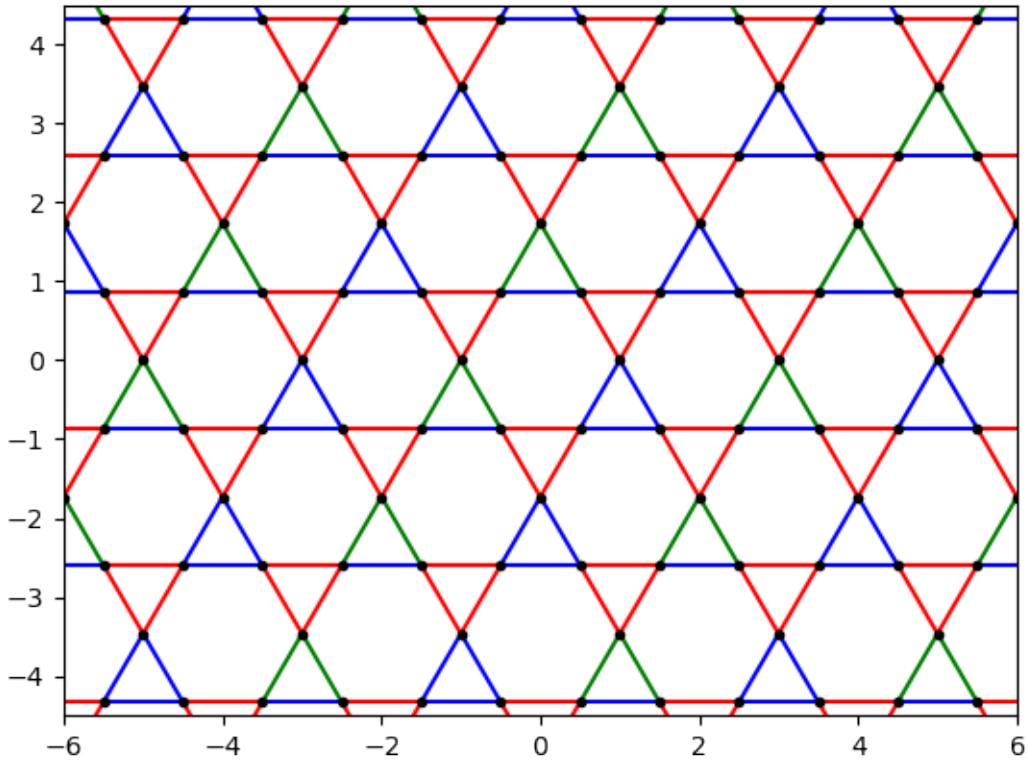

Figure 5: ansatz for the distorted Cr_5^+-ion lattice

6 Conclusion

Even though it is widely believed that a spin liquid state of matter exists, finding actual examples has proven to be difficult. We can not solve the Hamiltonian of many-spin systems analytically. This makes it hard to tell in which materials we should search for a spin liquid ground state.

Standard mean field theory decoupling fails in the case of spin liquids. We reviewed a slave-boson approach to this problem. The spin-raising and lowering operators were splitted into two pseudo-fermions. This allowed to develop a mean field theory which is in principle capable of describing spin liquid states. The Hilbert space of the slave-boson spin operators is bigger than the physical Hilbert space. There is a gauge freedom. Many mean field Hamiltonians, which look different, describe the same physical state. One consequence is that the symmetries of the physical system are encoded non-trivially. The symmetry groups of a lattice can be implemented as projective symmetry groups on mean field level. It is helpful to classify the PSGs of a given lattice, before starting with the actual analysis of mean field ground states.

We classified the $\mathbb{Z}_2$ PSGs of two lattice: of the kagome lattice and of a distorted version of the kagome lattice. The choice was motivated by experiments [4, 11]. Both lattices are likely to possess a spin liquid ground state. The symmetries of the kagome lattice can be implemented in 20 inequivalent ways, the symmetry group of the distorted lattice only in two different ways. We assumed that the invariant gauge group is $\mathbb{Z}_2$. This might not be true. And there is no guarantee that ansätze, associated with the PSGs we found, describe stable spin liquid phases when fluctuations are included.

7 Appendix

7.1 Appendix A: Local $SU(2)$ gauge structure

Proposition: Two ansätze contain the same physical information if and only if they differ by a local $SU(2)$ transformation.

One direction was shown by X.G. Wen [8, p. 377]. He explains why local $SU(2)$ equivalent ansätze produce the same spin wave functions and energy levels. I will repeat his proof, adding some details. This shows that we have to quotient out at least all local $SU(2)$ transformations if we want the ansätze to label physical systems 1-to-1. But this isn't enough to be certain about the gauge structure. There might be more general transformations that do not change the energy levels and spin wave function of an ansatz. The local $SU(2)$ transformations might only be a subgroup of this more general class of transformations. X.G. Wen also states in his book that the gauge freedom is at most local $SU(2)$, but he does not provide a proof [8, p. 377].

The reasoning in chapter 3, which allows to implement symmetry groups as projective symmetry groups, explicitly uses the other direction, though. We assumed that spin wave functions and energy states are invariant under a symmetry operation S of the lattice. From this assumption we concluded that the ansätze $\{U_{S(i)S(j)}\}$ and $\{U_{ij}\}$ must be local $SU(2)$ equivalent. Working only with a subgroup of the actual gauge group can lead to incorrect results, as is shown for example in [8, p. 375]. For this reason, the other direction is equally important. Before I can start, I will need a lot of preparation and new notation. This is why I have decided to put this chapter into the appendix.

After a transformation of fermionic operators all that is left are the anticommutation relations (CARs). It is important to know that operators which satisfy CARs induce an orthonormal basis on their Hilbert space, which behaves like an occupation number basis [18, 19, 26]. This is what allows to treat them as quasi-particles.

Linear operators $a_1, a_2, ..., a_n$ acting on a Hilbert space are said to satisfy *canonical anticommutation relations* (CARs) if

$$\forall ij: \quad a_i a_j^\dagger + a_j a_i^\dagger = \delta_{ij}\mathbb{1}, \qquad \text{and} \qquad \forall ij: \quad a_i a_j + a_j a_i = 0 \tag{7.1}$$

Lemma: *($a_j/a_j^\dagger$ act like lowering/raising operators)*

Let X be a Hilbert space and suppose $a_1, ..., a_n$ satisfy CARs. Then the following holds

(i) If $|\psi\rangle$ is a normed eigenvector of $a_j^\dagger a_j$ with eigenvalue 0, then $a_j^\dagger |\psi\rangle$ is a normed eigenvector of $a_j^\dagger a_j$ with eigenvalue 1. $a_j |\psi\rangle = 0$.

(ii) If $|\psi\rangle$ is a normed eigenvector of $a_j^\dagger a_j$ with eigenvalue 1, then $a_j |\psi\rangle$ is a normed eigenvector of $a_j^\dagger a_j$ with eigenvalue 0. $a_j^\dagger |\psi\rangle = 0$.

Proof: Omitted. The proof is straightforward, apply the CARs several times. □

Proposition: *(operators which satisfy CARs induce an orthonormal basis on X)* [26]

Let X be a finite dimensional Hilbert space. Suppose $a_1, ..., a_n$ and satisfy CARs. Then

(i) $X = V_1 \oplus V_2 \oplus ... \oplus V_m$ for some $m \in \mathbb{N}$ and each space V_i has dimension 2^n.

(ii) Each space V_i admits a vacuum state $|0_a\rangle$ and an orthonormal basis $\{|\underline{n}\rangle \mid \underline{n} \in \{0,1\}^n\}$ that behaves like an occupation number basis of $a_1, .., a_n$.

(iii) If $\dim(X) = 2^n$ then the vacuum state is unique up to a phase shift.

Proof: A sketch of the proof can be found here [26]. I added some details. First note that the operators $a_j^\dagger a_j$ are self-adjoint. For each j : $a_j^\dagger a_j a_j^\dagger a_j = a_j^\dagger a_j$. This holds because

$$a_j^\dagger a_j a_j^\dagger a_j = a_j^\dagger(\mathbb{1} - a_j^\dagger a_j)a_j = a_j^\dagger a_j - a_j^\dagger a_j^\dagger a_j a_j = a_j^\dagger a_j \tag{7.2}$$

I used $a_j^2 = 0$. Thus, the only possible eigenvalues of $a_j^\dagger a_j$ are 0 and 1.

The operators $a_j^\dagger a_j$ commute pairwise. Apply the first CAR repeatedly to check it. Next we want to find a vacuum state. I.e. we are looking for a vector $|0_a\rangle \in X$ such that $a_j |0_a\rangle = 0$ for all j. There is an algorithm to find the subspace of all possible vacuum states in X. I'll sketch the first steps. $a_1^\dagger a_1$ is a self-adjoint operator on a finite dimensional space. By the spectral theorem, X decomposes into the eigenspaces of $a_1^\dagger a_1$. All eigenvalues of $a_1^\dagger a_1$ must be 0 or 1. Hence,

$$X = \mathrm{Ker}\left(a_1^\dagger a_1 - 0\,\mathbb{1}\right) \oplus \mathrm{Ker}\left(a_1^\dagger a_1 - 1\,\mathbb{1}\right) \tag{7.3}$$

If $a_1^\dagger a_1$ has an eigenvector with eigenvalue 0 then it also has an eigenvector with eigenvalue 1 and vice versa. Thus, both subspaces are non-trivial. The essential observation for the next step is that each operator $a_2^\dagger a_2, ..., a_n^\dagger a_n$ preserves the eigenspaces of $a_1^\dagger a_1$. This follows directly from the fact that $a_j^\dagger a_j$ commute pairwise. Restrict all operators $a_1^\dagger a_1, ..., a_n^\dagger a_n$ to the subspace $\mathrm{Ker}(a_1^\dagger a_1)$. Certainly their restrictions obey CARs. Therefore, all results derived in the Hilbert space X also hold on $\mathrm{Ker}(a_1^\dagger a_1)$. Especially, $\mathrm{Ker}(a_1^\dagger a_1)$ decomposes into

$$\mathrm{Ker}(a_1^\dagger a_1) = \mathrm{Ker}\left(a_2^\dagger a_2|_{\mathrm{Ker}(a_1^\dagger a_1)} - 0\,\mathbb{1}\right) \oplus \mathrm{Ker}\left(a_2^\dagger a_2|_{\mathrm{Ker}(a_1^\dagger a_1)} - 1\,\mathbb{1}\right) \tag{7.4}$$

and both spaces are non-trivial. Restrict all operators to the first one and continue with $a_3^\dagger a_3$. This process yields a non-trivial subspace of X on which $a_j^\dagger a_j = 0$ for each j. Pick any normed vector $|0_a\rangle$ from this space. It follows from the previous lemma that $a_j |0_a\rangle = 0$ for all j.

For a tuple $\underline{n} \in \{0,1\}^n$ define

$$|\underline{n}\rangle = {a_1^\dagger}^{n_1} {a_2^\dagger}^{n_2} ... {a_n^\dagger}^{n_n} |0_a\rangle \tag{7.5}$$

$\{|\underline{n}\rangle\}$ is an orthonormal system on X. **Why?** Each vector $|\underline{n}\rangle$ is **normal**: Note that if $|\psi\rangle$ is an eigenvector of $a_j^\dagger a_j$ with eigenvalue 0 and $k \neq j$, then so is $a_k^\dagger |\psi\rangle$. From the previous lemma we know that normalization is preserved whenever we apply $a_j^\dagger$ to a normed vector in $\mathrm{Ker}(a_j^\dagger a_j)$. $|0_a\rangle$ is normed. Thus, by simple induction, each $|\underline{n}\rangle$ is normed. $\{|\underline{n}\rangle\}$ are pairwise **orthogonal**: Suppose $\underline{n} \neq \underline{n}'$. There exists j such that $n_j \neq n'_j$. Say $n_j = 1$ and $n'_j = 0$. $|0_a\rangle$ is an eigenvector of $a_j^\dagger a_j$ with eigenvalue 0. It is easy to see (using the first CAR repeatedly) that this does not change when we apply operators $a_k^\dagger$ to $|0_a\rangle$, as long as $k \neq j$. By simple induction, $|\underline{n}'\rangle$ is an eigenvector of $a_j^\dagger a_j$ with eigenvalue 0. On the other hand $|\underline{n}\rangle$ is an eigenvector of $a_j^\dagger a_j$ with eigenvalue 1. Eigenvectors of self-adjoint operators with distinct eigenvalues are orthogonal. $a_j^\dagger a_j$ is self-adjoint. Hence, $|\underline{n}\rangle \perp |\underline{n}'\rangle$.

Set $V_1 = \mathrm{span}\,\{|\underline{n}\rangle \,|\, \underline{n} \in \{0,1\}^n\}$. Clearly $\dim(V_1) = |\{|\underline{n}\rangle\}| = 2^n$. Using CARs it is easy to verify that the operators a_j act on $|\underline{n}\rangle$ as on occupation number basis vectors. Since V_1 is finite dimensional and thus closed, X decomposes into

$$X = V_1 \oplus V_1^\perp \tag{7.6}$$

It is clear that the operators a_j and $a_j^\dagger$ preserve V_1. This implies that they also preserve $V_1^\perp$. **Why?** Take any $|\psi\rangle \in V_1^\perp$. For all $|\phi\rangle \in V_1$:

$$\langle\phi|a_j\psi\rangle = \left\langle a_j^\dagger\phi \middle| \psi\right\rangle = 0 \qquad \text{and} \qquad \left\langle \phi \middle| a_j^\dagger\psi\right\rangle = \langle a_j\phi|\psi\rangle = 0 \tag{7.7}$$

since $a_j |\phi\rangle \in V_1$ and $a_j^\dagger |\phi\rangle \in V_1$. $|\phi\rangle$ was arbitrary. Thus, $a_j |\psi\rangle \in V_1^\perp$ and $a_j^\dagger |\psi\rangle \in V_1^\perp$.

So we can restrict all operators $a_1, ..., a_n$ to the subspace $V_1^\perp$. Their restrictions certainly satisfy CARs. If $V_1^\perp$ is non-trivial, proceed as before: Find a vacuum state, construct an orthonormal system in $V_1^\perp$ and decompose

$$V_1^\perp = V_2 \oplus V_2^\perp \tag{7.8}$$

After finitely many repetitions this process must terminate, since X is finite dimensional.

Next consider the case $\dim(X) = 2^n$. X is spanned by the first system of occupation number vectors. I.e. $X = V_1$ and $V_1^\perp = \{0\}$. We want to show that, up to a phase shift, there is only one vector $|0_a\rangle \in S_X$ satisfying $a_j |0_a\rangle = 0$ for all j. Let $|\tilde{0}_a\rangle \in S_X$ be any other such vector. $\{|\underline{n}\rangle\}$ is an orthonormal basis of X. Thus,

$$|\tilde{0}_a\rangle = \sum_{\underline{n}} \langle \underline{n}|\tilde{0}_a\rangle \, |\underline{n}\rangle \tag{7.9}$$

By systematically applying annihilation operators to both sides of equation (7.9), one finds that all coefficients $\langle \underline{n}|\tilde{0}_a\rangle = 0$, except $\langle 0_a|\tilde{0}_a\rangle$. To see it, start with the fully occupied state. Apply all annihilation operators on both sides. This will give $0 = \pm \langle \text{full}|\tilde{0}_a\rangle \, |0_a\rangle$. Thus, $\langle \text{full}|\tilde{0}_a\rangle = 0$. Continue with combinations of n-1 annihilation operators, and work your way down until you reach the 1-particle states. What is left will be $|0_a\rangle = \langle 0_a|\tilde{0}_a\rangle \, |0_a\rangle$. Both vacuum states are normed. Thus, they only differ by a phase. □

I will need more general transformations than local $SU(2)$ transformations. Let

$$\Psi = \begin{bmatrix} f_{1\uparrow} & f_{2\uparrow} & ... & f_{d\uparrow} & f^\dagger_{1\downarrow} & f^\dagger_{2\downarrow} & ... & f^\dagger_{d\downarrow} \end{bmatrix}^t, \quad \Psi^\dagger = \begin{bmatrix} f^\dagger_{1\uparrow} & f^\dagger_{2\uparrow} & ... & f^\dagger_{d\uparrow} & f_{1\downarrow} & f_{2\downarrow} & ... & f_{d\downarrow} \end{bmatrix} \tag{7.10}$$

For a unitary $2d \times 2d$ matrix W define a transformation of the form

$$\Psi \xrightarrow{W} W\Psi \qquad\qquad \Psi^\dagger \xrightarrow{W} \Psi^\dagger W^\dagger \tag{7.11}$$

I will call such a transformation *non-local* $U(2d)$. The local $SU(2)$ transformations are a subgroup of the non-local transformations. To see this, write W in block-form:

$$W = \left[\begin{array}{c|c} W_{\uparrow\uparrow} & W_{\uparrow\downarrow} \\ \hline W_{\downarrow\uparrow} & W_{\downarrow\downarrow} \end{array}\right] = \left[\begin{array}{ccc|ccc} W_{1\uparrow 1\uparrow} & ... & W_{1\uparrow d\uparrow} & W_{1\uparrow 1\downarrow} & ... & W_{1\uparrow d\downarrow} \\ ... & ... & ... & ... & ... & ... \\ W_{d\uparrow 1\uparrow} & ... & W_{d\uparrow d\uparrow} & W_{d\uparrow 1\downarrow} & ... & W_{d\uparrow d\downarrow} \\ \hline W_{1\downarrow 1\uparrow} & ... & W_{1\downarrow d\uparrow} & W_{1\downarrow 1\downarrow} & ... & W_{1\downarrow d\downarrow} \\ ... & ... & ... & ... & ... & ... \\ W_{d\downarrow 1\uparrow} & ... & W_{d\downarrow d\uparrow} & W_{d\downarrow 1\downarrow} & ... & W_{d\downarrow d\downarrow} \end{array}\right] \tag{7.12}$$

It is convenient to label the entries of W in the same way as the creation operators. Clearly, a non-local transformation W is a local $SU(2)$ transformation if and only if the four block matrices $W_{\_}$ are diagonal and $\det(W(i)) = W_{i\uparrow i\uparrow}W_{i\downarrow i\downarrow} - W_{i\downarrow i\uparrow}W_{i\uparrow i\downarrow} = 1$ for each i.

Lemma: *(non-local transformations are canonical)*

Let W be a unitary $2d \times 2d$ matrix. Consider the non-local transformation $\Psi \xrightarrow{W} W\Psi$:

$$\begin{bmatrix} f_{1\uparrow} \\ ... \\ f_{d\uparrow} \\ f^\dagger_{1\downarrow} \\ ... \\ f^\dagger_{d\downarrow} \end{bmatrix} = \left[\begin{array}{c|c} W_{\uparrow\uparrow} & W_{\uparrow\downarrow} \\ \hline W_{\downarrow\uparrow} & W_{\downarrow\downarrow} \end{array}\right] \begin{bmatrix} c_{1\uparrow} \\ ... \\ c_{d\uparrow} \\ c^\dagger_{1\downarrow} \\ ... \\ c^\dagger_{d\downarrow} \end{bmatrix}, \qquad \begin{bmatrix} f^\dagger_{1\uparrow} \\ ... \\ f^\dagger_{d\uparrow} \\ f_{1\downarrow} \\ ... \\ f_{d\downarrow} \end{bmatrix} = \left[\begin{array}{c|c} W^*_{\uparrow\uparrow} & W^*_{\uparrow\downarrow} \\ \hline W^*_{\downarrow\uparrow} & W^*_{\downarrow\downarrow} \end{array}\right] \begin{bmatrix} c^\dagger_{1\uparrow} \\ ... \\ c^\dagger_{d\uparrow} \\ c_{1\downarrow} \\ ... \\ c_{d\downarrow} \end{bmatrix} \tag{7.13}$$

The above transformation is canonical in the sense that for each pair $j\alpha$: $c^\dagger_{j\alpha}$ is the adjoint operator of $c_{j\alpha}$ and the operators $c_{i\alpha}$ satisfy canonical anticommutation relations.

