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Constraints on topological order in Mott Insulators

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We point out certain symmetry induced constraints on topological order in Mott Insulators (quantum magnets with an odd number of spin $\frac{1}{2}$ per unit cell). We show, for example, that the double semion topological order is incompatible with time reversal and translation symmetry in Mott insulators. This sharpens the Hastings-Oshikawa-Lieb-Schultz-Mattis theorem for 2D quantum magnets, which guarantees that a fully symmetric gapped Mott insulator must be topologically ordered, but is silent on which topological order is permitted. An application of our result is the Kagome lattice quantum antiferromagnet where recent numerical calculations of entanglement entropy indicate a ground state compatible with either toric code or double-semion topological order. Our result rules out the latter possibility.

Distinctions between phases of matter were traditionally based on symmetry considerations, since spontaneous symmetry breaking leads to distinct phases. However, with the discovery of the fractional Quantum Hall effects (FQHE), the role of topology in defining phases of matter was emphasized. Topologically ordered states in two dimensions (2D), such as FQHE phases and gapped quantum spin liquids, contain excitations with unusual (anyonic) statistics. Symmetries still have an important role to play in these systems, as the anyon excitations may carry fractional quantum numbers such as the fractional charge of Laughlin quasiparticles. The interplay of topology and symmetry leads to new and fundamental distinctions between states of matter. [1]

Charge conservation also allows us to define the filling ν of FQHE states. At fractional filling factors p/q , a featureless (translation invariant) state *must* have a non-trivial excitation of charge $1/q$. This is the simplest example of a constraint between the microscopic details (the fractional filling) and the emergent excitations (the fractional charge). Presumably this constraint helps stabilize the FQHE states over competing conventional orders which must break translation symmetry.

Gapped quantum spin liquids are close analogs of FQHE states. They also feature emergent anyon excitations and fractionalization of symmetry quantum numbers, although usually in the presence of time reversal symmetry. They are proposed to occur in two dimensional insulating quantum magnets, where frustration prevents the formation of a conventional ordered state[2]. Although a clearcut experimental example of a gapped spin liquid is currently lacking, numerical calculations have made a strong case for their existence in the $S = \frac{1}{2}$ antiferromagnet on the Kagome lattice[3, 4]. Experiments on the Kagome lattice material Herbertsmithite also observe a spin disordered state[5, 6]. Although bulk measurements do not observe an energy gap, this distinction has been attributed to disorder [7] or non-Heisenberg magnetic interactions[8–10], although other ground states have also been proposed[11].

The analog of fractional filling in quantum magnets is the Mott insulator, defined as an insulator with an odd number of $S = \frac{1}{2}$ moments per unit cell. In 1D, according to the Lieb-Schultz-Mattis argument, a $S = \frac{1}{2}$ antiferromagnetic chain must either be gapless or double the unit cell[12]. In 2D an analog of this result, the Hastings-Oshikawa-Lieb-Schultz-

Mattis (HOLSM) [13–17], states that at zero temperature, a Mott insulator must either be gapless, break spin / translation symmetry, or have emergent excitations with nontrivial mutual statistics. The last condition is not available in 1D, and corresponds to a topological quantum spin liquid phase, which is gapped and preserves all symmetries. Hence finding a symmetric, gapped state is indirect, but strong, evidence for a quantum spin liquid.

An intuitive way of visualizing this result is to think of a $S = \frac{1}{2}$ in terms of hard core bosons, where spin up is an empty site and spin down is a site occupied by a boson. A Mott insulator has a fractional (half odd integer) filling of bosons per unit cell. To obtain a featureless insulator, the bosons must fractionalize into half charged entities, which can then be uniformly assigned to lattice sites. When viewed directly from the spin language, this implies that to obtain a symmetric ground state, one needs $S = \frac{1}{2}$ excitations in the magnet which can screen the background spin in the unit cell. No local excitation (like a spin flip) carries $S = \frac{1}{2}$, so these excitations must be topological.

