**Modular matrices from universal wave-function overlaps in Gutzwiller-projected parton wave functions**

The MIT Faculty has made this article openly available. **Please share** how this access benefits you. Your story matters.

<table>
<thead>
<tr>
<th>Citation</th>
<th>Mei, Jia-Wei, and Xiao-Gang Wen. “Modular Matrices from Universal Wave-Function Overlaps in Gutzwiller-Projected Parton Wave Functions.” Phys. Rev. B 91, no. 12 (March 2015). © 2015 American Physical Society</th>
</tr>
</thead>
<tbody>
<tr>
<td>As Published</td>
<td><a href="http://dx.doi.org/10.1103/PhysRevB.91.125123">http://dx.doi.org/10.1103/PhysRevB.91.125123</a></td>
</tr>
<tr>
<td>Publisher</td>
<td>American Physical Society</td>
</tr>
<tr>
<td>Version</td>
<td>Final published version</td>
</tr>
<tr>
<td>Accessed</td>
<td>Fri Jan 25 02:53:53 EST 2019</td>
</tr>
<tr>
<td>Citable Link</td>
<td><a href="http://hdl.handle.net/1721.1/96153">http://hdl.handle.net/1721.1/96153</a></td>
</tr>
<tr>
<td>Terms of Use</td>
<td>Article is made available in accordance with the publisher’s policy and may be subject to US copyright law. Please refer to the publisher’s site for terms of use.</td>
</tr>
<tr>
<td>Detailed Terms</td>
<td></td>
</tr>
</tbody>
</table>
Modular matrices from universal wave-function overlaps in Gutzwiller-projected parton wave functions

Jia-Wei Mei\textsuperscript{1} and Xiao-Gang Wen\textsuperscript{1,2}
\textsuperscript{1}Perimeter Institute for Theoretical Physics, Waterloo, Ontario, Canada N2L 2Y5
\textsuperscript{2}Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

(Received 6 October 2014; revised manuscript received 22 February 2015; published 12 March 2015)

We implement the universal wave-function overlap (UWFO) method to extract modular $S$ and $T$ matrices for topological orders in Gutzwiller-projected parton wave functions (GPWFs). The modular $S$ and $T$ matrices generate a projective representation of $SL(2,Z)$ on the degenerate-ground-state Hilbert space on a torus and may fully characterize the $2+1$D topological orders, i.e., the quasiparticle statistics and chiral central charge (up to $E_8$ bosonic quantum Hall states). We use the variational Monte Carlo method to computed the $S$ and $T$ matrices of the chiral spin liquid (CSL) constructed by the GPWF on the square lattice, and we confirm that the CSL carries the same topological order as the $v = \frac{1}{2}$ bosonic Laughlin state. We find that the nonuniversal exponents in the UWFO can be small, and direct numerical computation can be applied on relatively large systems. The UWFO may be a powerful method to calculate the topological order in GPWFs.

DOI: 10.1103/PhysRevB.91.125123

PACS number(s): 75.10.Kt, 05.30.Pr, 73.43.--f

Topological order [1–3] connotes the pattern of long-range entanglement in gapped many-body wave functions [4–6]. It describes gapped quantum phases of matter that lie beyond the Landau symmetry breaking paradigm [7]. Local unitary transformations on many-body wave functions can remove local entanglement, however they preserve long-range topological entanglement. Therefore, a topological ordered state is not smoothly connected to a trivial (direct product) state by local unitary transformations [6]. Physically, topological order is described through topological quantum numbers, such as nontrivial ground-state structures and fractional excitations [1–3,8–10]. These topological properties are fully characterized by the quasiparticle (anyon in the bulk) statistics [8–10] and the chiral central charge, which encodes information about chiral gapless edge states [11,12].

Both the fusion rule and the topological spin of quasiparticles as well as the chiral central charge are characterized in the non-Abelian geometric phases encoded in the degenerate ground states [1–3,13–17], and vice versa. The non-Abelian geometric phases form a representation of $SL(2,Z)$ that is generated by $90^\circ$ rotation and Dehn twist on a torus; they are called modular $S$ and $T$ matrices, respectively [13,14]. The element of the modular $S$ matrix determines the mutual statistics of quasiparticles, while the element of the $T$ matrix determines the topological spin $\theta_a \in U(1)$ and the chiral central charge [13,14].

\[ N_{ab}^c = \sum_{\delta} N_{a\delta}^b N_{\delta c} \]

The central charge $c$ determines the thermal current of the edge state, $I_L = \frac{c}{2\pi} T^2$, at temperature $T$ [20] and is fixed up to $E_8$ bosonic quantum Hall states.

