Numerical detection of symmetry enriched topological phases with space group symmetry

Ling Wang,1,2 Andrew Essin,1,2 Michael Hermele,3 and Olexei Motrunich2

1Institute for Quantum Information and Matter,
California Institute of Technology, Pasadena, California 91125, USA
2Department of Physics, California Institute of Technology, Pasadena, California 91125, USA
3Department of Physics, 390 UCB, University of Colorado, Boulder CO 80309, USA

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Topologically ordered phases of matter, in particular so-called symmetry enriched topological (SET) phases, can exhibit quantum number fractionalization in the presence of global symmetry. In \( \mathbb{Z}_2 \) topologically ordered states in two dimensions, fundamental translations \( T_x \) and \( T_y \) acting on anyons can either commute or anticommute. This property, crystal momentum fractionalization, can be seen in a periodicity of the excited-state spectrum in the Brillouin zone. We present a numerical method to detect the presence of this form of symmetry enrichment given a projected entangled pair state (PEPS); we study the minima of spectrum of correlation lengths of the transfer matrix for a cylinder. As a benchmark, we demonstrate our method using a modified toric code model with perturbation. An enhanced periodicity in momentum clearly reveals the nontrivial anticommutation relation \( \{T_x, T_y\} = 0 \) for the corresponding quasiparticles in the system.

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Topological order is the name given to a variety of long range entangled but gapped phases of matter, in particular to phases that support anyonic excitations with unusual braiding statistics. Unlike phases that fall within the Landau symmetry-breaking paradigm, topological order is defined without any reference to symmetry. However, it is still very interesting to ask what further phenomena emerge in systems with symmetry, either spontaneously broken or unbroken. The term “symmetry enriched topological” (SET) phases was proposed to describe phases that have the same topological order but are distinct in the presence of a symmetry \([1, 3]\).

In two dimensions the excitations in a topological phase are point-like anyons. When a symmetry is present, what are their quantum numbers? It turns out that these can be fractional; most prominently, anyons in quantum Hall states typically have fractional electric charge (the quantum number corresponding to a \( U(1) \) symmetry of the system) \([4, 5]\). The values of these quantum numbers are highly constrained, notably by the “fusion rules” of the topological theory; in the Laughlin quantum Hall state with filling fraction 1/3, since three anyons give back an electron, the anyons must have charge \( e/3 \). Another example is the spin fractionalization in spin liquid phases of quantum magnets with a global \( SU(2) \) symmetry: a spinon quasiparticle carries a fractional number spin-1/2 whereas in conventional paramagnets or magnetically ordered states all quasiparticles carry integer spin \([6]\).

Can one distinguish SET phases given a wavefunction? The quantum numbers of the degenerate ground states and the projective quantum numbers of quasiparticles are the characteristic properties of the SET phases \([2, 7, 9]\). In the case of detecting the projective quantum number of an internal symmetry, the operation of the global internal symmetry generator can be factorized into a product of local operators, which can be transformed into operators acting only on the entanglement cut of the system, therefore one can detect the projective quantum number via measuring the commutator/anti-commutator of the boundary quasiparticles \([10, 11]\). However for the space group symmetry, such as the translation symmetries, the translation operator is written in a matrix product operator that can not be factorized, and in addition, there is no way to make an entanglement cut that preserves both \( T_x \) and \( T_y \) translations, therefore conventional techniques do not work. In this Letter, we address this question for space group symmetries in the context of projected entangled pair states (PEPSs) \([12]\).

