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Universal Wave-Function Overlap and Universal Topological Data from Generic Gapped Ground States

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We propose a way—universal wave-function overlap—to extract universal topological data from generic ground states of gapped systems in any dimensions. Those extracted topological data might fully characterize the topological orders with a gapped or gapless boundary. For nonchiral topological orders in (2 + 1)D, these universal topological data consist of two matrices $S$ and $T$, which generate a projective representation of $SL(2,\mathbb{Z})$ on the degenerate ground state Hilbert space on a torus. For topological orders with a gapped boundary in higher dimensions, these data constitute a projective representation of the mapping class group $MCG(M^d)$ of closed spatial manifold $M^d$. For a set of simple models and perturbations in two dimensions, we show that these quantities are protected to all orders in perturbation theory. These overlaps provide a much more powerful alternative to the topological entanglement entropy and allow for more efficient numerical implementations.

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Since the discovery of the fractional quantum Hall effect \cite{1,2} and the theoretical study of chiral spin liquids \cite{3,4}, it has been known that new kinds of orders beyond Landau symmetry breaking orders exist for gapped states of matter, called topological order \cite{5,6}. Topological order can be thought of as the set of universal properties of a gapped system, such as (a) the topology-dependent ground state degeneracy \cite{5,6} and (b) the non-Abelian geometric phases $S$ and $T$ of the degenerate ground states \cite{7,8,9,10}, which are robust against any local perturbations that can break any symmetries \cite{6}. This is just like superfluid order, which can be thought of as the set of universal properties, zero viscosity and quantized vorticity, that are robust against any local perturbations that preserve the $U(1)$ symmetry. It was proposed that the non-Abelian geometric phases of the degenerate ground states on the torus classify $(2 + 1)$D topological orders \cite{7}.

Interestingly, it turns out that nontrivial topological order is related to long-range quantum entanglement of the ground state \cite{10}. These long-range patterns of entanglement are responsible for the interesting physics, such as quasiparticle excitations with exotic statistics, completely robust edge states, as well as the universal ground state degeneracy and non-Abelian geometric phases mentioned above.

Our current understanding is that topological order in $2 + 1$ dimensions is characterized by a unitary modular tensor category (UMTC), which encodes particle statistics and gives rise to representations of the Braid group \cite{11}, and the chiral central charge $c_-$, which encodes information about chiral gapless edge states \cite{12,13}.

While the algebraic theory of $(2 + 1)$D topological order is largely understood, it is natural to ask whether it is possible to extract topological data from a generic nonfixed point ground state. One such proposal has been through using the non-Abelian geometric phases $S$ and $T$ \cite{7,8,9,10,11,12}. Another is using the entanglement entropy \cite{18,19}, which has the generic form in $2 + 1$ dimensions $S = aL - \gamma + O(1/L)$, where $\gamma$ is the topological entanglement entropy (TEE). It turns out that $\gamma = \log D$, where $D$ is the total quantum dimension and thus a universal topological property of the gapped phase. A generalization of TEE to higher dimensions was proposed in Ref. \cite{20}.

Here, we would like to propose a simple way to extract data from nonfixed point ground states that could potentially fully characterize the underlying Topological Quantum Field Theory (TQFT). We conjecture that for a system on a $d$-dimensional manifold $M^d$ of volume $V$ with the set of degenerate ground states $\{|\psi_{\alpha}\rangle\}_{\alpha=1}^V$, the overlaps of the degenerate ground states have the following form \cite{21,22}

$$
\langle \psi_\alpha | \hat{O}_A | \psi_\beta \rangle = e^{-\alpha V + a(1/V)} M^A_{\alpha,\beta},
$$

where $\hat{O}_A$, labeled by the index $A$, are transformations of the wave functions induced by the automorphism transformations of the space $M^d \rightarrow M^d$, $a$ is a nonuniversal constant, and $M^A$ is a universal unitary matrix [up to an overall $U(1)$ phase]. The $M^A$ form a projective representation of the automorphism group of the space $M^d$—AMG($M^d$), which is robust against any perturbations. We propose that such projective representations for different space topologies are universal topological data and that they might fully characterize topological orders with finite ground state degeneracy. The disconnected components of the automorphism group is the mapping class group $MCG(M^d) \equiv \pi_0[AMG(M^d)]$. We propose that projective representations of the mapping class group for
different space topologies are universal topological data and that they might fully characterize topological orders with a gapped boundary. (For a more general and a more detailed discussion, see Ref. [22]). For some more intuition behind our conjecture, see the Supplemental Material [23].