To fully characterize topological order, various numerical methods are proposed to access the modular $S$ and $T$ matrices from ground-state wave functions [21–26]. By braiding quasiholes, the modular $S$ and $T$ can be extracted from the Berry matrices [27–29]. Recently, one of us proposed the universal wave-function overlap (UWFO) method to calculate modular matrices [16,30]. For a given set $\{ |\psi_a \rangle \}_{a=1}^N$ of degenerate ground-state wave functions, it provides us with a practical method to extract the modular $S$ and $T$ matrices,

\[ S_{ab} = \langle \psi_a | \hat{S} | \psi_b \rangle = e^{-\alpha_{SL} L^2 + \alpha T^2} S_{ab}, \]

\[ T_{ab} = \langle \psi_a | \hat{T} | \psi_b \rangle = e^{-\alpha_{SL} L^2 + \alpha T^2} T_{ab}, \]

where $\hat{S}$ and $\hat{T}$ are the operators that generate the $90^\circ$ rotation and Dehn twist, respectively, on a torus with the $L^2$ lattice size. The exponentially small prefactor makes it difficult to numerically calculate the UWFO in (1). To avoid the exponential smallness, a gauge-symmetry preserved tensor renormalization method has been developed for the tensor-network wave functions [16,17], where the system size is effectively reduced as zero after the tensor renormalization.

Actually, in this paper, we will show that the nonuniversal exponent $\alpha_{T,S}$ can be small such that the UWFO can be directly numerically calculated on relatively large systems. We will take a chiral spin liquid (CSL) wave function on the square lattice [31] as an explicit example to extract the modular $S$ and $T$ matrices from the UWFO. We construct the set of ground states for a CSL by using Gutzwiller-projected parton wave functions (GPWF) [21,31–34]. We use the variational Monte Carlo method to calculate the UWFO for the CSL wave functions. The hopping parameters are set as $|t_1|/|t_0| = 0.5$ for the CSL on the $\pi$-flux square lattice, where $t_0$ and $t_1$ for nearest-neighbor and next-nearest-neighbor links, respectively. Due to $C_4$ symmetry, the overlap $S$ in Eq. (1) has a vanishing exponent $\alpha_S = 0$. $T$ in Eq. (1) has the relatively small nonuniversal complex exponent $\alpha_T = 0.04208 + 0.4809i$, and the direct
numeric computation is carried out on relatively large systems up to a 12 × 12 lattice size in this paper. The CSL is the lattice analogy of the \( v = \frac{1}{2} \) bosonic Laughlin state [31,32]. The parent Hamiltonians for CSL are also proposed in Refs. [35,36]. Our numerical results confirm the analogy by directly extracting the modular \( S \) and \( T \) matrices from the UWFO.

In the parton construction, the \( S = \frac{1}{2} \) spin operator is written in terms of fermionic parton operators, \( S^\sigma(z_i) = \frac{1}{2} f^\dagger_\sigma(z_i) \sigma_{\alpha \beta} f_{\alpha}(z_i) \). Here \( \sigma^\alpha (\sigma = x, y, z) \) is the Pauli matrices and \( f_{\alpha} (\alpha = \uparrow / \downarrow) \) is the isosite parton operator. We take the complex variables for the i-site coordinate, \( z_i = x_i + i y_i \), on a lattice. We have to impose the one-particle-per-site constraint for the partons, \( f^\dagger_\sigma(z_i) f_{\alpha}(z_i) + f^\dagger_\sigma(z_i) f_{\alpha}(z_i) = 1 \), such that the fermionic partons have the same Hilbert space on the i-site as the spin operators \( S^\sigma(z_i) \). The GPWF for the spin system can be read as

\[
|\Psi\rangle = \sum_{\{|z_i|\} } \mathcal{P}_G \Psi(|z_i^\dagger, z_i^\downarrow\rangle)|\{z_i\}\rangle,
\]

where \( |\{z_i\}\rangle \) is the spin configuration and \( \mathcal{P}_G \) is the Gutzwiller projection operator to impose the one-particle-per-site constraint for the fermionic partons.

