Magnetization plateaus of the quantum pyrochlore Heisenberg antiferromagnet

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We predict magnetization plateaus ground states for $S = 1/2$ Heisenberg antiferromagnets on pyrochlore lattices by formulating arguments based on gauge and spin-parity transformations. We derive a twist operator appropriate to the pyrochlore lattice, and show that it is equivalent to a large gauge transformation. Invariance under this large gauge transformation indicates the sensitivity of the ground state to changes in boundary conditions. This leads to the formulation of an Oshikawa-Yamanaka-Affleck–like criterion at finite external magnetic field, enabling the prediction of plateaus in the magnetization versus field diagram. We also develop an analysis based on the spin-parity operator, leading to a condition from which identical predictions are obtained of magnetization plateaus ground states. Both analyses are based on the non-local nature of the transformations, and rely only on the symmetries of the Hamiltonian. This suggests that the plateaus ground states can possess properties arising from non-local entanglement between the spins.

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I. INTRODUCTION

Geometrically frustrated lattices are widely expected to harbor exotic states of matter, including quantum spin-liquids [1–3], spin-ice [4–6], fractional excitations [6–8], and magnetization plateaus [9–12] at a finite external magnetic field. A plateau in the magnetization needs the existence of a finite spectral gap, and can sometimes involve a magnetic ground state with non-trivial entanglement [13–15]. A large number of theoretical and experimental studies have sought such exotic states on highly frustrated lattices like the kagome in two spatial dimensions (2D) and the pyrochlore in three dimensions (3D) [16–25]. While studies of the $S = 1/2$ kagome antiferromagnet at finite magnetic field have predicted as well as verified the existence of several magnetization plateaus [26–28], the pyrochlore counterpart has been much less studied. A notable work on the pyrochlore lattice involves a semi-classical (vector spin) symmetry-based analysis by Penc *et al.* [9]. There, the authors showed that a spin-lattice coupling may stabilize the 1/2-magnetization plateaus state. Such a plateau has been confirmed by recent experiments on the spinel ($CdCr_2O_4$) with $S = 3/2$ spins on the pyrochlore lattice formed by the network of the Cr sites [10,29]. Further, there are indications of magnetization plateaus in some recent experiments on spin-ice pyrochlore ($A_2B_2O_7$) systems with large easy-axis anisotropy as well [30].

A quantum mechanical treatment of the finite-field properties of the pyrochlore system is, however, lacking at present. We aim, therefore, to offer predictions of physical observables via a quantum mechanical formalism that relies solely on the symmetry properties of the Hamiltonian of interest, and without any perturbative expansions. Such treatments can sometimes offer non-trivial states of matter with topological properties, non-trivial plateaus states, etc. [31–35]. In the work of Haldane for ferromagnetic spin chains [36] as well as Tanaka *et al.* on antiferromagnetic spin chains [37], the Euclidean path integral approach has been employed for the calculation of non-trivial geometric phase factors (if any) in the probability amplitude for excitations above the ground state. This involves applying a gradual twist to the real-space order parameter in a system with periodic boundary conditions. As shown by Haldane, the topological quantization of such geometric phases can give rise to the gapping of the spectrum for the integer spin Heisenberg chains [36], while the spectrum of the half-integer spin chains remains gapless. Similar conclusions for half-integer spin chains can also be obtained from twist operator-based arguments relying on the sensitivity of the ground state to changes in boundary conditions: the Lieb-Schultz-Mattis (LSM) theorem [38] at zero external field, and its finite-field extension in the Oshikawa-Yamanaka-Affleck (OYA) criterion [33]. Such twist operations are equivalent to large gauge transformations, and can be visualized in terms of the adiabatic insertion of Aharanov-Bohm (AB) fluxes through the system [31,39]. The main purpose of this article is to develop such a formalism with the goal of predicting possible magnetization plateaus states in the quantum ($S = 1/2$) pyrochlore lattice. This is achieved by defining suitable twist and translation operators for the pyrochlore lattice, and applying them to obtain an OYA-like criterion for ground state properties in presence of a finite magnetic field.

While the LSM theorem and OYA criterion were originally obtained for 1D and quasi-1D systems, following the works of Oshikawa, Hastings, and others, these arguments have been extended to higher-dimensional systems with short-ranged interactions [32–35,38,40]. In general, applying the LSM argument in higher dimensions ($D > 1$) gives the energy of the variational twisted state as $\mathcal{O}(C/L)$ (where CL is the volume, and L is the length of the direction being twisted). Clearly, this energy is not small in the thermodynamic limit

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in a spatially isotopic system. By considering a strongly anisotropy limit such that $C/L \to 0$ [41], one can then apply the LSM argument once more. However, by relating the twist operator with a large gauge transformation, Oshikawa [32] showed that taking the LSM argument is valid well beyond the strong-anisotropy regime. Recent works have also extended the validity of the theorem to frustrated quantum spin systems [27,42]. This needs, for instance, a careful definition of the twist operator by taking into consideration the symmetries of the geometrically frustrated lattice [27].

