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Projective symmetry of partons in Kitaev's honeycomb model

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Low-energy states of quantum spin liquids are thought to involve partons living in a gauge-field background. We study the spectrum of Majorana fermions of Kitaev's honeycomb model on spherical clusters. The gauge field endows the partons with half-integer orbital angular momenta. As a consequence, the multiplicities reflect not the point-group symmetries of the cluster, but rather its projective symmetries, operations combining physical and gauge transformations. The projective symmetry group of the ground state is the double cover of the point group.

Quantum spin liquids are conjectured states of matter that have no long-range magnetic order and thus cannot be distinguished by their physical symmetries. The low-energy physics of spin liquids are often described in terms of partons—matter particles with fractional quantum numbers—interacting with emergent gauge fields[1–3]. Wen[4] proposed to classify spin liquids on the basis of *projective* symmetry, a combination of physical and gauge symmetries. Unfortunately, solvable models of spin liquids in more than one spatial dimension are hard to find. For this reason, partons and gauge fields in spin models have been typically introduced by fiat: spin variables are expressed in terms of Abrikosov fermions or Schwinger bosons and the resulting Hamiltonian, quartic in parton fields, is treated at the mean-field level. Although this approach can be justified in some limits, e.g., by taking the number of parton flavors $N \to \infty$[1–3], its applicability to physical spin models is debatable.

The association of projective symmetry with *ad hoc* fractionalization schemes[4–8] is unfortunate. It is therefore desirable to find clean applications of projective symmetry to exactly solvable models of spin liquids. To that end we show that the properties of partons in Kitaev's honeycomb spin model[9] are best characterized in the language of projective symmetry.

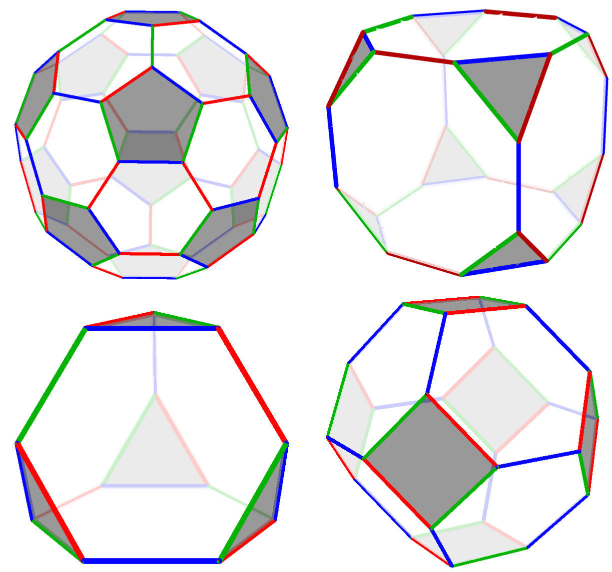

FIG. 1. Truncated tetrahedron, octahedron, cube, and icosahedron. Red, green, and blue edges have spin flavors x, y, and z, respectively. Shaded faces contain nonzero magnetic flux in the ground state.

Summary of main results. We study Kitaev's honeycomb spin model in a spherical lattice geometry realized by Archimedean solids , Fig. 1. The model is solvable by a fermionization procedure yielding a Hamiltonian quadratic in Majorana fermions c_n. Naturally, the spectrum of a highly symmetric cluster is degenerate. However, the multiplicities do not match the dimensions of the point-group irreps. For example, the group of tetrahedron T has irreps **1**, **1′**, **1″**, and **3**, labeled by their dimensions (we follow the notation of Grimus and Ludl [10]). Unexpectedly, Majorana modes on a truncated tetrahedron form doublets (Table I), which the point-group symmetries fail to explain.

The resolution of this paradox is tied to the presence of a gauge field felt by Majorana fermions. The net outward magnetic flux through plaquettes of the cluster is $\Phi = 4\pi g$, where g can be interpreted as the charge of a magnetic monopole at the cluster's center. The orbital angular momentum of a parton with unit electric charge is incremented by the angular momentum of the electromagnetic field g[11]. Because g is half-integer in the ground states of our clusters, the net angular momentum is converted from integer to half-integer. To accommodate states with half-integer angular momenta, we must enlarge the point group $T \subset SO(3)$ to its double cover $\tilde{T} \subset SU(2)$ and use the irreps for which a rotation through 2π yields a factor of -1[12]. The double group $\tilde{T}$ has three such irreps: **2**, **2′**, and **2″**. Hence the parton doublets. Similar scenarios apply to other spherical clusters: the projective symmetry group $\mathcal{G}$ of the ground state turns out to be the double cover $\tilde{G} \subset SU(2)$ of the corresponding point symmetry group $G \subset SO(3)$.