Proof: The first assertion follows directly from (7.13). The second follows from the fact that rows and columns of W form orthonormal systems. From (7.13) we find that

$$c_{i\uparrow} = \sum_{k\uparrow} W^*_{k\uparrow i\uparrow} \, f_{k\uparrow} + \sum_{k\downarrow} W^*_{k\downarrow i\uparrow} f^\dagger_{k\downarrow} \qquad \text{and} \qquad c_{i\downarrow} = \sum_{k\uparrow} W_{k\uparrow i\downarrow} \, f^\dagger_{k\uparrow} + \sum_{k\downarrow} W_{k\downarrow i\uparrow} \, f_{k\downarrow} f \tag{7.14}$$

The anticommutator $[\,\cdot\,,\cdot\,]_+$ is bilinear and symmetric. Thus,

$$\begin{aligned}\left[c_{i\uparrow}, c^\dagger_{j\uparrow}\right]_+ &= \sum_{k\uparrow}\sum_{l\uparrow} W^*_{k\uparrow i\uparrow} W_{l\uparrow j\uparrow} \left[f_{k\uparrow}, f^\dagger_{l\uparrow}\right]_+ + \sum_{k\downarrow}\sum_{l\uparrow} W^*_{k\downarrow i\uparrow} W_{l\uparrow j\uparrow} \left[f^\dagger_{k\downarrow}, f^\dagger_{l\uparrow}\right]_+ \\ &+ \sum_{k\uparrow}\sum_{l\downarrow} W^*_{k\uparrow i\uparrow} W_{l\downarrow j\uparrow} \left[f_{k\uparrow}, f_{l\downarrow}\right]_+ + \sum_{k\downarrow}\sum_{l\downarrow} W^*_{k\downarrow i\uparrow} W_{l\downarrow j\uparrow} \left[f^\dagger_{k\downarrow}, f_{l\downarrow}\right]_+ \\ &= \sum_{k\uparrow}\sum_{l\uparrow} W^*_{k\uparrow i\uparrow} W_{l\uparrow j\uparrow}\, \delta_{kl}\, \mathbb{1} + \sum_{k\downarrow}\sum_{l\downarrow} W^*_{k\downarrow i\uparrow} W_{l\downarrow j\uparrow}\, \delta_{kl}\, \mathbb{1} + 0 = W^\dagger_{-\,i\uparrow} W_{-\,j\uparrow}\, \mathbb{1} = \delta_{i\uparrow j\uparrow}\, \mathbb{1} \end{aligned} \tag{7.15}$$

$W_{-i\alpha}$ denotes the $i\alpha$th column vector of W. Similarly for the other relations. □

Remark: Take any complex $2d \times 2d$ matrix and consider a transformation of the form $\Psi \xrightarrow{W} W\Psi$. If the new operators should be adjoint to each other, then $\Psi^\dagger$ has to transform as $\Psi^\dagger \xrightarrow{W} \Psi^\dagger W^\dagger$. Suppose we also want the new operators to satisfy CARs. It follows from the anticommutation relations that the column vectors of W must be normed and pairwise orthogonal. I.e. in this case W has to be unitary. A non-local transformation, as defined in (7.11), is the most general linear transformation of Ψ that is canonical in the above sense.

We can use the global transformation above to diagonalize the mean field Hamiltonian which we found in the second chapter [19]. The spectral theorem states that every self-adjoint operator on a finite dimensional vector space can be diagonalized. In our case this would mean diagonalizing a $2^{2d} \times 2^{2d}$ matrix, since the Fock space has dimension 2^{2d}. Using CARs it is possible to reduce the problem to a $2d \times 2d$ matrix. Let

$$H: \quad \Gamma_{-1}(\mathcal{H}) \to \Gamma_{-1}(\mathcal{H}), \qquad\qquad H = \sum_{\langle ij\rangle} \left(\Psi^\dagger_i U_{ij} \Psi_j + \Psi^\dagger_j U^\dagger_{ij} \Psi_i\right) + \text{const.} \tag{7.16}$$

where U_{ij} are complex 2×2 matrices. The operators $f_{i\alpha} : \Gamma_{-1}(\mathcal{H}) \to \Gamma_{-1}(\mathcal{H})$ should be linear and should satisfy canonical anticommutation relations. Their occupation number basis should span $\Gamma_{-1}(\mathcal{H})$. These are the only requirements. Convince yourself, that any such operator can be written as

$$H = \Psi^\dagger\, U \Psi + \text{const.} \tag{7.17}$$

where

$$\Psi^\dagger = \begin{bmatrix} f^\dagger_{1\uparrow} & f^\dagger_{2\uparrow} & \dots & f^\dagger_{d\uparrow} & f_{1\downarrow} & f_{2\downarrow} & \dots & f_{d\downarrow} \end{bmatrix} \tag{7.18}$$

and U is a self-adjoint $2d \times 2d$ matrix. The spectral theorem states that there exists a unitary matrix W such that $D = W^\dagger U W$ is diagonal. By $\lambda_{1\uparrow}, ..., \lambda_{d\downarrow}$ denote the diagonal entries of D. Consider the non-local transformation $\Psi \xrightarrow{W} W\Psi$. Denote the transformed operators by $c_{i\alpha}$. As shown in the previous section, they satisfy CARs. Express H in new coordinates:

$$H = \tilde{\Psi}^\dagger\, W^\dagger U W\, \tilde{\Psi} + \text{const.} = \sum_{i\uparrow} \lambda_{i\uparrow}\, c^\dagger_{i\uparrow} c_{i\uparrow} + \sum_{i\downarrow} (-\lambda_{i\downarrow})\, c^\dagger_{i\downarrow} c_{i\downarrow} + \sum_{i\downarrow} \lambda_{i\downarrow} + \text{const.} \tag{7.19}$$

By $|\underline{n}_c\rangle$ (and $|\underline{n}_f\rangle$) denote occupation number vectors with respect to the operators $c_{i\alpha}$ (and $f_{i\alpha}$ respectively). $\Gamma_{-1}(\mathcal{H}) = \text{span}\{|\underline{n}_f\rangle\}$.

$$\dim(\Gamma_{-1}(\mathcal{H})) = 2^{|\{f_{i\alpha}\}|} = 2^{|\{c_{i\alpha}\}|} \tag{7.20}$$

Thus, the vectors $|\underline{n}_c\rangle$ span $\Gamma_{-1}(\mathcal{H})$. Each $|\underline{n}_c\rangle$ is an eigenvector of all operators $c^\dagger_{j\alpha} c_{j\alpha}$. Thus, they are eigenvectors of H. The energy levels are, up to a constant, given by all possible sums of the values $\lambda_{i\uparrow}, -\lambda_{i\downarrow}$. H is diagonal in the basis $\{|\underline{n}_c\rangle\}$. It is hard to obtain explicit expressions for $|\underline{n}_c\rangle$ in terms of the old basis $|\underline{n}_f\rangle$. Even if the transformation matrix W is known, the new vacuum state $|0_c\rangle$ still needs to be determined.

A natural question is: Suppose two ansätze $\{U_{ij}\}$ and $\{\tilde{U}_{ij}\}$ are related by a non-local transformation. I.e. there exists a unitary matrix W such that $\tilde{U} = W^\dagger U W$. Are their eigenstates related?

Define new operators $a_{j\alpha}$ by

$$\Psi_f = W\Psi_a \qquad \text{and} \qquad \Psi_f^\dagger = \Psi_a^\dagger W^\dagger \tag{7.21}$$

Let H be the mean field Hamiltonian of the ansatz $\{U_{ij}\}$ and $\tilde{H}$ the mean field Hamiltonian of $\{\tilde{U}_{ij}\}$. Note that

$$H = \Psi_f^\dagger U \Psi_f = \Psi_a^\dagger W^\dagger U W \Psi_a = \Psi_a^\dagger \tilde{U} \Psi_a \qquad \text{and} \qquad \tilde{H} = \Psi_f^\dagger \tilde{U} \Psi_f \tag{7.22}$$

up to a constant. From an algebraic point of view the problem of finding eigenstates is the same for H and $\tilde{H}$. The eigenstates of $\tilde{H}$ are occupation number vectors obtained from some set of creation operators. The same holds for H. It follows from (7.22) that there is a basis of eigenstates of H and one of $\tilde{H}$ such that

$$\left| \underline{m}_{MF}^{\{U_{ij}\}} \right\rangle = \sum_{\underline{n}} \left\langle \underline{n}_a \right| \underline{m}_{MF}^{\{U_{ij}\}} \left\rangle \right| \underline{n}_a \right\rangle = \sum_{\underline{n}} \left\langle \underline{n}_f \right| \underline{m}_{MF}^{\{\tilde{U}_{ij}\}} \left\rangle \right| \underline{n}_a \right\rangle \tag{7.23}$$

Now we have everything that we will need. We will start with the direction which is already sketched in Wen's book [8, p. 377].

Proposition: *(local $SU(2)$ equivalent ansätze carry the same physical information)*

Suppose $\{U_{ij}\}$ and $\{\tilde{U}_{ij}\}$ are local $SU(2)$ equivalent. That is there exists a local $SU(2)$ transformation W such that $\forall ij : \tilde{U}_{ij} = W(i)^\dagger U_{ij} W(j)$. Then the eigenstates of $H_{MF}^{\{U_{ij}\}}$ and of $H_{MF}^{\{\tilde{U}_{ij}\}}$ project onto the same spin wave functions in $\mathcal{H}_p$ and both Hamiltonians have the same energy levels.

Why? Write $H_{MF}^{\{U_{ij}\}} = H$ and $H_{MF}^{\{\tilde{U}_{ij}\}} = \tilde{H}$. Let

$$\Psi_i = W(i)\tilde{\Psi}_i, \qquad \text{with} \qquad \Psi_i = \begin{bmatrix} f_{i\uparrow} \\ f_{i\downarrow}^\dagger \end{bmatrix} \qquad \text{and} \qquad \tilde{\Psi}_i = \begin{bmatrix} a_{i\uparrow} \\ a_{i\downarrow}^\dagger \end{bmatrix} \tag{7.24}$$

Note that

$$H = \sum_{\langle ij \rangle} \left(\tilde{\Psi}_i^\dagger \tilde{U}_{ij} \tilde{\Psi}_j + \text{h.c.} \right) + \text{const.} \qquad \text{and} \qquad \tilde{H} = \sum_{\langle ij \rangle} \left(\Psi_i^\dagger \tilde{U}_{ij} \Psi_j + \text{h.c.} \right) + \text{const.} \tag{7.25}$$

Formally, H and $\tilde{H}$ look the same. The operators $f_{1\uparrow}, f_{1\downarrow}, .., f_{d\downarrow}$ and $a_{1\uparrow}, a_{1\downarrow}, .., a_{d\downarrow}$ both satisfy canonical anticommutation relations (CARs). Both Hamiltonians can be diagonalized by the same non-local $SU(2d)$ transformation. Hence, they will have the same energy levels. By $\{ |\, \underline{n}_f \rangle \,|\, \underline{n} \in \{0,1\}^d \}$ denote an occupation number basis of $\Gamma_{-1}(\mathcal{H})$ with respect to the operators $f_{j\alpha}$. By $|0_a\rangle$ denote a vacuum state of the operators $a_{j\alpha}$. As we have seen in the previous section, the eigenstates of H and $\tilde{H}$ are related:

$$\left| \underline{m}_{MF}^{\{U_{ij}\}} \right\rangle = \sum_{\underline{n}} \left\langle \underline{n}_f \right| \left. \underline{m}_{MF}^{\{\tilde{U}_{ij}\}} \right\rangle \, a_{1\uparrow}^{\dagger\ n_{1\uparrow}} a_{1\downarrow}^{\dagger\ n_{1\downarrow}} ... \, a_{d\downarrow}^{\dagger\ n_{d\downarrow}} \, |0_a\rangle \tag{7.26}$$

The eigenstates of H take the same form as the one of $\tilde{H}$, but with respect to a different orthonormal basis. This doesn't tell us yet that the states project onto the same vectors in $\mathcal{H}_p$. The vector $|0_f\rangle$ and the operators $f_{i\alpha_i}$, which are used in (2.46) to project to $\mathcal{H}_p$, are not gauge invariant.

By $|0_\Psi\rangle$ denote the unique state that satisfies

$$\forall i \in \text{lattice} : \qquad \Psi_i \, |0_\Psi\rangle = \begin{bmatrix} f_{i\uparrow} \, |0_\Psi\rangle \\ f_{i\downarrow}^\dagger \, |0_\Psi\rangle \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{7.27}$$

$|0_\Psi\rangle$ carries a down-spin on each site. Similarly define $|0_{\tilde{\Psi}}\rangle$. Fix any $\underline{\alpha} \in \{\uparrow, \downarrow\}^d$. Observe that

$$\langle\, 0_f | \prod_{i=1}^{d} f_{i\alpha_i} \, : \quad \Gamma_{-1}(\mathcal{H}) \to \mathbb{C} \qquad \text{and} \qquad \langle\, 0_\Psi | \prod_{\alpha_i = \uparrow} f_{i\downarrow}^\dagger f_{i\uparrow} \, : \quad \Gamma_{-1}(\mathcal{H}) \to \mathbb{C} \tag{7.28}$$

are the same function. To see this, convince yourself that $\prod_{\alpha_i=\uparrow} f^\dagger_{i\downarrow} f_{i\uparrow}$ will send the occupation number vector $|\,\underline{\alpha}\rangle$ to $|0_\Psi\rangle$ and every other occupation number vector to something orthogonal. It is clear that $|0_\Psi\rangle$ is gauge invariant. To see that $f^\dagger_{i\downarrow} f_{i\uparrow}$ is gauge invariant, compute

$$\begin{aligned} f^\dagger_{i\downarrow} f_{i\uparrow} &= \Big(W(i)_{21}\, a_{i\uparrow} + W(i)_{22}\, a^\dagger_{i\downarrow}\Big)\,\Big(W(i)_{11}\, a_{i\uparrow} + W(i)_{12}\, a^\dagger_{i\downarrow}\Big) \\ &= (W(i)_{11}W(i)_{22} - W(i)_{21}W(i)_{12})\; a^\dagger_{i\downarrow} a_{i\uparrow} = \det(W(i))\, a^\dagger_{i\downarrow} a_{i\uparrow} + 0 = a^\dagger_{i\downarrow} a_{i\uparrow} \end{aligned} \tag{7.29}$$

Together with (7.26), (7.28) and (2.46) it follows that corresponding eigenstates project indeed onto the same spin wave function in $\mathcal{H}_p$. □

Proposition: *(ansätze which carry the same physical information are local $SU(2)$ equivalent)*

Suppose two ansätze $\{U_{ij}\}$ and $\{\tilde{U}_{ij}\}$ share (up to a constant) the same energy levels with same multiplicity and suppose their eigenstates project to the same spin wave functions in $\mathcal{H}_p$. Then there exists a local $SU(2)$ transformation such that

$$\forall ij: \quad \tilde{U}_{ij} = W(i)^\dagger U_{ij} W(j) \tag{7.30}$$

Why? Let $H^{\{U_{ij}\}}_{MF} = H$ and $H^{\{\tilde{U}_{ij}\}}_{MF} = \tilde{H}$. Ignore constant terms. H and $\tilde{H}$ can be written as

$$H = \Psi^\dagger_f U \Psi_f \qquad \text{and} \qquad \tilde{H} = \Psi^\dagger_f \tilde{U} \Psi_f \tag{7.31}$$

Both Hamiltonians can be diagonalized by a non-local mixing of creation and annihilation operators. They share the same energy levels with same multiplicity. So there are unitary matrices R and T such that $R^\dagger U R = D = T^\dagger \tilde{U} T$ is diagonal. In consequence $\tilde{U} = T R^\dagger U R T^\dagger$. Set $W = T R^\dagger$. We have found a non-local transformation that transforms $\{U_{ij}\}$ into $\{\tilde{U}_{ij}\}$. It is sufficient to show that W takes the form of a local $SU(2)$ transformation. Define new operators $a_{i\alpha}$ by

$$\Psi_f = W \Psi_a \qquad \text{and} \qquad \Psi^\dagger_f = \Psi^\dagger_a W^\dagger \tag{7.32}$$

Then $H = \Psi^\dagger_a \tilde{U} \Psi_a$. The eigenstates of H and $\tilde{H}$ are related.

$$\Big|\, \underline{m}^{\{U_{ij}\}}_{MF} \Big\rangle = \sum_{\underline{n}} \Big\langle \underline{n}_f \,\Big|\, \underline{m}^{\{\tilde{U}_{ij}\}}_{MF} \Big\rangle\; a^{\dagger\; n_{1\uparrow}}_{1\uparrow} a^{\dagger\; n_{1\downarrow}}_{1\downarrow} \ldots a^{\dagger\; n_{d\downarrow}}_{d\downarrow}\; |0_a\rangle \tag{7.33}$$

(7.28) shows how to obtain the coefficients of the spin wave functions. The projection $\mathbb{P}_{\mathcal{H}_p}$ onto the physical subspace can be written as

$$\mathbb{P}_{\mathcal{H}_p} : \Gamma_{-1}(\mathcal{H}_p) \to \mathcal{H}_p \qquad\qquad \mathbb{P}_{\mathcal{H}_p} = \sum_{\underline{\alpha}\in\{\uparrow,\downarrow\}^d} |\,\underline{\alpha}_{\text{spin}}\rangle\langle 0_{\Psi_f}\,| \prod_{\alpha_i=\uparrow} f^\dagger_{i\downarrow} f_{i\uparrow} \tag{7.34}$$

Corresponding eigenstates of H and $\tilde{H}$ project onto the same spin wave function. In other words

$$\forall \underline{m}: \qquad \mathbb{P}_{\mathcal{H}_p} \Big|\, \underline{m}^{\{U_{ij}\}}_{MF} \Big\rangle = \mathbb{P}_{\mathcal{H}_p} \Big|\, \underline{m}^{\{\tilde{U}_{ij}\}}_{MF} \Big\rangle \tag{7.35}$$

Define a second linear function $\mathbb{P} : \Gamma_{-1}(\mathcal{H}) \to \mathcal{H}_p$.

$$\mathbb{P} = \sum_{\underline{\alpha}\in\{\uparrow,\downarrow\}^d} |\,\underline{\alpha}_{\text{spin}}\rangle\langle 0_{\Psi_a}\,| \prod_{\alpha_i=\uparrow} a^\dagger_{i\downarrow} a_{i\uparrow} \tag{7.36}$$

It follows from (7.33) that

$$\forall \underline{m}: \qquad \mathbb{P} \Big|\, \underline{m}^{\{U_{ij}\}}_{MF} \Big\rangle = \mathbb{P}_{\mathcal{H}_p} \Big|\, \underline{m}^{\{\tilde{U}_{ij}\}}_{MF} \Big\rangle = \mathbb{P}_{\mathcal{H}_p} \Big|\, \underline{m}^{\{U_{ij}\}}_{MF} \Big\rangle \tag{7.37}$$

The eigenstates of H form a basis of $\Gamma_{-1}(\mathcal{H})$. $\mathbb{P}_{\mathcal{H}_p}$ and $\mathbb{P}$ are linear. Thus, $\mathbb{P} = \mathbb{P}_{\mathcal{H}_p}$. But since $|\underline{\alpha}_{\text{spin}}\rangle$ are linear independent this can only hold if for each $\underline{\alpha} \in \{\uparrow,\downarrow\}^d$

$$\langle\, 0_{\Psi_f}| \prod_{\alpha_i=\uparrow} f^\dagger_{i\downarrow} f_{i\uparrow} : \quad \Gamma_{-1}(\mathcal{H}) \to \mathbb{C} \qquad \text{and} \qquad \langle\, 0_{\Psi_a}| \prod_{\alpha_i=\uparrow} a^\dagger_{i\downarrow} a_{i\uparrow} : \quad \Gamma_{-1}(\mathcal{H}) \to \mathbb{C} \tag{7.38}$$

are the same function. Especially, plugging in $\underline{\alpha} = (\downarrow, \downarrow, ..., \downarrow)$ gives $|\,0_\Psi\rangle := |\,0_{\Psi_f}\rangle = |\,0_{\Psi_a}\rangle$. Note that the operators $f^\dagger_{i\downarrow} f_{i\uparrow}$ and $f^\dagger_{i\uparrow} f_{i\downarrow}$ ($a^\dagger_{i\downarrow} a_{i\uparrow}$ and $a^\dagger_{i\uparrow} a_{i\downarrow}$ respectively) transfer between the different single occupied states in the basis $|\underline{n}_f\rangle$ (or $|\underline{n}_a\rangle$ respectively). (7.38) shows that the dual vectors of single occupied states are unchanged under W. Thus, $\mathcal{H}_p$ is invariant under W (*see the remark directly below the proof*).