Here, we extend the twist-operator formalism of Ref. [27] in deriving an OYA-like criterion for the possible existence of several fractional magnetization plateaus states in the $S = 1/2$ pyrochlore system. Besides this, we develop a spin-parity operator based analysis [43,44] of the system, and obtain predictions of magnetization plateaus identical to those found from the twist-operator method. This identifies spin-parity as a good quantum number for the identification of plateaus states. The rest of the work is organized as follows. In Sec. II, we discuss briefly the symmetries of the Hamiltonian. In Sec. III, we develop a twist-operator formalism and thereby derive an OYA-like criterion for possible plateaus states of the pyrochlore lattice. Section IV is devoted to the formulation of a spin-parity based criterion for magnetization plateaus, and a comparison made with those obtained from the twist-operator method. We conclude in Sec. V with a discussion of the results and some future directions. Details of some of the calculations are provided in the Appendices.

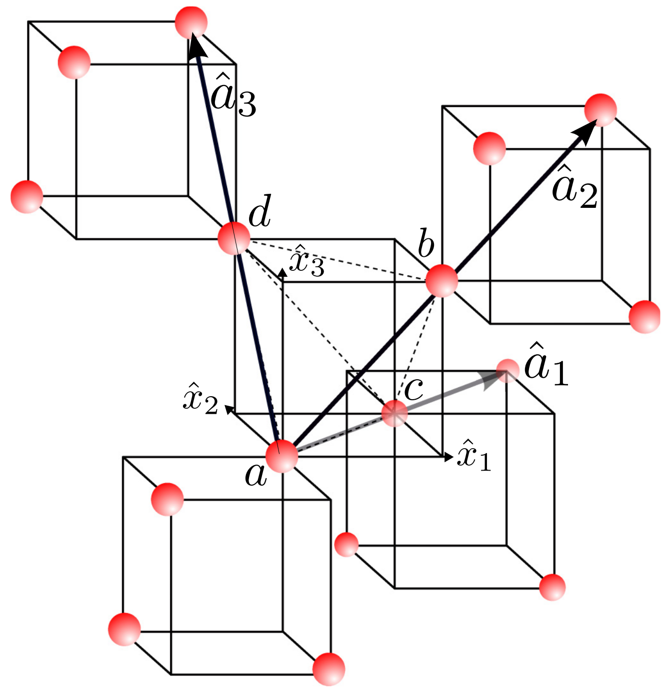

FIG. 1. Schematic diagram of the pyrochlore lattice with the basis vectors $\hat{a}_1$, $\hat{a}_2$, and $\hat{a}_3$ (defined in the main text). Red spheres represent sites with spin $S = 1/2$. The four vertices of a tetrahedron are different from one another with respect to their environment, indicating four sub-lattices through the indices a, b, c, and d. The dashed lines form a tetrahedron, signaling the geometric frustration present in the system.

II. HAMILTONIAN FOR THE PYROCHLORE LATTICE

The Hamiltonian for a system of spins on the three dimensional pyrochlore lattice with nearest neighbor (n.n.) antiferromagnetic Heisenberg exchange and an external magnetic field may be written as

$$H = \sum_{\langle \vec{r}\vec{r}' \rangle} J \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}'} - h \sum_{\vec{r}} S^z_{\vec{r}}, \tag{1}$$

where $\vec{r} \in (\vec{R}, j)$ with the lattice vector $\vec{R} = n_1\hat{a}_1 + n_2\hat{a}_2 + n_3\hat{a}_3$. Here, $\hat{a}_1$, $\hat{a}_2$, and $\hat{a}_3$ are the three non-orthogonal basis vectors of the pyrochlore lattice, and n_1, n_2, n_3 are coordinate numbers along their respective basis vectors (see Fig. 1). The basis vectors $(\hat{a}_1, \hat{a}_2, \hat{a}_3)$ can be defined in Cartesian coordinates $\{x_1, x_2, x_3\}$ as follows: $\frac{\hat{a}_1}{2} = \frac{1}{\sqrt{2}}(\hat{x}_1 + \hat{x}_2)$, $\frac{\hat{a}_2}{2} = \frac{1}{\sqrt{2}}(\hat{x}_1 + \hat{x}_3)$ and $\frac{\hat{a}_3}{2} = \frac{1}{\sqrt{2}}(\hat{x}_2 + \hat{x}_3)$. The four sub-lattice indices in a tetrahedron are given by the index $j \in \{a, b, c, d\}$. The coupling constant J is the n.n. spin-exchange coupling, while the external magnetic field (h) is applied along the direction perpendicular to the plane containing the basis vectors $\hat{a}_1$ and $\hat{a}_2$. For N_1, N_2, and N_3 being the number of units of each sub-lattice along the $\hat{a}_1$, $\hat{a}_2$, and $\hat{a}_3$ directions, respectively, the total number of sites in the lattice is $\mathcal{N} = 4N_1N_2N_3$. Below, we will consider periodic boundary conditions (PBC) along the $\hat{a}_1$ direction. Further, for δ denoting the distance between n.n. sites, $L_{\hat{a}_1} = 2\delta N_1$, $L_{\hat{a}_2} = 2\delta N_2$, and $L_{\hat{a}_3} = 2\delta N_3$ are the lengths along the $\hat{a}_1$, $\hat{a}_2$, and $\hat{a}_3$ directions, respectively. Hereafter, we will consider $\delta = 1$. In the following section, we will derive the twist operator for the pyrochlore lattice, and employ it in formulating an OYA-like criterion for predicting magnetization plateaus possible in this system.

