# Higher Berry structure of matrix product states 

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with
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Ref：arXiv：2305．08109．
Related papers：
－Adam Artymowicz，Anton Kapustin，Nikita Sopenko，arXiv：2305．06399．
－Marvin Qi，David T．Stephen，Xueda Wen，Daniel Spiegel，Markus J．Pflaum，Agnés Beaudry， Michael Hermele，arXiv：2305．07700．

## Berry phase Berry, 84

- The Berry phase is a $U(1)$-valued quantity defined from a one-parameter family of pure states in a 0 -dim system, a quantum mechanical system.
- Consider a one-parameter family of normalized states $|\psi(x)\rangle \in \mathbb{C}^{N},\langle\psi(x) \mid \psi(x)\rangle=1$, a circle $x \in C \cong S^{1}$.
- We introduce a triangulation $|C|=\left\{\left[x_{j}, x_{j+1}\right]\right\}_{j=1}^{n}$ of $C$.
- Because two nearest-neighbor states $\left|\psi\left(x_{j}\right)\right\rangle$ and $\left|\psi\left(x_{j+1}\right)\right\rangle$ are "close" to each other, implying $\left\langle\psi\left(x_{j}\right) \mid \psi\left(x_{j+1}\right)\right\rangle \neq 0$, the $U(1)$ phase of the inner product $\left\langle\psi\left(x_{j}\right) \mid \psi\left(x_{j+1}\right)\right\rangle$ is well-defined.



## Cont.

- For $|C|$, one can define a $U(1)$-valued quantity

$$
e^{i \gamma(|C|)}:=\prod_{j=1}^{n} \frac{\left\langle\psi\left(x_{j}\right) \mid \psi\left(x_{j+1}\right)\right\rangle}{\left|\left\langle\psi\left(x_{j}\right) \mid \psi\left(x_{j+1}\right)\right\rangle\right|} \in U(1) .
$$

- $e^{i \gamma(|C|)}$ is manifestly invariant under gauge transformations $\left|\psi\left(x_{j}\right)\right\rangle \mapsto\left|\psi\left(x_{j}\right)\right\rangle e^{i \xi_{j}}$.
- The Berry phase is defined as the limit

$$
e^{i \gamma(C)}=\lim _{\left|x_{j}-x_{j+1}\right| \rightarrow 0} e^{i \gamma(|C|)} .
$$

- In numerical calculations, the lattice formula $e^{i \gamma(|C|)}$ is usually sufficient.


## Berry "flux"

- Similarly, there is a lattice definition of the Berry curvature (field strength).
- For a 2-simplex $\Delta^{2}=(012)$ in the parameter space $\mathcal{M}$, we define the "Berry flux" $e^{i F\left(\Delta^{2}\right)}$ as the Berry phase of the boundary of $\Delta^{2}$.

$$
e^{i F\left(\Delta^{2}\right)}:=e^{i \gamma\left(\partial \Delta^{2}\right)} .
$$

- If the 2-simplex $\Delta^{2}$ is small enough, the flux piercing $\Delta^{2}$ is small $e^{i F\left(\Delta^{2}\right)} \sim 1$.
- Thus, $F\left(\Delta^{2}\right)$ can be considered as a $\mathbb{R}$-valued quantity $F\left(\Delta^{2}\right) \in \mathbb{R}$.

(figure from wikipedia)


## Chern number

- For a 2-submanifold $\Sigma \subset \mathcal{M}$ and its fixed triangulation $|\Sigma|$, a $\mathbb{Z}$-valued quantity (the first Chern number in the limit of $\operatorname{Area}\left(\Delta^{2}\right) \rightarrow 0$ ), is defined.

$$
\nu(|\Sigma|)=\frac{1}{2 \pi} \sum_{\Delta^{2} \in|\Sigma|} F\left(\Delta^{2}\right) \in \mathbb{Z}
$$

- The quantization $\nu(|\Sigma|) \in \mathbb{Z}$ is manifest:

$$
e^{2 \pi i \nu(|\Sigma|)}=\prod_{\Delta^{2} \in|\Sigma|} e^{i \gamma\left(\partial \Delta^{2}\right)} \equiv 1
$$



