Higher structures in matrix product states

Shuhei Ohyama[1,*] and Shinsei Ryu[2]
[1]*Center for Gravitational Physics and Quantum Information, Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan*
[2]*Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*

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For a parameterized family of invertible states (short-range-entangled states) in $(1+1)$ dimensions, we discuss a generalization of the Berry phase. Using translationally invariant, infinite matrix product states (MPSs), we introduce a gerbe structure, a higher generalization of complex line bundles, as an underlying mathematical structure describing topological properties of a parameterized family of MPSs. Furthermore, we introduce a generalization of a quantum mechanical inner product, which we call the "triple inner product," defined for three matrix product states. The triple inner product proves to extract a topological invariant, the Dixmier-Douady class over the parameter space.

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I. INTRODUCTION

A. The Berry phase and its higher generalization

Quantum mechanical phase degrees of freedom are known to have an interesting interplay with topology [1,2]. A canonical example is the Dirac monopole, where the presence of a magnetic monopole prevents quantum mechanical wave functions from being defined uniquely over the entire space. Instead, following the work by Wu and Yang [3], wave functions can be defined by introducing multiple patches, and at the intersection of two patches, wave functions from different patches are related by a transition function. The (large) gauge invariance results in the quantization of magnetic charges in units of the inverse of the fundamental charge. A magnetic monopole also arises in the context of the Berry phase, where a diabolic point of the Hamiltonian plays the role of the Dirac monopole of the Berry connection in a parameterized quantum system in which the wave function $|\psi(x)\rangle$ depends smoothly on some adiabatic parameter(s) x taken from a parameter space X. The mathematical structure underlying these situations is a principle U(1) bundle over the parameter space X. Such bundles are characterized and classified by a topological invariant, with the first Chern class taking its value in the second cohomology group of X, $H^2(X;\mathbb{Z})$.

The Berry phase also plays an important role in topological phenomena in many-body quantum physics such as quantum Hall states and Chern insulators [4,5] and the Thouless pump [6]. An important class of topological states is the so-called invertible states (short-range-entangled states) that are realized as a unique ground state of a gapped Hamiltonian. Invertible states can be protected by symmetry from being topologically trivial, i.e., symmetry-protected topological (SPT) phases, as known in topological insulators and the Haldane spin chain [7–10]. Topological invariants of these phases can be understood in terms of the Berry phase and wave function overlaps. For example, the first Chern number (the quantized Hall conductance) of Chern insulators (the quantum Hall effect) at the level of noninteracting electrons can be obtained from the Berry curvature and Berry connection in momentum space. This topological invariant can also be understood in terms of the Berry phase acquired by the wave function under adiabatic threading of magnetic flux. Similarly, for SPT phases protected by a discrete symmetry, the discrete phases acquired by wave functions through nonadiabatic discrete transformations can detect their topological invariants (see Ref. [11] for examples). In the path integral picture, all these topological invariants can be understood as topological terms, i.e., metric-independent terms, in topological quantum field theory.

Note that the discrete phases relevant to SPT phases are not associated with an adiabatic process, but with discrete transformations, unlike the regular notion of the Berry phase. Nevertheless, in this paper, we broaden the usage of the term "Berry phase" to indicate the phases of wave function overlaps that may encode topological information of topological states and processes. In a similar vein, we regard the transition functions in Wu and Yang's description of magnetic monopoles as an example of the Berry phase. In the setting of a parameterized family of wave functions, the transition functions can be extracted from the overlaps of two wave functions from different patches—they determine the topological class (the first Chern class).[1]

*shuhei.oyama@yukawa.kyoto-u.ac.jp

[1]Later in this paper, we introduce a generalization of the regular inner product, the triple inner product defined for three many-body quantum states (matrix product states). We will refer to the phase associated with the triple inner product as the higher Berry phase and discuss its topological properties. In particular, we will show that it determines the topological class (the Dixmier-Douady class) of a

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In recent years, it has been recognized that there are many-body systems in which the regular notion of the Berry phase fails to capture topological properties. Specifically, a family of invertible many-body quantum states that depends on some parameter $x \in X$, which we shall call invertible states over X for short, has been discussed [12–20]. Such a family can be topologically nontrivial and can be considered a generalization of the Thouless pump. It can also be considered a generalization of regular gapped phases (SPT phases) which can be regarded as a special case where the parameter space is a single point.[2] For example, it is known that there is a nontrivial family of $(d+1)$-dimensional systems with U(1) symmetry parameterized over S^d [13]. We, however, cannot use the ordinary Berry phase to detect its nontriviality in general. A cursory explanation is that the Berry connection and Berry curvature measure the nontriviality of $H^2(X;\mathbb{Z})$, so for example, when $d=3$, they cannot be nontrivial on S^3. Even worse, if not introduced carefully, the Berry connection and curvature may be ill defined in many-body quantum systems in the first place: For example, if we consider a chain of spins that are weakly interacting with each other and are each coupled to an adiabatically time-evolving magnetic field, the first Chern number diverges in the thermodynamic limit since each spin contributes independently.

In order to capture the topology of higher generalizations of the Thouless pumping, it has been realized that a "higher" generalization of the Berry phase, which takes its value in the higher cohomology group, $H^{d+2}(X;\mathbb{Z})$, is important [13,19,21]. Motivated by these developments, the purpose of this paper is to extend the ordinary Berry phase to $(1+1)$-dimensional quantum many-body systems and construct a topological invariant that takes its value in $H^3(X;\mathbb{Z})$. In this paper, the families of invertible states we consider do not preserve some symmetries, e.g., particle number conserving U(1).

B. Summary of the paper

In this paper, we identify a gerbe structure for parameterized families of invertible states in $(1+1)$ dimensions using translationally invariant, infinite matrix product states (MPSs). A gerbe is a higher generalization of complex line bundles and provides, as we will see, a natural framework to discuss the higher Berry phase. (We will give a brief overview of a gerbe in Sec. II B.) Specifically, we will show how we can construct a gerbe from a family of infinite MPSs. We also show how the data constituting the gerbe, and its topological invariant in particular, can be extracted from a (properly generalized) overlap of three MPSs. We call the overlap the triple inner product, which is depicted in Fig. 5 below. This is analogous to Wu and Yang's work, from which we can extract the ordinary Berry phase by taking the inner product of two wave functions that are physically the same but are taken from two different patches. In our generalization, we extract the higher Berry phase by taking the triple inner product of three states that are physically the same in three different patches. This triple inner product gives the so-called Dixmier-Douady class over the parameter space X that takes its value in $H^3(X;\mathbb{Z})$. This is the higher counterpart of the Chern class that classifies complex line bundles and takes its value in $H^2(Z;\mathbb{Z})$. Our formalism works for both the torsion and free parts of $H^3(X;\mathbb{Z})$, i.e., the cases when families of invertible states over X are classified by a finite order group and (copies of) the cyclic group $\mathbb{Z}$, respectively. For the free case, as we will discuss, it is essential to deal with MPSs whose rank (bond dimension) is not constant over the parameter space X. Finally, we will also discuss how this gerbe structure and the triple inner product are naturally described by using the language of noncommutative geometry, a star product and integration.

family of invertible states over X, without explicitly using a (higher generalization of) Berry connection.

[2]The phrase "invertible state parameterized by a single point" is a verbose mathematical expression, but being parameterized by a single point is equivalent to not being parameterized at all, and, physically, the "classification obtained when identified under continuous deformations" means nothing other than considering things that can be deformed into each other adiabatically as the same. Thus, when X is a point, the situation is nothing but "identifying invertible states through adiabatic deformation," which is precisely the standard classification problem for SPT phases.

II. CONSTRUCTION OF A GERBE FROM MPSs

A. Brief review of MPSs

This paper focuses on invertible states (short-range-entangled states) in $(1+1)$ dimensions. In particular, we study families of translationally invariant invertible states that depend on a parameter $x \in X$. Such a parameterized family can be called invertible states over X. Invertible states in $(1+1)$ dimensions are efficiently represented as MPSs, so we begin by reviewing the necessary ingredients of MPSs. Specifically, we deal with translationally invariant, infinite MPSs. For a more in-depth discussion, see, for example, Refs. [22–25].