For a 2D torus $T^2$ the mapping class group $\text{MCG}(T^2) = \text{SL}(2, \mathbb{Z})$ is generated by a $90^\circ$ rotation $\tilde{S}$ and a Dehn twist $\tilde{T}$. The corresponding $M^A$ are the unitary matrices $S, T$, which generate a projective representation of $\text{SL}(2, \mathbb{Z})$. Compared to the proposal in Ref. [7–9], here we do not need to calculate the geometric phase for a family of ground states and only have to consider a much simpler calculation—a particular overlap (with the cost of a nonuniversal contribution with volume scaling). We will calculate this for the simple example of the $\mathbb{Z}_N$ topological state studied in Refs. [24–28] and investigate the universality of this under perturbations such as adding string tension.

We note that a UMTC that describes the statistics of the excitations in $(2 + 1)$D, can also gives rise to a projective representation of $\text{SL}(2, \mathbb{Z})$. We propose that the universal wave-function overlap (1) computes this projective representation. The representation is generated by two elements $S$ and $T$ satisfying the relations

$$(ST)^3 = e^{i(2\pi/8)c} C, \quad S^2 = C, \quad (2)$$

where $C$ is a so-called charge conjugation matrix and satisfies $C^2 = 1$. Furthermore, we have that $(1/D) \sum a^2 \theta_a = e^{i(2\pi/8)c}$, where $d_a$ and $\theta_a$ are the quantum dimension and topological spin of quasiparticle $a$, respectively. This shows that the UMTC, or particle statistics, fixes the chiral central charge mod 8. This constitutes a projective representation of $\text{SL}(2, \mathbb{Z})$ on the ground state subspace on a torus, which encodes how the ground states transform under large automorphisms $\text{MCG}(T^2)$. We believe that our higher dimensional universal quantities (1) also encode information about the topological order in the ground state.

**Construction of degenerate set of ground states from local tensor networks.**—Since topological order exists even on topologically trivial manifolds, all of its properties should be available from a local wave function. But we need to sharpen what we mean by local wave functions, since wave functions typically depend on global data such as boundary conditions. Amazingly, there exists a surprisingly simple local representation of globally entangled states using tensor network language. In particular, a tensor network state (TNS) known as Projected Entangled Pair States (PEPS) is given by associating a tensor $T_{\alpha\beta\gamma}(a\beta\gamma\ldots)$ to each site $i$, where $\sigma_i$ is a physical index associated with the local Hilbert space, and $\alpha, \beta, \gamma$ are inner indices and connect to each other to form a graph. Using this representation, the wave function is given by

$$|\psi\rangle = \sum_{\{\sigma_i\}} \text{tTr}(T_{\alpha\beta\gamma}(1\beta\gamma\ldots)|\sigma_1, \sigma_2, \ldots). \quad (3)$$

where $\text{tTr}(\cdots)$ contracts the tensor indices in the tensor product network. By choosing the dimension of the inner indices large enough, one can approximate any state arbitrarily well. This particular representation is especially interesting for the study of gapped states since it automatically satisfies the area law, a property that gapped ground states are known to have [29,30]. One can think of the TNS as a parametrization of the interesting submanifold of the Hilbert space, where the ground states of the local gapped Hamiltonians live.

The local tensor representation of wave functions is however not enough; it must be equipped with a gauge structure [31]. Surprisingly, local variations of a tensor do not always correspond to local perturbations of the Hamiltonian and can change the global topological order. In order to approximate the ground state of a Hamiltonian with topological order with a gauge group $G$, it is important to search within the set of variational tensors with symmetry $G$. Arbitrarily small $G$ breaking variations might lead to tensor networks that can approximate local properties of a system well but give wrong predictions about the global properties.

In Ref. [32] a few concepts were introduced to characterize the symmetry structure of a TNS, in particular, the $d_{\text{space}}$-IGG, which is the group of intrinsically $d_{\text{space}}$-dimensional gauge transformations on the inner indices that leave the tensors invariant. It was in particular shown that in the case of the two-dimensional $\mathbb{Z}_2$ topological state we have $2$-IGG = $\mathbb{Z}_2$. Furthermore, it was shown that $2$-IGG contains information about string operators and can be used to construct the full set of degenerate ground states on the torus from a local tensor representation [33].

Thus, the local data we need are the local tensor + gauge structure. From this gauge structure we can twist the tensor to get the full set of ground states on a torus [32,34,35]. We shall call the natural basis we get from such a procedure the twist basis.