Landau levels on a sphere. Before turning our attention to Kitaev's lattice model, we illustrate the relevant concepts in a related continuum problem: Landau levels of a massive particle on a sphere[13]. It is convenient to treat it as a rigid rotor—a particle pivoted on a massless

Solid	Multiplicities	Φ	g	PSG
Truncated tetrahedron	2, 2, 2	2π	1/2	$\tilde{T}$
Truncated octahedron	4, 4, 4	6π	3/2	$\tilde{O}$
Truncated cube	4, 2, 4, 2	2π	1/2	$\tilde{O}$
Truncated icosahedron	6, 2, 4, 6, 2, 6, 4	6π	3/2	$\tilde{I}$

TABLE I. Multiplicities of Majorana modes (in the order of increasing energy $\epsilon > 0$), net magnetic flux Φ, monopole charge g, and projective symmetry group for Kitaev's spin model on some Archimedean solids.

rod of length r—with mutually orthogonal axes $\hat{\boldsymbol{\xi}}, \hat{\boldsymbol{\eta}}, \hat{\boldsymbol{\zeta}}$ affixed to it; in particular, $\hat{\boldsymbol{\zeta}} = \mathbf{r}/r$ points along the rod. Note that body components of orbital angular momentum L_ξ, L_η, and L_ζ commute with the global components L_x, L_y, and L_z, so we may use as basis vectors simultaneous eigenstates of L^2, L_z, and L_ζ[12]. The Hamiltonian is $H = L_\xi^2/2I_\xi + L_\eta^2/2I_\eta + L_\zeta^2/2I_\zeta$, where $I_\xi = I_\eta = mr^2$ and $I_\zeta = 0$. The vanishing of I_ζ requires setting $L_\zeta = 0$ in order to keep the energy finite, so $H = (L_\xi^2 + L_\eta^2)/2mr^2 = L^2/2mr^2$. In the presence of a magnetic field, the Hamiltonian is modified by replacing $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ with $\boldsymbol{\Lambda} = \mathbf{r} \times (\mathbf{p} - e\mathbf{A}) = \mathbf{L} - e\mathbf{r} \times \mathbf{A}$, where $\mathbf{A}$ is the vector potential.

Although magnetic field in this problem, $\mathbf{B}(\mathbf{r}) = g\mathbf{r}/r^3$, is spherically symmetric, the vector potential $\mathbf{A}(\mathbf{r})$ is not. We can undo the change induced in $\mathbf{A}(\mathbf{r})$ by a rotation if we follow it up with a gauge transformation[14]. The combined operation—a gauged rotation—leaves the vector potential, and thus the Hamiltonian, invariant. The generator of gauged rotations,

$$\mathbf{J} = \mathbf{L} - e\mathbf{r} \times \mathbf{A} - g\mathbf{r}/r = \boldsymbol{\Lambda} - g\hat{\boldsymbol{\zeta}}, \tag{1}$$

satisfies the standard algebra of angular momentum[13]. Its body-axis component $J_\zeta = L_\zeta - g = -g$. This constraint restricts g to integer and half-integer values and the length of the gauged angular momentum to $j = |g|, |g|+1, |g|+2, \ldots$ The Hamiltonian, expressed in terms of $\mathbf{J}$, reads

$$H = (\Lambda_\xi^2 + \Lambda_\eta^2)/2mr^2 = (\mathbf{J}^2 - g^2)/2mr^2. \tag{2}$$

Kitaev's lattice model. The Hamiltonian of Kitaev's spin model is[9]

$$H = -\sum_{\langle mn \rangle} J_{mn} S_m^{\alpha(mn)} S_n^{\alpha(mn)}, \tag{3}$$

where $\langle mn \rangle$ denotes a pair of nearest-neighbor sites m and n with a coupling constant J_{mn}. The spin component, or flavor, $\alpha(mn) = x$, y, or z depends on the link $\langle mn \rangle$. With spins $\mathbf{S}_n$ represented in terms of four Majorana fermions b_n^α, and c_n, $S_n^\alpha = ib_n^\alpha c_n$, the Hamiltonian becomes quadratic in c fermions:

$$H = -\sum_m \sum_n t_{mn} c_m c_n / 4. \tag{4}$$

Two b fermions sharing a link combine to form a Z_2 gauge variable $u_{mn} = ib_m^{\alpha(mn)} b_n^{\alpha(mn)} = -u_{nm}$. Link variables u commute with each other and with the Hamiltonian (4) and can therefore be treated as numbers $u_{mn} = \pm 1$. The hopping matrix of c Majorana fermions $t_{mn} = -2iJ_{mn}u_{mn}$ is pure imaginary, antisymmetric, and thus Hermitian.