Fix any i. Using the explicit expression of the transformation $\Psi \xrightarrow{W} W\Psi$ in (7.13), I find that

$$a^\dagger_{i\uparrow} a_{i\downarrow} = \sum_{k\uparrow}\sum_{l\downarrow} W_{k\uparrow i\uparrow} W_{l\uparrow i\downarrow}\, f^\dagger_{k\uparrow} f^\dagger_{l\downarrow} + \sum_{k\downarrow}\sum_{l\downarrow} W_{k\downarrow i\uparrow} W_{l\downarrow i\downarrow}\, f_{k\downarrow} f_{l\downarrow} + \sum_{k\uparrow}\sum_{l\downarrow} \left(W_{k\uparrow i\uparrow} W_{l\uparrow i\uparrow} - W_{k\uparrow i\downarrow} W_{l\downarrow i\uparrow}\right)\, f^\dagger_{k\uparrow} f_{l\downarrow} \tag{7.39}$$

W does not rotate $\mathcal{H}_p$. Especially $f^\dagger_{i\uparrow} f_{i\downarrow} |\,0_\Psi\rangle = a^\dagger_{i\uparrow} a_{i\downarrow} |\,0_\Psi\rangle$. Apply both sides of (7.39) to $|\,0_\Psi\rangle$:

$$f^\dagger_{i\uparrow} f_{i\downarrow} |\,0_\Psi\rangle = a^\dagger_{i\uparrow} a_{i\downarrow} |\,0_\Psi\rangle = 0 + \sum_{k\uparrow}\sum_{l\downarrow} \left(W_{k\uparrow i\uparrow} W_{l\uparrow i\uparrow} - W_{k\uparrow i\downarrow} W_{l\downarrow i\uparrow}\right)\, f^\dagger_{k\uparrow} f_{l\downarrow} \,|\,0_\Psi\rangle \tag{7.40}$$

The occupation number vectors $|\,\underline{n}_f\rangle$ are linear independent. It follows that W must satisfy

$$\begin{aligned} &W_{i\uparrow i\uparrow} W_{i\downarrow i\downarrow} - W_{i\uparrow i\downarrow} W_{i\downarrow i\uparrow} = 1 && \text{and} \\ &W_{k\uparrow i\uparrow} W_{l\uparrow i\uparrow} - W_{k\uparrow i\downarrow} W_{l\downarrow i\uparrow} = 0 && \text{if not } k = l = i \end{aligned} \tag{7.41}$$

The first condition is enough to deduce that W is a local $SU(2)$ transformation. I will need Hadamard's inequality. It states that for any complex $m \times m$ matrix N:

$$|\det(N)| \leq \prod_{i=1}^{m} \|N_{-i}\|_{\mathbb{C}^m} \tag{7.42}$$

where N_{-i} denotes the ith column vector of N. For each i consider the matrix

$$W(i) := \begin{bmatrix} W_{i\uparrow i\uparrow} & W_{i\uparrow i\downarrow} \\ W_{i\downarrow i\uparrow} & W_{i\downarrow i\downarrow} \end{bmatrix} \tag{7.43}$$

It is helpful to go back to (7.12) for a second to see where the entries of $W(i)$ live in the matrix W. Each column vector of W has norm 1. The entries of the column vectors of $W(i)$ belong to column vectors of W. Their norm must therefore be less than or equal to 1. On the other hand

$$|\det(W(i))| = |W_{i\uparrow i\uparrow} W_{i\downarrow i\downarrow} - W_{i\uparrow i\downarrow} W_{i\downarrow i\uparrow}| = 1 \tag{7.44}$$

Assume one of the column vectors of $W(i)$ has a norm strictly less than 1. Then Hadamard's inequality can not hold for $W(i)$, which is a contradiction. Thus, both column vectors of $W(i)$ have norm 1. This implies that all other entries of the column vectors $W_{-i\uparrow}$ and $W_{-i\downarrow}$ must be zero. i was arbitrary. Hence, the four $d \times d$ block matrices which form W are diagonal. Furthermore, $\det(W(i)) = 1$ for each i. W is a local $SU(2)$ transformation as claimed. □

Remark: It is not obvious from (7.38) that that $|\psi\rangle \xrightarrow{W} |\psi\rangle$ for each $|\psi\rangle \in \mathcal{H}_p$. It seems trivial only because Riesz' representation theorem is embedded so deeply into the bra-ket notation that one can use it without even noticing. Let X be a Hilbert space, let X' be the space of continuous linear functionals on X. The Fréchet-Riesz representation theorem [22, p. 246] tells that the mapping $X \to X'$, $\psi \mapsto \langle\psi|\cdot\rangle$ is antilinear, bijective and isometric. Thus, for each functional $f \in X'$ there exists a unique state $\psi \in X$ such that $f(\cdot) = \langle\psi|\cdot\rangle$. We can let the raising and lowering operators in (7.38) act to the left on the functionals $\langle 0_\Psi|\cdot\rangle$, $\langle 0_{\tilde{\Psi}}|\cdot\rangle$ respectively, by letting their adjoint act on 0_Ψ, $0_{\tilde{\Psi}}$ respectively. This shows the first assertion: $\langle\psi|\cdot\rangle = \langle W\psi|\cdot\rangle$ for all $\psi \in \mathcal{H}_p$. It is uniqueness that yields $\psi = W\psi$ for all $\psi \in \mathcal{H}_p$. The same functional can only have one representation.

7.2 Appendix B: Special unitary 2×2 matrices and $SO(3)$

It is impossible to deal effectively with projective symmetry groups without being comfortable with the $SU(2)$ group operation. The connection between $SU(2)$ and rotations in $\mathbb{R}^3$ is elegant and effective. This

is a small collection of the results which we will need for the PSG classification. We will use every result of this chapter repeatedly in appendix C and D. Introductions to $SU(2)$ can be found in any algebra book that contains a chapter about Lie groups. For references, see e.g. [27, 28, 29].

The group $SU(2)$ is

$$SU(2) := \left\{ W \,\middle|\, W \in \mathrm{Mat}(2\times 2, \mathbb{C}),\, W^\dagger = W^{-1},\, \det(W) = 1 \right\} \tag{7.45}$$

Note that this is indeed a group under matrix multiplication. $\mathbb{1}_{2\times 2} \in SU(2)$ is the identity and for each $U, V \in SU(2)$ it holds that $(UV)^\dagger = (UV)^{-1}$ and that $\det(UV) = \det(U)\det(V) = 1$.

Proposition 1: *(useful parametrizations of $SU(2)$)*

$SU(2)$ can alternatively be written as

$$SU(2) = \left\{ \begin{bmatrix} \alpha & -\beta^* \\ \beta & \alpha^* \end{bmatrix} \,\middle|\, \alpha, \beta \in \mathbb{C},\, |\alpha|^2 + |\beta|^2 = 1 \right\} \tag{7.46}$$

and

$$SU(2) = \left\{ \alpha_0\tau^0 + i\alpha_1\tau^1 + i\alpha_2\tau^2 + i\alpha_3\tau^3 \,\middle|\, \alpha_i \in \mathbb{R},\, \alpha_0^2 + \alpha_1^2 + \alpha_2^2 + \alpha_3^2 = 1 \right\} \tag{7.47}$$

and

$$SU(2) = \left\{ \exp\left(i\,\frac{\theta}{2}\,\hat{n}\cdot\vec{\tau} \right) \,\middle|\, \theta \in [0, 2\pi),\, \hat{n} \in \mathbb{R}^3,\, \|\hat{n}\| = 1 \right\} \tag{7.48}$$

Proof: Call the first set above A, the second one B and the third one C. First I will show that $SU(2) = A$. Take any matrix $g \in A$. Clearly $\det(g) = 1$. It is also easy to check that $gg^\dagger = \mathbb{1}_{2\times 2}$. Thus, $A \subset SU(2)$. Conversely, suppose $g \in SU(2)$.

$$g = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \qquad a, b, c, d \in \mathbb{C} \tag{7.49}$$

The condition $gg^\dagger = \mathbb{1}_{2\times 2}$ means that the row vectors of g must form an orthonormal basis of $\mathbb{C}^2$.

$$aa^* + cc^* = 1, \qquad bb^* + dd^* = 1, \qquad ab^* + cd^* = 0 \tag{7.50}$$

$\det(g) = 1$ gives

$$ad - bc = 1 \tag{7.51}$$

From (7.50):

$$c = \frac{-ab^*}{d^*} \tag{7.52}$$

Insert this in (7.51) and use $bb^* = 1 - dd^*$ to get

$$1 = ad + \frac{abb^*}{d^*} = ad + \frac{a(1 - dd^*)}{d^*} = \frac{a}{d^*} \tag{7.53}$$

Thus, $d = a^*$. Insert this again in (7.51) and use $aa^* = 1 - cc^*$ to find that $b = -c^*$. Hence, $g \in A$. Since g was arbitrary, $SU(2) \subset A$.

To see that $A = B$, observe that

$$\alpha_0\tau^0 + i\alpha\tau^1 + i\alpha_2\tau^2 + i\alpha_3\tau^3 = \begin{bmatrix} \alpha_0 + i\alpha_3 & \alpha_2 + i\alpha_1 \\ -\alpha_2 + i\alpha_1 & \alpha_0 - i\alpha_3 \end{bmatrix} \tag{7.54}$$

It remains to show that $C = B$. The exponential series of anything with finite norm converges absolutely. The limit is independent from the norm chosen on $\mathrm{Mat}(2\times 2, \mathbb{C})$. This holds because all norms on finite dimensional vector spaces generate the same topology. Furthermore, note that

$$(\hat{n}\cdot\vec{\tau})(\hat{n}\cdot\vec{\tau}) = \|\hat{n}\|^2\tau^0 + i\,(\hat{n}\times\hat{n})\cdot\vec{\tau} = \tau^0 \tag{7.55}$$

The notation is explained in the remark directly below the proof. In consequence for all even k: $(\hat{n}\cdot\vec{\tau})^k = \tau^0$ and for all odd k: $(\hat{n}\cdot\vec{\tau})^k = \hat{n}\cdot\vec{\tau}$. Hence,

$$\exp\left(i\,\frac{\theta}{2}\,\hat{n}\cdot\vec{\tau}\right) = \sum_{k=0}^{\infty}\frac{\left(i\,\frac{\theta}{2}\,\hat{n}\cdot\vec{\tau}\right)^k}{k!} = \sum_{k=0}^{\infty}\left(\frac{(-1)^k}{(2k)!}\left(\frac{\theta}{2}\right)^{2k}\right)\tau^0 + i\left(\sum_{k=0}^{\infty}\frac{(-1)^k}{(2k+1)!}\left(\frac{\theta}{2}\right)^{2k+1}\right)\hat{n}\cdot\vec{\tau}$$

$$= \cos\left(\frac{\theta}{2}\right)\tau^0 + i\,\sin\left(\frac{\theta}{2}\right)\hat{n}\cdot\vec{\tau} \tag{7.56}$$

Now it should be clear that $B \subset C$ and $C \subset B$. □

Remark: It is convenient to write a matrix $g \in SU(2)$ of the form

$$g = \alpha_0\tau^0 + i\alpha_1\tau^1 + i\alpha_2\tau^2 + i\alpha_3\tau^3 \qquad \text{as} \qquad g = \alpha_0\tau^0 + i\,\vec{\alpha}\cdot\vec{\tau} \tag{7.57}$$

The Pauli matrices satisfy the algebraic relation

$$\tau^i\tau^j = \delta_{ij}\tau^0 + i\,\epsilon_{ijk}\tau^k \tag{7.58}$$

(7.58) allows to derive the formula

$$(\vec{\alpha}\cdot\vec{\tau})(\vec{\beta}\cdot\vec{\tau}) = (\vec{\alpha}\cdot\vec{\beta})\,\tau^0 + i\,(\vec{\alpha}\times\vec{\beta})\cdot\vec{\tau} \tag{7.59}$$

Proposition 2: *(every $SU(2)$ matrix can be rotated to $i\tau^3$)*

Suppose $g \in SU(2)$ is of the form $g = i\vec{\alpha}\cdot\vec{\tau}$, $\vec{\alpha} \in S_{\mathbb{R}^3}$. Then there exists $R \in SU(2)$ such that $R^\dagger g R = i\tau^3$.

Proof: $R \in SU(2)$ if and only if there are numbers $a, b \in \mathbb{C}$ such that

$$R = \begin{bmatrix} a & -b^* \\ b & a^* \end{bmatrix} \qquad \text{and} \qquad |a|^2 + |b|^2 = 1 \tag{7.60}$$

R has to satisfy

$$R^\dagger g R = i\tau^3 \quad\Leftrightarrow\quad gR = Ri\tau^3 \quad\Leftrightarrow\quad g\begin{bmatrix} a & -b^* \\ b & a^* \end{bmatrix} = i\begin{bmatrix} a & b^* \\ b & -a^* \end{bmatrix} \tag{7.61}$$

Thus, we need to find $[a \quad b]^t \in \mathbb{C}^2$ such that

$$\left(g - i\tau^0\right)\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad \text{and} \qquad \left(g + i\tau^0\right)\begin{bmatrix} -b^* \\ a^* \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{7.62}$$

The determinant of $g - i\tau^0$ is

$$\det(g - i\tau^0) = \det\begin{bmatrix} i(\alpha_3 - 1) & \alpha_2 + i\alpha_1 \\ -(\alpha_2 - i\alpha_1) & -i(\alpha_3 + 1) \end{bmatrix} = \alpha_1^2 + \alpha_2^2 + (\alpha_3 - 1)(\alpha_3 + 1) = \|\vec{\alpha}\|^2 - 1 = 0 \tag{7.63}$$

In the same way one can find that $\det(g + i\tau^0) = 0$. This means that $\mathrm{Ker}(g - i\tau^0)$ and $\mathrm{Ker}(g + i\tau^0)$ are both non trivial. Pick any normed vector $[a \quad b]^t \in \mathrm{Ker}(g - i\tau^0)$.

$$\left(g - i\tau^0\right)\begin{bmatrix} a \\ b \end{bmatrix} = 0 \quad\Leftrightarrow\quad \left(g - i\tau^0\right)^*\begin{bmatrix} a^* \\ b^* \end{bmatrix} = 0 \quad\Leftrightarrow\quad \left(g - i\tau^0\right)^* i\tau^2(-i\tau^2)\begin{bmatrix} a^* \\ b^* \end{bmatrix} = 0$$

$$\Leftrightarrow\quad \left(g - i\tau^0\right)^* i\tau^2\begin{bmatrix} -b^* \\ a^* \end{bmatrix} = 0 \quad\Leftrightarrow\quad -i\tau^2\left(g - i\tau^0\right)^* i\tau^2\begin{bmatrix} -b^* \\ a^* \end{bmatrix} = -i\tau^2\,0 = 0 \tag{7.64}$$

A short calculation gives

$$-i\tau^2(g - i\tau^0)^* i\tau^2 = \tau^2 g^*\tau^2 + i\,\tau^2\tau^0\tau^2 = g + i\tau^0\,, \tag{7.65}$$

therefore $[a \quad b]^t$ satisfies both conditions in (7.62). Furthermore, $[a \quad b]^t$ is normed. Thus, there exists an $R \in SU(2)$ with $R^\dagger g R = i\tau^3$. □

Proposition 3: Suppose $g \in SU(2)$. Then $g^2 = \tau_0$ if and only if $g = \pm\tau^0$. And $g^2 = -\tau^0$ if and only if $g = i\,\vec{\alpha}\cdot\vec{\tau}$ for some $\vec{\alpha} \in S_{\mathbb{R}^3}$.

Proof: Let $g \in SU(2)$ be arbitrary. By proposition 1, g can be written as $g = \alpha_0\,\tau^0 + i\,\vec{\alpha}\cdot\vec{\tau}$ for some $\alpha_i \in \mathbb{R}$ with $\alpha_0^2 + \|\vec{\alpha}\|^2 = 1$.

$$g^2 = (\alpha_0\,\tau^0 + i\,\vec{\alpha}\cdot\vec{\tau})(\alpha_0\,\tau^0 + i\,\vec{\alpha}\cdot\vec{\tau}) = \alpha_0^2\,\tau^0 + i\,2\alpha_0\,\vec{\alpha}\cdot\vec{\tau} - \|\vec{\alpha}\|^2\,\tau^0 - i\,(\vec{\alpha}\times\vec{\alpha})\cdot\vec{\tau}$$

$$= (\alpha_0^2 - \|\vec{\alpha}\|^2)\,\tau^0 + i\,2\alpha_0\,\vec{\alpha}\cdot\vec{\tau} \tag{7.66}$$

$\{\tau^0, \tau^1, \tau^2, \tau^3\}$ is a basis of $\mathrm{Mat}(2\times 2, \mathbb{C})$. Thus, $g^2 = \tau^0$ is true if and only if $\alpha_0 = \pm 1$ and $\|\vec{\alpha}\| = 0$. Similarly, $g^2 = -\tau^0$ holds if and only if $\alpha_0 = 0$ and $\|\vec{\alpha}\| = 1$. □

Proposition 4: *(a and b commute iff they point in the same direction)*

Suppose $a = \alpha_0\tau^0 + i\vec{\alpha}\cdot\vec{\tau}$ and $b = \beta_0\tau^0 + i\vec{\beta}\cdot\vec{\tau}$ are $SU(2)$ matrices. a and b commute if and only if $\vec{\alpha}$ and $\vec{\beta}$ are linear dependent.

Proof: Using previous result compute

$$ab = (\alpha_0\beta_0 - \vec{\alpha}\cdot\vec{\beta})\,\tau^0 + i\,(\beta_0\vec{\alpha} + \alpha_0\vec{\beta} - \vec{\alpha}\times\vec{\beta})\cdot\vec{\tau}$$

$$ba = (\beta_0\alpha_0 - \vec{\beta}\cdot\vec{\alpha})\,\tau^0 + i\,(\alpha_0\vec{\beta} + \beta_0\vec{\alpha} - \vec{\beta}\times\vec{\alpha})\cdot\vec{\tau} \tag{7.67}$$

$\vec{\alpha}\cdot\vec{\beta} = \vec{\beta}\cdot\vec{\alpha}$ and $\vec{\alpha}\times\vec{\beta} = -\vec{\beta}\times\vec{\alpha}$. If $ab = ba$, then

$$0 = ab - ba = -2i\,(\vec{\alpha}\times\vec{\beta})\cdot\vec{\tau} \tag{7.68}$$

τ^μ are linearly independent. (7.68) can hold only if $\vec{\alpha}\times\vec{\beta} = 0$. This implies that $\vec{\alpha}$ and $\vec{\beta}$ are linearly dependent. Conversely, if $\vec{\alpha}$ and $\vec{\beta}$ are linearly dependent then $\vec{\alpha}\times\vec{\beta} = 0$ and a and b commute. □

Proposition 5: *(a and b anticommute iff both have no τ^0- component and $a \perp b$)*

Suppose $a = \alpha_0\,\tau^0 + i\,\vec{\alpha}\cdot\vec{\tau}$ and $b = \beta_0\,\tau^0 + i\,\vec{\beta}\cdot\vec{\tau}$ are $SU(2)$ matrices. a and b anticommute if and only if $\alpha_0 = \beta_0 = 0$ and $\vec{\alpha} \perp \vec{\beta}$.