As a start, let us consider a finite one-dimensional lattice with L sites, labeled by $j = 1, \dots, L$. Let $\mathfrak{h}_j$ be a local Hilbert space with dimension d (independent of j), where $\{|i\rangle\}_{i=1}^d$ is an orthonormal basis of $\mathfrak{h}_j$. The total Hilbert space of the chain is $\mathcal{H} := \bigotimes_{j=1}^L \mathfrak{h}_j$. A translationally invariant MPS is defined by a set of $n \times n$ matrices $\{A^i\}$ with the same index as the orthonormal basis. With periodic boundary conditions, the MPS generated by $\{A^i\}$ is given by

$$|\{A^i\}\rangle_L := \sum_{\{i_k\}} \mathrm{tr}(A^{i_1} \cdots A^{i_L})\,|i_1, \dots, i_L\rangle\,, \tag{1}$$

where $\sum_{\{i_k\}}$ represents a summation over all configurations of $(i_1, \dots, i_L)$, $\sum_{\{i_k\}} = \sum_{i_1} \cdots \sum_{i_L}$. MPSs with fixed boundary conditions can be defined similarly with boundary vectors specifying boundary conditions.

We are interested in invertible states in the thermodynamic limit, $L \to \infty$, where boundary conditions play no role. In this limit, the physical properties of the MPS are encoded in its transfer matrix, which is defined by

$$T_A := \sum_i A^{i*} \otimes A^i. \tag{2}$$

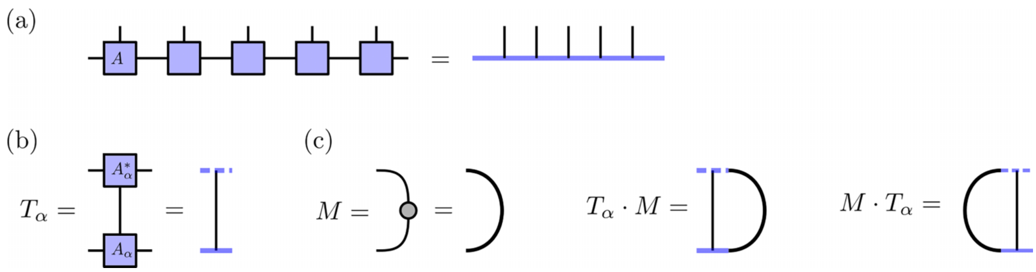

FIG. 1. (a) Matrix product states, (b) transfer matrices, and (c) the left and right actions of transfer matrices. When there is no confusion, we simplify our notation by not showing boxes representing tensors explicitly. The conjugate of the MPS matrix A is represented by dotted lines.

A transfer matrix T_A acts on $M \in \mathrm{Mat}_n(\mathbb{C})$ from the left and right as

$$T_A \cdot M := \sum_i A^i M A^{i\dagger}, \tag{3}$$

$$M \cdot T_A := \sum_i A^{i\dagger} M A^i, \tag{4}$$

respectively. We represent these actions pictorially in Fig. 1.

Invertible states are represented by a normal MPS, which can be defined, using a transfer matrix, as follows [22]: Let $\{A^i\}$ be a set of $n \times n$ matrices and r^R be the spectral radius of the transfer matrix for the first action of Eq. (6).[3] Then $\{A^i\}$ is normal if and only if the left action of the transfer matrix has a unique eigenvalue λ with eigenvalue $|\lambda| = r^R$ and the eigenvector Λ^R is a positive definite $n \times n$ matrix. We call an MPS generated by normal matrices a normal MPS. For normal matrices, it is known that the spectral radius r^L for the second action of Eq. (6) is equal to r^R, i.e., $r^R = r^L$. In addition, an eigenvector Λ^L with eigenvalue λ' such that $|\lambda'| = r^R$ is unique, and Λ^L is a positive-definite matrix.

For normal matrices, the eigenvalue equation $T_A \cdot \Lambda = \lambda\Lambda$ can be rewritten as

$$\sum_i A^i \Lambda A^{i\dagger} = \lambda\Lambda \quad \Longleftrightarrow \quad \sum_i A_c^i A_c^{i\dagger} = 1_n, \tag{5}$$

where $A_c^i := \frac{1}{\sqrt{\lambda}} \Lambda^{-\frac{1}{2}} A^i \Lambda^{\frac{1}{2}}$. We call $\{A_c^i\}$ the right canonical form of the normal matrices $\{A^i\}$. In this form, the spectral radius for the left action (3) is 1, and the eigenvector is modified, $\Lambda' \to \Lambda^{-\frac{1}{2}} \Lambda' \Lambda^{\frac{1}{2}}$, which is not the identity matrix in general. In the following, unless mentioned otherwise, we take our MPSs to be in the right canonical form and denote the eigenvectors with eigenvalue 1 for the left and right actions as Λ_A^R and Λ_A^L, respectively:

$$T_A \cdot \Lambda_A^R = \Lambda_A^R, \quad \Lambda_A^L \cdot T_A = \Lambda_A^L. \tag{6}$$

In the present case, Λ_A^R is just the identity matrix, but in the later generalization, the case where it is not the identity matrix will appear, so we assign a symbol to it in advance.

By using the left and right eigenvectors Λ_A^L and Λ_A^R, an infinite MPS is defined in the following manner [23,24,26]: For infinite systems, it is difficult to define the state itself since an MPS in an infinite system is formally given by

$$|\{A^i\}\rangle_\infty := \sum_{\{i_k\}} \cdots A^{i_1} \cdots A^{i_L} \cdots |\cdots i_1 \cdots i_L \cdots\rangle \tag{7}$$

and its coefficients have an ambiguous infinite product of matrices. In the infinite MPS formulation, we give up defining the state itself but define the expectation value of the state. An expectation value of a local observable contains infinitely many products of transfer matrices in the right and left directions (Fig. 2). Therefore, in the infinite size limit, the product only has a value on the eigenvector space of the transfer matrix with the maximum eigenvalue. So we close the right and left ends with Λ_A^L and Λ_A^R to define the expectation value. For example, the inner product of $|\{A^i\}\rangle_\infty$ is defined by

$$\langle\{A^i\}|\{A^i\}\rangle_\infty = \Lambda_A^L \cdot (T_A)^N \cdot \Lambda_A^R = \mathrm{tr}\big(\Lambda_A^L \Lambda_A^R\big) \tag{8}$$

for arbitrary $N \in \mathbb{N}$. In the right canonical form, $\Lambda_A^R = 1_n$, but the phase of Λ_A^L is not fixed. As a normalization condition for the infinite MPS, we fix the phase of Λ_A^L by $\mathrm{tr}(\Lambda_A^L) = 1$. Similarly, for example, the expectation values of local operators F_1 (acting on site 1) and G_{56} (acting on sites 5 and 6) are given by

$$\langle F_1 G_{56}\rangle := \Lambda_A^L \cdot T_A[F_1](T_A)^3 T_A[G_{56}] \cdot \Lambda_A^R, \tag{9}$$

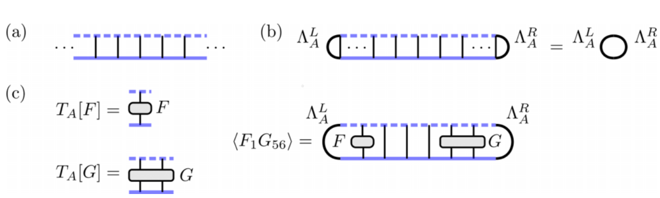

FIG. 2. (a) The inner product (norm) of infinite MPSs contains infinitely many products of the transfer matrices. (b) In the thermodynamic limit, only the eigenvector with the maximal eigenvalue survives. In the infinite MPS formalism, the inner product is defined by contracting the left end with the left eigenvector Λ_A^L and the right end with the right eigenvector Λ_A^R. By using the eigenvalue equation, this value is found to be equal to $\mathrm{tr}(\Lambda_A^L \Lambda_A^R)$. (c) In general, the expectation value of a local observable is defined by putting the left eigenvector on the left side of the operator with the leftmost support and the right eigenvector on the right side of the operator with the rightmost support.

[3] In this paper, we follow the terminology in [25]. We note that any injective tensor is proportional to a normal tensor. Conversely, any normal tensor becomes injective after blocking.

where $(T_A\,[F_1])_{(a,\,c),\,(b,d)} := \sum_{i,j} A^{i*}_{ab} F_1^{ij} A^j_{cd}$ and $(T_A\,[G_{56}])_{(a,d),(c,f)} := \sum_{i,j,k,l} \sum_{b,e} A^{i*}_{ab} A^{j*}_{bc} G^{ij,kl}_{56} A^k_{de} A^l_{ef}$.