III. TWIST OPERATORS AND THE OYA CRITERION

In defining twist operators appropriate to a geometrically frustrated lattice such as the pyrochlore, it is important to take notice of the following. As mentioned earlier, the twist operator is equivalent to a large gauge transformation operator. Thus, we place the system shown in Fig. 1 on a hypercylinder with PBC in the $\hat{a}_1$ direction. The application of an AB-flux along the axis of the cylinder induces a time-varying vector potential in the periodic direction ($\hat{a}_1$). As $\hat{a}_2$ and $\hat{a}_3$ are not orthogonal to $\hat{a}_1$, spins at different sites along basis vectors $\hat{a}_2$ and $\hat{a}_3$ differ in the phase induced by the equivalent AB-flux [27]. Further, a pyrochlore lattice can be considered as a collection of parallel layers of two-dimensional kagome lattices, with interpolating layers of two-dimensional triangular lattices [22]. In Fig. 1, we choose the kagome layers to lie in planes containing the basis vectors $(\hat{a}_1, \hat{a}_2)$, with the non-orthogonal basis vector $\hat{a}_3$ running between the parallel kagome layers. Thus, we construct the twist operator for the pyrochlore lattice along the direction $\hat{a}_1$ by using that developed recently for the kagome lattice [27].

We first write down, therefore, the twist operators for the four individual sub-lattices $j \in (a, b, c, d)$ as

$$\begin{aligned}
\hat{O}_a &= \exp\left[i\frac{2\pi}{N_1}\sum_{\vec{R}}\left(n_1 + \frac{n_2}{2} + \frac{n_3}{2}\right)\hat{S}^z_{\vec{R},a}\right],\\
\hat{O}_b &= \exp\left[i\frac{2\pi}{N_1}\sum_{\vec{R}}\left(n_1 + \frac{n_2}{2} + \frac{n_3}{2} + \frac{1}{4}\right)\hat{S}^z_{\vec{R},b}\right],\\
\hat{O}_c &= \exp\left[i\frac{2\pi}{N_1}\sum_{\vec{R}}\left(n_1 + \frac{n_2}{2} + \frac{n_3}{2} + \frac{1}{2}\right)\hat{S}^z_{\vec{R},c}\right],\\
\hat{O}_d &= \exp\left[i\frac{2\pi}{N_1}\sum_{\vec{R}}\left(n_1 + \frac{n_2}{2} + \frac{n_3}{2} + \frac{1}{4}\right)\hat{S}^z_{\vec{R},d}\right],
\end{aligned} \tag{2}$$

where $\hat{S}^z_{\vec{R},j}$ is the z-component of spin operator for jth sub-lattice at lattice vector $\vec{R}$, and N_1 is the number of units of a given sub-lattice along the $\hat{a}_1$ direction. Choosing site a as reference site within the unit-cell, the b and c sites differ by phases $\frac{1}{4}(2\pi/N_1)$ and $\frac{1}{2}(2\pi/N_1)$, respectively, from the geometry of the kagome lattice [27]. Further, as the projection of the b and d site on the $\hat{a}_1$ axis are identical, the d site has the same phase difference as the b site; this is the origin of the factors $\frac{1}{4}$ and $\frac{1}{2}$ in the twist operator definitions for the various sub-lattices given above. Also, the phase difference between spins belonging to nearest sites of the same sub-lattice and with fixed n_2 and n_3 coordinates is given by $2\pi/N_1$; the same for a fixed n_1 coordinate gives a phase difference of π/N_1. This is the origin of the phase terms $\frac{n_2}{2}$ and $\frac{n_3}{2}$ in the twist operators above.