Proof: If a and b anticommute, then

$$0 = ab + ba = 2(\alpha_0\beta_0 - \vec{\alpha}\cdot\vec{\beta})\,\tau^0 + 2i\,(\beta_0\,\vec{\alpha} + \alpha_0\,\vec{\beta})\cdot\vec{\tau} \tag{7.69}$$

I will prove by contradiction that $\alpha_0 = 0$. Assume $\alpha_0 \neq 0$. $\{\tau^0, \tau^1, \tau^2, \tau^3\}$ is a basis of $\mathrm{Mat}(2\times 2, \mathbb{C})$. Hence, $\beta_0\,\vec{\alpha} + \alpha_0\,\vec{\beta} = 0$. Together with $\alpha_0 \neq 0$ this gives $\vec{\beta} = -(\beta_0/\alpha_0)\,\vec{\alpha}$. Insert this in $\alpha_0\,\beta_0 - \vec{\alpha}\cdot\vec{\beta} = 0$ to find that $\alpha_0^2\,\beta_0 = -\beta_0\,\|\vec{\alpha}\|^2$. $\|\vec{\alpha}\|^2 = 1 - \alpha_0^2$ since $a \in SU(2)$. Thus, $\beta_0 = 0$. But then $\beta_0\,\vec{\alpha} + \alpha_0\,\vec{\beta} = 0$ can only hold if $\vec{\beta} = 0$, since $\alpha_0 \neq 0$. This implies $b = 0$, which contradicts $b \in SU(2)$. Hence, $\alpha_0 = 0$. Similarly one finds that $\beta_0 = 0$. It follows that $\vec{\alpha}\cdot\vec{\beta} = 0$. I.e. $\vec{\alpha} \perp \vec{\beta}$ per definition of orthogonality. It is easy to see the other direction. □

Proposition 6: *($SU(2)$ doubly covers $SO(3)$; i.e. $SU(2)/\mathbb{Z}_2 \cong SO(3)$)*

Suppose $g \in SU(2)$. $g = \alpha_0\tau^0 + i\,\vec{\alpha}\cdot\vec{\tau}$ for some numbers $\alpha_i \in \mathbb{R}$ with $\alpha_0^2 + \|\vec{\alpha}\|^2 = 1$. Suppose $R \in SU(2)$ is of the form

$$R = \exp\left(i\,\frac{\theta}{2}\,\hat{n}\cdot\vec{\tau}\right) = \cos\left(\frac{\theta}{2}\right)\,\tau^0 + i\sin\left(\frac{\theta}{2}\right)\,\hat{n}\cdot\vec{\tau} \tag{7.70}$$

Then

$$R^\dagger g R = \alpha_0\,\tau^0 + i\,\vec{\alpha}'\cdot\vec{\tau} \tag{7.71}$$

where $\vec{\alpha}' \in \mathbb{R}^3$ is $\vec{\alpha}$ rotated by the angle θ around the axis $\hat{n}$.

Proof: First compute $R^\dagger g R$. Using (7.59) and trigonometric addition formulas I find

$$R^\dagger g R = \left(\cos\left(\frac{\theta}{2}\right)\,\tau^0 - i\sin\left(\frac{\theta}{2}\right)\,\hat{n}\cdot\vec{\tau}\right)\left(\alpha_0\tau^0 + i\,\vec{\alpha}\cdot\vec{\tau}\right)\left(\cos\left(\frac{\theta}{2}\right)\,\tau^0 + i\sin\left(\frac{\theta}{2}\right)\,\hat{n}\cdot\vec{\tau}\right)$$

$$= \alpha_0\tau^0 + i\,\left(\cos(\theta)\,\vec{\alpha} - \sin(\theta)\,(\vec{\alpha}\times\hat{n}) + (1-\cos(\theta))\,(\vec{\alpha}\cdot\hat{n})\,\hat{n}\right)\cdot\vec{\tau} \tag{7.72}$$

On the other hand, $\vec{\alpha}'$ can be expressed in terms of a natural coordinate system. A good orthogonal basis to describe rotations around $\hat{n}$ is $\{\hat{n},\, \hat{n}\times\vec{\alpha},\, \hat{n}\times(\vec{\alpha}\times\hat{n})\}$. The bac-cab rule gives

$$\vec{\alpha} = (\vec{\alpha}\cdot\hat{n})\,\hat{n} + \hat{n}\times(\vec{\alpha}\times\hat{n}) \tag{7.73}$$

A rotation around the axis $\hat{n}$ does not change the $\hat{n}$-component of $\vec{\alpha}$. But it does change the other components:

$$\begin{aligned}\vec{\alpha}' &= (\vec{\alpha}\cdot\hat{n})\,\hat{n} + \cos(\theta)\,\hat{n}\times(\vec{\alpha}\times\hat{n}) + \sin(\theta)\,(\hat{n}\times\vec{\alpha}) \\ &= (\vec{\alpha}\cdot\hat{n})\,\hat{n} - \sin(\theta)\,(\vec{\alpha}\times\hat{n}) - \cos(\theta)\,\hat{n}\,(\hat{n}\cdot\vec{\alpha}) + \cos(\theta)\,\vec{\alpha}\,(\hat{n}\cdot\hat{n}) \\ &= \cos(\theta)\,\vec{\alpha} - \sin(\theta)\,(\vec{\alpha}\times\hat{n}) + (1-\cos(\theta))\,(\vec{\alpha}\cdot\hat{n})\,\hat{n}\end{aligned} \tag{7.74}$$

(7.74) is known as Rodrigue's rotation formula. $\vec{\alpha}'$ is exactly the vector we found before. □

Remark: Two $SU(2)$-matrices (R and $-R$) correspond to one rotation in $\mathbb{R}^3$. Rotations in $\mathbb{R}^3$ can be expressed as $SO(3)$ matrices. It is often much easier to think about the group operation in $SU(2)$ as of compositions of rotations rather than using the algebraic properties of τ^μ. Proposition 6 allows to prove 4 and 5 more easily. Proposition 2 is a direct corollary of 6 and the proof I have given before turns out to be redundant. To show why proposition 6 is so useful, I will give a second proof of proposition 5 using prop. 6: Suppose $a, b \in SU(2)$ anticommute, i.e. $ab = -ba$. Then $b^\dagger ab = -a$. This means that b rotates a to $-a$. It follows immediately that a has no τ^0- component, since rotations don't change the τ^0-component. Write b as

$$b = \cos\left(\frac{\theta}{2}\right)\,\tau^0 + i\sin\left(\frac{\theta}{2}\right)\,\hat{n}\cdot\vec{\tau} \tag{7.75}$$

Write $a = i\vec{\alpha}\cdot\vec{\tau}$. A rotation that changes $\vec{\alpha}$ to $-\vec{\alpha}$ must have an axis orthogonal to $\vec{\alpha}$ and must rotate $\vec{\alpha}$ by the angle $\theta = \pi$. Thus, $\hat{n}\perp\vec{\alpha}$ and $\cos(\theta/2) = 0$. This means a and b both have no τ^0-component and they are orthogonal. This is exactly the assertion of proposition 5. One can think about proposition 4 in the same way: Which rotations leave $\vec{\alpha}$ invariant? Either rotations around any axis, but with $\theta = 2\pi$, or rotations around $\vec{\alpha}$ by any angle.

Proposition 6 shows how each function $R^\dagger - R : SU(2)\to SU(2)$, $g\mapsto R^\dagger g R$ corresponds to a rotation in $\mathbb{R}^3$, where the correspondence isn't quite, but nearly, 1-to-1. This isn't good enough for the next chapter, though. For some transformation I will only have the freedom to apply one $SU(2)$ matrix R from the left or from the right. I.e. I will have to work with the functions $g\mapsto gR$ and $g\mapsto R^\dagger g$. If we restrict the matrices g to a plane orthogonal to R, then we can find a result similar to prop. 6.

Proposition 7: *(rotations of $SU(2)$ matrices restricted to a plane)*

Suppose $g\in SU(2)$ is of the form $g = i\vec{\alpha}\cdot\vec{\tau}$ and suppose $R\in SU(2)$ is

$$R = \cos\left(\frac{\theta}{2}\right)\,\tau^0 + i\,\sin\left(\frac{\theta}{2}\right)\,\hat{n}\cdot\vec{\tau} \tag{7.76}$$

with $\|\hat{n}\| = 1$ and $\vec{\alpha}\perp\hat{n}$. Then

$$gR = R^\dagger g = i\,\vec{\alpha}'\cdot\vec{\tau} \tag{7.77}$$

where $\vec{\alpha}'$ is $\vec{\alpha}$ rotated by the angle $\frac{\theta}{2}$ around the axis $\hat{n}$.

Proof: Compute

$$\begin{aligned}gR &= (i\vec{\alpha}\cdot\vec{\tau})\left(\cos\left(\frac{\theta}{2}\right)\,\tau^0 + i\,\sin\left(\frac{\theta}{2}\right)\,\hat{n}\cdot\vec{\tau}\right) = i\cos\left(\frac{\theta}{2}\right)\,\vec{\alpha}\cdot\vec{\tau} - \sin\left(\frac{\theta}{2}\right)\left((\hat{n}\cdot\vec{\alpha})\,\tau^0 + i(\vec{\alpha}\times\hat{n})\cdot\vec{\tau}\right) \\ &= i\left(\cos\left(\frac{\theta}{2}\right)\,\vec{\alpha} + \sin\left(\frac{\theta}{2}\right)\,(\hat{n}\times\vec{\alpha})\right)\cdot\vec{\tau}\end{aligned} \tag{7.78}$$

which is evidently the right vector. Thus, $-R : SU(2)\to SU(2)$ rotates any matrix $g = i\vec{\alpha}\cdot\vec{\tau}$ in the plane orthogonal to $\hat{n}$ by the same angle. Similarly for $R^\dagger - : SU(2)\to SU(2)$. It acts on every matrix of the above form in the same way. Proposition 6 shows that $R^\dagger - R = R^\dagger - \circ - R : SU(2)\to SU(2)$

rotates any matrix g in the plane by the total angle θ. Thus, $R^\dagger$ from the left must also rotate $i\vec{\alpha}\cdot\vec{\tau}$ by the angle $\frac{\theta}{2}$ around $\hat{n}$. □

Remark: The results of this chapter strongly connect to the fact that angular momentum generates representations of $SO(3)$ in quantum mechanical systems. For spins this means: Let $|\vec{\alpha},+\rangle$ be such that $(\vec{\alpha}\cdot\boldsymbol{S})\,|\vec{\alpha},+\rangle = \frac{1}{2}|\vec{\alpha},+\rangle$ where $\vec{\alpha}\in S_{\mathbb{R}^3}$. It is in this sense that a quantum spin has direction. $|\vec{\alpha},+\rangle$ is unique up to norm and phase. The state

$$e^{-i\theta\hat{n}\cdot\boldsymbol{S}}|\vec{\alpha},+\rangle = |\vec{\alpha}',+\rangle \tag{7.79}$$

satisfies $(\vec{\alpha}'\cdot\boldsymbol{S})|\vec{\alpha}',+\rangle = \frac{1}{2}|\vec{\alpha}',+\rangle$, where $\vec{\alpha}'$ is $\vec{\alpha}$ rotated by angle θ around the axis $\hat{n}$.

7.3 Appendix C: Classificationgg of kagome-based $\mathbb{Z}_2$ spin liquids

This chapter does not contain any physical ideas or explanations. I will determine all projective symmetry groups with invariant gauge $\mathbb{Z}_2$ and a symmetry group generated by D, P, T_x, T_y and time reversal symmetry T. The symmetry group belongs to the kagome lattice. For more details concerning spatial symmetries and time reversal symmetry, see Chapter 4.

D is the clockwise rotation of angle $2\pi/6$ around the point of origin (centre of the zeroth honeycomb cell). T_x and T_y are translation along the negative unit vectors. P is the projection which interchanges $\hat{x}$ and $\hat{y}$ (see figure 2).

7.3.1 Algebraic conditions

I will need to work with P and D in lattice coordinates. I label the atoms on the kagome lattice by lattice $= \mathbb{Z}\times\mathbb{Z}\times\{a,b,c\}$. Refer to figure 2 in chapter 4 to see which atom is which.

$$\begin{aligned} P:\text{lattice}\to\text{lattice},\quad & (x,y,a)\mapsto(y,x,c) & D:\text{lattice}\to\text{lattice},\quad & (x,y,a)\mapsto(x+y,-(x+1),b)\\ & (x,y,b)\mapsto(y,x,b) & & (x,y,b)\mapsto(x+y+1,-(x+1),c)\\ & (x,y,c)\mapsto(y,x,a) & & (x,y,c)\mapsto(x+y,-x,a) \end{aligned} \tag{7.80}$$

There are general algebraic conditions which every projective symmetry group with kagome symmetry group must satisfy. They arise from the commutation relations of the underlying symmetry group. It holds that

$$\begin{aligned} &T_xT_y = T_yT_x, && PT_x = T_yP, && PT_y = T_xP, && PD = D^{-1}P,\\ &DT_x = T_y^{-1}T_xD, && DT_y = T_xD, && P^2 = id, && D^6 = id \end{aligned} \tag{7.81}$$

The time reversal symmetry T commutes with all other symmetries (and gauge transformations).

$$TS = ST, \quad \text{for } S = T_x, T_y, P, D \tag{7.82}$$

and of course $T^2 = id$. The above relations translate directly into conditions for the projective symmetry group.

$$T_xT_yT_x^{-1}T_y^{-1} = id \quad\Rightarrow\quad (G_xT_xG_yT_yT_x^{-1}G_x^{-1}T_y^{-1}G_y^{-1}, id)\in IGG \tag{A1}$$

$$PT_xP^{-1}T_y^{-1} = id \quad\Rightarrow\quad (G_PPG_xT_xP^{-1}G_P^{-1}T_y^{-1}G_y^{-1}, id)\in IGG \tag{A2}$$

$$PT_yP^{-1}T_x^{-1} = id \quad\Rightarrow\quad (G_PPG_yT_yP^{-1}G_P^{-1}T_x^{-1}G_x^{-1}, id)\in IGG \tag{A3}$$

$$PDP^{-1}D = id \quad\Rightarrow\quad (G_PPG_DDP^{-1}G_P^{-1}G_DD, id)\in IGG \tag{A4}$$

$$DT_xD^{-1}T_x^{-1}T_y = id \quad\Rightarrow\quad (G_DDG_xT_xD^{-1}G_D^{-1}T_x^{-1}G_x^{-1}G_yT_y, id)\in IGG \tag{A5}$$

$$DT_yD^{-1}T_x^{-1} = id \quad\Rightarrow\quad (G_DDG_yT_yD^{-1}G_D^{-1}T_x^{-1}G_x^{-1}, id)\in IGG \tag{A6}$$

$$P^2 = id \qquad \Rightarrow \qquad (G_P P G_P P, id) \in IGG \tag{A7}$$

$$D^6 = id \qquad \Rightarrow \qquad (\,(G_D D)^6, id) \in IGG \tag{A8}$$

$$T^2 = id \qquad \Rightarrow \qquad (G_T T G_T T, id) \in IGG \tag{A9}$$

$$STS^{-1}T^{-1} = id \qquad \Rightarrow \qquad (G_S S G_T T S^{-1} G_S^{-1} T^{-1} G_T^{-1}, id) \in IGG \tag{A10-13}$$

The last line holds for $S = T_x, T_y, P, D$. I will determine all possible PSGs with invariant gauge group $\mathbb{Z}_2$. For those (A1) - (A13) impose the following restrictions on the $SU(2)$ matrices which form the gauge transformations:

$$\forall i \in \text{lattice}: \quad G_y(i)^\dagger G_x(i+\hat{y})^\dagger G_y(i+\hat{x}) G_x(i) = \eta_x \tau^0 \tag{A1}$$

$$\forall i \in \text{lattice}: \quad G_y(i)^\dagger G_P(i+\hat{y})^\dagger G_x(P(i)) G_P(i) = \eta_{Py} \tau^0 \tag{A2}$$

$$\forall i \in \text{lattice}: \quad G_x(i)^\dagger G_P(i+\hat{x})^\dagger G_y(P(i)) G_P(i) = \eta_{Px} \tau^0 \tag{A3}$$

$$\forall i \in \text{lattice}: \quad G_D(D(i)) G_P(D(i))^\dagger G_D(P^{-1}(i)) G_P(i) = \eta_{PD} \tau^0 \tag{A4}$$

$$\forall i \in \text{lattice}: \quad G_y(i-\hat{y}) G_x(i-\hat{y})^\dagger G_D(i-\hat{y}+\hat{x})^\dagger G_x(D^{-1}(i)) G_D(i) = \eta_{Dy} \tau^0 \tag{A5}$$

$$\forall i \in \text{lattice}: \quad G_x(i)^\dagger G_D(i+\hat{x})^\dagger G_y(D^{-1}(i)) G_D(i) = \eta_{Dxy} \tau^0 \tag{A6}$$

$$\forall i \in \text{lattice}: \quad G_P(P(i)) G_P(i) = \eta_P \tau^0 \tag{A7}$$

$$\forall i \in \text{lattice}: \quad G_D(D(i)) G_D(D^2(i)) G_D(D^3(i)) G_D(D^4(i)) G_D(D^5(i)) G_D(i) = \eta_D \tau^0 \tag{A8}$$

$$\forall i \in \text{lattice}: \quad G_T(i)^2 = \eta_T \tau^0 \tag{A9}$$

$$\forall i \in \text{lattice}: \quad G_T(i)^\dagger G_S(i)^\dagger G_T(S^{-1}(i)) G_S(i) = \eta_{xt,yt,Pt,Dt}\, \tau^0 \tag{A10-13}$$

where each $\eta = \pm 1$. The reason is that $\mathbb{Z}_2$ consists only of (id, id) and $(-id, id)$.

Remark: Every projective symmetry group with kagome symmetry group and invariant gauge group $\mathbb{Z}_2$ has to satisfy the above conditions. Until now, I wasn't able to prove the converse. I.e. that every group generated by pairs (G_S, S), $S \in \{T_x, T_y, P, D, T\}$, which satisfy conditions $(A1) - (A13)$, is a projective symmetry group with invariant gauge group $\mathbb{Z}_2$ and kagome symmetry group. So there might be none at all.