B. What is a gerbe, and why is it relevant?

The purpose of this paper is to discuss a higher generalization of the Berry phase for a parameterized family of $(1+1)$-dimensional invertible states. More specifically, we propose a gerbe as a proper mathematical structure that underlies the higher Berry phase and the topological classification of higher Thouless pumping. A gerbe is a higher generalization of a complex line bundle. In physics contexts, it has been used to describe, for example, the $(1+1)$-dimensional Wess-Zumino-Witten models, the $(2+1)$-dimensional Chern-Simons theories, the Kalb-Ramond B field and D-branes in string theory, and various anomalies in quantum field theory [27–30]. In this section, we introduce the mathematical definition of a gerbe. In the next section, we will then construct a gerbe from invertible states (MPSs) over X.

Before delving into gerbes, it is useful to recall the definition of a complex line bundle and its characterizing data, the transition functions. As mentioned in the Introduction, these underline the description of the regular Berry phase for a parameterized family of quantum mechanical states. Let X be a topological space and consider an open covering of X, $\{U_\alpha\}$, i.e., a set of open sets $\{U_\alpha\}$ such that $\bigcup_\alpha U_\alpha = X$. On each patch U_α, we have a trivial line bundle $L_\alpha \to U_\alpha$, and on each nonempty intersection $U_{\alpha\beta} := U_\alpha \cap U_\beta$, L_α and L_β are glued to each other by the transition function $e^{i2\pi\phi_{\alpha\beta}}$. They satisfy $e^{i2\pi\phi_{\beta\alpha}} = e^{-i2\pi\phi_{\alpha\beta}}$, and also, on triple intersections $U_{\alpha\beta\gamma} := U_\alpha \cap U_\beta \cap U_\gamma$,

$$e^{i2\pi\phi_{\alpha\beta}} e^{i2\pi\phi_{\beta\gamma}} e^{i2\pi\phi_{\gamma\alpha}} = 1. \tag{10}$$

The data $(\{U_\alpha\}, \{e^{i2\pi\phi_{\alpha\beta}}\})$ satisfying condition (10) topologically defines a complex line bundle. A transition function $\{e^{i2\pi\phi_{\alpha\beta}}\}$ is an element of the Čeck complex $C^1(X; \underline{\mathrm{U}(1)})$, and Eq. (10) is nothing but the cocycle condition. (Here, the underbar represents the sheaf cohomology.) Therefore, $e^{i2\pi\phi_{\alpha\beta}}$ defines the first Čeck cohomology class $[e^{i2\pi\phi_{\alpha\beta}}] \in H^1(X; \underline{\mathrm{U}(1)}) \simeq H^2(X;\mathbb{Z})$. Here, the isomorphism is given in the following way: Let us take a $\mathbb{R}$ lift $\hat{\phi}_{\alpha\beta\gamma}$ of $\phi_{\alpha\beta\gamma} \in \mathbb{R}/\mathbb{Z}$. Then, on $U_{\alpha\beta\gamma}$, $f_{\alpha\beta\gamma} := \hat{\phi}_{\alpha\beta} - \hat{\phi}_{\alpha\gamma} + \hat{\phi}_{\beta\gamma}$ takes its value in $\mathbb{Z}$ and satisfies the cocycle condition. Thus, it defines the second cohomology class $[f_{\alpha\beta\gamma}] \in H^2(X;\mathbb{Z})$, and this is a topological invariant of the complex line bundle, the so-called first Chern class.

Heuristically, we can generalize complex line bundles by assigning a complex line bundle $L_{\alpha\beta}$ on $U_{\alpha\beta}$, instead of a transition function $e^{i2\pi\phi_{\alpha\beta}}$. On $U_{\alpha\beta\gamma}$, as an analog of the cocycle condition $e^{i2\pi\phi_{\alpha\beta}} e^{i2\pi\phi_{\beta\gamma}} = e^{i2\pi\phi_{\alpha\gamma}}$, we consider an isomorphism $L_{\alpha\beta} \otimes L_{\beta\gamma} \simeq L_{\alpha\gamma}$. These isomorphisms have to satisfy a higher counterpart of the cocycle condition (10) on fourfold intersections. Formalizing these ideas, we can introduce a gerbe on X by specifying a datum $(\{U_\alpha\}, \{L_{\alpha\beta}\}, \{\sigma_{\alpha\beta\gamma}\})$ that satisfies the following conditions [31]: $\{U_\alpha\}$ is an open covering of a base space X, $L_{\alpha\beta}$ is a complex vector bundle over $U_{\alpha\beta}$, and $\sigma_{\alpha\beta\gamma} : L_{\alpha\beta} \otimes L_{\beta\gamma} \to L_{\alpha\gamma}$ is an isomorphism between complex vector bundles. They satisfy the commutative diagram

$$\begin{array}{ccc} L_{\alpha\beta} \otimes L_{\beta\gamma} \otimes L_{\gamma\delta} & \xrightarrow{1\otimes\sigma_{\beta\gamma\delta}} & L_{\alpha\beta} \otimes L_{\beta\delta} \\ {\scriptstyle \sigma_{\alpha\beta\gamma}}\downarrow & & \downarrow{\scriptstyle \sigma_{\alpha\beta\delta}\otimes 1} \\ L_{\alpha\gamma} \otimes L_{\gamma\delta} & \xrightarrow{\sigma_{\alpha\gamma\delta}} & L_{\alpha\delta}. \end{array} \tag{11}$$

Just like complex line bundles are classified by $H^2(X;\mathbb{Z})$, i.e., the first Chern class, it is known that gerbes on a topological space X are classified by the so-called Dixmier-Douady class that takes its value in $H^3(X;\mathbb{Z})$ [32]. On the other hand, $(1+1)$-dimensional invertible states over X are expected to be classified precisely by $H^3(X;\mathbb{Z})$ [21]. This is one of the primary reasons that we expect a gerbe to be an underlying mathematical structure for parameterized $(1+1)$-dimensional invertible states over X. By constructing a gerbe from a family of $(1+1)$-dimensional systems, we expect that we can extract a topological invariant that takes its value in $H^3(X;\mathbb{Z})$.

C. Definition of a constant-rank MPS gerbe

As we are interested in invertible states over X, we consider a family of infinite MPSs $\{A^i(x)\}$, in which the corresponding transfer matrix, left and right eigenvectors, etc., are also dependent on x. We will call this family MPSs over X. Following the definition of a gerbe presented above, we now construct a gerbe on X from MPSs over X. For simplicity, we will keep the rank (bond dimension) of MPSs constant at first. We will drop this condition later in Sec. II E.

To set the stage, we fix an open covering $\{U_\alpha\}_{\alpha\in I}$ of X and consider $n \times n$ normal MPS matrices $\{A^i_\alpha(x)\}$ on each U_α. As we mentioned before, we take $\{A^i_\alpha(x)\}$ in the canonical form. At the intersection of two patches $U_{\alpha\beta}$, we have two MPSs representing the same physical state defined at $x \in X$. By the fundamental theorem for (bosonic) MPSs [22], these two MPSs are related by a gauge transformation,

$$A^i_\alpha(x) = g_{\alpha\beta}(x) A^i_\beta(x) g^\dagger_{\alpha\beta}(x), \tag{12}$$

where $g_{\alpha\beta}$ is an element of the projective unitary group, $g_{\alpha\beta} \in \mathrm{PU}(n)$[4]. We call $g_{\alpha\beta}$ a transition function. Applying the fundamental theorem twice in the overlapping region of two patches, we get

$$A^i_\alpha = g_{\alpha\beta} g_{\beta\alpha} A^i_\alpha (g_{\alpha\beta} g_{\beta\alpha})^\dagger. \tag{13}$$

One of the consequences of the fundamental theorem is that the transition functions are unique up to a phase ambiguity. As a result, the product $g_{\alpha\beta} g_{\beta\alpha}$ differs from the identity matrix 1_n only by a phase, which can be represented as $e^{i\phi_{\alpha\beta}}$:

$$g_{\alpha\beta} g_{\beta\alpha} = e^{i\phi_{\alpha\beta}} 1_n \Longleftrightarrow g_{\beta\alpha} = e^{i\phi_{\alpha\beta}} g^\dagger_{\alpha\beta}. \tag{14}$$

Thus, the relation $g_{\beta\alpha} = g^\dagger_{\alpha\beta}$ does not hold in general. However, by redefining the phase of $g_{\alpha\beta}$, we can always make it hold. In the following, unless otherwise specified, we assume the relation $g_{\alpha\beta} = g^\dagger_{\beta\alpha}$.

[4]For simplicity, we omit the phase redundancy of MPSs.