Clearly this will place conditions on the types of topological order compatible with a symmetric state. The extensions of the Lieb-Schultz-Mattis theorem are silent on the detailed form of the topological order. Here we will show that one very natural seeming type of topological order, the double-semion state, is incompatible with a time reversal symmetric Mott insulator. Our method of proof can be readily generalized to other kinds of topological order and different symmetries. We leave that to future work.

This observation has an important consequence for interpreting recent numerical results on the Kagome antiferromagnet. Numerical calculations using the Density Matrix Renormalization Group have found a gapped phase with a featureless ground state i.e. one that preserves the spin, lattice and time reversal symmetry[3]. As the Kagome model is a Mott insulator with three $S = \frac{1}{2}$ per unit cell, this implies a quantum spin liquid phase. Subsequently, the topological entanglement entropy was calculated in this ground state and was found to be consistent with $\gamma = \ln 2$ [4, 18] the expected value for a spin liquid with Z_2 toric code topological order. Certain other topological orders are also compatible with this value but they break time reversal symmetry. The only other plau-

sible option is the double-semion theory, which is a twisted Z_2 topological order [19, 20]. Excitations in this phase are a semion, antisemion and a boson with mutual semionic statistics with the first two particles. Our argument demonstrates that double-semion topological order is incompatible with a fully symmetric Mott insulator. Given that the numerical results on the Kagome lattice antiferromagnet point to a symmetric ground state, we can exclude this topological order. The only remaining possibility which is consistent with all numerical results is the Z_2 toric code topological order.

This paper is organized as follows. First, we provide a summary of the central result and its application to the double-semion theory. We then give a more rigorous argument based on the action of symmetries on the minimally entangled ground states of an infinite cylinder. Finally, we discuss some numerical studies of ground states with double semion topological order in a Kagome Mott insulator, which provide a concrete illustration of the constraints described in this paper.

We will argue that in the presence of translation symmetry, there is always an Abelian anyon a in the system which **1**) is not transformed into another anyon type under the symmetries and **2**) can ‘screen’ the charge in the unit cell, meaning that a transforms under the symmetries in a manner that can combine with a missing unit cell in order to form a neutral object. One may visualize the system as a lattice of a -particles which screen the fractional charge of the unit cell. We then show that there are no anyons in the double-semion theory which satisfy criteria **1**, **2**), completing a ‘no-go’ argument.

There is an exception to our argument if translations permute the anyon types. This is impossible for the double-semion theory, so we defer all discussion of this case to the Supplementary Materials. [21]

The properties of a topological phase with respect to translation [22–27] can be captured by supposing there is an Abelian anyon of type ‘ a ’ sitting in each unit cell, generating a constant density of topological flux a . The anyons then experience magnetic flux owing to their mutual statistics with the anyon a . To be precise, [21] take an anyon b around a path enclosing one unit cell, accumulating a Berry phase

$$\eta_b = \frac{(T_y^{-1}T_x^{-1}T_yT_x)_b}{(T_y^{-1}T_yT_x^{-1}T_x)_b} = S_{ba}/S_{b\mathbb{1}}, \quad (1)$$

where x, y denote a basis for the Bravais lattice. The denominator has been included so that if the state is translationally symmetric, the non-universal components of each $T_{x/y}$ cancel, resulting in a robust phase. If there is constant topological flux a , then b has enclosed one a -flux, accumulating mutual statistics $S_{ba}/S_{b\mathbb{1}}$ where S is the topological S -matrix. On physical grounds, these phases should be consistent with fusion, $\eta_b\eta_c = \eta_{bc}$ (in a non-Abelian phase, all fusion channels for bc should share the same η). Setting $\eta_b = S_{ba}/S_{b\mathbb{1}}$ for some Abelian a is in fact the unique choice consistent with fusion, so measuring each η_b uniquely determines (and defines) the flux a .