\( \mathbb{Z}_2 \) topological phases with translation symmetry – We are interested in the topological order familiar from \( \mathbb{Z}_2 \) gauge theory, \( \mathbb{Z}_2 \) spin liquids, and the toric code. There are two bosonic anyon species, often called \( e \) and \( m \). Each sees the other with an Aharonov-Bohm phase of \(-1\) (they are mutual semions). When two-dimensional translation symmetry is present, the symmetry generators \( T_x \) and \( T_y \) may act nontrivially (projectively) on the anyons \([2, 13]\). A basis-independent characterization of these actions is given by the relations

\[
T_x e T_y T_x^{-1} T_y^{-1} = \eta_e = \pm 1,
\]

\[
T_x^m T_y^m T_x^{-m} T_y^{-m} = \eta_m = \pm 1,
\]

where \( T_x^e \) is the action of \( T_x \) on a single \( e \), etc. When one of these relations evaluates to \(-1\) we say that translations act projectively, or that the anyon has fractional crystal momentum or has nontrivial fractionalization class, a notion closely related to Wen’s projective symmetry group \([14]\).
One can interpret the nontrivial $e$ relation as the presence of an $m$ in each unit cell of the lattice, which the $e$ sees as a background $\pi$ magnetic flux. It is straightforward to show, based on this observation or directly from the relations above, that if $e$ has fractional crystal momentum, the spectrum (and density of states) of two-$e$ scattering states is periodic under $q \rightarrow q + (\pi, 0), (0, \pi), (\pi, \pi)$ \[13\] \[15\]. Assuming that $e$ is the excitation of lowest energy, the low-energy edge of the continuum of excited states will reveal the fractionalization class of $e$ in the dynamical structure factor of any operator that excites anyons. This is the main idea for detecting such SET states that we pursue in this paper. However, we access the low-energy edge of the excited states via the information contained in the ground state instead of the excitation spectrum due to a nice property given by the PEPS, which we will introduce below.

**PEPS and transfer matrix** – PEPS is an ansatz that represents the wavefunction by locally entangled virtual pairs and a projector that map the virtual system to the physical one \[16\]. It captures a wide range of phases including many with topological order \[17\] \[24\]. A one-dimensional version, the MPS \[25\], has been used to classify phases of symmetric, gapped spin systems based on the projective representation of the symmetry group \[26\] \[28\]. Here, we propose a method based on PEPS for the spectra of correlation lengths (SCL) of the system, which allows us to distinguish SET phases described by simple PEPSs.

In one-dimensional gapped systems, properties of the ground state wave function (the MPS) are completely determined by the transfer matrix if translation symmetry is present. The spectrum of correlation lengths, which is given by the negative of the logarithm of (normalized) eigenvalues ($\lambda$) of the transfer matrix \[25\], is intuitively related to the spectrum of excitations made by all possible local operators with momentum quantum number $k_x$, $\lambda = |\lambda e^{ik_x}|$, at the minima of the spectrum \[29\].

The SCL can be generalized in two dimensions, however the momentum quantum number in the $y$ direction $k_y$ is rigorously well defined as compared to the $k_x$ estimated from the complex phases of the transfer matrix eigenvalues, as in the one-dimensional case mentioned above. Consider a cylindrical geometry (as in Fig. 1), we can define the SCL of the transfer matrix of a cylinder. If translation symmetry in the $y$ direction is present, eigenvectors of the transfer matrix have well defined momentum quantum numbers $k_y$, and the minimum of the SCL is given by

$$\epsilon(k_x, k_y) = -\ln(|\lambda_{\text{max}}(k_x, k_y)|/\lambda_0),$$  \[2\]

where $\lambda_{\text{max}}(k_x, k_y) = e^{ik_y} |\lambda_{\text{max}}(k_x, k_y)|$ is the leading eigenvalue of the transfer matrix with momentum $k_y$ excluding ground states $\lambda_0$s (the largest eigenvalue among all sectors); in general it is a complex number with a phase $e^{ik_y}$ where $k_y$ is its momentum in the $x$ direction \[25\]. We conjecture that $\epsilon(k_x, k_y)$ at a given $(k_x, k_y)$ are analogous to the low-energy edge of the two-anyon scattering continuum described earlier. Thus, we propose that the minima of the SCL can be used to distinguish SET phases, by analogy with the dynamic structure factor. Next we will test this conjecture by examining the minima of the SCL of the transfer matrix.