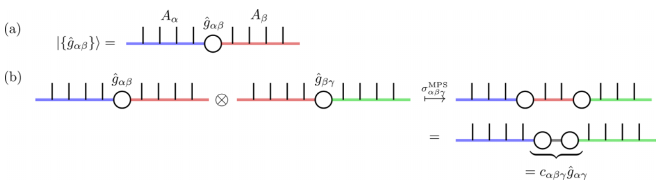

FIG. 3. Ingredients of an MPS gerbe. (a) A mixed-gauge MPS $|\{\hat{g}_{\alpha\beta}\}\rangle$ defined over $U_{\alpha\beta}$ and (b) the isomorphism $\sigma^{\mathrm{MPS}}_{\alpha\beta\gamma}$.

Let us take a U(n) lift $\{\hat{g}_{\alpha\beta}\}$ of $\{g_{\alpha\beta}\}$. From this unitary matrix $\{\hat{g}_{\alpha\beta}\}$, we define a state over $U_{\alpha\beta}$ by

$$|\{\hat{g}_{\alpha\beta}\}\rangle := \sum_{\{i_k\}} \cdots A^{i_1}_{\alpha} \times \cdots A^{i_p}_{\alpha} \hat{g}_{\alpha\beta} A^{i_{p+1}}_{\beta} \cdots A^{i_L}_{\beta} \cdots |\cdots i_1 \cdots i_L \cdots\rangle . \quad (15)$$

By using the identity $A^i_\alpha(x) g_{\alpha\beta}(x) = g_{\alpha\beta}(x) A^i_\beta(x)$, we can freely change the position of $\hat{g}_{\alpha\beta}$. Therefore, the right-hand side does not depend on $p \in \mathbb{Z}$. Although this state contains ambiguous infinite products in its coefficients, when calculating physical quantities (such as the higher Berry phase), as we will see below, we extract them by contracting the ends using the fixed point of suitable transfer matrices. The state $|\{\hat{g}_{\alpha\beta}\}\rangle$ is reminiscent of the so-called mixed-gauge MPS. At each point of $x \in U_{\alpha\beta}$, we can consider the one-dimensional complex vector space spanned by $|\{\hat{g}_{\alpha\beta}\}\rangle$. By bundling them over $U_{\alpha\beta}$, we also define a complex line bundle $L_{\hat{g}_{\alpha\beta}}$ over $U_{\alpha\beta}$. Finally, on a triple intersection $U_{\alpha\beta\gamma}$, we define the isomorphism

$$\sigma^{\mathrm{MPS}}_{\alpha\beta\gamma} : L_{\hat{g}_{\alpha\beta}} \otimes L_{\hat{g}_{\beta\gamma}} \to L_{\hat{g}_{\alpha\gamma}} : |\{\hat{g}_{\alpha\beta}\}\rangle \otimes |\{\hat{g}_{\beta\gamma}\}\rangle \mapsto |\{\hat{g}_{\alpha\beta}\hat{g}_{\beta\gamma}\}\rangle . \quad (16)$$

See Fig. 3 for pictorial representations of $|\{\hat{g}_{\alpha\beta}\}\rangle$ and $\sigma^{\mathrm{MPS}}_{\alpha\beta\gamma}$.

We claim that the datum $(\{U_\alpha\}, \{L_{\hat{g}_{\alpha\beta}}\}, \{\sigma^{\mathrm{MPS}}_{\alpha\beta\gamma}\})$ defines a gerbe on X. To see this, let us check the commutative diagram (11) for $(\{U_\alpha\}, \{L_{\hat{g}_{\alpha\beta}}\}, \{\sigma^{\mathrm{MPS}}_{\alpha\beta\gamma}\})$. First, let us note that a $c_{\alpha\beta\gamma} \in$ U(1) on $U_{\alpha\beta\gamma}$ exists so that

$$\hat{g}_{\alpha\beta}\hat{g}_{\beta\gamma} = c_{\alpha\beta\gamma}\hat{g}_{\alpha\gamma}. \quad (17)$$

We can show the existence of $c_{\alpha\beta\gamma}$ as follows: Using the fundamental theorem twice in the intersection of the three patches, moving from α to β and from β to γ, we obtain

$$A^i_\alpha = g_{\alpha\beta} g_{\beta\gamma} A^i_\gamma (g_{\alpha\beta} g_{\beta\gamma})^\dagger. \quad (18)$$

On the other hand, moving directly from α to γ, we get

$$A^i_\alpha = g_{\alpha\gamma} A^i_\gamma g^\dagger_{\alpha\gamma}. \quad (19)$$

One of the consequences of the fundamental theorem includes the uniqueness of the transformation function up to a phase ambiguity. Thus, $\hat{g}_{\alpha\beta}\hat{g}_{\beta\gamma}$ and $\hat{g}_{\alpha\gamma}$ differ only by a phase, i.e., Eq. (17). Next, since $|\{\hat{g}_{\alpha\beta}\hat{g}_{\beta\gamma}\}\rangle = c_{\alpha\beta\gamma}|\{\hat{g}_{\alpha\gamma}\}\rangle$, we can see that Eq. (11) is equivalent to $(\delta c)_{\alpha\beta\gamma\delta} := c_{\alpha\beta\gamma} c^*_{\alpha\beta\delta} c_{\alpha\gamma\delta} c^*_{\beta\gamma\delta} = 1$.[5] This equation is a higher analog of Eq. (10) and follows simply from the associativity of the matrix product. We thus establish $(\{U_\alpha\}, \{L_{\hat{g}_{\alpha\beta}}\}, \{\sigma^{\mathrm{MPS}}_{\alpha\beta\gamma}\})$ as a gerbe on X. In the following, we call $(\{U_\alpha\}, \{L_{\hat{g}_{\alpha\beta}}\}, \{\sigma^{\mathrm{MPS}}_{\alpha\beta\gamma}\})$ a constant-rank MPS gerbe. Here, the adjective "constant-rank" implies the bond dimension of MPS matrices is constant over the parameter space X. Furthermore, $c_{\alpha\beta\gamma}$ defines a second Čeck cohomology class $[c_{\alpha\beta\gamma}] \in H^2(X; \underline{\mathrm{U}(1)})$. To see this, we note that, since the defining equation for $\hat{g}_{\alpha\beta}$ imposes no constraints on the phase of $\hat{g}_{\alpha\beta}$, we can freely transform the phase of $\hat{g}_{\alpha\beta}$. Under the phase transformation of $\hat{g}_{\alpha\beta}$,

$$\hat{g}_{\alpha\beta} \mapsto e^{i\chi_{\alpha\beta}}\hat{g}_{\alpha\beta}, \quad (20)$$

the function $c_{\alpha\beta\gamma}$ changes as

$$c_{\alpha\beta\gamma} \mapsto c_{\alpha\beta\gamma} e^{i\chi_{\alpha\beta}} e^{i\chi_{\beta\gamma}} e^{-i\chi_{\alpha\gamma}} = c_{\alpha\beta\gamma}(\delta e^{i\chi})_{\alpha\beta\gamma}. \quad (21)$$

We can freely multiply it by $(\delta e^{i\chi})_{\alpha\beta\gamma}$ using any arbitrarily defined function $e^{i\chi_{\alpha\beta}}$ on $U_{\alpha\beta}$. This is precisely the transformation due to the coboundary degree of freedom. Therefore, $[c_{\alpha\beta\gamma}] \in H^2(X; \underline{\mathrm{U}(1)})$. The standard isomorphism $H^2(X; \underline{\mathrm{U}(1)}) \simeq H^3(X; \mathbb{Z})$ then gives a corresponding class in $H^3(X; \mathbb{Z})$, which is a topological invariant of the gerbe.[6] This class is known as the Dixmier-Douady class [33]. Due to the isomorphism, we also call the cohomology class $[c_{\alpha\beta\gamma}]$ the Dixmier-Douady class.