For example, consider the FQHE at $\nu = 1/m$; the anyons are labeled by their charge $Q_b = eb/m$. When an anyon b en-

circles one magnetic unit cell it acquires an Aharonov-Bohm phase $\eta_b = e^{2\pi i \frac{b}{m}}$. Since $S_{ba} = e^{2\pi i ba/m} / \sqrt{m}$, we see that the background topological flux is $a = 1$, the $Q_a = e/m$ quasi-particle.

In the presence of other symmetries, there are two constraints on the allowed background flux a . First **(1)**, note that in general applying a global symmetry G can turn one anyon type into another, $G : b \rightarrow Gb$. The flux a must be left invariant under any symmetry G which commutes with the translations $T_{x/y}$, otherwise the phases η_b will break the symmetry G .

Second **(2)**, we will later prove that the anyon a transforms under the symmetries so as to screen the microscopic unit cell. For concreteness we discuss three cases, each of which is applicable to the Mott insulator: i) if there is half-integral spin per unit cell, a must have half-integral spin (it is a ‘spinon’); ii) if there is fractional U(1) charge n/m per unit cell, then a must have fractional charge n/m (as for the Laughlin quasiparticles); and iii) if each unit cell transforms as a Kramer’s doublet $\mathcal{T}^2 = -1$, then a must transform as a Kramer’s doublet.

Cases i - iii imply there must be non-trivial topological order: since the charges assigned to a are fractional, they cannot be carried by any local (trivial) excitation, which is the content of the HOLS M theorem. But from **(1)** we have learned something in addition to HOLS M: a cannot be permuted by the symmetries. This small addition is sufficient to rule out the double-semion theory.

The double-semion topological order can be viewed as a topological phase of bosons which is comprised of a pair of opposite $m = \pm 2$ bosonic Laughlin states ($U(1)_2 \times U(1)_{-2}$). It can be described by a two component Abelian Chern Simons theory $\mathcal{L} = \frac{2}{4\pi} \epsilon^{\mu\nu\lambda} (a_{1\mu} \partial_\nu a_{1\lambda} - a_{2\mu} \partial_\nu a_{2\lambda})$ and has the same quantum dimension and ground state degeneracy on the torus (4) as the Z_2 toric code topological order. The quasiparticle content is $\{1, s\} \times \{1, s'\} = \{1, s, s', b\}$ where s (s') is the semion (antisemion) and $b = ss'$ is a boson, with mutual semionic statistics with the first two particles.

The topological spins of the semions are $\theta_{s/s'} = \pm i$. Under time reversal, the topological spin is conjugated, $\theta_{\mathcal{T}s} = \theta_s^*$, so time reversal exchanges the semions: $\mathcal{T}s = s'$. This constrains the allowed realizations of SO(3), U(1) and time reversal symmetry in a way we show is incompatible with scenarios i-iii). In all cases we assume that both time reversal and translation symmetry are respected.

i) SO(3). There are two ways to realize SO(3) in the double-semion model. First, we can assign trivial (integral) spin to each anyon. But for case i) we need at least one anyon to transform as $S = \frac{1}{2}$, and the unique possibility is that $\{1, b\}$ have integral spin while $\{s, s'\}$ have half-integral spin. Clearly s, s' must have the same spin, as they are related by time reversal. Since $bs = s'$, b cannot have half-integral spin in order to preserve consistency with fusion. There is no anyon a which carries $S = \frac{1}{2}$ and isn’t permuted by \mathcal{T} .

ii) $U(1)$. Since $b^2 = s^2 = s'^2 = 1$, fusion requires that each anyon either has $U(1)$ charge Q of 0 or $\frac{q}{2}$ (modulo the unit of charge q in this theory). Fusion and time-reversal require $Q_s = Q_{s'} = Q_s + Q_b$, so $Q_b = 0$ is neutral. There are two possibilities: $Q_{s/s'} = 0$, or $Q_{s/s'} = \frac{q}{2}$. In either case, there is no anyon a which carries $Q = \frac{n}{m}q$ and is not permuted by \mathcal{T} .