7.3.2 Translation symmetries

Result: There always exists a gauge in which

$$\forall x \forall y \forall z: \quad G_y(x,y,z) = \tau^0, \qquad \text{and} \qquad \forall x \forall y \forall z: \quad G_x(x,y,z) = \eta_x^y\, \tau^0 \tag{7.83}$$

Why? $IGG(H) = \mathbb{Z}_2 = \{(id, id), (-id, id)\}$. Let W be a local $SU(2)$ transformation. $H \xrightarrow{W} \tilde{H}$. The projective symmetry group of $\tilde{H}$ is isomorphic to the projective symmetry group of H. Recall that in the new gauge W

$$\tilde{G}_x = W G_x T_x W^{-1} T_x^{-1} \tag{7.84}$$

The matrices $W G_x T_x W^{-1} T_x^{-1}(i)$ can be found like this:

$$\Psi_i \xrightarrow{T_x^{-1}} \Psi_{i+\hat{x}} \xrightarrow{W^{-1}} W(i+\hat{x})^\dagger \Psi_{i+\hat{x}} \xrightarrow{T_x} W(i+\hat{x})^\dagger \Psi_i \xrightarrow{WG_x} W(i+\hat{x})^\dagger G_x(i) W(i) \Psi_i \tag{7.85}$$

Thus, $G_x(i)$ and $G_y(i)$ transform under W as

$$\tilde{G}_x(i) = W(i+\hat{x})^\dagger G_x(i) W(i), \qquad \tilde{G}_y(i) = W(i+\hat{y})^\dagger G_y(i) W(i) \tag{7.86}$$

Fix z. Choose an arbitrary matrix $W_z \in SU(2)$. Set $W(0,0,z) = W_z$.

$$\tau^0 = W((0,0,z)+\hat{x})^\dagger G_x(0,0,z)W(0,0,z) \quad \Leftrightarrow \quad W(1,0,z) = G_x(0,0,z)W(0,0,z) \tag{7.87}$$

So set $W(1,0,z) = G_x(0,0,z)W_z$. Continue with the next unit cell $0+2\hat{x}$.

$$\tau^0 = W(2,0,z)^\dagger G_x(1,0,z)W(1,0,z) \quad \Leftrightarrow \quad W(2,0,z) = G_x(1,0,z)G_x(0,0,z)W(0,0,z) \tag{7.88}$$

In general, set $W(x,0,z) = G_x(x-1,0,z)G_x(x-2,0,z)...G_x(0,0,z)W_z$ for $x > 0$. Then

$$\forall x \geq 0: \quad \tilde{G}_x(x,0,z) = \tau^0 \tag{7.89}$$

The same works in the $-\hat{x}$ direction. Set

$$W(x,0,z) = G_x(x,0,z)^\dagger G_x(x+1,0,z)^\dagger ... G_x(-1,0,z)^\dagger W_z \tag{7.90}$$

for $x < 0$. Then

$$\forall x < 0: \quad \tilde{G}_x(x,0,z) = \tau^0 \tag{7.91}$$

We found $SU(2)$ matrices $W(i)$ on the row of unit cells $\{(x,0,z)\,|\,x \in \mathbb{Z}\}$ such that $\forall x: \tilde{G}_x(x,0,z) = \tau^0$. Do the same with G_y on each column of unit cells $\{(x_0,y,z)\,|\,y \in \mathbb{Z}\}$. Start with the already fixed matrix $W(x_0,0,z) \in SU(2)$ and proceed as above, but in $\hat{y}$-direction. Then

$$\forall x \forall y: \tilde{G}_y(x,y,z) = \tau^0 \qquad \text{and} \qquad \forall x: \tilde{G}_x(x,0,z) = \tau^0 \tag{7.92}$$

z was arbitrary. Do the above for every z. Then W is completely determined and in the new gauge

$$\forall x \forall y \forall z: G_y(x,y,z) = \tau^0 \qquad \text{and} \qquad \forall x \forall z: G_x(x,0,z) = \tau^0 \tag{7.93}$$

I will continue in this gauge. It remains to find which options there are to choose $G_x(x,y,z)$ for $y \neq 0$. When I insert (7.93) into algebraic condition (A1), I find that

$$\forall i: \quad G_x(i+\hat{y}) = \eta_x G_x(i) \tag{7.94}$$

Thus, up to gauge transformations, there are only two different PSGs for $\mathbb{Z}_2$-spin liquids which have only translation symmetry. Namely

$$G_y(i) = \tau^0, \quad G_x(i) = \tau^0 \qquad \text{and} \qquad G_y(i) = \tau^0, \quad G_x(i) = (-1)^y \tau^0 \tag{7.95}$$

This is exactly what was claimed at the beginning of this section. □

7.3.3 Time reversal symmetry

Result: Without changing G_x and G_y, we can switch to a gauge in which

$$\forall x \forall y \forall z: \quad G_T(x,y,z) = \eta_{xt}^x \eta_{yt}^y \, g_{Tz} \tag{7.96}$$

where $g_{Tz} = G_T(0,0,z)$. Furthermore, g_{Tz} must obey

$$\forall z: \quad g_{Tz}^2 = \eta_T \tau^0 \tag{7.97}$$

Why? T commutes with all other symmetries. The matrices of G_T must satisfy

$$G_T(i)^\dagger G_x(i)^\dagger G_T(i+\hat{x})G_x(i) = \eta_{xt}\tau^0 \quad \text{and} \quad G_T(i)^\dagger G_y(i)^\dagger G_T(i+\hat{y})G_y(i) = \eta_{yt}\tau^0 \tag{A10/11}$$

for all lattice vectors i. In the gauge from the previous section, this becomes

$$G_T(i+\hat{x}) = \eta_{xt}\, G_T(i) \qquad \text{and} \qquad G_T(i+\hat{y}) = \eta_{yt}\, G_T(i) \tag{7.98}$$

The matrices of G_T in one unit cell determine all others recursively. (7.98) can be solved by setting

$$\forall i \in \text{lattice}: \quad G_T(x,y,z) = \eta_{xt}^x \eta_{yt}^y \, g_{Tz} \tag{7.99}$$

where $g_{Tz} = G_T(0,0,z)$. The constraint

$$\forall z: \quad g_{Tz}^2 = \eta_T \tau^0 \tag{7.100}$$

comes from algebraic condition (A9). □

7.3.4 Mirror symmetry

Results: We can switch to a gauge in which

$$\forall x\forall y\forall z : G_P(x,y,z) = \eta_{Px}^x \eta_{Py}^y \eta_x^{xy}\, g_{Pz}, \qquad \forall x\forall y\forall z : \quad G_T(x,y,z) = \eta_{xt}^{x+y}\, g_{Tz} \tag{7.101}$$

$g_T = i\tau^3$. Additionally, I find the condition

$$\forall z : \quad g_{Tz}^\dagger g_{Pz}^\dagger g_{TP^{-1}(z)}\, g_{Pz} = \eta_{Pt}\tau^0 \tag{7.102}$$

Why? Insert (7.83) into (A2) and (A3) to get

$$\forall i : \quad G_P(i+\hat{y}) = \eta_{Py}\eta_x^x\, G_P(i) \qquad \text{and} \qquad \forall i : \quad G_P(i+\hat{x}) = \eta_{Px}\eta_x^y\, G_P(i) \tag{7.103}$$

Again, choosing matrices $G_P(i)$ in one unit cell determines all matrices $G_P(i)$ on the lattice recursively. (7.103) can be solved by

$$\forall x\forall y\forall z : \quad G_P(x,y,z) = \eta_{Px}^x \eta_{Py}^y \eta_x^{xy}\, g_{Pz} \tag{7.104}$$

where $g_{Pz} = G_P(0,0,z)$. (A12) imposes an additional constraint on G_T. Recall that

$$G_T(i)^\dagger G_P(i)^\dagger G_T(P^{-1}(i)) G_P(i) = \eta_{Pt}\tau^0 \tag{A12}$$

Insert (7.104) into (A12) to get

$$\eta_{xt}^{x+y}\eta_{yt}^{y+x}\, g_{Tz}^\dagger\, g_{Pz}^\dagger g_{TP^{-1}(z)} g_{Pz} = \eta_{Pt}\tau^0 \tag{7.105}$$

The right hand side is independent of x and y, so the left hand side has to be too. This can only hold if $\eta_{xt} = \eta_{yt}$. It follows that

$$\forall x\forall y\forall z : \quad G_T(x,y,z) = \eta_{xt}^{x+y}\, g_{Tz} \qquad \text{and} \qquad \forall z : \quad g_{Tz}^\dagger g_{Pz}^\dagger g_{TP^{-1}(z)} g_{Pz} = \eta_{Pt}\tau^0 \tag{7.106}$$

□

7.3.5 Rotation symmetry

Result: There always exists a gauge in which

$$\begin{aligned} \forall x\forall y : \quad & G_D(x,y,a) = \eta_x^{f_a(x,y)} \eta_{Dxy}^{x+y}\, g_{Da}, \quad G_D(x,y,b) = \eta_x^{f_b(x,y)} \eta_{Dxy}^{x+y} g_{Db} \\ & G_D(x,y,c) = \eta_x^{f_c(x,y)} \eta_{Dxy}^{x+y} \eta_{Dy} g_{Dc} \end{aligned} \tag{7.107}$$

with $f_a(x,y) = f_c(x,y) = xy + \frac{1}{2}(y^2+y)$ and $f_b(x,y) = xy + \frac{1}{2}(y^2-y)$.

Why? It is helpful to write down D^{-1} explicitly.

$$\begin{aligned} D^{-1} : \text{lattice} \to \text{lattice}, \qquad & (x,y,a) \mapsto (-y, x+y, c) \\ & (x,y,b) \mapsto (-(y+1), x+y+1, a) \\ & (x,y,c) \mapsto (-(y+1), x+y, b) \end{aligned} \tag{7.108}$$

Insert (7.83) in (A6) to get

$$\forall x\forall y\forall z : \quad \eta_x^y\, G_D(x+1,y,z)^\dagger G_D(x,y,z) = \eta_{Dxy}\tau^0 \tag{7.109}$$

and in (A5) to get

$$\begin{aligned} \forall x\forall y : \quad & \eta_x^{y-1} G_D(x+1,y-1,a)^\dagger \eta_x^{x+y} G_D(x,y,a) = \eta_{Dy}\tau^0 \\ \forall x\forall y : \quad & \eta_x^{y-1} G_D(x+1,y-1,b)^\dagger \eta_x^{x+y+1} G_D(x,y,b) = \eta_{Dy}\tau^0 \\ \forall x\forall y : \quad & \eta_x^{y-1} G_D(x+1,y-1,c)^\dagger \eta_x^{x+y} G_D(x,y,c) = \eta_{Dy}\tau^0 \end{aligned} \tag{7.110}$$

Knowing $G_D(i)$ in one unit cell determines all the matrices matrices $G_D(i)$ recursively. The solution for $z = a$ and $z = c$ is different from the solution for $z = b$. For atom a, rearrange (7.109) and (7.110) to

$$\begin{aligned} \forall x \forall y: \quad & G_D(x+1,y,a) = \eta_x^y \eta_{Dxy} G_D(x,y,a) \\ \forall x \forall y: \quad & G_D(x,y+1,a) = \eta_x^{x+y+1} \eta_{Dxy} \eta_{Dy} G_D(x,y,a) \end{aligned} \tag{7.111}$$

A sensible ansatz to solve this system is

$$G_D(x,y,a) = \eta_x^{f(x,y)} \eta_{Dxy}^{g(x,y)} \eta_{Dy}^{h(x,y)} g_{Da} \tag{7.112}$$

where f, g and h are some $\mathbb{Z}/2\mathbb{Z}$-valued functions and $g_{Da} = G_D(0,0,a)$. (7.111) then implies

$$\begin{aligned} & f(x+1,y) = f(x,y) + y, && g(x+1,y) = g(x,y) + 1, && h(x+1,y) = h(x,y) \\ & f(x,y+1) = f(x,y) + x + y + 1, && g(x,y+1) = g(x,y) + 1, && h(x,y+1) = h(x,y) + 1 \end{aligned} \tag{7.113}$$

I found the following solution. Set

$$f(x,y) = xy + \frac{1}{2}(y^2 + y), \qquad g(x,y) = x + y, \qquad h(x,y) = y \tag{7.114}$$

It is easy to check that they indeed satisfy the above conditions (modulo 2). Solve $G_D(x,y,c)$ in the same way. For atom b, (7.109) and (7.110) read as

$$\begin{aligned} \forall x \forall y: \quad & G_D(x+1,y,a) = \eta_x^y \eta_{Dxy} G_D(x,y,b) \\ \forall x \forall y: \quad & G_D(x,y+1,a) = \eta_x^{x+y} \eta_{Dxy} \eta_{Dy} G_D(x,y,b) \end{aligned} \tag{7.115}$$

Using the same ansatz

$$G_D(x,y,b) = \eta_x^{f(x,y)} \eta_{Dxy}^{g(x,y)} \eta_{Dy}^{h(x,y)} g_{Db} \tag{7.116}$$

I find the solution

$$f(x,y) = xy + \frac{1}{2}(y^2 - y), \qquad g(x,y) = x + y, \qquad h(x,y) = y \tag{7.117}$$

To summarise,

$$\forall x \forall y \forall z: \quad G_D(x,y,z) = \eta_x^{f_z(x,y)} \eta_{Dxy}^{x+y} \eta_{Dy}^{y} \, g_{Dz} \tag{7.118}$$

where $f_a(x,y) = f_c(x,y) = xy + \frac{1}{2}(y^2 + y)$ and $f_b(x,y) = xy + \frac{1}{2}(y^2 - y)$.

The last step is to switch the gauge again. Consider a gauge transformation W of the form

$$W(x,y,z) = \eta_{Dy}^{x+y} \, \tau^0 \tag{7.119}$$

W will not alter (G_T, T) and (G_P, P). It will change (G_x, T_x) and (G_y, T_y) either not or only by a global minus sign. This makes no difference for the resulting projective symmetry group. G_D transforms under W like this:

$$G_D(i) \xrightarrow{W} W(D^{-1}(i))^\dagger \, G_D(i) \, W(i) \tag{7.120}$$

Hence, in the new gauge:

$$\begin{aligned} \forall x \forall y: \quad G_D(x,y,a) &= \eta_{Dy}^{x+y-y} \, \eta_x^{f_a(x,y)} \eta_{Dxy}^{x+y} \eta_{Dy}^{y} \, g_{Da} \, \eta_{Dy}^{x+y} = \eta_{Dy}^{2(x+y)} \eta_x^{f_a(x,y)} \eta_{Dxy}^{x+y} \\ &= \eta_x^{f_a(x,y)} \eta_{Dxy}^{x+y} g_{Da} \end{aligned} \tag{7.121}$$

In the same way for atom b and c. The transformation gives $G_D(x,y,c)$ an additional global minus sign in the case $\eta_{Dy} = -1$. I will continue in this gauge. □

7.3.6 The remaining algebraic conditions

Results: There is a gauge in which $\forall x \forall y \forall z$:

$$G_D(x,y,z) = \eta_x^{h_z(x,y)} g_{Dz} \qquad G_T(x,y,z) = g_{Tz} \qquad G_P(x,y,z) = \eta_x^{xy} g_{Pz} \tag{7.122}$$

where $h_a(x,y) = h_c(x,y) = x + y + xy + \frac{1}{2}(y^2 + y)$ and $h_b(x,y) = x + y + xy + \frac{1}{2}(y^2 - y)$. G_x and G_y are the same as before. Additionally, I find the conditions

$$\begin{aligned}
&g_{Pb}^2 = \eta_P \tau^0 && g_{Pa} g_{Pc} = \eta_P \tau^0 && g_{Db} g_{Pb}^\dagger g_{Dc} g_{Pa} = \eta_{PD} \tau^0 \\
&g_{Dc} g_{Pc}^\dagger g_{Db} g_{Pb} = \eta_{PD} \tau^0 && g_{Da} g_{Pa}^\dagger g_{Da} g_{Pc} = \eta_{PD} \tau^0 && \forall z : \; g_{Tz}^\dagger g_{Dz}^\dagger g_{TD^{-1}(z)} g_{Dz} = \eta_{Dt} \tau^0 \\
&(g_{Da} g_{Db} g_{Dc})^2 = \eta_x \eta_D \tau^0
\end{aligned} \tag{7.123}$$

Why? It remains to check algebraic conditions (A4), (A7), (A13) and (A8). I will start with (A4).

$$\forall i \in \text{lattice} : \qquad G_D(D(i)) G_P(D(i))^\dagger G_D(P^{-1}(i)) G_P(i) = \eta_{PD} \tau^0 \tag{A4}$$

For $i = (x,y,a)$, this reads as

$$\eta_x^{f_b(x+y,-(x+1))} \eta_{Dxy}^{y-1} g_{Db} \eta_{Px}^{x+y} \eta_{Py}^{-(x+1)} \eta_x^{-(x+y)(x+1)} g_{Pb}^\dagger \eta_x^{f_c(y,x)} \eta_{Dxy}^{y+x} \eta_{Dy} g_{Dc} \eta_{Px}^x \eta_{Py}^y \eta_x^{xy} g_{Pa} = \eta_{PD} \tau^0 \tag{7.124}$$

Collect exponents. Since each ηs is either $+1$ or -1, exponents can be treated as $\mathbb{Z}/2\mathbb{Z}$-valued functions. The result is

$$\forall x \forall y : \quad \eta_x^{x+1} \eta_{Px}^y \eta_{Py}^{x+y+1} \eta_{Dxy}^{x+1} g_{Db} g_{Pb}^\dagger g_{Dc} g_{Pa} = \eta_{Dy} \eta_{PD} \tau^0 \tag{7.125}$$

The right hand side is independent of x and y. So the left hand side must be constant in x and y too. This can only hold if $\eta_{Px} = \eta_{Py}$. Then

$$\forall x \forall y : \quad \eta_x^{x+1} \eta_{Py}^{x+1} \eta_{Dxy}^{x+1} g_{Db} g_{Pb}^\dagger g_{Dc} g_{Pa} = \eta_{Dy} \eta_{PD} \tau^0 \tag{7.126}$$

For $i = (x,y,b)$, condition (A4) reads

$$\eta_x^{f_c(x+y+1,-(x+1))} \eta_{Dxy}^y \eta_{Dy} g_{Dc} \eta_{Py}^y \eta_x^{-(x+1)(x+y+1)} g_{Pc}^\dagger \eta_x^{f_b(y,x)} \eta_{Dxy}^{y+x} g_{Db} \eta_{Py}^{x+y} \eta_x^{xy} g_{Pb} = \eta_{PD} \tau^0 \tag{7.127}$$

which gives

$$\forall x \forall y : \quad \eta_x^x \eta_{Py}^x \eta_{Dxy}^x g_{Dc} g_{Pc}^\dagger g_{Db} g_{Pb} = \eta_{Dy} \eta_{PD} \tau^0 \tag{7.128}$$

For $i = (x,y,c)$, condition (A4) is

$$\eta_x^{f_a(x+y,-x)} \eta_{Dxy}^y g_{Da} \eta_{Py}^y \eta_x^{-x(x+y)} g_{Pa} \eta_x^{f_a(y,x)} \eta_{Dxy}^{y+x} g_{Da} \eta_{Py}^{x+y} \eta_x^{xy} = \eta_{PD} \tau^0 \tag{7.129}$$

and after collecting terms

$$\forall x \forall y : \quad \eta_x^x \eta_{Py}^x \eta_{Dxy}^x g_{Da} g_{Pa}^\dagger g_{Da} g_{Pc} = \eta_{PD} \tau^0 \tag{7.130}$$

The last equation must be constant in x on both sides. Note that

$$\eta_x^x \eta_{Py}^x \eta_{Dxy}^x = \eta_{Py}^x (\eta_x \eta_{Dxy})^x \tag{7.131}$$

Thus,

$$\eta_{Py} = \eta_x \eta_{Dxy} \qquad \Leftrightarrow \qquad \eta_{Dxy} = \eta_x \eta_{Py} \tag{7.132}$$

Furthermore, this yields the following three conditions

$$\eta_{Dy} g_{Db} g_{Pb}^\dagger g_{Dc} g_{Pa} = \eta_{PD} \tau^0, \quad \eta_{Dy} g_{Dc} g_{Pc}^\dagger g_{Db} g_{Pb} = \eta_{PD} \tau^0 \quad \text{and} \quad g_{Da} g_{Pa}^\dagger g_{Da} g_{Pc} = \eta_{PD} \tau^0 \tag{7.133}$$

Before I continue, consider the gauge transformation

$$W(x,y,z) = \eta_{Py}^x \tau^0 \tag{7.134}$$

It does not change G_T and G_y. It can change G_x only by a global sign. W transforms G_P like this:

$$G_P(x,y,z) = \eta_{Py}^{x+y}\eta_x^{xy} g_{Pz} \xrightarrow{W} \eta_{Py}^{y}\tau^0\eta_{Py}^{x+y}\eta_x^{xy} g_{Pz}\eta_{Py}^{x}\tau^0 = \eta_x^{xy} g_{Pz} \tag{7.135}$$