The GPWF can be put on a torus by implying the equivalence conditions \( z \sim z + 1 \) and \( z \sim z + \tau \), where \( \tau = \tau_x + i \tau_y \) is a complex number. The principal region of a torus is bounded by the four points \( z = \frac{1}{2}(\pm 1 \pm \tau) \). Here the top and bottom and left and right sides are identified, respectively.

\[
\begin{align*}
\mathcal{P}_G & \Psi(|z_i^\dagger, z_i^\downarrow\rangle) = e^{i\frac{\pi}{\tau_y}}(Z - Z_0^\dagger |\tau\rangle \theta^\dagger_{\tau_y} (Z^\dagger - Z_0^\dagger |\tau\rangle) \\
& \times \mathcal{P}_G \prod_{i<j} \theta^\dagger_{\tau_y} (z_i^\uparrow - z_j^\downarrow |\tau\rangle) \prod_{k<l} \theta^\dagger_{\tau_y} (z_k^\uparrow - z_l^\downarrow |\tau\rangle),
\end{align*}
\]

where \( \theta_{\alpha,\beta}(z |\tau\rangle) \) is the theta function and \( Z_0 \) is the center-of-mass coordinate. Different ground states are specified by the different zeros, \( Z_0 \), in the center-of-mass wave functions. The zeros are determined by the general boundary conditions [37,38]. The modular \( S \) and \( T \) matrices for the ideal GPWF in Eq. (4) can be analytically calculated by deformation of the mass matrix [14],

\[
S = \frac{1}{\sqrt{2}} (1 1 1) , \quad T = e^{-i \frac{\pi}{\tau_y}} (1 0 e^{i \frac{\pi}{\tau_y}})
\]

with the central charge \( c = 1 \), the same as those for the \( v = \frac{1}{2} \) bosonic Laughlin state.

In Ref. [31], the generic GPWF for a CSL is written as

\[
\mathcal{P}_G \Psi(|z_i^\dagger, z_i^\downarrow\rangle) = \mathcal{P}_G \det \varphi_{\sigma}(z_i^\dagger) \det \varphi_{\sigma}(z_i^\downarrow) ,
\]

where \( \det \varphi_{\sigma}(z_i^\dagger / z_i) \) is the determinate wave function for the fermionic partons filling the valence bands of the tight-binding model,

\[
H_{MF} = - \sum_{i,j,\sigma} t(z_i, z_j) f^\dagger_{\sigma}(z_i) f_{\sigma}(z_j) + H.c. ,
\]

on the \( \pi \)-flux square lattice with both nearest-neighbor and next-nearest-neighbor hopping amplitude [31]. There are \( \frac{\pi}{\tau_y} \) fluxes in every triangle in the plaquette, e.g., \( \Delta_{123} \) in \( \Delta_{123} \) in Fig. 1, \( \Phi(\Delta_{123}) = \arg(t_{12}, t_{23}, t_{13}) = \frac{\pi}{\tau_y} \). Different ground-state wave functions can be obtained by different general boundary conditions. For the spin operator, the boundary condition is

\[
S^\sigma(z_i + 1) = e^{i\phi^\sigma} S^\sigma(z_i) , \quad S^\sigma(z_i + \tau) = e^{i\phi^\sigma} S^\sigma(z_i) .
\]

Due to fractionalization in the GPWF [39,40], the partron has the boundary condition

\[
f^\dagger_{\sigma}(z_i + 1) = e^{i\frac{\pi}{\tau_y}} f^\dagger_{\sigma}(z_i) , \quad f^\dagger_{\sigma}(z_i + \tau) = e^{i\frac{\pi}{\tau_y}} f^\dagger_{\sigma}(z_i) ,
\]

with \( \sigma = \pm 1 \) for \( f^\dagger_{\uparrow / \downarrow} \). When we increase \( \Phi_{1/2} \) from 0 to 2\( \pi \), the spin operators are invariant, however the parton wave functions do not go back to themselves and lead to another ground state for the GPWF. Therefore, we have different ground states for a CSL labeled by the spin fluxes in the holes of a torus \( |\Phi^\uparrow, \Phi^\downarrow\rangle \),

\[
|\Psi_{\alpha}\rangle = \{|00\rangle, |02\pi\rangle, |2\pi0\rangle, |2\pi2\pi\rangle\}
\]

with \( \alpha = 1,2,3,4 \). Actually only two of them are linearly independent.