iii) *Time reversal*. Under \mathcal{T} the two semions are exchanged, $\mathcal{T} : s \leftrightarrow s'$, while the boson b is unchanged. Furthermore, the boson b must be assigned $\mathcal{T}^2 = 1$ because it is composed of a pair of particles (s, s') with trivial mutual statistics which are transformed into one another under time reversal. Leaving a detailed argument to the Supplementary Materials [21], intuitively when \mathcal{T}^2 acts on b it is equivalent to taking s around s' , which leads to unit phase i.e. $\mathcal{T}^2 = +1$, and hence no Kramers degeneracy. Again, there is no anyon a which is a Kramer's doublet.

To justify criteria 1, 2 we consider the action of braiding, time reversal, and translation on the degenerate ground states of an infinitely long cylinder. There is a special 'minimally entangled' (ME) basis [28] for the degenerate ground states in which each of these operations permutes the basis states. These permutations are subject to certain conditions which impose the two constraints 1, 2 on the background anyon flux a . We restrict to Abelian theories to simplify the discussion, but the result is general.

A topological theory with m anyon types has m degenerate ground states on an infinitely long cylinder[29]. To construct the ME basis, [28] define periodic coordinate y and infinite coordinate x . Let \mathcal{F}_y^a denote the adiabatic process of creating a pair of anyons b/\bar{b} from the vacuum, taking b around the cylinder in the $+y$ direction, and reannihilating the pair, as illustrated in Fig. 1 [30, 31]. \mathcal{F}_x^b is a similar process in which a pair b/\bar{b} is dragged out to $x = \pm\infty$. The $\mathcal{F}_{x/y}^b$ are a set of unitary matrices acting on the ground state manifold. \mathcal{F}_x^b threads topological flux b through the cylinder, while the \mathcal{F}_y^b are like Wilson loops which detect the topological flux. Their commutation relations are determined by the mutual statistics $S_{bc}/S_{b\mathbb{1}}$ and the fusion group N_{bc}^d :

$$\begin{aligned} \mathcal{F}_y^b \mathcal{F}_x^c &= \frac{S_{bc}}{S_{b\mathbb{1}}} \mathcal{F}_x^c \mathcal{F}_y^b : \\ \mathcal{F}_{x/y}^b \mathcal{F}_{x/y}^c &\propto \mathcal{F}_{x/y}^{b \cdot c}, \quad b \cdot c = \sum_d N_{bc}^d d \quad (\text{Abelian fusion}) \end{aligned} \quad (2)$$

The ME basis simultaneously diagonalizes each \mathcal{F}_y^b . [28, 32, 33] The ME basis has definite topological flux threading the cylinder, reducing the entanglement entropy between the two regions $x < 0$ and $x > 0$. In contrast, for the non-MES, the Wilson loop - Wilson loop correlation functions generated by \mathcal{F}_y^b have long-range order along the length of the cylinder, generating additional entanglement entropy (they are long-range ordered 'cat states' if we view the cylinder as a 1D system). By choosing a basis which diagonalizes \mathcal{F}_y^b , each basis state is a local minima of the entanglement.

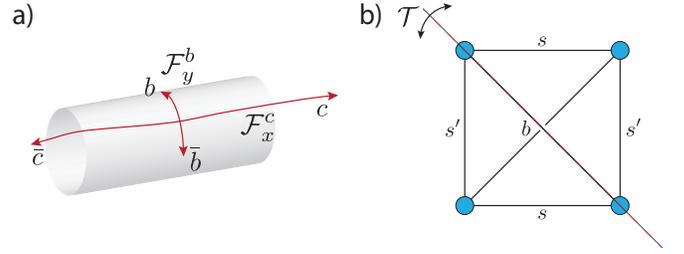


FIG. 1. **a)** The adiabatic processes $\mathcal{F}_{x/y}^b$. **b)** The 4 minimally entangled basis states are represented as the node of a graph. The process \mathcal{F}_x^c , with $c = 1, b, s, s'$, permutes these basis state, illustrated with labeled edges. The action of time reversal \mathcal{T} is also a permutation of the MES; the only permutation consistent with fusion acts as a mirror reflection across the diagonal, since it must exchange $\mathcal{T} : s \leftrightarrow s'$