A constant-rank MPS gerbe is a proper mathematical structure to describe invertible states over X when we are interested in the torsion part of $H^3(X; \mathbb{Z})$, i.e., a finite order subgroup of $H^3(X; \mathbb{Z})$. Such cases were studied in detail in Ref. [19]. In general, however, the rank of MPS matrices may not be constant over the parameter space X [34]. Moreover, constant-rank MPS matrices cannot describe nontrivial models which take their values in the free part, i.e., (copies of) the infinite cyclic group $\mathbb{Z}$, of $H^3(X; \mathbb{Z})$. Let us briefly explain this point. Since $\hat{g}_{\alpha\beta}\hat{g}_{\beta\gamma} = c_{\alpha\beta\gamma}\hat{g}_{\alpha\gamma}$ holds as a unitary matrix, the following equation is obtained by taking the determinant of both sides:

$$\det(\hat{g}_{\alpha\beta}) \det(\hat{g}_{\alpha\gamma})^* \det(\hat{g}_{\beta\gamma}) = c^n_{\alpha\beta\gamma}. \quad (22)$$

This equation implies that $c^n_{\alpha\beta\gamma}$ is closed cocycle and $[c^n_{\alpha\beta\gamma}]$ is trivial in $H^2(X; \underline{\mathrm{U}(1)})$, i.e., $[c^n_{\alpha\beta\gamma}] = 1 \in H^2(X; \underline{\mathrm{U}(1)})$. Therefore, the topological class of $(\{U_\alpha\}, \{L_{\hat{g}_{\alpha\beta}}\}, \{\sigma^{\mathrm{MPS}}_{\alpha\beta\gamma}\})$ is in the torsion part of $H^3(X; \mathbb{Z})$. We can also show this point using differential forms. By taking the logarithm, determinant, and exterior derivative of both sides of $\hat{g}_{\alpha\beta}\hat{g}_{\beta\gamma} = c_{\alpha\beta\gamma}\hat{g}_{\alpha\gamma}$,

$$d\log\det(\hat{g}_{\alpha\beta}) - d\log\det(\hat{g}_{\alpha\gamma}) + d\log\det(\hat{g}_{\beta\gamma}) = d\log(c_{\alpha\beta\gamma}). \quad (23)$$

This implies $(w_\alpha := 0, d\log\det(\hat{g}_{\alpha\beta}), c_{\alpha\beta\gamma})$ is a third smooth Deligne cocycle [19,32]. Since this cocycle is flat, i.e., $\eta_\alpha := dw_\alpha = 0$, the topological class of $(\{U_\alpha\}, \{L_{\hat{g}_{\alpha\beta}}\}, \{\sigma^{\mathrm{MPS}}_{\alpha\beta\gamma}\})$ is trivial in the free part of $H^3(X; \mathbb{Z})$. This property is

[5]Here, δ is the coboundary operator of the Čeck cohomology.

[6]Here, the isomorphism is given in the following way: Let us take a $\mathbb{R}$ lift $w_{\alpha\beta\gamma}$ of $c_{\alpha\beta\gamma}$, i.e., $c_{\alpha\beta\gamma} = e^{i2\pi w_{\alpha\beta\gamma}}$. Then, on $U_{\alpha\beta\gamma\delta}$, $d_{\alpha\beta\gamma\delta} := w_{\alpha\beta\gamma} - w_{\alpha\beta\delta} + w_{\alpha\gamma\delta} - w_{\beta\gamma\delta}$ takes its value in $\mathbb{Z}$ and satisfies the cocycle condition. Thus, it defines the third cohomology class $[d_{\alpha\beta\gamma\delta}] \in H^3(X; \mathbb{Z})$.

completely determined by the Dixmier-Douady class and independent of the choice of the higher connections. This is due to the mathematical fact that the topological class of a $PU(n)$ bundle can only take its value in the torsion part of $H^3(X;\mathbb{Z})$ [35]. Therefore, we need to handle a family of MPS matrices with a nonconstant rank and construct a gerbe from such matrices.[7] We discuss this point in Sec. II E.

D. Triple inner product of MPSs

Before delving into nonconstant-rank MPSs, let us discuss one more ingredient, still using constant-rank MPSs. Specifically, we demonstrate how the data that make up the MPS gerbe, such as the transition functions and the Dixmier-Douady class, relate to certain overlaps of MPSs. We show that the Dixmier-Douady class can be obtained from the triple inner product, defined below, for three MPSs. This is reminiscent of Wu and Yang's work on U(1) magnetic monopoles, where a topological invariant, the Chern class, can be obtained from the inner product of two wave functions from different patches. In this discussion, we present an alternative formulation in which the MPS gerbe's data are expressed in terms of (triple) wave function overlaps. Moreover, in the following section, we will see that this formulation also naturally generalizes to the definition of a gerbe from MPSs over X with a nonconstant rank.

Let us start with the transfer matrix at $x \in U_\alpha$, which is defined as

$$T_\alpha(x) = \sum_i A_\alpha^{i*}(x) \otimes A_\alpha^i(x). \tag{24}$$

As reviewed in Sec. II A, $T_\alpha(x)$ acts on $\mathrm{Mat}_n(\mathbb{C})$ from the left and right as $T_\alpha(x) \cdot M := \sum_i A_\alpha^i(x) M A_\alpha^{i\dagger}(x)$ and $M \cdot T_\alpha(x) := \sum_i A_\alpha^{i\dagger}(x) M A_\alpha^i(x)$, respectively, for arbitrary $M \in \mathrm{Mat}_n(\mathbb{C})$. We represent this action pictorially in Fig. 1. The transfer matrix $T_\alpha(x)$ has unique right and left eigenvectors $\Lambda_\alpha^R(x)$ and $\Lambda_\alpha^L(x)$ with eigenvalue 1:

$$T_\alpha(x) \cdot \Lambda_\alpha^R(x) = \Lambda_\alpha^R(x), \quad \Lambda_\alpha^L(x) \cdot T_\alpha(x) = \Lambda_\alpha^L(x). \tag{25}$$

A primary tool in this section is a mixed transfer matrix [37], which we define from $\{A_\alpha^i(x)\}$ and $\{A_\beta^i(x)\}$ as

$$T_{\alpha\beta}(x) := \sum_i A_\beta^{i*}(x) \otimes A_\alpha^i(x) \tag{26}$$

over $U_{\alpha\beta}$. A crucial observation is that the spectrum of $T_{\alpha\beta}(x)$ is identical to that of $T_\alpha(x)$, and in particular, $T_{\alpha\beta}(x)$ has unique left and right eigenvectors with eigenvalue 1. Let us check this point. From now on, we omit the dependence on x. Let $\Lambda_\alpha^{R,k}$ be the kth eigenvector of T_α with eigenvalue $\lambda_\alpha^{R,k}$, $T_\alpha \cdot \Lambda_\alpha^{R,k} = \lambda_\alpha^{R,k}\Lambda_\alpha^{R,k}$. Then $\Lambda_{\alpha\beta}^{R,k} := \Lambda_\alpha^{R,k}\hat{g}_{\alpha\beta}$ is the eigenvector of $T_{\alpha\beta}$ with the same eigenvalue $\lambda_\alpha^{R,k}$:

$$\begin{aligned} T_{\alpha\beta} \cdot \Lambda_{\alpha\beta}^{R,k} &= \sum_i A_\alpha^i\left(\Lambda_\alpha^{R,k}\hat{g}_{\alpha\beta}\right)\left(\hat{g}_{\beta\alpha}A_\alpha^{i\dagger}\hat{g}_{\beta\alpha}^\dagger\right) = \lambda_\alpha^{R,k}\Lambda_\alpha^{R,k}\hat{g}_{\beta\alpha}^\dagger \\ &= \lambda_\alpha^{R,k}\Lambda_{\alpha\beta}^{R,k}. \end{aligned} \tag{27}$$

[7]According to mathematics, another way to avoid this obstacle is to consider the case of $n = \infty$ [36]. However, it is practically difficult to deal with MPSs of infinite rank.

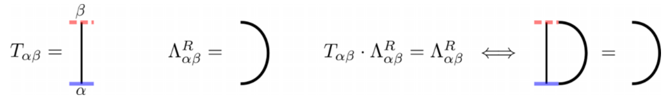

FIG. 4. The mixed transfer matrix $T_{\alpha\beta}$ and its right eigenvalue equation.

