A fractionalised "$Z_2$" classical Heisenberg spin liquid

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Quantum spin systems are by now known to exhibit a large number of different classes of spin liquid phases. By contrast, for classical Heisenberg models, only one kind of fractionalised spin liquid phase, the so-called Coulomb or $U(1)$ spin liquid, has until recently been identified: this exhibits algebraic spin correlations and impurity moments, ‘orphan spins’, whose size is a fraction of that of the underlying microscopic degrees of freedom. Here, we present two Heisenberg models exhibiting fractionalisation in combination with exponentially decaying correlations. These can be thought of as a classical continuous spin version of a $Z_2$ spin liquid. Our work suggests a systematic search and classification of classical spin liquids as a worthwhile endeavour.

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Fractionalisation is one of the several unusual properties generally observed in systems evading low-temperature conventional symmetry breaking ordered states in favor of unconventional topological orders. On account of such exotic behavior, much attention has been devoted to the identification of systems exhibiting such new topological physics. Frustrated magnets [1–3] have played a prominent role, where several spin liquids (SL) [4, 5] starting in the late 90s [6] were identified [7–9].

While by now a multitude of quantum SL have been discovered [10] and classified [11], the situation with classical Heisenberg SL is comparatively much sparser. The first Heisenberg spin liquid to be identified unambiguously, the antiferromagnet on the pyrochlore lattice [7, 12] is a $U(1)$ spin liquid exhibiting pinch-points in its structure factor indicating algebraically decaying correlations [7, 12–15], as well as fractionalisation of its microscopic degrees of freedom: disorder in the form of dilution creates new, weakly-interacting, magnetic degrees of freedom which possess a half of the microscopic magnetic moments of the Heisenberg model [16, 17].

Such fractionalisation is perhaps the cleanest signature of spin-liquidity in such a classical setting, as definitions in terms of topological field theory are frustrated by the bulk gapless excitations due to the continuous classical nature of the Heisenberg spins.

Given the by now overwhelming variety of known quantum spin liquids (for an example, see Ref. 18), it may therefore come as a surprise that no corresponding richness appears to exist for classical Heisenberg magnets: the $U(1)$ case is the only one studied in detail. It turns up in many settings, such as the checkerboard and pyrochlore lattices (for $n \neq 2$ component spins) [7, 12], the kagome (for $n > 3$ component spins) [19, 20], or the SCGO ‘pyrochlore slab’ [21].

Here we ask the question whether this absence of evidence of other types of spin liquid is evidence of absence. The answer is that there is indeed more diversity than has been so far recognised: we identify a new SL class which does not exhibit algebraic correlations in the $T \to 0$ limit, and nonetheless displays spin fractionalisation.

In the following, we consider two Heisenberg models, defined on variants of the $(3, 4, 6, 4)$—Archimedean lattice (known as the ruby lattice; for a nice introduction to Archimedean lattices see Ref. 22) and of the kagome lattice, Fig. 1. When viewed as corner-sharing networks of clusters, these lattices do not allow the conventional mapping from spin to flux variables to obtain an emergent $U(1)$ gauge field [15]. We provide the solution of the corresponding classical $O(n)$ models in the large-$n$ limit and show numerically that this captures well the behaviour of the Heisenberg $n = 3$ model. These solutions cleanly exhibit the features mentioned above, including the exponential decay of spin correlations alongside the appearance of fractional moments in the presence of dilution with non-magnetic impurities. We close with a discussion of the broader picture, in particular exhibiting the connection of this new SL to a known class of quantum $Z_2$ SL.

Model.— Practically all Heisenberg models with a SL phase are defined on a lattice consisting of clusters, such
that all pairwise interactions within a cluster $\alpha$ have equal strength [15]. This implies

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j = \frac{J}{2} \sum_{\alpha} (\vec{S}_\alpha)^2 + \text{const.}, \quad (1)$$

with $\vec{S}_\alpha = \sum_{i \in \alpha} \vec{S}_i$, the total spin of a cluster. For an antiferromagnetic Heisenberg model, any state satisfying the local constraints $\vec{S}_\alpha = 0$ is a ground state.