We will in the following consider the $\mathbb{Z}_N$ topological state. We can construct a local tensor for this state in the following way. Let the physical spins live on the links of the lattice, and give each link an orientation as in Fig. 1(b). Put a tensor $T_{\alpha\beta\gamma\delta}(\sigma_1, \sigma_2, \ldots)$ on each site and require that

$$[a] = [a][a][a] = [a][a][a] = [a][a][a]. \quad (4)$$

where $[a]$ is a local tensor.

![FIG. 1.](image-url) (a) Lattice under consideration, with the spins living on the links. (b) Tensor network for $\mathbb{Z}_N$ gauge theory. The lattice is chosen with the orientation shown. The tensors live on the lattice sites and the dots represent the physics indices. (c) Symmetry of the $\mathbb{Z}_N$ tensor.
$T_{\alpha \beta}^{(\alpha \beta)} = 1$, if $\beta + \gamma - \alpha - \delta = 0 \mod N$, (4)

otherwise $T_{\alpha \beta}^{(\alpha \beta)} = 0$. This tensor has a $\mathbb{Z}_N$ symmetry given by the tensors [see Fig. 1(c)]

$$\alpha \rightarrow \alpha + 2\pi i, \quad \beta \rightarrow \beta = \delta_{\alpha \beta} e^{-2\pi i \alpha}.$$}

$\mathbb{Z}_N$ topological order.—Equipped with the ground states from the local tensors, one can calculate the overlap (1) to extract the universal topological properties. As a simple example, let us calculate the overlap (1) for the case of $\mathbb{Z}_N$ topological state on the lattice in Fig. 1(a).

For this simple example we will not use the tensor product representation for simplicity, since it can be calculated directly. See Ref. [37] for the calculation of Eq. (1) using the tensor network and gauge structure. Let there be a local Hilbert space $\mathcal{H}_a \cong C[\mathbb{Z}_N] \cong C^N$ associated with each link $a \in \Omega$ with basis $\{|\sigma_a\rangle\}_{\sigma_a \in \mathbb{Z}_N}$.

We will represent a spin configuration $\{|\sigma_a\rangle, \sigma_a = \ldots\}$ on a string picture, where the state on link $a \in \Omega$ is represented by an oriented string of type $\sigma_a \in \mathbb{Z}_N$ with a chosen orientation, and $|0\rangle$ corresponds to no string. There is a natural isomorphism $\mathcal{H}_a \cong \mathcal{H}_a^*$ for link $a$ and its reversed orientation $a^*$ by $|\sigma_a\rangle \mapsto |\sigma_a^\prime\rangle = |\bar{\sigma}_a\rangle$.

The ground state Hilbert space of the $\mathbb{Z}_N$ topological order consists of an equal superposition of all closed-string configurations that satisfy the $\mathbb{Z}_N$ fusion rules.

The string-net ground state Hilbert space on $\mathbb{T}^2$ can be algebraically constructed in the following way. Let $\Lambda^N_\Delta$ denote the set of triangular plaquettes and for each $p \in \Lambda^N_\Delta$ define the string operator $B_p^\Delta$ that acts on the links bounding $p$, with clockwise orientation, by $|\sigma\rangle \mapsto |\sigma + 1 \mod N\rangle$. The set of all contractable closed loop configurations can be thought of as the freely generated group $G_{\text{free}}^\Delta = \langle \{B_p^\Delta\}_{p \in \Lambda^N_\Delta} \rangle$, modulo the relations $(B_p^\Delta)^N \sim 1, \prod_{p \in \Lambda^N_\Delta} B_p^\Delta \sim 1$, and $B_p^\Delta B_q^\Delta \sim B_q^\Delta B_p^\Delta$, denoted as $G^\Delta_{\text{free}} = G_{\text{free}}^\Delta/\sim$. Similarly we let the subgroup $G^\Delta_0 \subset G^\Delta_{\text{free}}$ correspond to closed loop configurations on the square lattice links. For the ground states on the torus, we need to introduce two new operators $W_x$ and $W_y$, corresponding to noncontractable loops along the two cycles of $T^2$. These satisfy $(W_i^\Delta)^N = 1, i = x, y$. With these, we can construct the group $G^\Delta_0$, corresponding to closed string configurations with $(\alpha, \beta)$ windings along the cycle $(x, y)$, modulo $N$. Similarly, let $G_\Delta$ be the group of all possible closed string configurations on the torus. These states are orthonormal $\langle g_{ab} | g_{ab} \rangle = \delta_{g_{ab}, g_{ab}}$.