Therefore, there is a one-to-one correspondence between the eigenvectors of T_α and $T_{\alpha\beta}$ with the same eigenvalue. Similarly, for a left eigenvector $\Lambda_\alpha^{L,k}$ of T_α with eigenvalue $\lambda_\alpha^{L,k}$, $\Lambda_{\alpha\beta}^{L,k} := \hat{g}_{\beta\alpha}\Lambda_\alpha^{L,k}$ is a left eigenvector of $T_{\alpha\beta}$ with the eigenvalue $\lambda_\alpha^{L,k}$:

$$\begin{aligned} \Lambda_{\alpha\beta}^{L,k} \cdot T_{\alpha\beta} &= \sum_i \left(\hat{g}_{\beta\alpha}A_\alpha^{i\dagger}\hat{g}_{\beta\alpha}^\dagger\right)\hat{g}_{\beta\alpha}\Lambda_\alpha^{L,k}A_\alpha^i = \lambda_\alpha^{L,k}\hat{g}_{\beta\alpha}\Lambda_\alpha^{L,k} \\ &= \lambda_\alpha^{L,k}\Lambda_{\alpha\beta}^{L,k}. \end{aligned} \tag{28}$$

We define the right and left eigenstates of $T_{\alpha\beta}$ with eigenvalue 1 by

$$\Lambda_{\alpha\beta}^R := \Lambda_\alpha^R\hat{g}_{\alpha\beta} = \hat{g}_{\alpha\beta}\Lambda_\beta^R, \quad \Lambda_{\alpha\beta}^L := \hat{g}_{\beta\alpha}\Lambda_\alpha^L = \Lambda_\beta^L\hat{g}_{\beta\alpha}. \tag{29}$$

We represent the eigenvalue equations pictorially in Fig. 4. In the right canonical form, $\Lambda_\alpha^R = 1_n$. We also fix the phase of Λ_α^L by the condition $\mathrm{tr}(\Lambda_\alpha^L) = 1$. This is the normalization condition of the infinite MPS. Note that the phases of $\Lambda_{\alpha\beta}^R$ and $\Lambda_{\alpha\beta}^L$ are still redundant, but their redefinition can be absorbed in the $U(n)$ lift of the transition functions.

We are now ready to define the triple inner product. On a triple intersection $U_{\alpha\beta\gamma}$, consider the "boomerang" diagram in Fig. 5. Here, three infinite MPSs, representing the same physical state at $x \in X$, from three different patches are "glued" together as in Fig. 5. Observe how "bra" and "ket" MPS matrices are arranged depending on which "wing" they are located. At the infinities of the three wings, the tensor network is capped off by putting either left or right eigenvectors. The products of the mixed transfer matrices are easily computed in the thermodynamic limit, and we can check that the boomerang diagram computes the Dixmier-Douady class; the

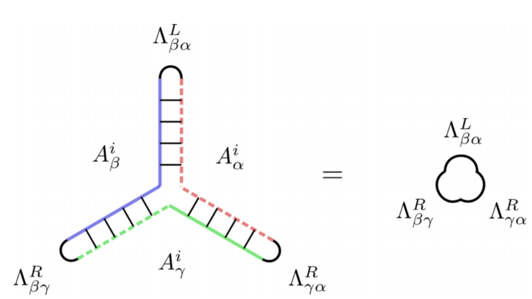

FIG. 5. The triple inner product of three MPSs, $\{A_\alpha^i\}$, $\{A_\beta^i\}$, and $\{A_\gamma^i\}$, from different patches U_α, U_β, and U_γ, respectively. The right side of the middle wing and the right side of the bottom right wing represent the matrix A_α^i; the left side of the middle wing and the left side of the bottom left wing represent the matrix A_β^i, and the right side of the bottom left wing and the left side of the bottom right wing represent the matrix A_γ^i. The dotted lines represent the complex conjugation of the MPS matrices.

boomerang diagram equals

$$\mathrm{tr}\big(\Lambda^L_{\beta\alpha}\Lambda^R_{\beta\gamma}\Lambda^R_{\gamma\alpha}\big) = \mathrm{tr}\big(\Lambda^L_{\alpha}\hat{g}_{\alpha\beta}1_n\hat{g}_{\beta\gamma}1_n\hat{g}_{\gamma\alpha}\big) = c_{\alpha\beta\gamma}. \quad (30)$$

We define the triple inner product of three MPSs as the boomerang diagram and the higher Berry phase as the Dixmier-Douady class. The ordinary Berry phase can be obtained from the ordinary inner product of two wave functions that are physically the same but taken from two different patches. As the natural generalization of this method, the higher Berry phase in (1 + 1)-dimensional systems can be obtained from the triple inner product of three MPSs that are physically the same but taken from three different patches. Note that with the mixed transfer matrix and the triple inner product, it is not necessary to deal with the transition functions explicitly. Instead, the data necessary to define the (constant-rank) MPS gerbe are encoded in the mixed transfer matrix and the triple inner product.

Finally, we note that there are some ambiguities in the definition of an MPS gerbe and a triple inner product. For example, a gerbe can be constructed by using $\Lambda^L_{\beta\alpha}$ instead of $\Lambda^R_{\alpha\beta}$ in the definition of the line bundle on $U_{\alpha\beta}$. In our choice, $|\{A^i_\alpha\}\rangle$, $|\{\hat{g}_{\alpha\beta}\}\rangle$, and the modulus of the triple inner product are all normalized to be 1, while in other choices we would need to adjust normalization (by properly rescaling $\Lambda^L_{\beta\alpha}$). Our choice would be natural in this sense.

E. Definition of a nonconstant-rank MPS gerbe

In Secs. II C and II D, we assumed that the rank of the MPS matrices is constant over the parameter space X. As a generalization of this situation, we consider a family of MPS matrices with nonconstant rank. To that end, we first introduce the notion of essentially normal matrices: let $\{A^i\}$ be a set of $n\times n$ matrices. Then $\{A^i\}$ is essentially normal if and only if there is an invertible matrix X such that

$$XA^iX^{-1} = \begin{pmatrix}\tilde{A}^i & 0\\ Y^i & 0\end{pmatrix} \quad (31)$$

for some $\tilde{n}\times\tilde{n}$ matrices $\{\tilde{A}^i\}$ and $(n-\tilde{n})\times\tilde{n}$ matrices Y^i. Also, we impose the right canonical form condition, $\sum_i A^iA^{i\dagger} = 1_n$. In terms of $\{\tilde{A}^i\}$ and Y_i, this means that

$$\sum_i \tilde{A}^i\tilde{A}^{i\dagger} = 1_{\tilde{n}}, \quad \sum Y^iY^{i\dagger} = 1_{n-\tilde{n}},$$
$$\sum_i Y^i\tilde{A}^{i\dagger} = 0, \quad \sum_i \tilde{A}^iY^{i\dagger} = 0. \quad (32)$$

We call $\tilde{n}$ an essential rank of the essentially normal matrices and $\{\tilde{A}^i\}$ the normal part of the essentially normal matrices. Usually, we eliminate the lower triangular component Y^i by hand because it does not affect the state. However, such cases appear naturally when considering a family of MPS matrices.

Let $\{U_\alpha\}$ be an open covering of X, and let us consider a family of essentially normal MPS matrices. Assume that the rank of MPS matrices is constant on each patch. Let $\{A^i_\alpha\}$ be $n_\alpha\times n_\alpha$ essentially injective matrices whose essential rank $\tilde{n}_\alpha(x)$ can be dependent on $x\in U_\alpha$. We also assume that $\tilde{n}_\alpha(x) = \tilde{n}_\beta(x)$ on a nonempty intersection $U_{\alpha\beta}$. Let us consider the mixed transfer matrix

$$T_{\alpha\beta} = \sum_i A^{i*}_\beta \otimes A^i_\alpha. \quad (33)$$

The mixed transfer matrix $T_{\alpha\beta}$ acts on $M\in \mathrm{Mat}_{n_\alpha\times n_\beta}(\mathbb{C})$ from the left as

$$T_{\alpha\beta}\cdot M = \sum_i A^i_\alpha M A^{i\dagger}_\beta \quad (34)$$

and acts on $M\in \mathrm{Mat}_{n_\beta\times n_\alpha}(\mathbb{C})$ from the right as

$$M\cdot T_{\alpha\beta} = \sum_i A^{i\dagger}_\beta M A^i_\alpha. \quad (35)$$

Then we can show that both the maximal left and right eigenvalues of the mixed transfer matrix are 1, and the right and left eigenvectors $\Lambda^R_{\alpha\beta}$ and $\Lambda^L_{\alpha\beta}$ are unique and are given by

$$\Lambda^R_{\alpha\beta} := \begin{pmatrix}\tilde{\Lambda}^R_{\alpha\beta} & 0\\ 0 & \sum_i Y^i_\alpha\tilde{\Lambda}^R_{\alpha\beta}Y^{i\dagger}_\beta\end{pmatrix}, \quad \Lambda^L_{\alpha\beta} := \begin{pmatrix}\tilde{\Lambda}^L_{\alpha\beta} & 0\\ 0 & 0\end{pmatrix}, \quad (36)$$

respectively, where $\tilde{\Lambda}^R_{\alpha\beta}$ and $\tilde{\Lambda}^L_{\alpha\beta}$ are right and left eigenvectors with eigenvalue 1 of the mixed transfer matrix of the normal part of $\{A^i_\alpha\}$ and $\{A^i_\beta\}$.