As spin components at different sites commute, we can combine all four twist operators into one: $\hat{O} = \hat{O}_a\hat{O}_b\hat{O}_c\hat{O}_d$. The final form of the twist operator for the pyrochlore lattice is then

$$\begin{aligned}
\hat{O} = \exp\Bigg[i\frac{2\pi}{N_1}\Bigg(&\sum_{\vec{r}}\left(n_1 + \frac{n_2}{2} + \frac{n_3}{2}\right)\hat{S}^z_{\vec{r}}\\
&+\sum_{\vec{R}}\left(\frac{1}{4}\hat{S}^z_{\vec{R},b} + \frac{1}{2}\hat{S}^z_{\vec{R},c} + \frac{1}{4}\hat{S}^z_{\vec{R},d}\right)\Bigg)\Bigg].
\end{aligned} \tag{3}$$

We note that the terms $\exp[i\frac{2\pi}{N_1}\sum_{\vec{r}}(\frac{n_3}{2}\hat{S}^z_{\vec{r}})]$ and $\exp[i\frac{2\pi}{N_1}\sum_{\vec{R}}(\frac{1}{4}\hat{S}^z_{\vec{R},d})]$ in Eq. (3) are extra with respect to the twist operator for the kagome lattice formulated in Ref. [27]. The first of these phases arises due to the contribution from the third non-orthogonal basis vector $\hat{a}_3$. The second phase, on the other hand, is simply due to fourth sub-lattice (d) of the pyrochlore system.

Defining $\hat{T}_{\hat{a}_1}$ as a translation operator along $\hat{a}_1$ direction, such that $\hat{T}_{\hat{a}_1}\vec{S}_{n_1,n_2,n_3}\hat{T}^\dagger_{\hat{a}_1} = \vec{S}_{n_1+1,n_2,n_3}$, yields the following identity for the pyrochlore lattice (the detailed steps of which are shown in Appendix A):

$$\hat{T}_{\hat{a}_1}\hat{O}\hat{T}^\dagger_{\hat{a}_1} = \hat{O}\,\exp\left[-i2\pi\,(4N_2N_3)\left(\hat{m} - \frac{\hat{S}^z_{\boxtimes}}{4}\right)\right], \tag{4}$$

where $\hat{m} = \hat{S}^z_{\mathrm{Tot}}/(4N_1N_2N_3)$ is the magnetization per site operator, with $\hat{S}^z_{\mathrm{Tot}} = \sum_{\vec{r}}\hat{S}^z_{\vec{r}}$ being the total magnetization operator, and $\hat{S}^z_{\boxtimes}$ is the z-component of the four spins in a tetrahedron. For a finite magnetic field, one can now predict the possibility of magnetization plateaus by deriving an OYA-like criterion [33] from this relation in term of the fractional magnetization per site m/m_s, where $m_s = 1/2$ is the saturation magnetization per site:

$$\frac{Q_m}{2}\left(\frac{m}{m_s} - \frac{S^z_{\boxtimes}}{2}\right) = n, \tag{5}$$

where Q_m (= 4, 8, 12, 16, . . . , etc.) [45,46] is the magnetic unit cell and n is an integer. In obtaining Eq. (5) from Eq. (4), we have rewritten $4N_2N_3 = qQ_m$, where $Q_m = 4p$ and $N_2N_3 = pq$ (p and q are any non-zero positive integer). The factor q is absorbed by noting that the phase factor in Eq. (4) is known mod(2π). Thus, for $S^z_{\boxtimes} = 2$ and $Q_m = 4$ (the fundamental lattice unit cell), the criterion predicts possible magnetization plateaus at $m/m_s = 0$ and 1/2 for $n = -2$ and -1, respectively. On the other hand, for $Q_m = 8$, 12, and 16 we have more plateaus possible at 0, 1/8, 1/6, 1/4, 1/3, 3/8, 2/3, 5/8, 3/4, 5/6, and 7/8. In keeping with Ref. [27], these plateaus are likely good candidate ground states in the search for topological order in a three-dimensional geometrically frustrated spin-1/2 system. We will see below that identical predictions are obtained for magnetization plateaus based on arguments employing a spin-parity operator for the pyrochlore lattice.