We work with Archimedean solids obtained from Platonic solids by truncation, Fig. 1. Without loss of generality, we use ferromagnetic coupling constants, $J_1 > 0$ on edges inherited from Platonic solids and $J_2 > J_1 > 0$ on the edges resulting from truncation.

The product of link variables around a loop gives the Z_2 magnetic flux $W = (-iu_{12})(-iu_{23})\ldots(-iu_{L1})$. The allowed values of the flux depend on the perimeter L of the loop: $W = \pm 1$ for even L and $\pm i$ for odd L[9,15]. Distinct physical states of the spin model can be fully specified by the values of Z_2 fluxes on all plaquettes and by the state of the c Majorana fermions in this static magnetic background. Different gauge representations $\{u\}$ of the same flux pattern $\{W\}$ are related by a gauge transformation

$$u'_{mn} = \Lambda_m u_{mn} \Lambda_n, \quad c'_n = \Lambda_n c_n, \quad \Lambda_n = \pm 1. \tag{5}$$

The physics of the Z_2 gauge field in Kitaev's model has been explored in Refs. 16–19.

The Hamiltonian of the Majorana operators (4) can be reduced to a diagonal form,

$$H = \sum_k \epsilon_k (\gamma_k^\dagger \gamma_k - \gamma_k \gamma_k^\dagger)/2, \tag{6}$$

where $\gamma_k = \frac{1}{2}\sum_n \psi_n^{(k)} c_n$ and $\gamma_k^\dagger$ are annihilation and creation operators of (complex) fermion eigenmodes and $\epsilon_k \geq 0$ are their excitation energies. The one-particle wavefunctions $\psi_n^{(k)}$ and the eigenvalues ϵ_k can be found by solving the one-particle Schrödinger equation $-\sum_n t_{mn}\psi_n = \epsilon\psi_m$ with a pure imaginary hopping amplitude $t_{mn} = -2iJ_{mn}u_{mn}$[9]. Eigenvalues of t_{mn} come in pairs $\pm\epsilon$: if wavefunction ψ_n has the eigenvalue $+\epsilon$ then its complex conjugate ψ_n^* has the eigenvalue $-\epsilon$. Positive eigenvalues are the excitation energies of the Majorana eigenmodes in Eq. (6). The Z_2 flux $W = e^{i\Phi}$ translates into a $U(1)$ flux Φ experienced by these fermions. The allowed values of Φ depend on the loop length L: 0 and π for L even, $\pm\pi/2$ for L odd.

The flux pattern in the ground state can be found from the following heuristic rules[15]. A loop with an odd perimeter L is indifferent to the value of its flux $\Phi = \pm\pi/2$. For even L, there is a preferred value: $\Phi = 0$ if $L = 2 \bmod 4$ and $\Phi = \pi$ if $L = 0 \bmod 4$. For example, the ground state of the honeycomb model has zero flux on all hexagons[9].

Projective symmetry group. We next construct the projective symmetry group (PSG) for the truncated tetrahedron. In the ground state, its hexagons have no flux, whereas all triangles have the same flux $\Phi = +\pi/2$ or $-\pi/2$. The net flux $\Phi = \pm 2\pi$ means a half-integer

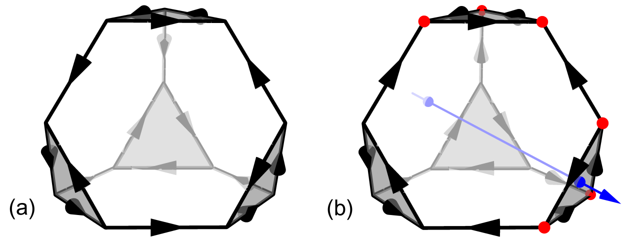

FIG. 2. (a) A ground state of Kitaev's model on a truncated tetrahedron. Arrows show directions for which the phase of the hopping amplitudes $\arg t = -\pi/2$. (b) The same state rotated through $\frac{2\pi}{3}$ about the indicated threefold symmetry axis. The hopping amplitudes can be restored by a Z_2 gauge transformation on vertices labeled with dots.