Using (7.132), I find that G_D takes the form

$$\begin{aligned} &G_D(x,y,a) = \eta_x^{x+y+f_a(x,y)}\eta_{Py}^{x+y} g_{Da}, \quad G_D(x,y,b) = \eta_x^{x+y+f_b(x,y)}\eta_{Py}^{x+y} g_{Db}, \\ &G_D(x,y,c) = \eta_x^{x+y+f_c(x,y)}\eta_{Py}^{x+y}\eta_{Dy} g_{Dc} \end{aligned} \tag{7.136}$$

before the transformation W. Thus, in the new gauge G_D is

$$\begin{aligned} &G_D(x,y,a) = \eta_x^{x+y+f_a(x,y)} g_{Da}, \quad G_D(x,y,b) = \eta_x^{x+y+f_b(x,y)}\eta_{Py} g_{Db}, \\ &G_D(x,y,c) = \eta_x^{x+y+f_c(x,y)}\eta_{Py}\eta_{Dy} g_{Dc} \end{aligned} \tag{7.137}$$

Since we have not chosen $g_{Db}, g_{Dc} \in SU(2)$ yet, let them absorb the unnecessary signs η_{Dy} and η_{Py}. Condition (A7) gives no new constraints for the ηs, but

$$g_{Pb}^2 = \eta_P\tau^0, \quad g_{Pa}g_{Pc} = \eta_P\tau^0 \quad \text{and} \quad g_{Pc}g_{Pa} = \eta_P\tau^0 \tag{7.138}$$

The condition (A13) is

$$\forall i \in \text{lattice}: \quad G_T(i)^\dagger G_D(i)^\dagger G_T(D^{-1}(i)) G_D(i) = \eta_{Dt}\,\tau^0 \tag{A13}$$

If I insert $i = (x,y,a)$, this reads as

$$\forall x \forall y: \quad \eta_{xt}^{y} g_{Ta}^\dagger g_{Da}^\dagger g_{Tc} g_{Da} = \eta_{Dt}\tau^0 \tag{7.139}$$

which can only hold if

$$\eta_{xt} = 1 \qquad \text{and} \qquad g_{Ta}^\dagger g_{Da}^\dagger g_{Tc} g_{Da} = \eta_{Dt}\tau^0 \tag{7.140}$$

Similar for the atoms b and c:

$$g_{Tb}^\dagger g_{Db}^\dagger g_{Ta} g_{Db} = \eta_{Dt}\tau^0 \qquad \text{and} \qquad g_{Tc}^\dagger g_{Dc}^\dagger g_{Tb} g_{Dc} = \eta_{Dt}\tau^0 \tag{7.141}$$

(A8) gives no further constraints on the choice of ηs, but the three equivalent conditions

$$(g_{Db}g_{Dc}g_{Da})^2 = \eta_x\eta_D\tau^0, \quad (g_{Dc}g_{Da}g_{Db})^2 = \eta_x\eta_D\tau^0 \quad \text{and} \quad (g_{Da}g_{Db}g_{Dc})^2 = \eta_x\eta_D\tau^0 \tag{7.142}$$

as claimed. □

7.3.7 Gauge inequivalent choices in the zeroth unit cell

This is going to be tedious. I will proceed in the following scheme: I will set some of the ηs to $+1$ or -1 and then show that **if** we have a projective symmetry group which satisfies conditions $(1)-(9)$ for the given combination of ηs, **then** we can always find a new gauge in which the projective symmetry group takes some simple form. After I have done this for all possible combinations of $\eta_P, \eta_{PD}, ..., \eta_x\eta_D = \pm 1$, I have found all projective symmetry groups on the kagome lattice up to the choice of gauge. The conditions on $g_T, g_{Pz}, g_{Dz} \in SU(2)$ are:

(1) $g_{Tz}^2 = \eta_T\tau^0$ (2) $g_{Pb}^2 = \eta_P\tau^0$ (3) $g_{Pa}g_{Pc} = \eta_P\tau^0$

(4) $g_{Db}g_{Pb}^\dagger g_{Dc}g_{Pa} = \eta_{PD}\tau^0$ (5) $g_{Dc}g_{Pc}^\dagger g_{Db}g_{Pb} = \eta_{PD}\tau^0$ (6) $g_{Da}g_{Pa}^\dagger g_{Da}g_{Pc} = \eta_{PD}\tau^0$

(7) $g_{Tz}^\dagger g_{Dz}^\dagger g_{TD^{-1}(z)} g_{Dz} = \eta_{Dt}\tau^0$ (8) $g_{Tz}^\dagger g_{Pz}^\dagger g_{TP^{-1}(z)} g_{Pz} = \eta_{Pt}\tau^0$ (9) $(g_{Da}g_{Db}g_{Dc})^2 = \eta_x\eta_D\tau^0$

We can use those conditions to further simplify the projective symmetry groups. We will use the results and the language that we developed in appendix B throughout this section. Some general remarks before

I start. Consider a gauge transformation F of the form $F(x,y,z) = F_z \in SU(2)$. F will not alter G_x and G_y. It will act on G_D and G_P like this

$$\begin{aligned} g_{Pa} &\xrightarrow{F} F_c^\dagger g_{Pa} F_a & g_{Pb} &\xrightarrow{F} F_b^\dagger g_{Pb} F_b & g_{Pc} &\xrightarrow{F} F_a^\dagger g_{Pc} F_c \\ g_{Da} &\xrightarrow{F} F_c^\dagger g_{Da} F_a & g_{Db} &\xrightarrow{F} F_a^\dagger g_{Db} F_b & g_{Dc} &\xrightarrow{F} F_b^\dagger g_{Dc} F_c \end{aligned} \tag{7.143}$$

and G_T like this

$$g_{Ta} \xrightarrow{F} F_a^\dagger g_{Ta} F_a, \qquad g_{Tb} \xrightarrow{F} F_b^\dagger g_{Tb} F_b, \qquad G_T(x,y,c) \xrightarrow{F} F_c^\dagger g_{Tc} F_c \tag{7.144}$$

Thus, if each F_z commutes with g_{Tz}, then F will leave G_T unchanged.

I will start with the case $\eta_T = -1$. Then for each z it holds that $g_{Tz}^2 = -\tau^0$. This tells that each g_{Tz} has no τ^0 component.

Fact: Suppose $g \in SU(2)$. Then $g^2 = \tau_0$ if and only if $g = \pm\tau^0$. And $g^2 = -\tau^0$ if and only if $g = i\,\vec{\alpha}\cdot\vec{\tau}$ for some $\vec{\alpha} \in S_{\mathbb{R}^3}$. (Proposition 3 in appendix B).

Furthermore, we can use a gauge transformation of the form (7.143) to transform each matrix g_{Tz} to $i\tau^3$. This is because of the

Fact: Suppose $g \in SU(2)$ is of the form $g = i\,\vec{\alpha}\cdot\vec{\tau}$, $\vec{\alpha} \in S_{\mathbb{R}^3}$. Then there exists $R \in SU(2)$ such that $R^\dagger g R = i\tau^3$. (Proposition 2 in appendix B). □

Switch to a gauge in which $g_{Tz} = i\tau^3$ for each z. Write $g_T = g_{Tz} = i\tau^3$. I don't want to alter G_T anymore. So I can only use transformations where each F_z commutes with $i\tau^3$.

Fact: Let $a = \alpha_0\,\tau^0 + i\,\vec{\alpha}\cdot\vec{\tau}$ and $b = \beta_0\,\tau^0 + i\,\vec{\beta}\cdot\vec{\tau}$ be $SU(2)$-matrices. a and b commute if and only if $\vec{\alpha}$ and $\vec{\beta}$ are linearly dependent. (Proposition 4 in appendix C).

Thus, I still have the freedom to transform with $F_z = \alpha_0\tau^0 + i\alpha_3\tau^3$. These are exactly the $SU(2)$ matrices which correspond to rotations around the z-axis. A precise description of what this means can be found in appendix B. Furthermore, if the matrices g_{Pz}, g_{Dz} and g_T satisfied $(2)-(9)$ just before a gauge transformation F, then so do the transformed matrices $\tilde{g}_{Pz}, \tilde{g}_{Dz}, \tilde{g}_T$. This can be checked easily by plugging $g_{Pa} = F_c \tilde{g}_{Pa} F_a^\dagger$, $g_{Pb} = F_b \tilde{g}_{Pb} F_b^\dagger$, ... into $(2)-(9)$. More precisely:

Suppose g_T, g_{Pz}, g_{Dz} satisfy condition $(1)-(9)$. Suppose F is a gauge transformation which transforms g_T, g_{Pz}, g_{Dz} as in (7.143). Additionally, suppose that all matrices F_z commute with g_T. Then the transformed matrices will satisfy $(1)-(9)$. Lastly, I will need

Fact: Let $a = \alpha_0\,\tau^0 + i\,\vec{\alpha}\cdot\vec{\tau}$ and $b = \beta_0\,\tau^0 + i\,\vec{\beta}\cdot\vec{\tau}$ be $SU(2)$-matrices. a and b anticommute if and only if $\alpha_0 = \beta_0 = 0$ and $\vec{\alpha} \perp \vec{\beta}$. (Proposition 5 in appendix B).

We are ready to start. Unfortunately, there is no better way to do this than case distinction.

Case 1: $\eta_T = -1, \eta_P = 1, \eta_{PD} = 1$. Then

$$\forall z: \quad g_{Pz} = g_{Dz} = \tau^0 \tag{7.145}$$

up to the choice of gauge and global signs.

Why? By $(2): g_{Pb}^2 = \tau^0$. So $g_{Pb} = \pm\tau^0$. $(3): g_{Pc} = g_{Pa}^\dagger$. Insert this in (6) to get $g_{Da} = \pm g_{Pa}$. (4) and (5) are equivalent. (4) together with (2) and (6) gives $g_{Db}g_{Dc}g_{Da} = \pm\tau^0$. Thus, $\eta_x\eta_D = 1$ and (9) is automatically satisfied. Since $g_{Pb} = \pm\tau^0$, $\eta_{Pt} = 1$. This means that all g_{Pz} commute with g_T. Using $g_{Da} = \pm g_{Pa}$, we find that g_{Da} commutes with g_T. Thus, $\eta_{Dt} = 1$ is forced. This means that all g_{Dz} commute with g_T. $g_T = i\tau^3$. Hence, each g_{Pz} and g_{Dz} can only have τ^0- and τ^3-components. We go into the **sub-case 1.1.1:** $g_{Pb} = \tau^0$ and $g_{Da} = g_{Pa}$. Set $F_a = g_{Pa}^\dagger$, $F_c = \tau^0$ and $F_b = g_{Dc}$. F does not change g_T. In the new gauge $\forall z: g_{Pz} = g_{Dz} = \tau^0$. Next, consider **sub-case 1.1.2:** $g_{Pb} = \tau^0$ and $g_{Da} = -g_{Pa}$. The same transformation gives $\forall z: g_{Pz} = \tau^0$, $g_{Db} = g_{Dc} = \tau^0$ and $g_{Da} = -\tau^0$. Use a transformation of the form $F_b = -\tau^0$ and $F_a = F_c = \tau^0$ to switch the sign of g_{Db} and g_{Dc}. Continue with **sub-case 1.2.1:** $g_{Pz} = -\tau^0$ and $g_{Da} = g_{Pa}$. Set $F_c = \tau^0$, $F_a = -g_{Pa}$ and $F_b = g_{Dc}$ and $F_c = \tau^0$. In the gauge F, $\forall z: g_{Pz} = -\tau^0$, $g_{Db} = g_{Dc} = \tau^0$ and $g_{Da} = -\tau^0$. Again, switch the sign of g_{Db} and g_{Dc}. Finally, **sub-case 1.2.2:** $g_{Pb} = -\tau^0$ and $g_{Pa} = -g_{Da}$. The same transformation as in sub-case 1.2.1 will give $\forall z: g_{Pz} = -\tau^0$ and $\forall z: g_{Dz} = \tau^0$. □

Case 2: $\eta_T = -1, \eta_P = 1, \eta_{PD} = -1, \eta_{Dt} = 1$. Then

$$\forall z: \quad g_{Pz} = \tau^0, \qquad g_{Da} = i\tau^3, \qquad g_{Db} = \tau^0, \qquad g_{Dc} = -\tau^0 \tag{7.146}$$

up to gauge and global signs.

Why? (2) gives $g_{Pb}^2 = \pm\tau^0$. Thus, $\eta_{Pt} = 1$ and (8) is satisfied. From (3) we know that $g_{Pc} = g_{Pa}^\dagger$. Insert this into (6) to get $(g_{Da}g_{Pa}^\dagger)^2 = -\tau^0$. Hence, $\exists\, \vec{\alpha} \in S_{\mathbb{R}^3}$ such that $g_{Da}g_{Pa}^\dagger = i\vec{\alpha}\cdot\vec{\tau}$. I.e. $g_{Da} = (i\,\vec{\alpha}\cdot\vec{\tau})\, g_{Pa}$. Insert this into (7):

$$g_T^\dagger g_{Pa}^\dagger(-i\vec{\alpha}\cdot\vec{\tau})g_T(i\vec{\alpha}\cdot\vec{\tau})g_{Pa} = \tau^0 \qquad \Leftrightarrow \qquad (-i\vec{\alpha}\cdot\vec{\tau})g_T(i\vec{\alpha}\cdot\vec{\tau})g_{Pa}g_T^\dagger g_{Pa}^\dagger g_T = g_T \tag{7.147}$$

(8) : $g_{Pa}g_T^\dagger g_{Pa}^\dagger g_T = \tau^0$. Thus, $i\vec{\alpha}\cdot\vec{\tau}$ commutes with g_T. This can only hold if $\vec{\alpha}$ and $\hat{e}_z$ are linearly dependent. Thus, $g_{Da}g_{Pa}^\dagger = \pm i\tau^3$. Insert this into (4) to find that $g_{Da}g_{Db}g_{Dc} = \pm i\tau^3$. In consequence $\eta_x\eta_D = -1$ is forced and (9) is satisfied. **Sub-case 2.1.1:** $g_{Pb} = \tau^0$, $g_{Da}g_{Pa}^\dagger = i\tau^3$. Switch to a new gauge F. Set $F_a = g_{Pa}^\dagger$, $F_b = F_c = \tau^0$. In this gauge $g_{Pz} = \tau^0$ and $g_{Da} = i\tau^3$. (4) : $g_{Db} = -g_{Dc}^\dagger$. The transformed matrices still satisfy conditions (1) – (9). Transform a second time with $F_b = g_{Db}^\dagger$, $F_a = F_c = \tau^0$ to get (7.146). **Sub-case 2.1.2:** $g_{Pb} = \tau^0$, $g_{Da}g_{Pa}^\dagger = -i\tau^3$. Same two transformations as in sub-case 2.1.1 give

$$\forall z: \quad g_{Pz} = \tau^0, \qquad g_{Da} = -i\tau^3, \qquad g_{Db} = \tau^0, \qquad g_{Dc} = -\tau^0 \tag{7.148}$$

Transform additionally with $F_b = -\tau^0$ to get $g_{Da} = -i\tau^3, g_{Db} = -\tau^0$ and $g_{Dc} = \tau^0$. **Sub-case 2.2.1:** $g_{Pb} = -\tau^0$, $g_{Da}g_{Pa}^\dagger = i\tau^3$. Can be transformed to (7.146), except that G_P gets a global sign. **Sub-case 2.2.2:** $g_{Pb} = -\tau^0$, $g_{Da}g_{Pa}^\dagger = -i\tau^3$. Can be transformed to (7.146) with an additionally global sign for G_P, similar transformation as before. □

Case 3: $\eta_T = -1, \eta_P = 1, \eta_{PD} = -1, \eta_{Dt} = -1$. Then

$$\forall z: \quad g_{Pz} = \tau^0, \qquad \forall z: \quad g_{Dz} = i\tau^1 \tag{7.149}$$

up to global signs and gauge.

Why? $g_{Pb} = \pm\tau^0$. Thus, $\eta_{Pt} = 1$ and each g_{Pz} commutes with g_T. $\eta_{Dt} = -1$ implies that each g_{Dz} anticommutes with g_T. Insert $g_{Pc} = g_{Pa}^\dagger$ into (6) to find that $(g_{Da}g_{Pa}^\dagger)^2 = -\tau^0$. **Sub-case 3.1:** $g_{Pb} = \tau^0$. Since all g_{Pz} commute with g_T, we are allowed to transform as follows. Set $F_a = g_{Pa}^\dagger$ and $F_b = F_c = \tau^0$. In the new gauge $g_{Pa} = g_{Pc} = \tau^0$. Thus, $g_{Da}^2 = -\tau^0$ and $g_{Db}g_{Dc} = g_{Dc}g_{Db} = -\tau^0$. $\eta_x\eta_D = -1$ is forced and equation (9) is satisfied. We can use a gauge transformation to rotate g_{Da} to $i\tau^1$ without changing g_{Pz}. g_{Db} and g_{Dc} both anticommute with g_T. Thus, they only have τ^1- and τ^2-components. Say $g_{Db} = i\alpha_1\tau^1 + i\alpha_2\tau^2$, $\|\vec{\alpha}\| = 1$. Consider a gauge transformation of the form $F_a = F_c = \tau^0$. $F_b = \alpha_1\tau^0 - i\alpha_2\tau^3$. F will only change g_{Db} and g_{Dc}:

$$\tilde{g}_{Db} = F_a^\dagger g_{Db}F_b = (i\alpha_1\tau^1 + i\alpha_2\tau^2)(\alpha_1\tau^0 - i\alpha_2\tau^3) = i(\alpha_1^2 + \alpha_2^2)\tau^1 + i(\alpha_2\alpha_1 - \alpha_1\alpha_2)\tau^2 = i\tau^1 \tag{7.150}$$

using that $\|\vec{\alpha}\| = 1$. Since $g_{Db} = -g_{Dc}^\dagger$, it follows that $g_{Dc} = i\tau^1$. **Sub-case 3.2:** $g_{Pb} = -\tau^0$. Switch to a gauge in which $g_{Pa} = g_{Pc} = -\tau^0$. Again we find that $g_{Da}^2 = -\tau^0$ and $g_{Db}g_{Dc} = g_{Dc}g_{Db} = -\tau^0$. In the same way as in the sub-case before, transform each g_{Dz} to $i\tau^1$. □

Case 4: $\eta_T = -1, \eta_P = -1, \eta_{PD} = 1, \eta_{Pt} = 1, \eta_{Dt} = 1$. Then

$$g_{Pa} = \tau^0, \qquad g_{Pb} = i\tau^3, \qquad g_{Pc} = -\tau^0, \qquad g_{Da} = i\tau^3, \qquad g_{Db} = \tau^0, \qquad g_{Dc} = i\tau^3 \tag{7.151}$$

up to gauge and global signs.

Why? $\eta_P = -1$ implies that g_{Pb} has no τ^0-component. Since g_{Pb} commutes with g_T ($\eta_{Pt} = 1$) we have that $g_{Pb} = \pm i\tau^3$. **Sub-case 4.1:** $g_{Pb} = i\tau^3$. We know that g_{Pa} and g_{Pc} commute with g_T. We can switch to a gauge in which $g_{Pa} = \tau^0$. (3) : $g_{Pa} = -g_{Pc}^\dagger$. Thus, $g_{Pc} = -\tau^0$ in this gauge. From condition (6) we get that $g_{Da}^2 = -\tau^0$. This means that g_{Da} has no τ^0-component. From (4) and (5) we know that $g_{Dc}g_{Db} = i\tau^3$. g_{Da} commutes with g_T. Thus, $g_{Da} = \pm i\tau^3$. g_{Db} has no τ^1- and τ^2-components and commutes with g_T and g_{Pb}. Transform with $F_b = g_{Db}^\dagger$. F will only change g_{Db} and g_{Dc}. In the new gauge $g_{Db} = \tau^0$ and in consequence $g_{Dc} = i\tau^3$. If $g_{Da} = i\tau^3$, leave it like this. If $g_{Da} = -i\tau^3$ use $F_b = -\tau^0$ to switch the sign of g_{Db} and g_{Dc} too. $\eta_x\eta_D = 1$ and (9) is satisfied. **Sub-case 4.2:**

$g_{Pb} = -i\tau^3$. Switch to a gauge in which $g_{Pa} = -\tau^0$ and $g_{Pc} = \tau^0$. As before: $g_{Da}^2 = -\tau^0$ which implies that g_{Da} has no τ^0-component. g_{Da} commutes with g_T and in consequence $g_{Da} = \pm i\tau^3$. Continue as in sub-case 4.1. □

Case 5: $\eta_T = -1, \eta_P = -1, \eta_{PD} = 1, \eta_{Pt} = 1, \eta_{Dt} = -1$. Then

$$g_{Pa} = \tau^0, \qquad g_{Pb} = i\tau^3, \qquad g_{Pc} = -\tau^0, \qquad g_{Da} = i\tau^1, \qquad g_{Db} = i\tau^1, \qquad g_{Dc} = i\tau^2 \tag{7.152}$$

up to gauge and global signs.