For the generic GPWF in Eq. (6), we use the UWFO in Eq. (1) to exact the modular matrices \( S \) and \( T \). To carry out the UWFO, we need calculate the following overlaps:

\[
P_{ab} = \langle \Psi_b | \Psi_a \rangle , \quad \hat{S}_{ab} = |\Psi_a \rangle |\Psi_b\rangle , \quad \hat{T}_{ab} = |\Psi_a \rangle |\Psi_b\rangle^\dagger ,
\]

where \( |\Psi_a\rangle \) is the state in Eq. (8) and \( |\Psi_b\rangle = \hat{S} |\Psi_b\rangle , |\Psi_b^\dagger\rangle = \hat{T} |\Psi_b\rangle \), where \( \hat{S} \) and \( \hat{T} \) are the 90° rotation and Dehn twist.
transformations in Eq. (3) on a torus. The \( P \) matrix has rank 2 with the numerical tolerance less than \( 10^{-3} \) implying twofold ground-state degeneracy. Given GPWFs, we implement the “sign trick” \([41]\) to calculate the overlap,

\[
\langle \Psi_a | \Psi_b \rangle = \sum_{\{z_i\}} \psi_a^*(z_i) \psi_b(z_i) 
\]

\[
\equiv \langle \Psi_a | \Psi_b \rangle_{\text{amp}} \langle \Psi_a | \Psi_b \rangle_{\text{sgn}}, \tag{10}
\]

where \( \psi_a(z_i) \) is the amplitude wave function of the spin configuration \( \{z_i\} \) in \( |\Psi_a\rangle \), and the sign term

\[
\langle \Psi_a | \Psi_b \rangle_{\text{sgn}} = \sum_{\{z_i\}} \rho_{ab} \psi_a^*(z_i) \psi_b(z_i) 
\]

\[
\equiv \langle \Psi_a | \Psi_b \rangle_{\text{sgn}} \tag{11}
\]

is calculated using the Monte Carlo method according to the weight \( \rho_{ab} = |\psi_a(z_i)|^2 \langle \psi_b(z_i) | \psi_b(z_i) \rangle \). The amplitude term is the normalization factor for weight \( \rho_{ab} \),

\[
\langle \Psi_a | \Psi_b \rangle_{\text{amp}} = \sum_{\{z_i\}} |\psi_a(z_i)|^2 \psi_b(z_i). \tag{12}
\]

Actually, we are only interested in the ratios of amplitudes. For example, for the \( P \) matrix in Eq. (9), we evaluate the matrix-element amplitude ratios

\[
\frac{\langle \Psi_a | \Psi_b \rangle_{\text{amp}}}{\langle \Psi_b | \Psi_b \rangle_{\text{amp}}} = \sum_{\{z_i\}} \rho_{ab;11} \sqrt{\frac{|\psi_a^*(z_i)|^2 |\psi_b(z_i)|^2}{|\psi_b(z_i)|^2 |\psi_b(z_i)|^2}} \tag{13}
\]

according to the Monte Carlo sampling weight \( \rho_{ab;11} = \sqrt{|\psi_a^*(z_i)|^2 |\psi_b(z_i)|^2} \). We then diagonalize the modular \( S \) and \( T \) matrices. We first diagonalize the \( P \) matrix,

\[
P = U^\dagger P_{\lambda} U, \quad U = (u_1, u_2, u_3, u_4). \tag{14}
\]

Only two eigenvectors (e.g., \( u_3 \) and \( u_4 \)) have nonzero eigenvalues around 2. These two states \( (u_3, u_4) \) are the linearly independent ground states. In terms of the normalized \( \tilde{U} = (u_3, u_4) \), the overlaps for \( \tilde{S} \) and \( \tilde{T} \) in Eq. (9) turn out to be \( 2 \times 2 \) square matrices,

\[
S_{12}^{12} = \tilde{O} \tilde{S}_{12} \tilde{O}^\dagger, \quad T_{12}^{12} = \tilde{O} \tilde{T}_{12} \tilde{O}^\dagger. \tag{15}
\]

Generally, \( T^1 \) is not diagonal since \( u_3 \) and \( u_4 \) are not the minimum entangled states or eigenstates of the Wilson loop operators \([21]\). We then diagonalize \( T_1 \) to obtain the minimum entangled states \( v_1 \) and \( v_2 \),

\[
T^1 = V^\dagger T^1 V, \quad S^1 = V^\dagger S^1 V, \quad V = (v_1, v_2). \tag{16}
\]

where \( T^1 \) is diagonal and the phases of \( V \) are fixed according to the conditions \( S_{12} = S_2^1 \) and \( S_{12}^1 > 0 \).