As there are some experimental indications of plateaus obtained in $S = 3/2$ pyrochlore systems [10,29], we comment briefly here on magnetization plateaus that are similarly obtained from the twist-operator approach for this system as well. From Eq. (4), following the same steps as required to reach Eq. (5) and with $S^z_{\boxtimes} = 6$, we obtain an OYA-like criterion for the $S = 3/2$ pyrochlore system

$$\frac{3Q_m}{2}\left(\frac{m}{m_s} - 1\right) = n, \tag{6}$$

where Q_m (= 4, 8, 12, 16, . . . , etc.) is the magnetic unit cell [as in Eq. (5)], $m_s = 3/2$ is the saturation magnetization per site, and n is an integer. For $Q_m = 4$, criteria for plateaus at $m/m_s = 1/2, 2/3$, and 5/6 are satisfied for $n = -3, -2$, and -1, respectively. Further, a plateau at $m/m_s = 3/4$ is obtained for an extended unit cell of $Q_m = 8$ and $n = -3$. While a plateau at $m/m_s = 1/2$ has been verified in the spinel materials $CdCr_2O_4$ [10] and $ZnCr_2O_4$ [29], there are only preliminary indications of plateaus at $m/m_s = 2/3, 3/4$, and 5/6 thus far [29].

IV. SPIN-PARITY AND MAGNETIZATION PLATEAUS

In the previous section, we predicted possible magnetization plateaus for the quantum pyrochlore system with the help of a symmetry-based OYA criterion. The twist-operator employed in reaching these predictions is observed to be non-local in nature, respects various spin and lattice symmetries of the Hamiltonian, and the operation involves a global sensitivity to changes in boundary conditions. The spin-parity transformation also involves a global change via a spin-flip (i.e., rotation by π in the xy plane) of all spins, and respects the spin and lattice symmetries of the Hamiltonian [43,44]. It is, therefore, interesting to see whether predictions of plateaus can be made in geometrically frustrated quantum spin systems with the help of the spin-parity operator. Therefore, we devoted the current section to an analysis based on the spin-parity transformation. We will see that this formalism predicts similar plateaus states for the $S = 1/2$ pyrochlore system as obtained earlier from the twist operator analysis. We will comment on the origin of this similarity at the end of this section.

The spin-parity operations $S^x_{\vec{r}} \to -S^x_{\vec{r}}$, $S^y_{\vec{r}} \to -S^y_{\vec{r}}$, and $S^z_{\vec{r}} \to S^z_{\vec{r}}$ leave the Hamiltonian (1) invariant. The operation corresponds to a π-rotation of all spins ($\vec{S}_i = \frac{1}{2}\vec{\sigma}_i$, where σ's are Pauli spin matrices) about the z-axis and can be written as [43,44]

$$\mathcal{S} = \exp\left[i\frac{\pi}{2}\sum_{\vec{r}}\sigma^z_{\vec{r}}\right] = \prod_{\vec{r}} i\sigma^z_{\vec{r}} = \mathcal{W}\times\mathcal{Z}, \tag{7}$$

where $\mathcal{W} = \exp[i\frac{\pi}{2}\mathcal{N}]$ and $\mathcal{Z} = \prod_{\vec{r}}\sigma^z_{\vec{r}}$, with $\mathcal{N}$ the total number of sites in the lattice. Then, we can rewrite $\mathcal{Z}$ as

$$\mathcal{Z} = \exp\left[i\pi\left(\hat{S}^z_{\text{Tot}} - \mathcal{N}S\right)\right] = \exp[i\pi\mathcal{N}(\hat{m} - S)], \tag{8}$$

where $\hat{S}^z_{\text{Tot}} = \frac{1}{2}\sum_{\vec{r}}\sigma^z_{\vec{r}}$ is the total magnetization operator of the system, $S = 1/2$, and $\hat{m} = \frac{1}{\mathcal{N}}\sum_{\vec{r}}\hat{S}^z_{\vec{r}}$ is magnetization per site operator. The operator $\mathcal{Z}$ is clearly a global operator, and takes values ± 1 corresponding to two topologically different parity sectors of the many-body Hilbert space. It is straightforward to show that the spin-parity operator $\mathcal{Z}$ commutes with the Hamiltonian H: $[\mathcal{Z}, H] = 0$ (see Appendix B for details). Thus, the eigenvalues of $\mathcal{Z}$ are good quantum numbers. Therefore, from the quantization condition of Eq. (8), we have

$$\mathcal{N}(m - S) = n, \tag{9}$$

where n is any integer.

Thus far, we have not invoked any notion of a specific lattice geometry in reaching Eq. (9). In order to make conclusions specific to the pyrochlore lattice, we note that since the four lattice sites of a tetrahedron form the minimum unit cell of a pyrochlore lattice with periodic boundary conditions in all directions, we must impose the condition: $\mathcal{N} = 4N_1N_2N_3$. For $S = 1/2$, the magnetization (m) values satisfying the condition Eq. (9) correspond to states with a well-defined parity. If protected by a spectral gap, we expect that such states correspond to non-trivial topologically ordered spin liquid ground states and exhibit plateaus in the magnetization vs. field plot. We will now show that, upon imposing the condition