Lattices of corner-sharing clusters include kagome, checkerboard, and pyrochlore [3]. Here, the clusters themselves occupy a bipartite lattice. At least within the limit that spins have an infinite number of components (the so-called large-$n$ limit [20]; a finite number of components may, in some cases, lead to an entropic selection of part of the ground states [6, 7, 12, 23], and to a loss of the low temperature liquid phase), one finds a classical SL phase with algebraic correlations at zero temperature and a correlation length that diverges as $T \to 0$ [14, 15].

Such models have long been studied, and the concomitant SL phase has always turned out to host an emergent $U(1)$ gauge field in its Coulomb phase. This yields characteristic pinch-points in the $T = 0$ structure factor [15].

Here, we consider generalizations of such models by identifying cases where the clusters themselves do not occupy a bipartite lattice. Does this change lead to loss of liquidity fractionalisation and/or pinch points?

Two options in 2d of corner-sharing, non-bipartite lattices of clusters are shown on Fig. 1. The left panel illustrates the ruby lattice, where the clusters (square plaquettes) occupy a kagome lattice. The right panel in turn illustrates a variant of the well-known kagome lattice, where all spins within a hexagonal plaquette interact equally with one another forming a corner-sharing network of hexagons. This we will simply refer to as kagome lattice in the following.

A detailed study of these classical Heisenberg models seems to be missing in the literature, but the quantum XXZ model on the kagome lattice considered here has prominently been studied in Ref. 24, where the presence of a $\mathbb{Z}_2$ quantum SL phase was found. Indeed, this quantum SL is intimately related to the resonating valence bond liquid (RVB) of the triangular quantum model, as it corresponds to a dimer model where each site hosts exactly three, rather than just a single, dimer [25].

Fractionalisation and liquidity.— The most direct way of establishing fractionalisation is to consider the behaviour of the model under dilution with nonmagnetic ions (vacancies). Removing all but one spin of a given plaquette, a local paramagnetic moment, so-called orphan [26], emerges in the system, which is robust down to the zero temperature limit. The local moment in the models currently known, is of size $1/2$ [17] or $1/3$ [27].

For the $U(1)$ SLs, an effective theory for such objects yields that, in the zero temperature limit, they effectively behave as Coulomb vector charges, since they exhibit a Coulomb interaction with a thermal screening length, $\xi_{th}$, that diverges as $1/\sqrt{T}$. [17, 28] It is possible to apply the hybrid field theory developed in these works for the orphans surrounded by a bath of large-$n$ spins to the models considered here.

We indeed find that the presence of fractionalised 1/2-orphan moments also occurs in models considered here. Monte Carlo simulations verify this fact for the Heisenberg case, see Fig. 2. This is our first central result, as it confirms that low temperature correlations of these Heisenberg models are not simply those of a trivial paramagnet, but instead reflect a richer structure, to which we turn next.

From the hybrid field theory, one can derive an orphan interaction in terms of correlators of the pristine system, the so-called charge-charge correlations between the total spin of the two $\alpha$ clusters located at the respective orphan plaquette positions, $(\vec{S}_\alpha(\vec{r}_1) \cdot \vec{S}_\alpha(\vec{r}_2))$.

We find that these correlators are extremely short ranged, Fig. 3, with orphan-interactions decaying exponentially quickly – rather than algebraically as is the case for Coulomb orphans. The exponentially decaying orphan-correlations were also verified directly in Heisenberg Monte Carlo simulations.

This exponential decay results from a feature of the adjacency matrix spectrum of the lattices studied here, which crucially is gapped. As explained in more details on the Appendix, this gap replaces the divergent correlation length of the bipartite $U(1)$ case with

$$\xi_{gap} \propto 1/\sqrt{T + \gamma} \quad (2)$$

with $\gamma > 0$. We confirm this prediction directly from our
numerical solution of the large-\(n\) equations, Fig. 3, which features a finite correlation length even in the \(T \to 0\) limit, smaller than a nearest neighbor distance, \(a\).