The $N^2$-dimensional ground state Hilbert space is then spanned by the following vectors $\{|\alpha \beta\rangle = |G^\Delta_0|^{-1/2} \sum_{g_{ab} \in G^\Delta} |g_{ab}\rangle\}$, where $\alpha, \beta = 0, \ldots, N - 1$. The construction can trivially be extended to higher-genus surfaces. This is the string-net basis for the $\mathbb{Z}_N$ gauge theory. The ground states in the twist basis corresponding to the tensor (4) are just the eigenbasis of the operators $W_x$ and $W_y$. These are given by

$$\langle \psi_{ab} \rangle = \frac{1}{\sqrt{|G^\Delta|}} \sum_{g_{ab} \in G^\Delta} e^{i\alpha a_0(g) + i\beta b_0(g)} |g\rangle,$$

where $\gamma = e^{-2\pi i / N}$ and $a_i$ count how many times the string configuration $g$ wraps around the $i$th cycle. Note that $W_x |\psi_{ab}\rangle = e^{2\pi i / N a} |\psi_{ab}\rangle$ and $W_y |\psi_{ab}\rangle = e^{2\pi i / N b} |\psi_{ab}\rangle$. For later use, note that $|G^\Delta_0| = N|\Lambda_\Delta^0|^{-1} = N^{2L^2 - 1}$, $|G^\Delta| = N|\Lambda_\Delta^0|^{-1} = N^{L^2 - 1}$, $|G_\Delta| = N^2 |G^\Delta_0|$, and $|G_\Box| = N^2 |G^\Delta_0|$. The $S$ and $T$ matrices from the ground state.—We can now define two nonlocal operators on our Hilbert space $\hat{S}_S, \hat{S}_T: \mathcal{H} = \mathcal{H}$ as in Fig. 2, mimicking the generators of the torus mapping class group in the continuum. Here, $\hat{S}_S$ maps any spin configuration to the 90 deg rotated configuration. $\hat{S}_T$ corresponds to a shear transformation and is defined as in Fig. 2. It is clear that since we are on the lattice, these operators will not preserve the subspace of closed string configurations. We can easily calculate the matrix elements of $\hat{S}_T$ and $\hat{S}_S$ between ground states. In both cases, only $|G_\Box\rangle$ configurations have a nonzero overlap with the undeformed ground state. For the $S$ transformation we find the overlap (see Fig. 3)

$$\langle \psi_{ab} | \hat{S}_S | \psi_{\bar{a} \bar{b}} \rangle = \delta_{a, \bar{b}} \delta_{\bar{b}, -\bar{a}} |G_\Box| = S_{ab, \bar{a} \bar{b}} e^{-\log(N)L^2},$$

where we have defined the modular $S$ matrix $S_{ab, \bar{a} \bar{b}} = \delta_{a, \bar{b}} \delta_{\bar{b}, -\bar{a}}$. Similarly we have $\langle \psi_{ab} | \hat{S}_T | \psi_{\bar{a} \bar{b}} \rangle = T_{ab, \bar{a} \bar{b}} e^{-\log(N)L^2}$, where the modular $T$ matrix is given by $T_{ab, \bar{a} \bar{b}} = \delta_{a, \bar{a}} \delta_{\bar{b}, b}$. One can readily check that these satisfy Eq. (2) with $c_2 = 0 \mod 8$ and $G_{ab, \bar{a} \bar{b}} = \delta_{a, -a} \delta_{b, \bar{b}}$. Thus, this forms a projective representation of the modular group $SL(2, \mathbb{Z})$.

In order to use Verlinde’s formula and generate the relevant UMTC, we need to put the modular matrices in the

FIG. 2 (color online). Definition of $S$ and $T$ transformations. The $S$ transformation corresponds to rotating configurations 90 deg, while $T$ corresponds to a shear transformation. Note that this transformation does not leave the space of closed loop configurations invariant.
FIG. 3 (color online). In the string-net basis, a modular $S$ transformation flips the topological sectors $(\alpha, \beta) \rightarrow (\beta, -\alpha \mod N)$, while a $T$ transformation has the effect $(\alpha, \beta) \rightarrow (\alpha, \alpha + \beta \mod N)$.