**Modified toric code model** – To construct the simplest $\mathbb{Z}_2$ spin liquid which realizes all possible projective quantum numbers of the translation symmetry, we consider the toric code Hamiltonian on a square lattice

$$H = -K_x \sum_s A_s - K_m \sum_p B_p,$$  \[3\]

where $A_s = \prod_{\ell \in s} \sigma^x_{\ell}$ is defined on the vertex $s$, $B_p = \prod_{\ell \in p} \sigma^x_{\ell}$ is defined on the plaquette $p$, and the sum runs over all vertices and all plaquettes. This Hamiltonian has four degenerate ground states \[30\]. Depending on the signs of $K_m$ and $K_x$, the quasi-particles $e$, $m$, if created, will move in a background of $0$- or $\pi$-flux. That is, $\eta_e = \text{deg}$. 

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**FIG. 1:** (a) Schematic representation of a PEPS on a cylinder of size $L_x \times L_y$. (b) When multiplying bra and ket of PEPS, we sum over the physical degrees of freedom, group the virtual indices of a bond, and arrive at the double tensor of a single site. (c) Placing $L_y$ double tensors on a ring and tracing out the virtual degrees on the shared bonds, we form the transfer matrix of the cylinder.

**FIG. 2:** A demonstration of the PEPS wavefunction of the toric code model in the $\sigma^x$ basis. Green lines denote the star operator $A_s$, and the plaquette operator $B_p$, and dark red lines denote the position of the 4-index $T$ tensor and the 3-index $g$ tensor, which are placed at the vertices and bonds of the dual lattice (denoted in dashed lines).
satisfies the position of the bond. We ask that the wave function \( \psi \) where

\[
\epsilon(0,k_y) = \frac{1}{2} \ln \left( \frac{1}{\lambda_0} \right) + O \left( \frac{1}{\lambda_0^2} \right),
\]

which is a good description of the perturbed state for \( h \ll K_c \), or \( w \approx 1 \). Throughout this paper, we use \( w = 0.9 \), which corresponds to \( h \ll |K_m|,|K_c| \) and is deep in the topologically ordered phase. For the phase diagram of the modified PEPS as a function of \( w \) in case of \( K_m < 0 \) and \( K_c > 0 \) (Supplemental Material [31]).

Numerical detection of the projective quantum number under translation symmetries – We take the PEPS wave functions described above and calculate the SCL of the transfer matrix [see Fig. 1(b)] for different signs of \( K_m \) and \( K_c \). The transfer matrix of a cylinder with translation symmetry \( T_y \) can be block-diagonalized in momentum basis, which means each left and right eigenvector has a well defined momentum quantum number \( k_y \). We start by explicitly writing the transfer matrix in real space into a block diagonal form in momentum space (Supplemental Material [31]). Once we have obtained the transfer matrix in momentum basis, we diagonalize each block with momentum \( k_y = 2\pi m/L_y, m = 0, 1, \cdots, L_y - 1 \), find the minima of the normalized SCL \( \epsilon(k_x,k_y) = -\ln(|\lambda_{\text{max}}(k_x,k_y)|/\lambda_0) \), and plot \( \epsilon(k_x,k_y) \) as a function of \( k_y \) for \( k_x = 0 \) and \( \pi \). Fig. 3 illustrates the minima of the SCL for \( K_m > 0 \) and \( K_c > 0 \), in which case, all eigenvalues of the transfer matrix are real and positive. The results for \( K_m < 0, K_c > 0 \) and \( L_y \) even are presented in Fig. 4. \( \epsilon(0,k_y) \) corresponds to the largest real and positive eigenvalue \( \lambda \) at each \( k_y \) excluding the two degenerate \( \lambda_0 \) at \( k_y = 0 \), while \( \epsilon(\pi,k_y) \) corresponds to the smallest real and negative eigenvalue \( \lambda \) at each \( k_y \). In the case of odd \( L_y \) for \( K_m < 0 \) and \( K_c > 0 \), matrices at each \( k_y \) further form into two non-commuting blocks, encoding the fact that applying the transfer matrix flips the eigenvalue of \( \prod_l \sigma_l^y \), where the product is over a loop encircling the system in the y-direction. This corresponds to a breaking of translation symmetry (\( T_x \)) in a one-dimensional limit (\( L_x \to \infty \) with \( L_y \) fixed). All eigenvalues of the transfer matrix come in \( \pm \) pairs, thus
$\lambda$ real and negative $k$ sector $K$