Why? $g_{Pb}^2 = -\tau^0$ and g_{Pb} commutes with g_T. Thus, $g_{Pb} = \pm i\tau^3$. If $g_{Pb} = -i\tau^3$ transform to a gauge in which $g_{Pa} = \tau^0$ and $g_{Pc} = -\tau^0$. If $g_{Pb} = -i\tau^3$ transform to $g_{Pa} = -\tau^0$ and $g_{Pc} = \tau^0$. This is possible because g_{Pa} and g_{Pc} both commute with g_T. As in case 4 it follows that $g_{Da}^2 = -\tau^0$ and $g_{Dc}g_{Db} = i\tau^3$. Each g_{Dz} anticommutes with g_T. Use F_a and F_c to rotate g_{Da} to $i\tau^1$. Then transform a second time, in the same way as described in case 3 to get $g_{Db} = i\tau^1$. Automatically, $g_{Dc} = -i\tau^3 i\tau^1 = \tau^3\tau^1 = i\tau^2$. $\eta_x\eta_D = -1$ is forced and (9) is satisfied. □

Case 6: $\eta_T = -1, \eta_P = -1, \eta_{PD} = 1, \eta_{Pt} = -1, \eta_{Dt} = 1, \eta_x\eta_D = 1$. Then

$$g_{Pa} = i\tau^1, \qquad g_{Pb} = i\tau^1, \qquad g_{Pc} = i\tau^1, \qquad g_{Da} = \tau^0, \qquad g_{Db} = \tau^0, \qquad g_{Dc} = \tau^0 \tag{7.153}$$

up to gauge and global signs.

Why? Each g_{Dz} commutes with g_T. Transform twice to get $g_{Da} = g_{Db} = \tau^0$. Since $\eta_x\eta_D = 1$, we get from (9) that $g_{Dc}^2 = \pm\tau^0$. Use F_a to switch the sign of g_{Da} and g_{Db} if $g_{Dc} = -\tau^0$. Each matrix g_{Pz} anticommutes with g_T. $\exists R \in SU(2)$ such that $R^\dagger g_{Pb} R = i\tau^1$. Set $F_a = F_b = F_c = R$. In the new gauge $g_{Pb} = i\tau^1$ and all matrices g_{Dz} remain the same. From (5) we get $g_{Pc} = g_{Pb}$ and from (4) $g_{Pa} = -g_{Pc}^\dagger$. Thus, $g_{Pa} = g_{Pb} = g_{Pc} = i\tau^1$ and (6) is satisfied. □

Case 7: $\eta_T = -1, \eta_P = -1, \eta_{PD} = 1, \eta_{Pt} = -1, \eta_{Dt} = 1, \eta_D = -1$. Then

$$g_{Pa} = i\tau^2, \qquad g_{Pb} = i\tau^1, \qquad g_{Pc} = i\tau^2, \qquad g_{Da} = \tau^0, \qquad g_{Db} = \tau^0, \qquad g_{Dc} = i\tau^3 \tag{7.154}$$

up to gauge and global signs.

Why? Each matrix g_{Dz} commutes with g_T. Transform twice to get $g_{Da} = g_{Db} = \tau^0$. Since $\eta_D = -1$, $g_{Dc} = \pm i\tau^3$. If $g_{Dc} = -i\tau^3$ use F_a to switch the sign of g_{Da} and g_{Db}. Rotate g_{Pb} to $i\tau^1$ in the same way as in case 6. Equation (4) determines $g_{Pa} = i\tau^2$ and since $g_{Pa} = -g_{Pc}^\dagger$, $g_{Pc} = i\tau^2$. □

Case 8: $\eta_T = -1, \eta_P = -1, \eta_{PD} = 1, \eta_{Pt} = -1, \eta_{Dt} = -1$. Then

$$\forall z: \quad g_{Pz} = i\tau^1, \qquad g_{Da} = i\tau^2, \qquad g_{Db} = i\tau^1, \qquad g_{Dc} = -i\tau^1 \tag{7.155}$$

up to gauge and global signs.

Why? This is the most difficult case, so I'll present some more details. All g_{Dz} and g_{Pz} live in the τ^1-τ^2-plane since they all anticommute with g_T. Rotate each g_{Pz} to $i\tau^1$. Equation (4) then becomes $g_{Db}(i\tau^1)^\dagger g_{Dc} i\tau^1 = \tau^0$. g_{Dc} anticommutes with g_T. Thus, $g_{Dc} = i\gamma_1\tau^1 + i\gamma_2\tau^2$ for some $\gamma_1, \gamma_2 \in \mathbb{R}$. Let $g_{Db} = i\beta_1\tau^1 + i\beta_2\tau^2$. Note that

$$(i\tau^1)^\dagger(i\gamma_1\tau^1 + i\gamma_2\tau^2)i\tau^1 = i\gamma_1\tau^1 - i\gamma_2\tau^2 \tag{7.156}$$

since $i\tau^1$ corresponds to a rotation of angle π around the $\hat{e}_x$-axis. So (4) reads as

$$(i\beta_1\tau^1 + i\beta_2\tau^2)(i\gamma_1\tau^1 - i\gamma_2\tau^2) = \tau^0 \tag{7.157}$$

This can only hold if $\gamma_1 = -\beta_1$ and $\gamma_2 = \beta_2$. I will need proposition 7 as stated in the appendix. There exists $R \in SU(2)$ such that $R^\dagger g_{Db} = -i\tau^1$. R will rotate any $SU(2)$-matrix in the τ^1-τ^2-plane by the same angle. And there exists $L \in SU(2)$ such that $g_{Dc}L = +i\tau^1$. L will rotate any matrix in the τ^1-τ^2-plane by the same angle as R, but in the opposite direction. Figure (6) should explain what is going on. Set $F_a = R$ and $F_c = L$, $F_b = \tau^0$. The gauge transformation F will only change g_{Db} and g_{Dc}. This because both R and L act on g_{Pa}, g_{Pc} and g_{Da} and their effects cancel each other out. Finally, equation (6) gives $(g_{Da}g_{Pa}^\dagger)^2 = -\tau^0$. This only holds if $g_{Da}g_{Pa}^\dagger$ has no τ^0-component. Thus, $g_{Da} = \pm i\tau^2$. These two options differ only by a global sign for G_D. $\eta_x\eta_D = -1$ is forced and (9) is satisfied. □

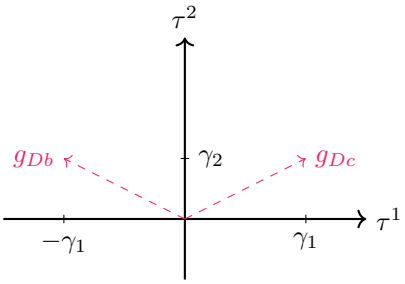

Figure 6: g_{Db} and g_{Dc} in case 8

Case 9: $\eta_T = -1, \eta_P = -1, \eta_{PD} = -1, \eta_{Pt} = -1$. Then

$$\forall z: \quad g_{Pz} = i\tau^1, \qquad \forall z: \quad g_{Dz} = i\tau^1 \tag{7.158}$$

up to gauge and global signs.

Why? Each g_{Pz} commutes with g_T. Rotate them all to $i\tau^1$. From equation (6) we get that $(g_{Da}g_{Pa}^\dagger)^2 = \tau^0$. This can only hold if $g_{Da}g_{Pa}^\dagger = \pm\tau^0$. Thus, $g_{Da} = \pm i\tau^1$. This forces $\eta_{Dt} = -1$ and in consequence all g_{Dz} anticommute with g_T. Let $g_{Db} = i\beta_1\tau^1 + i\beta_2\tau^2$ and $g_{Dc} = i\gamma_1\tau^1 + i\gamma_2\tau^2$. In the same way as in case 8 condition (4) gives

$$i\beta_1\tau^1 + i\beta_2\tau^2 = i\gamma_1\tau^1 - i\gamma_2\tau^2 \tag{7.159}$$

This implies $\gamma_1 = \beta_1$ and $\gamma_2 = -\beta_2$, since $\{\tau^0, \tau^1, \tau^2, \tau^3\}$ is a basis of $SU(2)$. Use F_a and F_c to rotate both g_{Db} and g_{Dc} to $i\tau^1$ without changing anything else. This works in the same way as described in case 8. $g_{Da} = \pm i\tau^1$ and the two options only differ by a global sign for G_D. One can use F_b to switch the sign of g_{Db} and g_{Dc} in the case $g_{Da} = -i\tau^1$. $\eta_x\eta_D = -1$ is forced and (9) is satisfied. □

Case 10: $\eta_T = -1, \eta_P = -1, \eta_{PD} = -1, \eta_{Pt} = 1$. Then

$$g_{Pa} = \tau^0, \qquad g_{Pb} = i\tau^3, \qquad g_{Pc} = -\tau^0, \qquad g_{Da} = \tau^0, \qquad g_{Db} = -i\tau^3, \qquad g_{Dc} = \tau^0 \tag{7.160}$$

up to gauge and global signs.

Why? g_{Pb} commutes with g_T. This means it has no τ^1- and no τ^2-component. Since $g_{Pb}^2 = -\tau^0$, $g_{Pb} = \pm i\tau^3$. If $g_{Pb} = i\tau^3$ then switch to a gauge in which $g_{Pa} = \tau^0$ and $g_{Pc} = -\tau^0$. Else, transform to $g_{Pa} = -\tau^0$ and $g_{Pc} = \tau^0$. In the new gauge it follows from (6) that $g_{Da}^2 = \tau^0$. Thus, $g_{Da} = \pm\tau^0$ and $\eta_{Dt} = 1$ is forced. Each matrix g_{Dz} commutes with g_T. Transform with $F_c = F_a = g_{Dc}^\dagger$. This will only change g_{Db} and g_{Dc}. In the new gauge $g_{Dc} = \tau^0$. From (4) we get $g_{Db}i\tau^3 = \tau^0$. Thus, $g_{Db} = -i\tau^3$. $g_{Da} = \pm\tau^0$. The two options differ only by a global sign for G_D. $\eta_x\eta_D = -1$ is forced and (9) is satisfied. □

These were all the possible cases with $\eta_T = -1$. It remains to consider PSGs with $\eta_T = 1$. In this case each $g_{Tz}^2 = \tau^0$. This can only hold if each $g_{Tz} = \pm\tau^0$ (prop. 3 in appendix B). Note that condition (7) leads to a contradiction, if some of the matrices g_{Tz} are τ^0 and some are $-\tau^0$. Thus, either $\forall z: g_{Tz} = \tau^0$ or $\forall z: g_{Tz} = -\tau^0$. Both options yield the same conditions (2) − (9) for g_{Dz} and g_{Pz}. Furthermore, they only differ by a global sign for G_T. Since $IGG = \mathbb{Z}_2$ and since $PSG = SG \cdot IGG$, they will both generate the same PSGs. Thus, without loss of generality we may assume that $\forall z: g_{Tz} = \tau^0 =: g_T$. I will continue in this gauge.

Case 11: $\eta_T = 1, \eta_P = 1, \eta_{PD} = 1$. Then

$$\forall z: \quad g_{Pz} = g_{Dz} = \tau^0 \tag{7.161}$$

up to gauge and global signs.

Proof: $g_{Pb}^2 = \tau^0$ implies that $g_{Pb} = \pm\tau^0$. Equation (3) gives $g_{Pc} = g_{Pa}^\dagger$. Insert this in (6) to get $(g_{Da}g_{Pa}^\dagger)^2 = \tau^0$. This can only be true if $g_{Da} = \pm g_{Pa}$. Thus, equation (5) and (4) read as $g_{Da}g_{Db}g_{Dc} = \pm\tau^0$. So $\eta_x\eta_D = 1$ is forced and (9) is satisfied. (7) and (8) are automatically satisfied, $\eta_{Dt} = \eta_{Pt} = 1$ is forced. If $g_{Pb} = \tau^0$ and $g_{Da} = g_{Pa}$, choose $F_c = \tau^0$, $F_a = g_{Pa}^\dagger$ and $F_b = g_{Dc}$. The only critical part

is the transformation of g_{Pc} and g_{Db}. $F_a^\dagger g_{Pc} F_c = (F_c^\dagger g_{Pa} F_a)^\dagger = \tau^0$, since $g_{Pc} = g_{Pa}^\dagger$. And $F_a^\dagger g_{Db} F_b = g_{Da} g_{Db} g_{Dc} = \tau^0$ because of condition (4). Thus, in this gauge $\forall z: g_{Pz} = g_{Dz} = \tau^0$. If $g_{Pb} = -\tau^0$ and $g_{Da} = g_{Pa}$, choose $F_c = -\tau^0$, $F_a = g_{Pa}^\dagger$ and $F_b = g_{Dc}$. In this gauge $\forall z: g_{Pz} = g_{Dz} = -\tau^0$. If $g_{Pb} = \tau^0$ and $g_{Da} = -g_{Pa}$, choose $F_c = -\tau^0$, $F_a = -g_{Pa}^\dagger$ and $F_b = g_{Dc}$. Then $\forall z: g_{Pz} = \tau^0$ and $\forall z: g_{Dz} = -\tau^0$. Finally, if $g_{Pb} = -\tau^0$ and $g_{Da} = -g_{Pa}$, choose $F_c = -\tau^0$, $F_a = g_{Pa}^\dagger$ and $F_b = -g_{Dc}$. In this gauge $\forall z: g_{Pz} = -\tau^0$ and $\forall z: g_{Dz} = \tau^0$. □

Case 12: $\eta_T = 1, \eta_P = 1, \eta_{PD} = -1$. Then

$$\forall z: g_{Pz} = \tau^0, \qquad g_{Da} = i\tau^3, \qquad g_{Db} = -\tau^0 \qquad \text{and} \qquad g_{Dc} = \tau^0 \tag{7.162}$$

up to gauge and global signs.

Proof: $\eta_{Pt} = \eta_{Dt} = 1$ is forced and equations (7) and (8) are satisfied. (2) gives $g_{Pb} = \pm\tau^0$. From (3) we know that $g_{Pc} = g_{Pa}^\dagger$. Insert this in (6) to get $(g_{Da} g_{Pa}^\dagger)^2 = -\tau^0$. This can only hold if $g_{Da} g_{Pa}^\dagger = i\,\vec{\alpha}\cdot\vec{\tau}$ for some $\vec{\alpha} \in S_{\mathbb{R}^3}$. Thus, $g_{Pa} = (-i\vec{\alpha}\cdot\vec{\tau})\, g_{Da}$. Insert this in (4) or (5) to get $g_{Da} g_{Db} g_{Dc} = \pm i\vec{\alpha}\cdot\vec{\tau}$, where the minus sign holds in the case $g_{Pb} = \tau^0$ and the plus sign in the case $g_{Pb} = -\tau^0$. In consequence, $\eta_x \eta_D = -1$ is forced and equation (9) is satisfied. There always exists a matrix $R \in SU(2)$ such that $R^\dagger i\vec{\alpha}\cdot\vec{\tau} R = i\tau^3$. I will need R later. If $g_{Pb} = +\tau^0$, set $F_c = R$, $F_a = g_{Pa}^\dagger R$ and $F_b = g_{Dc} R$. Transforming with F yields the proposed result. In the case $g_{Pb} = -\tau^0$, set $F_c = -R$, $F_a = g_{Pa}^\dagger R$ and $F_b = g_{Dc} R$. □

Case 13: $\eta_T = 1, \eta_P = -1,\ \eta_{PD} = 1, \eta_x \eta_D = 1$. Then

$$\forall z: g_{Pz} = i\tau^3, \qquad \forall z: g_{Dz} = \tau^0 \tag{7.163}$$

up to gauge and global signs.

Proof: $\eta_{Dt} = \eta_{Pt} = 1$ is forced, (7) and (8) are satisfied. $g_{Pb}^2 = -\tau^0$. Thus, $g_{Pb} = i\,\vec{\alpha}\cdot\vec{\tau}$ for some $\vec{\alpha} \in S_{\mathbb{R}^3}$. Use F_a and F_c to transform g_{Db} and g_{Dc} to τ^0. Use F_b to transform g_{Pb} to $i\tau^3$. (4) gives that in this gauge $g_{Pa} = i\tau^3$. (3) tells that $g_{Pc} = -g_{Pa}^\dagger$. Thus, $g_{Pc} = i\tau^3$. (9) : $g_{Da}^2 = \tau^0$. Thus, $g_{Da} = \pm\tau^0$. In the case $g_{Da} = -\tau^0$, use $F_b = -\tau^0$ to switch the sign of g_{Db} and g_{Dc} without changing g_{Pz}. (6) is satisfied. □

Case 14: $\eta_T = 1, \eta_P = -1, \eta_{PD} = 1, \eta_x \eta_D = -1$. Then

$$\forall z: g_{Pz} = i\tau^3, \qquad g_{Da} = i\tau^1, \qquad g_{Db} = \tau^0, \qquad g_{Dc} = \tau^0 \tag{7.164}$$

up to gauge and global signs.

Proof: Do exactly the same steps as in case 13. After the transformations, (9) becomes $g_{Da}^2 = -\tau^0$. Thus, $g_{Da} = i\,\vec{\alpha}\cdot\vec{\tau}$ for some $\vec{\alpha} \in S_{\mathbb{R}^3}$. (6) reads as $(g_{Da} i\tau^3)^2 = -\tau^0$. This can only hold if $g_{Da} i\tau^3$ has no τ^0-component. Consequently, g_{Da} can have no τ^3-component. It must live in the τ^1-τ^2-plane. Thus, it is possible to rotate g_{Da} without changing the other matrices. Choose a gauge in which $g_{Da} = i\tau^1$. □

Case 15: $\eta_T = 1, \eta_P = -1, \eta_{PD} = -1$. Then

$$\forall z: g_{Pz} = i\tau^3, \qquad g_{Da} = i\tau^3, \qquad g_{Db} = \tau^0, \qquad g_{Dc} = -\tau^0 \tag{7.165}$$

up to gauge and global signs.

Proof: $\eta_{Dt} = \eta_{Pt} = 1$ is forced and (7) and (8) are satisfied. (2) : $g_{Pb}^2 = -\tau^0$. Thus, $g_{Pb} = i\,\vec{\alpha}\cdot\vec{\tau}$ for some $\vec{\alpha} \in S_{\mathbb{R}^3}$. It follows from (3) that $g_{Pa} = -g_{Pc}^\dagger$. Insert this into (6) to get $(g_{Da} g_{Pa}^\dagger)^2 = \tau^0$. This implies that $g_{Da} = \pm g_{Pa}$. Insert this into (5) : $g_{Dc} g_{Da} g_{Db} = \pm i\,\vec{\alpha}\cdot\vec{\tau}$. Thus, $\eta_x \eta_D = -1$ is forced and (9) is satisfied. Use F_b to rotate g_{Pb} to $i\tau^3$. Use F_c and F_a to transform g_{Db} and g_{Dc} to τ^0 without changing $g_{Pb} = i\tau^3$. It follows from (5) that in this gauge $g_{Pc} = -i\tau^3$. Thus, because of (4), $g_{Pa} = -g_{Pc}^\dagger = -i\tau^3$. Recall that (6) implies $g_{Da} = \pm g_{Pa}$. In the case $g_{Da} = -g_{Pa}$ you can use $F_b = -\tau^0$ to switch also the sign of g_{Db} and g_{Dc} without changing g_{Pz}.Thus, the two options only differ by a global sign for G_D. Lastly, transform with $F_c = -\tau^0$ to switch the signs of g_{Pa}, g_{Pc}, g_{Da} and g_{Dc}. □

7.4 Appendix D: Classification of Cr_5^+-ion lattice based $\mathbb{Z}_2$ spin liquids

Again, this chapter does not contain any physical motivations or explanations. I will only show the calculation which leads to the classification of $\mathbb{Z}_2$ PSGs on the distorted kagome lattice shown in chapter 5. Everything will work pretty much the same as for the kagome lattice.