This can be readily checked as follows. Let M be an $n_\alpha\times n_\beta$ matrix and consider the following decomposition:

$$M = \begin{pmatrix}\Lambda & Z\\ X & \Lambda'\end{pmatrix}, \quad (37)$$

where Λ, X, Z, and Λ' are $\tilde{n}_\alpha\times\tilde{n}_\alpha$, $(n_\alpha-\tilde{n}_\alpha)\times\tilde{n}_\alpha$, $\tilde{n}_\alpha\times(n_\beta-\tilde{n}_\alpha)$, and $(n_\alpha-\tilde{n}_\alpha)\times(n_\beta-\tilde{n}_\alpha)$, respectively. Then, the right eigenvalue equation $T_{\alpha\beta}\cdot M = M$ reads

$$\sum_i \begin{pmatrix}\tilde{A}^i_\alpha\Lambda\tilde{A}^{i\dagger}_\beta & \tilde{A}^i_\alpha\Lambda Y^{i\dagger}_\beta\\ Y^i_\alpha\Lambda\tilde{A}^{i\dagger}_\beta & Y^i_\alpha\Lambda Y^{i\dagger}_\beta\end{pmatrix} = \begin{pmatrix}\Lambda & Z\\ X & \Lambda'\end{pmatrix}. \quad (38)$$

From the upper left block, we see that Λ must be the right eigenvector, $\Lambda = \Lambda^R_{\alpha\beta} = g_{\alpha\beta}$. We also see from the lower left block $\sum_i Y^i_\alpha\Lambda\tilde{A}^{i\dagger}_\beta = \sum_i Y^i_\alpha g_{\alpha\beta}\tilde{A}^{i\dagger}_\beta = \sum_i Y^i_\alpha\tilde{A}^{i\dagger}_\alpha g^\dagger_{\alpha\beta} = 0$, where we used the right canonical condition (32). We can show similarly that $\sum_i\tilde{A}^i_\alpha\Lambda Y^{i\dagger}_\beta = g_{\alpha\beta}\sum_i\tilde{A}^i_\beta Y^{i\dagger}_\beta = 0$. We thus conclude the first equation in (36). For the left eigenequation $M\cdot T_{\alpha\beta} = M$, we consider a similar decomposition (37), which leads to

$$\sum_i \begin{pmatrix}\big(\tilde{A}^{i\dagger}_\beta\Lambda + Y^{i\dagger}_\beta X\big)\tilde{A}^i_\alpha + \big(\tilde{A}^{i\dagger}_\beta Z + Y^{i\dagger}_\beta\Lambda'\big)Y^i_\alpha & 0\\ 0 & 0\end{pmatrix}$$
$$= \begin{pmatrix}\Lambda & Z\\ X & \Lambda'\end{pmatrix}. \quad (39)$$

The solution is given by the second equation in (36), $X = Z = \Lambda' = 0$ and $\Lambda = \tilde{\Lambda}^L_{\alpha\beta}$.

We are now ready to define a gerbe from a family of essentially normal matrices, including the case where the rank is not constant over the parameter space. It is defined, as a natural generalization of a constant-rank MPS gerbe, as follows: We

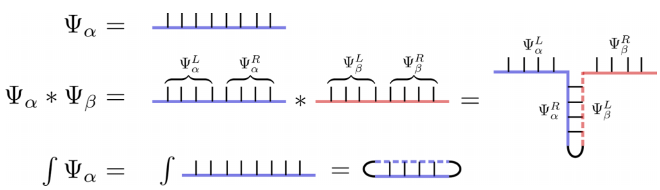

FIG. 6. Matrix product states, star product, and integration. Along the dotted lines, the relevant MPS tensors are conjugated, i.e., A^*.

define a state over $U_{\alpha\beta}$ by

$$\left|\{\Lambda^R_{\alpha\beta}\}\right\rangle := \sum_{\{i_k\}} \cdots A^{i_1}_\alpha \cdots A^{i_p}_\alpha \Lambda^R_{\alpha\beta} A^{i_{p+1}}_\beta \times \cdots A^{i_L}_\beta \cdots |\cdots i_1 \cdots i_{i_L} \cdots\rangle \tag{40}$$

and a complex line bundle over $U_{\alpha\beta}$ by

$$L^{\rm MPS}_{\alpha\beta} := \mathbb{C}\left|\{\Lambda^R_{\alpha\beta}\}\right\rangle. \tag{41}$$

On a triple intersection, we define an isomorphism

$$\sigma^{\rm MPS}_{\alpha\beta\gamma} : L^{\rm MPS}_{\alpha\beta} \otimes L^{\rm MPS}_{\beta\gamma} \to L^{\rm MPS}_{\alpha\gamma} : \left|\{\Lambda^R_{\alpha\beta}\}\right\rangle \otimes \left|\{\Lambda^R_{\beta\gamma}\}\right\rangle \mapsto \left|\{\Lambda^R_{\alpha\beta}\Lambda^R_{\beta\gamma}\}\right\rangle = c_{\alpha\beta\gamma}\left|\{\Lambda^R_{\alpha\gamma}\}\right\rangle. \tag{42}$$

Then, $\mathcal{G}^{\rm MPS} := (\{U_\alpha\}, \{L^{\rm MPS}_{\alpha\beta}\}, \{\sigma^{\rm MPS}_{\alpha\beta\gamma}\})$ is a gerbe on X. We call $\mathcal{G}^{\rm MPS}$ a nonconstant-rank MPS gerbe, or an MPS gerbe for short. The triple inner product can also be defined following the constant-rank case. We can compute the Dixmier-Douady class by the same diagram as in Fig. 5: The boomerang diagram equals

$$\mathrm{tr}\big(\Lambda^L_{\beta\alpha}\Lambda^R_{\beta\gamma}\Lambda^R_{\gamma\alpha}\big) = c_{\alpha\beta\gamma}. \tag{43}$$

Since $\{\Lambda^L_{\alpha\beta}\}$ includes the projection onto the normal part and $\{\Lambda^R_{\alpha\beta}\}$ is block diagonal, Eq. (43) reduces to

$$\mathrm{tr}\big(\Lambda^L_{\beta\alpha}\Lambda^R_{\beta\gamma}\Lambda^R_{\gamma\alpha}\big) = \mathrm{tr}\big(\tilde\Lambda^L_{\beta\alpha}\tilde\Lambda^R_{\beta\gamma}\tilde\Lambda^R_{\gamma\alpha}\big). \tag{44}$$

Namely, $c_{\alpha\beta\gamma}$ is nothing but the Dixmier-Douady class for the MPS matrices projected onto the normal part.

III. STAR PRODUCT AND INTEGRATION

In this section, we introduce two operations for infinite MPSs: the star product ($*$) and integration ($\int$). As we will see, these operations are useful for describing the structures introduced in the preceding sections. Our definitions are largely inspired by, and essentially identical to, the noncommutative geometry in string field theory [38].

Let us first introduce a multiplication law $*$ for two infinite MPSs (Fig. 6). In this section, we denote an MPS constructed from $\{A^i_\alpha\}$ as Ψ_α. For two MPSs Ψ_α and Ψ_β from different patches U_α and U_β, the product $\Psi_\alpha * \Psi_\beta$ is defined by first splitting Ψ_α and Ψ_β into their left and right pieces, denoted by Ψ^L_α and Ψ^R_α and Ψ^L_β and Ψ^R_β, respectively. In the product $\Psi_\alpha * \Psi_\beta$, Ψ^R_α and Ψ^L_β are glued, i.e., contracted. In this process, the MPS matrices $\{A^i_\beta\}$ on the left part of Ψ_β are first converted to their conjugates $\{A^{i*}_\beta\}$ (bras) and then contracted with the right part of Ψ_α. The star product is associative, $(\Psi_\alpha * \Psi_\beta) * \Psi_\gamma = \Psi_\alpha * (\Psi_\beta * \Psi_\gamma)$, but not commutative. Intuitively, we regard physical indices in Ψ^L_α and Ψ^R_α as row (input) and column (output) indices of an infinite matrix, or a semi-infinite matrix product operator. Accordingly, the star product can be interpreted as matrix multiplication of two infinite-dimensional matrices.