**FIG. 4:** The minima of SCL at momentum $k$ in (a) $K$ that the minima of the SCL are indeed doubly periodic $L$ and corresponds to the smallest real and positive $\lambda$ in sector $k_y$, except $\lambda_0$. (b) $\epsilon(k_y)$ corresponds to the smallest real and negative $\lambda$ in sector $k_y$. (c) The splitting $\Delta(L_y) = \epsilon_{(\pi,0)} - \epsilon_{(\pi,\pi)}$ as illustrated in (b) vanishes exponentially as a function of length $L_y$.

$\epsilon_{(0,\pi,k_y)}$ are identical, as presented in Fig. [3](#). We find that the minima of the SCL are indeed doubly periodic when $K_m < 0$, but not when $K_m > 0$.

For the case of $K_e < 0$ and $K_m < 0$ ($K_m > 0$), the resulting $\epsilon_{(0,k_y)}$ are exactly the same as above, because the low-energy excitations are dictated by coupling $K_m$ regardless of the sign of $K_e$. Note that when $K_e < 0$, $\epsilon_{(\pi,k_y)}$ is not accessible, because the transfer matrix at any $L_y$ consists of adjacent two columns of the lattice, thus all eigenvalues are positive.

If we want the projective quantum number of $m$-particles, we can take a perturbed Hamiltonian as

$$H'' = -K_e \sum_s A_s - K_m \sum_p B_p + h' \sum_l \sigma_l^z$$

instead, and correspondingly choose a PEPS representation defined in the $\sigma^z$ basis, where acting with a local operator $\text{diag}(w,1)$ is equivalent to adding a perturbation $\delta H = h' \sum_l \sigma_l^z$. The low-energy excitations are two $m$-particles and the sign of $K_e$ determines whether the $m$-particle hops in a background of 0- or $\pi$-flux on the dual lattice. Once the projective quantum numbers $\eta_e$ and $\eta_m$ are known, one completely determines SET class of the state if the symmetry group consists only of translation.

**Conclusion** – We have presented a numerical method to distinguish symmetry enriched topological (SET) phases with fractionalized translation symmetry. This method uses the spectrum of correlation lengths (SCL) of the transfer matrix on a cylinder to represent qualitatively the excitation spectrum of the system as a function of $k_y$ for special $k_x = 0, \pi$, if the ground state wave function is available in terms of projected entangled pair state (PEPS). From the fact that the nontrivial fractional quantum numbers of quasi-particles under translation symmetries will be manifest as enhanced Brillouin zone periodicity in the dispersion relation, one can read out the projective quantum number of the low energy quasiparticles from the behavior of the minima of SCL. We bench-marked this method with the toric code model under perturbation. Modifying the sign of the coupling coefficients in front of operator $A_s$ and $B_p$ and the perturbation terms, we were able to generate topologically ordered ground states with preferred $e$-particle or $m$-particle low-energy excitations in a background of either 0 or $\pi$ magnetic flux, which realizes all symmetry classes with this topological order and symmetry [2]. We expressed the ground states of the modified toric code Hamiltonians as bond-dimension $D = 2$ PEPSs and calculated the minima of the SCL of the transfer matrix on a cylinder, and the pattern of SCL revealed the fractional quantum numbers of the low energy quasiparticles under translation symmetries.