$$\mathcal{N} = 4N_1N_2N_3 = q\tilde{Q}_m, \tag{10}$$

where $\tilde{Q}_m = 4p$ is the magnetic unit cell, $N_1N_2N_3 = pq$ (p, q belongs to the set of non-zero positive integers). Together with $S = 1/2$, Eq. (9) gives the same predictions for the positions of magnetization plateaus for pyrochlore lattice as obtained from the OYA criterion [Eq. (5)]. The fundamental unit cell of the pyrochlore lattice is $\tilde{Q}_m = 4$ (for $p = 1$) and various enlarged unit cells are $\tilde{Q}_m = 8, 12, 16, \ldots$, etc. (for $p = 2, 3, 4, \ldots$) [45,46]. Then, we can rewrite Eq. (9) as

$$\frac{q\tilde{Q}_m}{2}\left(\frac{m}{m_s} - 1\right) = n, \tag{11}$$

where $m_s = 1/2$ is the saturation magnetization per site.

We find two cases for the possible plateaus states of the minimum unit cell $\tilde{Q}_m = 4$. First, we define $\mathcal{Z}_{Py}$ as the spin-parity operator relevant to the pyrochlore lattice, and obtained from Eq. (8) by imposing the condition Eq. (10). Then, for $\mathcal{Z}_{Py} = -1$, such that n is an odd integer from Eq. (8). When put into Eq. (11), this implies that q is an odd integer, and thus

$$2\left(\frac{m}{m_s} - 1\right) = 2k + 1, \quad k \in \text{integer}. \tag{12}$$

For $k = -1$, this gives a possible magnetization plateaus at $m/m_s = 1/2$. Similarly, for $\mathcal{Z}_{Py} = 1$, such that n is an even integer, Eq. (11) implies that if q is odd

$$2\left(\frac{m}{m_s} - 1\right) = 2w, \quad w \in \text{integer}. \tag{13}$$

For $w = -1$, we obtain a possible plateau at $m/m_s = 0$. Finally, if q is even integer

$$2\left(\frac{m}{m_s} - 1\right) = l, \quad l \in \text{integer}. \tag{14}$$

If l is either odd or even, we obtain the $m/m_s = 1/2$ and $m/m_s = 0$ plateau, respectively (as before). The analysis can also be extended to the case of the enlarged unit cells, i.e., $\tilde{Q}_m = 8, 12, 16, \ldots$, obtaining possible plateaus states at $m/m_s = 0, 1/8, 1/6, 1/4, 1/3, 3/8, 2/3, 5/8, 3/4, 5/6,$ and $7/8$. We find, therefore, predictions that are identical to those obtained earlier from the twist operator analysis, and end by commenting on the origin of this similarity. The similarity in predictions arises from the fact that both the twist ($\hat{O}$) and the spin-parity operators ($\mathcal{Z}_{Py}$) analyses involve a sensitivity to changes in boundary conditions: the former by a twist that is distributed gradually among the spins, and the latter by a twist identical to all the spins. This can be seen from the following relation between the matrix elements obtained from Eqs. (4) and (8) acting on the ground state $|\psi_0\rangle$,

$$\langle\psi_0|\left(\hat{O}^\dagger\hat{T}_{\hat{a}_1}\hat{O}\hat{T}^\dagger_{\hat{a}_1}\right)^{\frac{N_1}{2}}|\psi_0\rangle = \langle\psi_0|\mathcal{Z}_{Py}|\psi_0\rangle. \tag{15}$$

This relation indicates that the final result of the application of both types of twists is equivalent in terms of the global rotations they apply on the ground state of the spin system. The resulting OYA-like relations, Eqs. (5) and (9), obtained from these global rotations should, therefore, lead to identical predictions on possible gapped plateaus ground states.

V. DISCUSSION

In conclusion, we have predicted possible magnetization plateaus ground states for the $S = 1/2$ pyrochlore lattice with arguments based on an OYA-like criterion and the spin-parity operator. Our analysis shows that for the fundamental lattice unit cell (i.e., a tetrahedron), $m/m_s = 0$ and $1/2$ are the two possible plateaus states, while other plateaus with fractional magnetization arise with the enlargement of the unit cell. Similar results have been obtained for magnetization plateaus in the spin-1/2 kagome system [11,12,27]. We have also obtained results from the twist-operator approach for $S = 3/2$ pyrochlore systems that predict plateaus at $m/m_s = 1/2, 2/3, 3/4$, and $5/6$. While a plateau at $m/m_s = 1/2$ has been observed in certain spinels [10,29], there are only preliminary results on plateaus at other fractions [29].

It is important to note that our analysis does not depend on the perturbative expansion of any coupling, instead relying only on the symmetries of the Hamiltonian. Given that the operators employed in reaching these predictions are nonlocal (i.e., global) in nature, we expect that the properties of the corresponding ground states will be topologically distinct. For instance, some recent theoretical studies on the spin-1/2 kagome lattice have also revealed the topological nature of magnetization plateaus ground states [13,14].