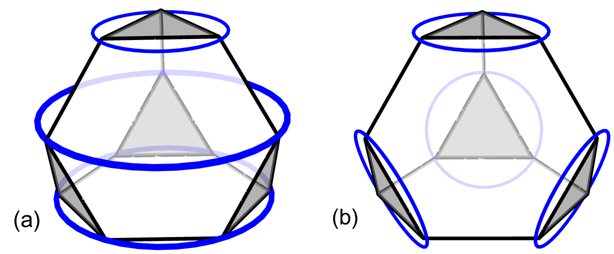

FIG. 3. Unprimed (a) and primed (b) rotations about a threefold axis.

monopole charge $g = \Phi/(4\pi) = \pm 1/2$. A gauge configuration $\{u\}$ for one of the two ground states is shown in Fig. 2(a). The presence of a gauge field endows edges with a sense of direction and thereby reduces the symmetry.

Consider rotation $R(\frac{2\pi}{3}, \hat{\mathbf{n}})$ about threefold axis $\hat{\mathbf{n}}$ [Fig. 2(b)] that reverses the sign for some of the gauge variables u_{mn} and the corresponding hopping amplitudes t_{mn}. As in Haldane's problem, the flux pattern remains unchanged and we may restore the original u and t by a gauge transformation (5). One such transformation—let us call it $\Lambda(\frac{2\pi}{3}, \hat{\mathbf{n}})$—has $\Lambda_n = -1$ on sites marked with red dots in Fig. 2(b) and $+1$ on the remaining sites. The combined operation of gauged rotation,

$$\mathcal{R}(\tfrac{2\pi}{3}, \hat{\mathbf{n}}) = \Lambda(\tfrac{2\pi}{3}, \hat{\mathbf{n}})\, R(\tfrac{2\pi}{3}, \hat{\mathbf{n}}), \tag{7}$$

leaves the hopping matrix invariant[14]. The complementary gauge transformation, $\Lambda'_n = -\Lambda_n$, also restores the gauge configuration. This is a general result: every point-group symmetry R generates two gauged symmetries: ΛR and $-\Lambda R$.

The $\frac{2\pi}{3}$ gauged rotation (7) has a peculiar property: applying it three times yields not the identity but rather multiplication by -1[14]. If we identify this operation with a 2π gauged rotation then we find a result reminiscent of half-integer spin, $\mathcal{R}(2\pi, \hat{\mathbf{n}}) \equiv \mathcal{R}^3(\frac{2\pi}{3}, \hat{\mathbf{n}}) = -1$. Alternatively, we may define the gauged 2π rotation as a combination of the ordinary rotation $R(2\pi, \hat{\mathbf{n}}) = 1$ with the global gauge transformation $\Lambda(2\pi, \hat{\mathbf{n}}) = -1$: $\mathcal{R}(2\pi, \hat{\mathbf{n}}) \equiv \Lambda(2\pi, \hat{\mathbf{n}}) R(2\pi, \hat{\mathbf{n}}) = -1$. Then the gauged symmetries satisfy the composition rule for rotations, $\mathcal{R}^3(\frac{2\pi}{3}, \hat{\mathbf{n}}) = \mathcal{R}(2\pi, \hat{\mathbf{n}})$.

The PSG for the ground-state flux sector is obtained as follows. We first construct two gauged rotations $\mathcal{R}(\frac{2\pi}{3}, \hat{\mathbf{n}}_1)$ and $\mathcal{R}(\frac{2\pi}{3}, \hat{\mathbf{n}}_2)$ about two different threefold axes $\hat{\mathbf{n}}_1$ and $\hat{\mathbf{n}}_2$ from ordinary rotations as described above. We then use the multiplication table of $SU(2)$ rotations (more precisely, of its subgroup $\tilde{T}$) to generate new elements and label them accordingly, e.g., $\mathcal{R}(\frac{2\pi}{3}, \hat{\mathbf{n}}_2)\mathcal{R}^{-1}(\frac{2\pi}{3}, \hat{\mathbf{n}}_1) = \mathcal{R}(\pi, \hat{\mathbf{n}}_3)$, where $\hat{\mathbf{n}}_3$ is a twofold axis. We check that each new element $\mathcal{R}(\phi, \mathbf{n})$ is indeed a gauged rotation, i.e., a composition of the corresponding ordinary rotation $R(\phi, \mathbf{n}) \in T$ and of a Z_2 gauge transformation $\Lambda(\phi, \mathbf{n})$ defined in Eq. (5). Lastly we check that the multiplication tables of the newly constructed group and of $\tilde{T}$ are the same. This program establishes that the PSG of the ground-state flux sectors is indeed $\tilde{T}$, the double cover of the point group T. Similar results are obtained with the other Archimedean solids (Table I).