This method can be generalized to detect projective
quantum numbers of SET phases under a broader symmetry group including translations and other space group symmetries.

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[31] See Supplemental Material for PEPS construction of the ground state of toric code model with $K_x < 0$; the phase diagram of the PEPS by tuning parameter $w$ for $K_m < 0$ and $K_c > 0$; and details of diagonalizing the transfer matrix of a cylinder in momentum basis.
[33] N. Schuch, D. Poilblanc, J. I. Cirac and D. Pérez-García,
the dual lattice as in Fig. 6(a). Assuming that each tensor at four positions
affected by the operation of $A_s$ on one plaquette of the dual lattice. (b) To meet the condition $A_s |\psi\rangle = -|\psi\rangle$, we choose
$a = -1$ on the vertical bonds of every other column of the dual lattice (as marked by $-1$) and $a = 1$ for all other bonds
(without mark).

Topological Order in the Projected Entangled-Pair States

APPENDIX

PEPS for the ground state of toric code model with $K_e < 0$

In this section, we will discuss how to write a PEPS ground state for the toric code model with $K_e < 0$ while keeping the bond dimension $D = 2$.

We want to write the PEPS in the $\sigma_z$ basis since our perturbation $h \sum_i \sigma_i^z$ is simple in this basis. The PEPS is composed of a 4-index tensor $T_{\alpha\beta\gamma\delta}$ of bond dimension $D = 2$

$$T_{\alpha\beta\gamma\delta} = \begin{cases} 1, & (0,0) \ (\alpha + \beta + \gamma + \delta) \% 2 = 0 \\ 0, & (1,1) \ (\alpha + \beta + \gamma + \delta) \% 2 = 1, \end{cases}$$  

for $K_m > 0$ ($K_m < 0$), and a 3-index tensor $g^s_{\alpha\alpha'}$

$$g^s_{\alpha\alpha'} = \begin{cases} a, & \alpha = \alpha' = s = 0 \\ 1, & \alpha = \alpha' = s = 1 \\ 0, & \text{otherwise}. \end{cases}$$

Here $a$ is a number and can be different at different positions in order to satisfy the following condition when $K_e < 0$

$$A_s |\psi\rangle = -|\psi\rangle.$$  

(10)

The action of $A_s$ is to flip four spins on the plaquette of the dual lattice as in Fig. 6(a). Assuming that each $g$-tensor at four positions $s_0, s_1, s_2, s_3$ in Fig. 6(a) shares the same constant $a$, then Eq. (10) means that $a^{4-2n} = -1$ for $n = 0, 1, \cdots, 4$, where $n$ is the number of down spins in that plaquette. However, there is no solution for the set of equations $a^0 = a^{\pm 2} = a^{\pm 4} = -1$. In conclusion, one has to break the translation symmetry and let $a$ be different at different positions in one plaquette. We can choose a pattern as in Fig. 6(b) to satisfy Eq. (10) for every $s$. This choice maintains the translation invariance in the $y$ direction but doubles the unit cell in the $x$ direction; in such a case the transfer matrix consists of two adjacent columns instead of just one. We find that the minima of the SCL $\epsilon_{(0,k_y)}$ for $K_e < 0$ $K_e > 0$ as a function of $w$ at special points $(0,0)$ and $(\pi, \pi)$ for the cylinder perimeters $L_y = 8, 10, 12, 14$. For various fixed $w$, $\gamma_{(0,0)}$ is plotted against $L_y$ in (b) a semi-log plot and (c) a log-log plot.