To further check the absence of any ordering tendency in the Heisenberg \(n = 3\) case (due to some order-by-disorder mechanism in the \(T \to 0\) limit), we directly study the spin structure factor. The Monte Carlo result for the ruby lattice Heisenberg model is presented in Fig. 4, obtained from a combination of parallel tempering, microcanonical and heat bath moves. This also displays the analytical large-\(n\) \(T = 0\) result, as well as the Ising \(n = 1\) case at \(T = 0\) mentioned below (results for the kagome case are analogous). These differ quantitatively, but not qualitatively from each other.

Our simulations reach lattice sizes of \(L \times L\) unit cells, with \(L = 36\) on the ruby lattice (and \(L = 24\) on the kagome lattice; not shown), and the peak heights saturate at large \(L\). This is consistent with quickly decaying correlations – the pair spin correlations computed in our simulations are observed to decay exponentially.

Crucially, and this our next central result, the structure factors do not present the non-analyticities, such as pinch-points, known to occur in the \(U(1)\) liquids on lattices with corner-sharing structure.

Discussion.— We have presented two Heisenberg models exhibiting (i) orphan fractionalisation, (ii) exponentially decaying correlations down to \(T \to 0\), and (iii) absence of order-by-disorder. Together, these establish the existence of a new type of classical SL.

In order to embed this in the known lore of spin liquidity, let us consider the corresponding Ising models at zero temperature. These are related to dimer coverings on non-bipartite lattices by the following map.

Ising variables sitting on the ruby (kagome) lattice, can also be seen as variables sitting on the bonds of a kagome (triangular) lattice. Say that only those bonds with an up spin have a dimer. Therefore the Ising model ground states are equivalent to a double dimer covering, or loop model, on the kagome lattice for the ruby lattice; and to the triple dimer covering of the triangular lattice mentioned above, for the kagome lattice model.

Such dimer models on non-bipartite lattices often present only short-range correlations [25], which we have confirmed by computing correlations with a worm loop Monte Carlo algorithm. The corresponding structure factor presented on Fig. 4 shows qualitative agreement to the Heisenberg and large-\(n\) results. Again, no non-analyticities, such as pinch-points, are discernible, reflecting the short-range nature of the spin correlations.

Despite this evidence for absence of ordering, the system is still not simply in a trivial paramagnetic phase. In fact, an emergent \(\mathbb{Z}_2\) gauge structure is a well-established possibility for such dimer models [25]. The \(\mathbb{Z}_2\) gauge structure arises from the fact that the set of possible ground states split into winding sectors, such that local moves within the ground state do not connect configurations with different winding parities. This is usually seen by considering a non-contractible line on a torus/cylinder the system is defined on, and determining the parity of the number of dimers crossing this line. Allowed moves consist of loops visiting alternately occupied and non occupied bonds, and exchanging these; such a local rearrangement cannot change the winding parity.

While the \(U(1)\) spin liquids on the bipartite lattices of clusters are endowed with a winding number of dimers, the non-bipartite case considered here only allows for a \(\mathbb{Z}_2\) winding parity. Thence, by analogy to the classical Heisenberg magnet on the pyrochlore lattice, which retains the \(U(1)\) gauge structure of the corresponding Ising model (spin ice) [14], the cases considered here are classical Heisenberg analogies of \(\mathbb{Z}_2\) spin liquids.

We believe that the reason their existence has so far been overlooked may have to do with the fact that non-\(U(1)\) frustrated systems in settings considered so far have very different Ising and Heisenberg low-T behaviors, e.g.,...
the Ising triangular antiferromagnet, algebraic ground state ensemble, is replaced in the Heisenberg case by a magnetically ordered ground state.

We have thus shown that classical fractionalisation can occur beyond the $U(1)$ case. The effect of dilution at low temperatures is therefore to create very short-ranged interacting spin-texture complexes, which fluctuate as simple paramagnets with fractional moment of $S/2$.