Parton multiplets. The number of vertices in a truncated Platonic solid equals the order of the corresponding point group $G \subset SO(3)$. States of a fermion living on the vertices transform under the regular representation of the group G. These states can be uniquely labeled by group elements as follows. Assign the identity element e to an arbitrary vertex; the rest of the vertices are labeled by the group element $R \in G$ that takes vertex e into them. (We now regard symmetries as active transformations.) A symmetry $R_2 \in G$ acts on state $|R_1\rangle$ as left multiplication:

$$R_2|R_1\rangle = |R_2 R_1\rangle. \tag{8}$$

For the truncated tetrahedron and its group $G = T$, the regular representation is decomposed into irreps as follows: $\mathbf{12} = \mathbf{1} + \mathbf{1}' + \mathbf{1}'' + 3 \times \mathbf{3}$.

The same applies to the double cover $\tilde{G}$ of group G, except that each fermion state is now represented by group elements $\mathcal{R} \in \tilde{G}$ twice, as $\pm|\mathcal{R}\rangle$. The one-fermion states are decomposed into only those irreps of $\tilde{G}$ for which a 2π rotation equals multiplication by -1. For the double tetrahedral group $\tilde{T}$, $\mathbf{12} = 2\times\mathbf{2} + 2\times\mathbf{2}' + 2\times\mathbf{2}''$. Thus we expect six doublets for a complex fermion on a truncated tetrahedron. For a Majorana fermion, states obtained by complex conjugation are identified and we obtain three doublets, as is indeed the case (Table I). For the double octahedral group $\tilde{O}$, $\mathbf{24} = 2 \times \tilde{\mathbf{2}} + 2 \times \tilde{\mathbf{2}}' + 4 \times \tilde{\mathbf{4}}$. Majorana fermions on a truncated cube indeed come in multiplets of 2, 2, 4, and 4. On a truncated octahedron, the doublets are "accidentally" degenerate (Table I). For the buckyball (the icosahedral group I), $\mathbf{60} = 2 \times \tilde{\mathbf{2}} + 2 \times \tilde{\mathbf{2}}' + 4 \times \tilde{\mathbf{4}} + 6 \times \tilde{\mathbf{6}}$; we expect Majorana multiplets with dimensions 2, 2, 4, 4, 6, 6, 6, in agreement with direct diagonalization (Table I).

Parton spectrum. Symmetries $R \in G$ (or $\mathcal{R} \in \tilde{G}$) used so far represent rotations about axes fixed in space. It is convenient to introduce a second set of "primed" operations R' (or their gauged versions $\mathcal{R}'$) representing rotations about axes that themselves rotate:

$$R_2'|R_1\rangle = |R_1 R_2\rangle = R_1 R_2 R_1^{-1}|R_1\rangle. \tag{9}$$

If R_2 is a rotation about the axis nearest to vertex e then $R_1 R_2 R_1^{-1}$ is an equivalent rotation about the axis nearest to vertex R_1, Fig. 3. The primed operations are direct analogs of rotations about axes attached to a rigid body, which also follow right multiplication[20]. The groups of primed and unprimed rotations are isomorphic: the multiplication table for R' is the same as that of R^{-1}. Primed and unprimed rotations commute: $R_3 R_2'|R_1\rangle = |R_3 R_1 R_2\rangle = R_2' R_3|R_1\rangle$.