7.4.1 Algebraic conditions

The lattice sites are labelled by $\mathbb{Z} \times \mathbb{Z} \times \{a, b, c, e, f, g\}$. Figure 3 in chapter 4 shows which label belongs to which atom. I will need to work with T_x, T_y and R in lattice coordinates.

$$\begin{aligned} T_x &: \text{lattice} \to \text{lattice}, & (x, y, z) &\mapsto (x-1, y, z) \\ T_y &: \text{lattice} \to \text{lattice}, & (x, y, z) &\mapsto (x, y-1, z) \\ R &: \text{lattice} \to \text{lattice}, & (x, y, z) &\mapsto (y, -(x+y+1),\, z-1) \end{aligned} \tag{7.166}$$

In lattice coordinates, R corresponds to D^2 from the kagome lattice symmetry group. You can use this to check the above and to check the following commutation relations. The symmetry group satisfies

$$\begin{aligned} T_xT_y &= T_yT_x & RT_x &= T_y^{-1}R & RT_y &= T_y^{-1}T_xR & R^3 &= id \\ T_xT &= TT_x & T_yT &= TT_y & TR &= RT & T^2 &= id \end{aligned} \tag{7.167}$$

As before, they can be translated into conditions, which any projective symmetry group with Cr_5^+ - lattice symmetry group must satisfy.

$$T_xT_yT_x^{-1}T_y^{-1} = id \quad \Rightarrow \quad (G_xT_xG_yT_yT_x^{-1}G_x^{-1}T_y^{-1}G_y^{-1}, id) \in IGG \tag{B1}$$

$$RT_xR^{-1}T_y = id \quad \Rightarrow \quad (G_RRG_xT_xR^{-1}G_R^{-1}G_yT_y, id) \in IGG \tag{B2}$$

$$RT_yR^{-1}T_x^{-1}T_y = id \quad \Rightarrow \quad (G_RRG_yT_yR^{-1}G_R^{-1}T_x^{-1}G_x^{-1}G_yT_y, id) \in IGG \tag{B3}$$

$$R^3 = id \quad \Rightarrow \quad (G_RRG_RRG_RR, id) \in IGG \tag{B4}$$

$$T_xTT_x^{-1}T^{-1} = id \quad \Rightarrow \quad (G_xT_xG_TTT_x^{-1}G_x^{-1}T^{-1}G_T^{-1}, id) \in IGG \tag{B5}$$

$$T_yTT_y^{-1}T^{-1} = id \quad \Rightarrow \quad (G_yT_yG_TTT_y^{-1}G_y^{-1}T^{-1}G_T^{-1}, id) \in IGG \tag{B6}$$

$$RTR^{-1}T^{-1} = id \quad \Rightarrow \quad (G_RRG_TTR^{-1}G_R^{-1}T^{-1}G_T^{-1}, id) \in IGG \tag{B7}$$

$$T^2 = id \quad \Rightarrow \quad (G_TTG_TT, id) \in IGG \tag{B8}$$

I only determine the PSGs with invariant gauge group $\mathbb{Z}_2$. The algebraic conditions translate into the following conditions for the $SU(2)$ matrices:

$$\forall i \in \text{lattice}: \quad G_y(i)^\dagger G_x(i+\hat{y})^\dagger G_y(i+\hat{x})G_x(i) = \eta_x\tau^0 \tag{B1}$$

$$\forall i \in \text{lattice}: \quad G_y(i-\hat{y})G_R(i-\hat{y})^\dagger G_x(R^{-1}(i))G_R(i) = \eta_{Rx}\tau^0 \tag{B2}$$

$$\forall i \in \text{lattice}: \quad G_y(i-\hat{y})G_x(i-\hat{y})^\dagger G_R(i-\hat{y}+\hat{x})^\dagger G_y(R^{-1}(i))G_R(i) = \eta_{Ry}\tau^0 \tag{B3}$$

$$\forall i \in \text{lattice}: \quad G_R(R(i))G_R(R^2(i))G_R(i) = \eta_R\tau^0 \tag{B4}$$

$$\forall i \in \text{lattice}: \quad G_T(i)^\dagger G_x(i)^\dagger G_T(i+\hat{x})G_x(i) = \eta_{xt}\tau^0 \tag{B5}$$

$$\forall i \in \text{lattice}: \quad G_T(i)^\dagger G_y(i)^\dagger G_T(i+\hat{y})G_y(i) = \eta_{yt}\tau^0 \tag{B6}$$

$$\forall i \in \text{lattice}: \quad G_T(i)^\dagger G_R(i)^\dagger G_T(R^{-1}(i))G_R(i) = \eta_{Rt}\tau^0 \tag{B7}$$

$$\forall i \in \text{lattice}: \quad G_T(i)G_T(i) = \eta_T\tau^0 \tag{B8}$$

Each η can take the value $+1$ and -1. This is because $\mathbb{Z}_2 = \{(id, id), (-id, id)\}$.

7.4.2 Translation symmetries and time reversal symmetry

The implementation of the translation symmetries T_x and T_y and the time reversal symmetry T works in exactly the same way as for the kagome lattice. (B1), (B5), (B6) and (B8) correspond directly to

(A1), (A10), (A11) and (A9). There always exists a gauge in which

$$G_x(x,y,z) = \eta_x^y \tau^0, \qquad G_y(x,y,z) = \tau^0, \qquad G_T(x,y,z) = \eta_{xt}^x \eta_{yt}^y g_{Tz} \tag{7.168}$$

where $g_{Tz} = \pm\tau^0$ if $\eta_T = 1$ and $g_{Tz} = i\tau^3$ for each z if $\eta_T = -1$. I will continue in this gauge.

7.4.3 Rotation symmetry

Results: There is a gauge in which

$$G_R(x,y,z) = \eta_x^{\frac{1}{2}(x^2-x)+xy} g_{Rz}, \qquad G_T(x,y,z) = g_{Tz} \tag{7.169}$$

Furthermore, g_{Rz} have to satisfy

$$\forall z: \quad g_{Tz}^\dagger g_{Rz}^\dagger g_{TR^{-1}(z)} g_{Rz} = \eta_{Rt}\tau^0 \qquad \text{and} \qquad \forall z: \quad g_{RR(z)}\, g_{RR^2(z)}\, g_{Rz} = \eta_R \eta_x\, \tau^0 \tag{7.170}$$

Why? It is helpful to write down R^{-1} explicitly.

$$R^{-1}: \quad \text{lattice} \to \text{lattice}, \qquad (x,y,z) \mapsto (-(x+y+1),\, x,\, z+1) \tag{7.171}$$

Insert (7.168) into (B2) and (B3) to get

$$G_R(x,y,z) = \eta_x^x \eta_{Rx}\, G_R(x,y-1,z), \qquad G_R(x,y,z) = \eta_x^{y-1} \eta_{Ry}\, G_R(x+1,y-1,z) \tag{7.172}$$

Shift indices to find the recursive conditions

$$G_R(x+1,y,z) = \eta_x^{x+y} \eta_{Rx} \eta_{Ry}\, G_R(x,y,z) \tag{7.173}$$

$$G_R(x,y+1,z) = \eta_x^x \eta_{Rx}\, G_R(x,y,z) \tag{7.174}$$

It is clear that the choice of $G_R(0,0,z) \in SU(2)$ for each z determines $G_R(i)$ for all $i \in$ lattice. A good ansatz to solve the above system is

$$G_R(x,y,z) = \eta_x^{f(x,y)} \eta_{Rx}^{g(x,y)} \eta_{Ry}^{h(x,y)}\, g_{Rz} \tag{7.175}$$

with $g_{Rz} \in SU(2)$. f, g and h are $\mathbb{Z}/2\mathbb{Z}$ - valued functions. Conditions (7.173) and (7.174) then become

$$f(x+1,y) = x + y + f(x,y) \qquad f(x,y+1) = x + f(x,y) \tag{7.176}$$

$$g(x+1,y) = 1 + g(x,y) \qquad g(x,y+1) = 1 + g(x,y) \tag{7.177}$$

$$h(x+1,y) = 1 + h(x,y) \qquad h(x,y+1) = h(x,y) \tag{7.178}$$

I find the following solution

$$f(x,y) = \frac{1}{2}\, x(x-1) + xy, \qquad g(x,y) = x + y, \qquad h(x,y) = x \tag{7.179}$$

It is easy to check that they satisfy the requirements. Arithmetic in the exponents is modulo 2, since the ηs only take the values ± 1. Consider a gauge transformation W of the form

$$W(x,y,z) = \eta_{Rx}^y \eta_{Ry}^{x+y}\, \tau^0 \tag{7.180}$$

W will not change G_T and G_x and G_y only by global signs.

$$G_R(i) \xrightarrow{W} W(R^{-1}(i))^\dagger G_R(i) W(i) \tag{7.181}$$

Thus, in the new gauge W:

$$G_R(x,y,z) = \eta_{Rx}^x \eta_{Ry}^{-(x+y+1)+x} \tau^0\, \eta_x^{\frac{1}{2}(x^2-x)+xy} \eta_{Rx}^{x+y} \eta_{Ry}^x g_{Rz}\, \eta_{Rx}^y \eta_{Ry}^{x+y}\, \tau^0 = \eta_x^{\frac{1}{2}(x^2-x)+xy} \eta_{Ry} g_{Rz} \tag{7.182}$$

Since g_{Rz} are not chosen yet, let them absorb η_{Ry}. I will continue in this gauge. Insert (7.182) into algebraic condition (B7):

$$\eta_{xt}^{x}\eta_{yt}^{y}g_{Tz}^{\dagger}\,\eta_{x}^{f(x,y)}\,g_{Rz}^{\dagger}\eta_{xt}^{-(x+y+1)}\eta_{yt}^{x}g_{TR^{-1}(z)}\,\eta_{x}^{f(x,y)}\,g_{Rz}=\eta_{Rt}\tau^{0} \tag{7.183}$$

After collecting exponents (modulo 2) this reads

$$\eta_{xt}^{y+1}\eta_{yt}^{x+y}g_{Tz}^{\dagger}g_{Rz}^{\dagger}g_{TR^{-1}(z)}g_{Rz}=\eta_{Rt}\tau^{0} \tag{7.184}$$

The right hand side is constant in x, so the left hand side has to be too. This can only hold if $\eta_{xt}=1$. The left hand side is constant as a function of y and $\eta_{xt}=1$. Thus, $\eta_{yt}=1$. Furthermore, it follows that

$$\forall z:\quad g_{Tz}^{\dagger}g_{Rz}^{\dagger}g_{TR^{-1}(z)}g_{Rz}=\eta_{Rt}\tau^{0} \tag{7.185}$$

it remains to consider algebraic condition (B4). After collecting exponents modulo 2 one finds that (B4) gives no new constraint for η_x, η_{Rx} and η_{Ry}. But (B4) gives a new constraint on g_{Rz}:

$$\forall z:\qquad g_{RR(z)}\,g_{RR^{2}(z)}\,g_{Rz}=\eta_{R}\eta_{x}\,\tau^{0} \tag{7.186}$$

as claimed. □

7.4.4 Gauge inequivalent choices in the zeroth unit cell

The conditions on g_{Rz} and g_{Tz} are

$$(1)\quad g_{Tz}^{\dagger}g_{Rz}^{\dagger}g_{TR^{-1}(z)}g_{Rz}=\eta_{Rt}\tau^{0}\qquad(2)\quad g_{RR(z)}\,g_{RR^{2}(z)}\,g_{Rz}=\eta_{R}\eta_{x}\,\tau^{0}\qquad(3)\quad g_{Tz}^{2}=\eta_{T}\tau^{0} \tag{7.187}$$

Consider a gauge transformation of the form $F(x,y,z)=F_z\in SU(2)$. F does not change G_x and G_y. If each F_z commutes with g_T, then F doesn't change G_T. F acts on G_R like this:

$$G_R(i)\xrightarrow{F}F(R^{-1}(i))^{\dagger}G_R(i)F(i) \tag{7.188}$$

Which is the same as

$$\begin{aligned}
&g_{Ra}\xrightarrow{F}F_b^{\dagger}g_{Ra}F_a && g_{Rb}\xrightarrow{F}F_c^{\dagger}g_{Rb}F_b && g_{Rc}\xrightarrow{F}F_a^{\dagger}g_{Rc}F_c\\
&g_{Re}\xrightarrow{F}F_f^{\dagger}g_{Re}F_e && g_{Rf}\xrightarrow{F}F_g^{\dagger}g_{Rf}F_f && g_{Rg}\xrightarrow{F}F_e^{\dagger}g_{Rg}F_g
\end{aligned} \tag{7.189}$$

If the matrices g_T, g_{Rz} satisfied (1) and (2) before the transformation F, then so will the transformed matrices. To see this, simply plug the transformed matrices into $(1)-(3)$. The transformation matrices will cancel each other out. I will proceed in the following scheme: I will set some of the ηs to $+1$ or -1 and then show that **if** we have a projective symmetry group which satisfies conditions $(1)-(3)$ for the given combination of ηs, **then** we can always find a new gauge in which the projective symmetry group takes some simple form. After I have done this for all possible combinations of $\eta_{Rt}, \eta_R\eta_x, \eta_T=\pm1$, I have found all possible projective symmetry groups up to the choice of gauge.

Start with the case $\eta_T=-1$. $g_{Tz}^2=-\tau^0$. Thus, each g_{Tz} can not have a τ^0-component (prop. 3, appendix B). Switch to a gauge in which $g_{Tz}=g_T=i\tau^3$ for all z (prop. 2, appendix B). I will continue in this gauge.

Case 1: $\eta_T=-1, \eta_{Rt}=-1$ leads to a contradiction.

Why? The main argument of this proof comes from prop. 5, appendix B. **Fact**: Suppose $a=\alpha_0\,\tau^0+i\,\vec{\alpha}\cdot\vec{\tau}$ and $b=\beta_0\,\tau^0+i\,\vec{\beta}\cdot\vec{\tau}$ are $SU(2)$ matrices. a and b anticommute if and only if $\alpha_0=\beta_0=0$ and $\vec{\alpha}\perp\vec{\beta}$.

$\eta_{Rt}=-1$ implies that each matrix g_{Rz} anticommutes with $g_T=i\tau^3$. This can only hold if they have no τ^0- and no τ^3-component. Say, $g_{Ra}=i\vec{\alpha}\cdot\vec{\tau}$ and $g_{Rc}=i\vec{\beta}\cdot\vec{\tau}$ with $\alpha_3=\beta_3=0$. Condition (2) gives $g_{Rb}=\eta_R\eta_x\,g_{Rc}^{\dagger}g_{Ra}^{\dagger}$. But

$$\eta_R\eta_x\,g_{Rc}^{\dagger}g_{Ra}^{\dagger}=\eta_R\eta_x\,(-i\vec{\beta}\cdot\vec{\tau})(-i\vec{\alpha}\cdot\vec{\tau})=-\eta_R\eta_x\,\left(\left(\vec{\alpha}\cdot\vec{\beta}\right)\,\tau^0+i\,\left(\vec{\alpha}\times\vec{\beta}\right)\cdot\vec{\tau}\right) \tag{7.190}$$

Since $\vec{\alpha}$ and $\vec{\beta}$ both live in the τ^1-τ^2-plane, $\vec{\alpha} \times \vec{\beta}$ will certainly point in τ^3-direction. Thus, g_{Rb} has only τ^0- and τ^3-components. This contradicts that g_{Rb} anticommutes with g_T. □

Case 2: $\eta_T = -1, \eta_{Rt} = 1, \eta_R \eta_x = 1$. Then $\forall z : g_{Rz} = \tau^0$up to gauge. **Why?** All matrices g_{Rz} commute with g_T. Transform with $F_a = g_{Ra}^\dagger$, $F_c = g_{Rb}$ $F_e = g_{Re}^\dagger$ and $F_g = g_{Rf}$. After the transformation $g_{Ra} = g_{Rb} = g_{Re} = g_{Rf} = \tau^0$. Condition (2) forces $g_{Rc} = \tau^0$ and $g_{Rg} = \tau^0$. □

Case 3: $\eta_T = -1, \eta_{Rt} = 1, \eta_R \eta_x = -1$. Then $\forall z : g_{Rz} = -\tau^0$ up to gauge. **Why?** All matrices g_{Rz} commute with g_T. Transform with $F_a = -g_{Ra}^\dagger$, $F_b = \tau^0$, $F_c = -g_{Rb}$, $F_e = -g_{Re}^\dagger$, $F_f = \tau^0$ and $F_g = -g_{Rf}$. Then $g_{Rz} = -\tau^0$ for $z = a, b, e, f$. Condition (2) forces $g_{Rc} = g_{Rg} = -\tau^0$. □

Note that case 3 yields the same projective symmetry group as case 2. This is because whenever $(G_S, S) \in PSG$ for any symmetry S then also $(-G_S, S) \in PSG$. ($PSG = IGG \cdot SG$ and $IGG = \mathbb{Z}_2$).

Continue with $\eta_T = 1$. $g_{Tz}^2 = \tau^0$ for each z. This can only hold if $g_{Tz} = \pm\tau^0$. Condition (1) can never be satisfied, if not all matrices g_{Tz} have the same sign. Thus, either $\forall z : g_{Tz} = \tau^0$ or $\forall z : g_{Tz} = -\tau^0$. Those two options differ only by a global sign for G_T, which makes no difference for the resulting PSG. Without loss of generality assume $g_{Tz} = \tau^0 = g_T$ for all z.

Case 4: $\eta_T = 1, \eta_R \eta_x = 1$. Then $\forall z : g_{Rz} = \tau^0$. **Why?** $\eta_{R_t} = 1$ is forced and condition (1) is satisfied. Transform in the same way as in case 2. □

Case 5: $\eta_T = 1, \eta_R \eta_x = -1$. Then $\forall z : g_{Rz} = -\tau^0$ up to gauge. **Why?** Parallel to case 3. $\eta_{R_t} = 1$ is forced and condition (1) is satisfied. Transform in the same way as in case 3. □

Note that case 5 yields the same PSG as case 4, since the result differs only by a global sign for G_R.

To summarise: The final form of the PSGs is

$$G_T(x,y,z) = g_{Tz}, \qquad G_y(x,y,z) = \tau^0,$$
$$G_x(x,y,z) = \eta_x^y \, \tau^0, \qquad G_R(x,y,z) = \eta_x^{\frac{1}{2}\, x(x-1)+xy} \, g_{Rz} \tag{7.191}$$

The gauge inequivalent choices for the matrices g_{Rz} and g_{Tz} are summarised in table 3.

g_{Tz}	g_{Ra}	g_{Rb}	g_{Rc}	g_{Re}	g_{Rf}	g_{Rg}	$\eta_T, \eta_{Rt}, \eta_R\eta_x$	Case
τ^0	τ^0	τ^0	τ^0	τ^0	τ^0	τ^0	$+,+,+$	4/5
$i\tau^3$	τ^0	τ^0	τ^0	τ^0	τ^0	τ^0	$-,+,+$	2/3

Table 3: gauge-inequivalent choices for g_{Rz} up to global signs

There are $2 \times 2 = 4$ different $\mathbb{Z}_2$ PSGs on the distorted kagome lattice with time reversal.

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Berlin, January 3, 2025 .....