FIG. 7: (a) The ground state gap $\gamma_{(k_x,k_y)}$ for coupling $K_m < 0$ $K_e > 0$ as a function of $w$ at special points $(0,0)$ and $(\pi, \pi)$ for the cylinder perimeters $L_y = 8, 10, 12, 14$. For various fixed $w$, $\gamma_{(0,0)}$ is plotted against $L_y$ in (b) a semi-log plot and (c) a log-log plot.
Phase diagram of the PEPS wavefunction by tuning parameter $w$ for $K_m < 0$ and $K_e > 0$

This section studies the phase diagram of the PEPS wavefunction by tuning parameter $w$ [in the local operator $\text{diag}(w, 1)$] from 1 to 0 for $K_m < 0$, $K_e > 0$. In one limit, when $w \approx 1$, the state is deep in the topologically ordered phase. In the opposite limit, $w \to 0$, all spins tend to point down, but the constraint Eq. [S] requires that each plaquette has an odd number of up spins. These conditions together lead to a state where all configurations with one spin up in each plaquette contribute equally.

When $w$ is in between 0 and 1, one can imagine that the entropy contributed from the massive number of configurations that meet Eq. [S] is competing with the Zeeman energy, and a valence bond solid order could emerge. As one varies $w$ from 1 to 0, the PEPS wavefunction could go through a phase transition from the topologically ordered phase to a valence bond solid phase. Inside the valence bond solid phase, translation symmetry is spontaneously broken in the thermodynamic limit, but at any finite size, the ground states are degenerate. We expect that two degenerate eigenvalues with $\pm 1$ will appear as the leading eigenvalues of the transfer matrix; whereas in the topological phase, both leading eigenvalues are $+1$.

We now try to identify this phase transition using techniques discussed in the paper. We define $\gamma(k_x, k_y)$, which roughly represents the gap to the ground state at momentum $(k_x, k_y)$, using eigenvalues of the transfer matrix:

$$
\gamma(k_x, k_y) = \begin{cases} 
-\ln(|\lambda^L_{(k_x, k_y)}|/\lambda_0), & k_x = k_y = 0 \\
-\ln(|\lambda^\text{max}_{(k_x, k_y)}|/\lambda_0), & \text{otherwise}
\end{cases},
$$

[in the sector $(0, 0)$ we take the subleading eigenvalue $\lambda^L_{(k_x, k_y)}$; otherwise the leading eigenvalue $\lambda^\text{max}_{(k_x, k_y)}$]. $\gamma(k_x, k_y)$ is different from $\epsilon(k_x, k_y)$ defined earlier in that the splitting of $\lambda_0$, doubly degenerate in the thermodynamic limit in the topological phase, is explicitly calibrated by $\gamma(0, 0)$. We plot $\gamma(k_x, k_y)$ at special points $(0, 0)$ and $(\pi, \pi)$ as a function of $w$ for cylinder perimeters $L_y = 8, 10, 12, 14$ in Fig. [7](a). Note that all other gaps lie well above these two within the plotted range. We do not see a crossing of $\gamma(0, 0)$ and $\gamma(\pi, \pi)$ as we vary $w$. Instead, we find that they approach each other, with $\gamma(\pi, \pi)$ slightly larger than $\gamma(0, 0)$ when $w$ is close to 0. In order to examine finite size effects we plot $\gamma(0, 0)$ as a function of $L_y$ at various fixed $w$, in a semi-log plot [in Fig. [7](b)] and a log-log plot [in Fig. [7](c)]. The results are inconclusive; we cannot identify any critical point where a topological phase turns into a valence bond solid phase due to very large correlation length and insufficient system $L_y$ size available.

Diagonalizing the transfer matrix of a cylinder in momentum basis

In the general case, the transfer matrix, denoted as $E$, of a cylinder of circumference $L_y$ can be thought of as a Hamiltonian for a system composed of local degrees of freedom with Hilbert space dimension $D^2$ ($D$ is the bond dimension of PEPS) where each degree of freedom is composed of two virtual degrees of freedom. These local degrees of freedom are arranged in a ring with $L_y$ “sites”. Note that the transfer matrix is generally non-hermitian. The matrix elements of the transfer matrix in real space can be computed by specifying a basis vector $|a\rangle$ (which denotes compactly configuration of all $L_y$ local degrees of freedom) and multiplying it by the transfer matrix

$$
E|a\rangle = \sum_b h_{ba}|b\rangle,
$$

where $h_{ba} = \langle b | E | a \rangle$ is the matrix element.