For Abelian b , the process \mathcal{F}_x^b permutes the MES in a manner consistent with fusion. We represent this permutation as a graph, shown in Fig. 1 for the double-semion theory. Each node of the graph is an MES; nodes are connected by an edge ' b ' if the two MES are related by \mathcal{F}_x^b .

Time-reversal or an onsite symmetry (such as spin rotations) G must also permute the MES: these symmetries leave the entanglement entropy invariant, so under G the MES remain local minima of the entanglement entropy. When G acts on an anyon, it can also be transformed into some other anyon, $G : b \rightarrow Gb$. Since $G\mathcal{F}_y^b G^{-1} \propto \mathcal{F}_y^{Gb}$ while $\mathcal{F}_y^b \mathcal{F}_y^c \propto \mathcal{F}_y^{b \cdot c}$, there are constraints on the allowed permutations of the MES.

As an example, consider time-reversal \mathcal{T} in the double-semion model, where \mathcal{T} leaves the anyons $\mathbb{1}, b$ invariant, but exchanges the semions, $\mathcal{T} : s \leftrightarrow s'$. Referring to Fig. 1, we see that the permutation \mathcal{T} must act like a reflection across the diagonal, exchanging s edges and s' .

Finally we consider translations T_x along the length of the cylinder, taking an entanglement point of view on the LSM theorem. Again, T_x can only permute the MES, because the MES are the unique basis states which are not long-range correlated along the length x of the cylinder, and T_x cannot generate long-range correlations. In fact, T_x is equivalent to threading topological flux $\mathcal{F}_x^{aL_y}$, where a is the anyon in each unit cell and L_y is the circumference of the cylinder, because T_x transfers L_y of the a through the cylinder. The commutator $\mathcal{F}_y^{b^{-1}} T_x^{-1} \mathcal{F}_y^b T_x$ is equivalent to an anyon b encircling an annular region of $1 \times L_y$ unit cells. As discussed, the result is a robust phase $\eta_b^{L_y}$. Using Eq.(1), $\eta_b = S_{ba}/S_{b\mathbb{1}}$, combined with Eq. (2) and the non-degeneracy of braiding, we find $T_x \propto \mathcal{F}_x^{aL_y}$.

To understand the further constraints on the permutation T_x (and hence on the special anyon a) we examine the entanglement properties for bipartitions at different x . Let ρ_x be the reduced density matrix for the system to the left of x (leaving the dependence on the particular MES implicit). If the state is symmetric (there is always at least one MES which is symmetric [21]), then under \mathcal{T} or an $SO(3)$ spin rotation R , ρ_x

transforms as

$$\mathcal{T} : \rho_x \rightarrow U_{\mathcal{T};x} \rho_x^* U_{\mathcal{T};x}^\dagger, \quad R : \rho_x \rightarrow U_{R;x} \rho_x U_{R;x}^\dagger \quad (3)$$

where $U_{\mathcal{T};x}, U_{R;x}$ are unitary matrices. It is known that the U are a *projective* representation of the symmetries. [34–36] For \mathcal{T} there are two possibilities,

$$U_{\mathcal{T};x} U_{\mathcal{T};x}^* = \gamma_x, \quad \gamma_x = \pm 1 \quad (4)$$

independent of whether the microscopic degrees of freedom transform as $\mathcal{T}^2 = \pm 1$. For rotations R , the $U_{R;x}$ can either be decomposed into integral representations of $\text{SO}(3)$, which we denote by $S_x = 1$, or half-integral representation of $\text{SO}(3)$, which we denote $S_x = -1$.