To our knowledge, this is the first analytical work for the $S = 1/2$ pyrochlore system that predicts the existence of plateaus in the magnetization. It will be interesting to test these predictions numerically by looking for signatures in, for instance, exact diagonalization (ED) studies of small clusters. Extending our work to the case of spinel systems (in which both A and B sites are magnetic) should be interesting, as magnetization plateaus [47] and spin liquid ground states [48,49] in such systems are under investigation. Finally, it will be challenging to adapt either the functional RG method [50] or the renormalization group method used recently in studying the $m/m_s = 1/3$ plateau of the kagome system [14] to the plateaus we have predicted here for the pyrochlore.

Note added in proof. We take note of a recent arxiv posting by Dr. S. Pujari [46], where connections between different magnetization plateau states of the kagome (analyzed in Ref. [27]) and pyrochlore lattices presented earlier are discussed. This appears to arise from the possibility that the pyrochlore lattice can accommodate stable closely packed hexagonal modes in a commensurate fashion within its alternating kagome layers, and have the remaining sites as fully polarized (including those on the intervening alternating triangular layers). The link is especially interesting, given that the known exact ground state wave function for the $m/m_s = 7/9$ plateau of the kagome system is linked with the ground state of the pyrochlore lattice plateau at $m/m_s = 5/6$.

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APPENDIX A: LSM CALCULATION

Here, we present a calculation of the non-commutativity between twist and translation operators defined in Sec. III:

$$\begin{aligned}
\hat{T}_{\hat{a}_1}\hat{O}\hat{T}_{\hat{a}_1}^\dagger &= \hat{T}_{\hat{a}_1}\ \exp\left[i\frac{2\pi}{N_1}\left(\sum_{\vec{r}}\left(n_1+\frac{n_2}{2}+\frac{n_3}{2}\right)\hat{S}^z_{\vec{r}}+\sum_{\vec{R}}\left(\frac{1}{4}\hat{S}^z_{\vec{R},b}+\frac{1}{2}\hat{S}^z_{\vec{R},c}+\frac{1}{4}\hat{S}^z_{\vec{R},d}\right)\right)\right]\hat{T}_{\hat{a}_1}^\dagger\\
&= \hat{T}_{\hat{a}_1}\ \exp\left[i\frac{2\pi}{N_1}\sum_{n_2,n_3,j}\left(\hat{S}^z_{(1,n_2,n_3),j}+2\hat{S}^z_{(2,n_2,n_3),j}+\cdots+(N_1-1)\hat{S}^z_{(N_1-1,n_2,n_3),j}+N_1\hat{S}^z_{(N_1,n_2,n_3),j}\right)\right]\hat{T}_{\hat{a}_1}^\dagger\\
&\quad\times\ \exp\left[i\frac{2\pi}{N_1}\left(\sum_{\vec{r}}\left(\frac{n_2}{2}+\frac{n_3}{2}\right)\hat{S}^z_{\vec{r}}+\sum_{\vec{R}}\left(\frac{1}{4}\hat{S}^z_{\vec{R},b}+\frac{1}{2}\hat{S}^z_{\vec{R},c}+\frac{1}{4}\hat{S}^z_{\vec{R},d}\right)\right)\right]\\
&= \exp\left[i\frac{2\pi}{N_1}\sum_{n_2,n_3,j}\left(\hat{S}^z_{(2,n_2,n_3),j}+2\hat{S}^z_{(3,n_2,n_3),j}+\cdots+(N_1-1)\hat{S}^z_{(N_1,n_2,n_3),j}+N_1\hat{S}^z_{(N_1+1,n_2,n_3),j}\right)\right]\\
&\quad\times\ \exp\left[i\frac{2\pi}{N_1}\left(\sum_{\vec{r}}\left(\frac{n_2}{2}+\frac{n_3}{2}\right)\hat{S}^z_{\vec{r}}+\sum_{\vec{R}}\left(\frac{1}{4}\hat{S}^z_{\vec{R},b}+\frac{1}{2}\hat{S}^z_{\vec{R},c}+\frac{1}{4}\hat{S}^z_{\vec{R},d}\right)\right)\right]\\
&= \hat{O}\ \exp\left[i\frac{2\pi}{N_1}\sum_{n_2,n_3,j}N_1\hat{S}^z_{(1,n_2,n_3),j}\right]\exp\left[-i\frac{2\pi}{N_1}\sum_{\vec{r}}\hat{S}^z_{\vec{r}}\right]\\
&= \hat{O}\ \exp\left[i2\pi\sum_{n_2,n_3,j}\hat{S}^z_{(1,n_2,n_3),j}\right]\exp\left[-i\frac{2\pi}{N_1}\hat{S}^z_{\mathrm{Tot}}\right]\\
&= \hat{O}\ \exp\left[-i\frac{2\pi}{N_1}\left(\hat{S}^z_{\mathrm{Tot}}-N_1N_2N_3\hat{S}^z_{\boxtimes}\right)\right],
\end{aligned}\tag{A1}$$