The transfer matrix commutes with translations $T$ in the $y$ direction and hence can be diagonalized simultaneously with $T$. The eigenvalues of $T$ have the form $e^{i k}$ where $k = 2 \pi m / L_y$, $m = 0, 1, \ldots, L_y - 1$. We construct the corresponding eigenspace $V_k$ as follows.

First, we consider classes of real-space configurations that are related to each other by an action of $T$: $|a\rangle$ and $|a'\rangle$ belong to the same class if $|a'\rangle = T^\ell|a\rangle$ for some $\ell$. It is easy to see that we can specify each class by one representative member $|a\rangle$, while all other members are given by $T^\ell|a\rangle$, $\ell = 0, 1, \ldots, R - 1$, where $R$ is the smallest number such that $T^R|a\rangle = |a\rangle$: the “periodicity” $R$ must be less than or equal to $L_y$ since $T^{L_y} = 1$. For a given momentum $k$, if $k R_a$ is an integer multiple of $2 \pi$, then out of the states in this class we can construct a single normalized eigenstate of $T$ with eigenvalue $e^{i k}$ as follows:

$$
|a_k\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{L_y-1} e^{-i k r} T^r |a\rangle,
$$

where $N_a$ is the normalization constant

$$
N_a = L_y^2 / R_a.
$$

On the other hand, if $k R_a$ is not an integer multiple of $2 \pi$, we cannot construct such an eigenstate from the states in this class; thus this class of configurations is not compatible with the momentum $k$ and is not included as a basis state for $V_k$. By going over all classes that are compatible with $k$, we construct a complete basis of $V_k$, which we call the momentum basis.

We calculate the transfer matrix elements in the basis
of $V_k$ as follows

$$
E|a_k\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{L_y-1} e^{-ikrT^r} E|a\rangle
$$

$$
= \sum_{b'} h_{b'} a \frac{1}{\sqrt{N_a}} \sum_{r=0}^{L_y-1} e^{-ikrT^r} |b'\rangle.
$$

(15)

where $|b'\rangle$ runs over all real-space basis states. Each such $|b'\rangle$ belongs to some class whose representative we denote as $|b\rangle$, and hence there is $l_{b'}$ such that

$$
|b'\rangle = T^{-l_{b'}} |b\rangle.
$$

(16)

Substituting this in Eq. (15), we have

$$
E|a_k\rangle = \sum_{b'} h_{b'} a e^{-ikl_{b'}} \frac{1}{\sqrt{N_b}} |b_k\rangle,
$$

(17)

where the summation runs over all real-space basis states $|b'\rangle$ and not only the representative $b$. Note that for each momentum-space basis state $|b_k\rangle$, the matrix element $\langle a_k|E|b_k\rangle$ obtains contributions from all $b'$ that belong to the class which corresponds to $|b_k\rangle$.

After finding the matrix elements $\langle b_k|E|a_k\rangle$ in the basis in $V_k$, we can separately diagonalize the block diagonal transfer matrix for each momentum $k$ and obtain the corresponding $\epsilon_{k_y}$.

In the present case, the transfer matrix actually simplifies since the structure of the $T$ and $g$ tensors are such that the labels $\alpha\alpha'$ of the double tensor must coincide at each “site” in the transfer matrix; $\alpha_i = \alpha'_i$ and $\beta_i = \beta'_i$ ($i = 0, 1, \ldots, L_y - 1$), thus the size of Hilbert space is reduced from $D^{2L_y}$ to $D^{L_y}$. 