quasiparticle basis [38]. This is done as follows: for the $\mathbb{Z}_N$ theory there are noncontractable magnetic operators on the dual lattice satisfying $(\Gamma^a)^N = 1$, and with the commutation relations $W_x \Gamma_x = e^{-i2\pi/|N|} \Gamma_x W_x$ and $W_y \Gamma_y = e^{-i2\pi/|N|} \Gamma_y W_y$. The basis we are after corresponds to having a well-defined magnetic and electric flux through one direction of the torus. In the eigenbasis of $W_y$ and $\Gamma_y$, $|\phi_{mn}\rangle$, we find

$$S_{mn, \bar{m} \bar{n}} = \frac{1}{N} e^{-i2\pi/(N)(m \bar{n} + n \bar{m})},$$

$$T_{mn, \bar{m} \bar{n}} = \delta_{m, \bar{m}} \delta_{n, \bar{n}} e^{-i2\pi/(N)mn},$$

the well-known modular matrices for the $\mathbb{Z}_N$ model.

Perturbed $\mathbb{Z}_N$ model.—We will now consider a local perturbation to the $\mathbb{Z}_N$ topological state. One interesting perturbation is to add a magnetic field of the form

$$h \Gamma = \frac{J}{2} \sum_{\sigma \in \Omega} (Z_\alpha + Z'_\alpha),$$

where $Z_\alpha = \sigma _\alpha = e^{i2\pi/(N)\sigma _\alpha}$ [40]. This perturbation breaks the exact solvability of the model, but essentially corresponds to introducing string tension to each closed string configuration. This can be implemented by a local deformation of the ground states of the form

$$|\psi_{ab}\rangle_A = \frac{1}{\sqrt{|G_\Delta|}} \sum_{g \in G_\Delta} A^{-L(g)} e^{i\alpha_{ab}(g) + \beta \gamma_{ab}(g)} |g\rangle,$$

where $A$ is a variational parameter. Furthermore, $L(g) = \sum_{\sigma \in \Omega} \frac{1}{2} \left|1 - \cos \left(2\pi/(N)\sigma_g\right)\right|$, which is just the total string length for $N = 2$.

Performing an $S$ transformation, we find the overlap

$$A (|\psi_{ab}\rangle \hat{\mathcal{S}} |\psi_{\bar{a} \bar{b}}\rangle)_A = \frac{1}{|G_\Delta|} \sum_{g \in G_\Delta} A^{-L(g)} \sum_{\beta = 0}^{N-1} \sum_{\sigma \in \Omega} A^{-L(g)} |\sigma\rangle.$$
this direction is now essentially local. By such a local perturbation, one can break the ground state degeneracy from $N^d$ down to $N^2$. One can directly show that the generators for an $\text{SL}(2,Z) \leq \text{SL}(3,Z)$ subgroup exactly reduce to the 2D $S$ and $T$ matrices [42].

Conclusion.—In this Letter we have conjectured a universal wave-function overlap (1) for gapped systems in $d$ dimensions, which gives rise to projective representations of the mapping class group $\text{MCG}(M^d)$, for any manifold $M^d$. These quantities contain more information than the topological entanglement entropies [18–20], and might characterize the topological order completely, as in two dimensions [7]. In a following paper [37], we will numerically study the overlaps (1) for simple two-dimensional models and show that the universal quantities are very robust against perturbations and unambiguously characterize phase transitions. In Ref. [42] we study the universal quantities (1) for three-dimensional systems.

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[33] A related concept for a finite group $G$ is $G$-injective PEPS [34]. A $G$-injective tensor is a tensor that is invariant under a $G$ action on all inner indices simultaneously, together with the property that one can achieve any action on the virtual indices by acting on the physical indices. It was shown that these tensors are ground states of a parent Hamiltonian with TEE $\gamma = \log |G|$. This class of PEPS describes the universality class of quantum double models $D(G)$. Recently, this was generalized to $(G,\omega)$-injective PEPS [35], where the action of $G$ is twisted by a 3-cocycle of $\omega$ of $G$. It was shown that these PEPS describe topological order in the universality class of Dijkgraaf-Witten TQFTs [36] and only depend on the cohomology class $[\omega] \in H^3(G,\mathbb{U}(1))$ of $\omega$.
[38] In general, we do not have a gauge theory and need another way to find the modular matrices in the right basis. One way is to find a basis that satisfies certain special properties. In Ref. [39] it was shown for several examples that this basis is unique and leads to the right form of $S$ and $T$.
[40] See Ref. [27] for an analysis of models of this type.