As the hopping matrix t commutes with unprimed rotations, we may guess that it can be expressed in terms of primed rotations. Indeed, for the truncated tetrahedron, it is a superposition of gauged rotations through $+\pi$ about the nearest twofold axis $\hat{\mathbf{n}}_1$ and through $+\frac{2\pi}{3}$ and $-\frac{2\pi}{3}$ about the nearest threefold axis $\hat{\mathbf{n}}_2$:

$$t = -2i[J_1\mathcal{R}'(\pi, \hat{\mathbf{n}}_1) - J_2\mathcal{R}'(\tfrac{2\pi}{3}, \hat{\mathbf{n}}_2) + J_2\mathcal{R}'(-\tfrac{2\pi}{3}, \hat{\mathbf{n}}_2)]. \tag{10}$$

Because primed rotations form group $\tilde{T}$, we may use its irreps to block-diagonalize the hopping matrix. The block that corresponds to irrep λ is obtained by replacing $\mathcal{R}'(\phi, \hat{\mathbf{n}})$ in Eq. (10) with the irrep matrix $\mathcal{D}^{(\lambda)}(-\phi, \hat{\mathbf{n}})$. Matrices for irrep $\mathbf{2}$ of $\tilde{T}$ coincide with matrices of finite rotation of the fundamental (spin-$\frac{1}{2}$) irrep of $SU(2)$: $\mathcal{D}^{(\mathbf{2})}(-\phi, \hat{\mathbf{n}}) = e^{i(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})\phi/2}$, where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices. Taking the axes to be $\hat{\mathbf{n}}_1 = (0,0,1)$ and $\hat{\mathbf{n}}_2 = (1,1,1)/\sqrt{3}$, we obtain a 2×2 block $t^{(\mathbf{2})} = -2J_1\sigma_z + 2J_2(\sigma_x + \sigma_y + \sigma_z)$, whose positive eigenvalue $\epsilon = 2\sqrt{J_1^2 - 2J_1J_2 + 3J_2^2}$ matches the energy of one of the Majorana doublets obtained by direct diagonalization of the hopping matrix. Irreps $\mathbf{2}'$ and $\mathbf{2}''$ of $\tilde{T}$ cannot be expressed in terms of $SU(2)$ rotation matrices. However, their direct sum $\mathbf{2}' + \mathbf{2}''$ coincides with the 4-dimensional (spin-$\frac{3}{2}$) irrep of $SU(2)$, so we may again use $SU(2)$ rotation matrices to obtain a 4×4 block. Parton energies are roots of the characteristic polynomial $P(\epsilon) = \epsilon^4 - (3J_1^2 + 2J_1J_2 + 2J_2^2)\epsilon^2 + 16(J_1 + J_2)^2 J_2^2$. They reproduce the energies of the two remaining Majorana doublets. This diagonalization procedure also works correctly for the ground states of the other spherical clusters listed in Table I.

We can gain an additional insight into the spectrum of Majorana fermions by making a direct connection to Haldane's continuum model discussed above. If the hopping matrix t on a cluster were real and positive, the state with the lowest energy $\epsilon < 0$ would be $\psi_n = 1$, a lattice analog of the s state, followed by analogs of states with angular momenta $\ell = 1, 2, \ldots$ with multiplicities $2\ell + 1$ until the continuum approximation breaks down[21]. In the presence of a magnetic flux $\Phi = 4\pi g$ through the cluster, the energy eigenstates on the sphere have angular momenta $j = |g|, |g|+1, |g|+2, \ldots$ in the order of increasing energy with multiplicities $2j+1$. The same can be expected for the eigenstates of the hopping matrix with energies $\epsilon < 0$. Because the positive eigenvalues of the Majorana hopping matrix mirror the negative ones, we expect that the parton multiplet with the highest energy $\epsilon > 0$ will have angular momentum $j = |g|$, followed by multiplets with $j = |g|+1, |g|+2, \ldots$ until the continuum approximation breaks down. Indeed, e.g., on the buckyball, $g = 3/2$, the highest-energy partons form a quartet ($j = 3/2$) and a sextet ($j = 5/2$), see Table I. The octet ($j = 7/2$) is split into a doublet and a sextet by deviations from spherical symmetry due to the lattice.

We have shown that parton excitations in Kitaev's honeycomb model on highly symmetric spherical clusters have half-integer orbital angular momenta due to a nontrivial gauge background resembling the field of a magnetic monopole with a half-integer charge.

The structure of parton multiplets can be understood in the framework of projective symmetries, which combine physical and gauge transformations. For all spherical clusters we have examined, the projective symmetry group for the ground state is the double cover $\tilde{G}$ of the point group G. As far as we know, this is the first application of projective symmetries in a solvable model of a spin liquid.

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