Since the CSL wave function has 90° rotation symmetry, the exponent in \( S^1 \) in Eq. (16) vanishes, \( \alpha_S = 0 \), which is confirmed in the numerical calculations. The UWFO of the \( T \) matrix has a complex exponent \( \alpha_T \) in the prefactor. The real part of the exponent \( \text{Re}(\alpha_T) \) is easily obtained from the amplitude of the

FIG. 2. (Color online) \( L^2 \)-dependent of amplitude and phase of \( T' \) in Eq. (16) are shown in (a) and (b), respectively. Here \( \text{Log}(\text{Amp}) \equiv \log(|T'_{11}|) \) and \( \frac{\beta}{\pi} \equiv \frac{\text{arg}(T_{11})}{2\pi} + k \) with \( k = 3.5, 8, 11 \) for \( L = 6, 8, 10, 12 \). In (c), we plot \( -\frac{\pi}{2} \text{Im}(\alpha_T) = 0.07632, 0.07654, 0.07664, 0.07676 \). The red dashed line is for \( c = 1 \). In (c), the numerical error bars are included and smaller than the symbols’ sizes.

\( T' \) in Eq. (16) by fitting \( \log(\text{amp}) \equiv \log(|T'_{11}|) \) with respect to \( L^2 \), \( \text{Re}(\alpha_T) = 0.04208 \), as shown in Fig. 2(a). The phase \( \theta \) is defined up to \( 2\pi \), \( \frac{\beta}{\pi} \equiv \frac{\text{arg}(T_{11})}{2\pi} + k \) with \( k \in \mathbb{Z} \). For \( L = 6, 8, 10, 12 \), the corresponding integers are \( k = 3.5, 8, 11 \). From the fitting in Fig. 2(b), we obtain \( \text{Im}(\alpha_T) = 0.4809 \). The central charge is sensitive to the exact value of
square lattice with three orbitals per site. A rotation symmetry, the exponents $\alpha_{S,T}$ in Eq. (1) are both finite. On the square lattice, we can also use the Kadanoff block renormalization procedure to reduce the system size $L^2 \rightarrow L^2$. Then the exponents in the prefactors of the UWFO can be significantly reduced. Many local unitary transformations on the lattice can potentially reduce the exponents in the UWFO. If different ground-state sectors have the same topological spins, we can follow Ref. [15] to identify the minimum entangled states to diagonalize the modular $T$ matrix. The UWFO method is easily generalized to the 3+1D topological orders in the GPWFs. The GPWF for quantum dimer models in three dimensions has already been constructed in Ref. [42]. In three dimensions, the modular group of the 3-torus is $SL(3,Z)$ generated by

$$\hat{S} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad \hat{T} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (18)$$

We can use the UWFO to directly study the topological information in 3+1D [16].

In conclusion, we use the universal wave-function overlap method to exact the modular $S$ and $T$ matrices for the topological order in the Gutzwiller-projected parton wave function for the chiral spin liquid state on the square lattice. The chiral spin liquid is the lattice analogy of the $v = \frac{1}{2}$ bosonic Laughlin state, and the analogy is directly confirmed by the modular $S$ and $T$ matrices from the universal wave-function overlap. The exponents in the prefactors of the wave-function overlaps are found to be small, and the variational Monte Carlo calculations are carried out on relatively large systems. The Monte Carlo calculations of the universal wave-function overlap can be easily generalized to other Bravais lattices and 3+1D topological orders.

X.-G.W. is supported by NSF Grant No. DMR-1005541 and NSFC 11274192. He is also supported by the BMO Financial Group and the John Templeton Foundation. Research at the Perimeter Institute is supported by the Government of Canada through Industry Canada and by the Province of Ontario through the Ministry of Research.