To see the connection with the MPS gerbe, we consider three MPSs, Ψ_α, Ψ_β, and Ψ_γ, defined on patches U_α, U_β, and U_γ, respectively. First, we can readily check that the product $\Psi_\alpha * \Psi_\beta$ is nothing but the mixed-gauge MPS $|\{\Lambda^R_{\alpha\beta}\}\rangle$. Following the notation in this section, we simply write $|\{\Lambda^R_{\alpha\beta}\}\rangle \equiv \Psi_{\alpha\beta}$. We also note that an infinite canonical MPS is an idempotent of the star product, $\Psi_\alpha * \Psi_\alpha = \Psi_\alpha$. Second, the product of $\Psi_{\alpha\beta}$ and $\Psi_{\beta\gamma}$ is given by

$$\Psi_{\alpha\beta} * \Psi_{\beta\gamma} = \Psi_\alpha * \Psi_\beta * \Psi_\beta * \Psi_\gamma = c_{\alpha\beta\gamma}\Psi_{\alpha\gamma}. \tag{45}$$

Hence, the star product is nothing but $\sigma^{\rm MPS}_{\alpha\beta\gamma}$. We note that mixed-gauge MPSs are closed under the multiplication $*$.

To see how the triple inner product arises, we also introduce an integration $\int$. To define the integration of Ψ_α, $\int\Psi_\alpha$, we "fold" Ψ_α and contract Ψ^L_α and Ψ^R_α (Fig. 6). With this rule, we can see, for example,

$$\int \Psi_\alpha = \mathrm{tr}\left(\Lambda^L_\alpha\Lambda^R_\alpha\right) = 1,$$
$$\int \Psi_\alpha * \Psi_\beta = \mathrm{tr}\left(\Lambda^L_{\alpha\beta}\Lambda^R_{\alpha\beta}\right) = \mathrm{tr}\left(\Lambda^L_\beta\hat{g}_{\beta\alpha}\hat{g}_{\alpha\beta}\Lambda^R_\beta\right) = 1. \tag{46}$$

Namely, $\int\Psi_\alpha$ is the norm of Ψ_α, and $\int\Psi_\alpha * \Psi_\beta$ is the overlap between Ψ_α and Ψ_β. It is also evident that $\int\Psi_\alpha * \Psi_\beta = \int\Psi_\beta * \Psi_\alpha$. As before, regarding the physical indices in Ψ^L_α and Ψ^R_α as row and column indices, the integration is interpreted as the matrix trace. Finally, we can readily see that the integral of the triple product $\Psi_\alpha * \Psi_\beta * \Psi_\gamma$ is the triple inner product (Fig. 7),

$$\int \Psi_\alpha * \Psi_\beta * \Psi_\gamma = c_{\alpha\beta\gamma}. \tag{47}$$

The cyclicity $\int\Psi_\alpha * \Psi_\beta * \Psi_\gamma = \int\Psi_\beta * \Psi_\gamma * \Psi_\alpha$ is evident from the cyclicity of $c_{\alpha\beta\gamma}$. Thus, the star product and integration reproduce the essential ingredients of the MPS gerbe. We note that the triple inner product can also be viewed as the regular inner product of two nonuniform states, $\Psi_{\alpha\beta}$ and $\Psi_{\beta\gamma}$.

Before leaving this section, several comments are in order.

(1) It appears that there is some flexibility in the definition of the star product and the integration. For example, when we glue two MPSs Ψ_α and Ψ_β, we can take the conjugate of Ψ^R_α while keeping Ψ^L_β intact. As for the integration, we also have at least two choices, i.e., taking the conjugation of Ψ^L_α or Ψ^R_α. To be consistent with the "regular rule" of matrix multiplication and trace, one would choose to take the conjugate of Ψ^R_α both in $\Psi_\alpha * \Psi_\beta$ and $\int\Psi_\alpha$; in this convention, the left (right) part of an MPS is always regarded as the row (column) indices (both in the star product and trace). This choice results in a different definition of an MPS gerbe and

$\Psi_\alpha * \Psi_\beta * \Psi_\gamma =$

$\int \Psi_\alpha * \Psi_\beta * \Psi_\gamma =$

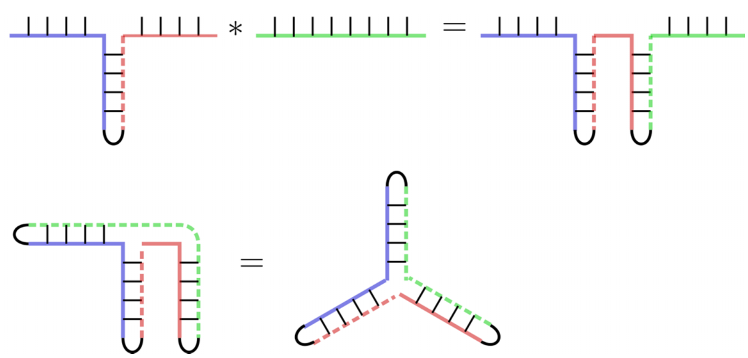

FIG. 7. The star product of three MPSs, Ψ_α, Ψ_β, and Ψ_γ, and the triple inner product.

a triple inner product as noted at the end of Sec. II D. (The idempotent property $\Psi_\alpha * \Psi_\alpha = \Psi_\alpha$, however, is lost in this choice.) We also note that, while we have focused on the right canonical form, we can adopt a different canonical form, the mixed canonical form, in particular.

(2) The notations and ideas behind these definitions are from noncommutative geometry [39]: $\Psi_\alpha, \Psi_\beta, \ldots$ can be thought of as an analog of differential forms, and the star product is an analog of the wedge product. As differential forms, we should be able to integrate Ψ_α. The star product and integration are some of the ingredients that constitute noncommutative geometry. To fully define noncommutative geometry, we need additional structures, the derivative, and $\mathbb{Z}_2$ grading. In string field theory, the derivative is given by the so-called Becchi-Rouet-Stora-Tyutin (BRST) operator that is used to select physical states. The $\mathbb{Z}_2$ grading is provided by the number of ghosts. While we do not need such structures for the purpose of this paper, i.e., to discuss the topological properties of gapped translationally invariant ground states, we may speculate that the full noncommutative geometry structure may be useful once we consider a wider class of states, e.g., excited states.

(3) We noted that an infinite MPS is an idempotent of the star product, i.e., projector, $\Psi_\alpha * \Psi_\alpha = \Psi_\alpha$. This is similar to the fact that in string field theory, the matter part of the full string field satisfies the same equation [40–43] and describes a D-brane (D25-brane), an extended object in string theory. This is reminiscent of the fact that invertible states in $(1+1)$ dimensions can be expressed as boundary states in boundary conformal field theory [44]. Furthermore, a mixed-gauge MPS $\Psi_{\alpha\beta}$ can be interpreted as a boundary condition changing operator [45,46], and the star product $\Psi_{\alpha\beta} * \Psi_{\beta\gamma} = c_{\alpha\beta\gamma}\Psi_{\alpha\gamma}$ represents the fusion of two boundary condition changing operators. With proper regularization (Euclidean evolution), the triple inner product corresponds to the partition function on a strip with boundary conditions specified by α, β, and γ, i.e., with the insertion of a boundary condition changing operator between α and β, say.[8]

[8]To describe a parameterized family of invertible states we expect that these boundary conditions preserve only the conformal symmetry and not any larger symmetry.

IV. DISCUSSION

In this paper, we identified a gerbe structure for a family of infinite MPSs over a parameter space X. We also introduced, as a generalization of the ordinary Berry phase for overlaps of two wave functions, the triple inner product for three infinite MPSs and showed that it extracts the Dixmier-Douady class, which is a topological invariant of an MPS gerbe and hence a family of invertible states over X. Our formalism works for both the torsion and free parts of $H^3(X;\mathbb{Z})$. In particular, for the free case, we showed how to handle nonconstant-rank MPSs over X.

The relation between the triple inner product and the Dixmier-Douady class is one of the upshots of this paper. In principle, this relation can provide a practical way to calculate the topological invariant for a given family of $(1+1)$-dimensional invertible states. An important next step would be to find an explicit "algorithm" for this and study examples.

In addition, it is interesting to consider the triple inner product of a larger class of MPSs, such as finite and/or nontranslationally invariant MPSs. In particular, it may be interesting to study finite MPSs with periodic boundary conditions. We also note that a wave function overlap for three many-body states, similar to our triple inner product, has been discussed as a numerical tool to extract universal data of $(1+1)$-dimensional lattice quantum systems at criticality [47–49].

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