We make use of the odd number of $S = \frac{1}{2}$ per unit cell by calculating the dependence of γ_x, S_x on the location of the cut x . Consider a cylinder with odd, but arbitrarily large, circumference, so that each ring of the cylinder transforms as $\mathcal{T}^2 = -1$ and with half-integral spin. Since the reduced density matrices for ρ_x, ρ_{x+1} differ by the addition of a single ring, it is straightforward to prove [36] that

$$\gamma_{x+1} = -\gamma_x, \quad S_{x+1} = -S_x. \quad (5)$$

Intuitively, every time the entanglement cut passes a spin, the entanglement invariants flip, since the spins transform with $\gamma = S = -1$ themselves. However, the cuts at $x, x+1$ are related by the translation T_x , so the state must double the unit cell - this is a version of the LSM theorem. A similar phenomena occurs whenever the unit-cell transforms projectively under a symmetry.[36] The case of $U(1)$ at fractional filling is somewhat distinct, but the conclusion equivalent [21].

Tying these strings together, we argued that T_x is a permutation equivalent to threading some Abelian flux, $T_x \propto \mathcal{F}_x^{aL_y}$. For odd L_y , T_x flips the entanglement invariants, so a must be non-trivial. When an anyon a crosses an entanglement cut during the process \mathcal{F}_x^a , the entanglement invariants γ_x/S_x flip *if and only if* a transforms as $\mathcal{T}^2 = -1$ / with half-integral spin. More generally, we conclude that a must transform with the same projective representation or $U(1)$ fractional charge as the unit cell; this is the precise meaning of criteria **2**), that a can ‘screen’ the charge of the unit cell. Criteria **1**) follows from $T_x \mathcal{T} = \mathcal{T} T_x$.

Returning to the double-semion model, examining Fig.1 we see that the only non-trivial choice consistent with time-reversal is $T_x \propto \mathcal{F}_x^{bL_y}$. But the bosonic excitation must have integral spin and $\mathcal{T}^2 = 1$, so when a boson b passes an entanglement cut at x it does *not* flip the entanglement invariants γ_x, S_x . But if \mathcal{F}_x^b leaves these invariants unchanged, while T_x flips them, we arrive at a contradiction.

Several recent works have examined the possibility of double-semion quantum spin liquids on lattices including the Kagome model. These works were partially motivated by numerical evidence that there is a chiral spin liquid adjacent to the $S = \frac{1}{2}$ Kagome Heisenberg anti-ferromagnetic phase, with tentative evidence that the two phases may be related by a

continuous transition. [37–40] There is a natural scenario for a continuous phase transition between a double-semion theory and a chiral spin-liquid. [41]

These theoretical studies found exactly solvable quantum-dimer models with double-semion topological order.[42–44] In the dimer picture, these double-semion states preserve translation, time reversal, and $\text{SO}(3)$. But this is not a counter example to our no-go argument, because the dimer picture loses track of the $S = \frac{1}{2}$ nature of the constituent spins.

In fact, Ref. 43 provides intriguing evidence for the no-go argument. A dimer wavefunction can be translated into a $S = \frac{1}{2}$ wavefunction, but this requires choosing a particular dimer reference configuration. While the reference configuration breaks translation invariance, when this procedure is applied to the RVB state with the topological order of the Z_2 toric-code, the resulting state is translation invariant. However, when applied to the double-semion RVB, there is an *observable* doubling of the unit cell which could not be removed within the variational space considered. In light of the no-go argument it appears this is an intrinsic feature of the $S = \frac{1}{2}$ Kagome model.

In conclusion, we have argued that symmetries enforce a new type of constraint on the topological order of a Mott insulator. Like Lieb-Schultz-Mattis and its extensions, this result is a helpful ally in the hunt for spin liquids since local order parameters cannot be used to distinguish between topological orders.

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