where $\hat{S}^z_{\boxtimes} = \hat{S}^z_{(1,1,1),a} + \hat{S}^z_{(1,1,1),b} + \hat{S}^z_{(1,1,1),c} + \hat{S}^z_{(1,1,1),d}$ is the vector sum of the z-component of the four sub-lattice spins in a boundary tetrahedron ($n_1 \equiv 1$ corresponds to a boundary spin). $\hat{S}^z_{\mathrm{Tot}} = \sum_{\vec{r}} \hat{S}^z_{\vec{r}}$ is the total magnetization operator, and we have used periodic boundary conditions along $\hat{a}_1$ such that site $N_1 + 1 \equiv$ site 1.

APPENDIX B: COMMUTATION RELATIONS

We present here the calculation of the commutation relation $[\mathcal{Z}, H]$, which is equivalent to calculating the two commutators, $[\prod_{\vec{r}} \sigma^z_{\vec{r}},\, \sigma^z_{\vec{r}}]$ and $[\prod_{\vec{r}} \sigma^z_{\vec{r}},\, \vec{\sigma}_{\vec{r}} \cdot \vec{\sigma}_{\vec{r}'}]$. Of these, the first commutation relation is exactly zero, as it involves only the z-component of Pauli matrices. The second commutator can be computed as follows:

$$
\begin{aligned}
&\left[\prod_{\vec{r}} \sigma^z_{\vec{r}},\, \sigma^x_{\vec{r}}\sigma^x_{\vec{r}'}\right] \\
&= \left[\prod_{\vec{r}} \sigma^z_{\vec{r}}, \sigma^x_{\vec{r}}\right]\sigma^x_{\vec{r}'} + \sigma^x_{\vec{r}}\left[\prod_{\vec{r}} \sigma^z_{\vec{r}}, \sigma^x_{\vec{r}'}\right] \\
&= \big(0 + \cdots + \sigma^z_{\vec{r}_1} \cdots [\sigma^z_{\vec{r}}, \sigma^x_{\vec{r}}] \cdots \sigma^z_{\vec{r}_{\mathcal{N}}} + \cdots + 0\big)\sigma^x_{\vec{r}'} \\
&\quad + \sigma^x_{\vec{r}}\big(0 + \cdots + \sigma^z_{\vec{r}_1} \cdots [\sigma^z_{\vec{r}'}, \sigma^x_{\vec{r}'}] \cdots \sigma^z_{\vec{r}_{\mathcal{N}}} + \cdots + 0\big) \\
&= \sigma^z_{\vec{r}_1} \cdots (i\sigma^y_{\vec{r}}) \cdots (i\sigma^y_{\vec{r}'}) \cdots \sigma^z_{\vec{r}_{\mathcal{N}}} \\
&\quad + \sigma^z_{\vec{r}_1} \cdots (-i\sigma^y_{\vec{r}}) \cdots (i\sigma^y_{\vec{r}'}) \cdots \sigma^z_{\vec{r}_{\mathcal{N}}} \\
&= 0.
\end{aligned}
\tag{B1}
$$

In the above, we have used the following Pauli matrix identities: $[\sigma^\alpha_n, \sigma^\beta_m] = i\epsilon^{\alpha\beta\gamma}\delta_{nm}\sigma^\gamma_n$, where $\{\alpha, \beta, \gamma\} \in \{x, y, z\}$, $\epsilon^{\alpha\beta\gamma}$ is the antisymmetric tensor, and δ_{nm} is the δ function between site n and m. In the same way, we find that

$$
\left[\prod_{\vec{r}} \sigma^z_{\vec{r}},\, \sigma^y_{\vec{r}}\sigma^y_{\vec{r}'}\right] = \left[\prod_{\vec{r}} \sigma^z_{\vec{r}},\, \sigma^z_{\vec{r}}\sigma^z_{\vec{r}'}\right] = 0. \tag{B2}
$$

Thus, we can conclude that

$$
\left[\prod_{\vec{r}} \sigma^z_{\vec{r}},\, \vec{\sigma}_{\vec{r}} \cdot \vec{\sigma}_{\vec{r}'}\right] = 0. \tag{B3}
$$

Bringing together both commutators, we find that

$$
[\mathcal{Z},\, H] = 0, \tag{B4}
$$

i.e., the spin-parity operator commutes very generally with the Hamiltonian for the $S = 1/2$ Heisenberg antiferromagnet in a field.

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