The necessary conditions for the appearance of such fractional moments are as yet unknown. More generally, the abundance of lattice geometries, and the possible influence of further terms in the Hamiltonian, e.g., anisotropic interactions, remain to be studied. For instance, a recently studied SL of Ref. 29, with anisotropic interactions on the pyrochlore lattice, exhibits ‘pinch lines’; while a a new Heisenberg spin liquid on the $J_1-J_2-J_3$ honeycomb has been shown to exhibit fractionalised moments of $1/3$, albeit ultimately also exhibiting pinch-points [27].

A general search may thus reveal many further suprises, and a proper classification of classical spin-liquid behavior – known or yet to be discovered – is a task that calls for further research.

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Appendix.— Spin correlations at large-$n$ are:

$$
\langle S_\mu^- S_\nu^- \rangle = (\hat{M}^{-1})_{\mu\nu},
$$

where $\mu, \nu$ indicate any two atoms in the basis, and the matrix $\hat{M}$ is related to the interaction matrix, $V$, by:

$$
\hat{M} = \beta J \hat{V} + \lambda \hat{\mathcal{F}},
$$

with Lagrange multiplier $\lambda$ enforcing spin normalization.

Charge-charge correlations, e.g., in the modified kagome lattice model (where only a single dispersive band contribute to these correlators), are:

$$
\langle S_\xi^- S_\xi^- \rangle = \frac{\nu_{\text{kag}} T}{\lambda T + \nu_{\text{kag}}},
$$

where $\nu_{\text{kag}}$ is the eigenvalue of the dispersive band:

$$
\nu_{\text{kag}} = 3 + (\cos q_x \cdot \hat{a}_1 + \cos q_y \cdot \hat{a}_2 + \cos q_z \cdot \hat{a}_3),
$$

In general, the denominator of the charge-charge correlations expressions hosts terms of the form $(\lambda' + \nu_i(q))$, with $\lambda' = \lambda/\beta J = \lambda T', J$, and $\nu_i(q)$ describing the dispersive bands. This is so, since the matrix inversion involved in computing the correlations is given by $G = (\hat{M}^{-1})_{\mu\nu} = g_{\mu\nu}(q)/\det(\hat{M}(q))$, and in general

$$
\det(\frac{\hat{M}}{\beta J}) = \lambda^{n_g} \prod_i (\lambda' + \nu_i(q)),
$$

where $n_g$ denotes the number of ground state flat bands. The eigenvalues generally depend on a function $s_q$ reflecting the symmetries of the lattice at hand. In the two models considered here,

$$
\lambda' = \cos q_x \cdot \hat{a}_1 + \cos q_y \cdot \hat{a}_2 + \cos q_z \cdot \hat{a}_3.
$$

For computing correlations in real space at large distances, $R \to \infty$, one can expand the symmetric functions $s_q$ around $q = 0$; in our case,

$$
\lambda' = -1.5 + (q_x^2 + q_y^2),
$$

FIG. 4: Spin structure factors on the ruby lattice: a) analytical result from the large-$n$ approach at zero temperature; b) Monte Carlo result for a system with Heisenberg spins at inverse temperature $\beta J = 20$ and $N = 7776$ spins ($L = 36$); c) result from a worm Monte Carlo simulation at $T = 0$ Ising model, for a system with $N = 10584$ spins ($L = 42$).
with $\vec{q}'$ possibly rescaled in relation to $\vec{q}$, in order to include irrelevant prefactors. For the case of the kagome charge-charge correlations,

$$C = \sum_{BZ} \langle S_7(-\vec{q})S_7(\vec{q}) \rangle \exp(i\vec{q} \cdot \hat{r}R) \sim \int d^2\vec{q} \exp(i\vec{q} \cdot \hat{r}R) \frac{\nu_{kag}T}{\lambda T + \Delta + (q_x'^2 + q_y'^2)}$$  \hspace{0.5cm} (10)

where $\Delta$ is related to $\nu_{kag}$, and hence the band gap. Thus, the correlations have an asymptotic behavior $\exp(-R/\xi)$, with

$$\xi \sim \frac{1}{\sqrt{T + \gamma}}$$  \hspace{0.5cm} (11)