## To 1-dim invertible states in quantum spin systems

- We want to discuss generalizing the story above to invertible ( $\cong$ short-range entangled $\cong$ unique gapped) states in 1-dim quantum spin systems.
- The essential difference is that a 1-dim system is inherently infinite-dimensional:

$$
\mathcal{H}_{\text {total }}=\bigotimes_{x \in \mathbb{Z}} \mathcal{H}_{x}, \quad \mathcal{H}_{x} \cong \mathbb{C}^{d} .
$$

- One can try the same definition of the Berry phage in 0-dim systems to 1 -dim systems but with finite system size with length $L$.
- However, the inner product between two different invertible states decays exponentially

$$
\left\langle\psi \mid \psi^{\prime}\right\rangle \sim e^{-\alpha L} .
$$

- So the $U(1)$ phase is of $\left\langle\psi \mid \psi^{\prime}\right\rangle$ might be numerically ill-defined...
- This suggests we must reconstruct the "higher Berry phase" in a way suitable for 1-dim infinite systems.


## Kapustin=Spodyneiko

- Kapustin and Spodyneiko proposed "higher Berry curvature" in $d$-dim systems.

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## Higher-dimensional generalizations of Berry curvature

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(0) (Received 20 February 2020; accepted 14 May 2020; published 11 June 2020)

- In the form of correlation functions of the local Hamiltonians $h_{x}$ and its external derivatives $d h_{x}$, they constructed a $\Omega^{(d+2)}(\mathcal{M})$-valued quantity $((d+2)$-differential form), a generalization of the Berry curvature in $d$-dim.
- I am not going into detail, but let me explain the relationship with the $\Omega$-spectrum structure of the space of invertible states.


## $\Omega$-spectrum proposal [Kitaev, 11, 13, 15, ... in videos]

- A proposal on the topological structure behind the space of invertible states.
- Let $F_{d}$ be the "space of $d$-dim invertible states" (which has not been rigorously defined yet).
- Proposal: The sequence of the spaces $\left\{F_{d}\right\}_{d \in \mathbb{Z}}$ forms an $\Omega$-spectrum of the generalized cohomology theory. Namely, there is a homotopy equivalence

$$
\Omega F_{d+1} \sim F_{d}
$$

where

$$
\left.\Omega F_{d+1}=\left\{S^{1} \rightarrow F_{d+1}| | \Psi(0)\right\rangle=|\Psi(2 \pi)\rangle=|1\rangle\right\}
$$

is the based loop space of $F_{d+1}$. (|1 $\rangle$ is a trivial tensor product state.)

- Physically, $\Omega F_{d+1}$ is the "space of adiabatic cycles in $(d+1)$-dim".
- Implication: The adiabatic cycles in $(d+1)$-dim are classified by the invertible phases in $d$-dim.

$$
\pi_{0}\left(\Omega F_{d+1}\right)=\pi_{0}\left(F_{d}\right) .
$$

This is consistent with physics: Thouless pump, Floquet cycle,...

- For free fermions, $\pi_{0}\left(\Omega^{k} F_{d+k}\right)=\pi_{0}\left(F_{d}\right)$ is well-established [Teo-Kane '10].

What is the space of invertible states in 1-dim quantum spin systems? puzzle

- For 0-dim,

$$
E_{0} \sim \mathbb{C} P^{N-1}\left(=\mathbb{C}^{N} / \mathbb{C}^{\times}\right) \hookrightarrow \mathbb{C} P^{\infty}=B U(1) \sim K(\mathbb{Z}, 2)
$$

the classifying space of $U(1)$. The embedding is given by

$$
\psi=\left(\psi_{1}, \ldots \psi_{N}\right) \mapsto\left(\psi_{1}, \ldots, \psi_{N}, 0\right)
$$

- If the $\Omega$-spectrum structure is true,

$$
E_{0} \sim \Omega E_{1} \quad \Rightarrow \quad E_{1} \sim K(\mathbb{Z}, 3)
$$

is consistent.

- What is $K(\mathbb{Z}, 3)$ ?
$\rightarrow$ the classifying space of infinite projective unitary group $B P U(\infty) \sim K(\mathbb{Z}, 3)$.
- Where is $P U(\infty)$-bundle structure in 1-dim invertible states?
- A family of matrix product states (MPSs) is a $P U(D)$-bundle.

Haegeman=Mariën=Osborne=Verstraete 14

- MPS should be a good starting point.


## Matrix product state (MPS) Vidal, Perez-Garcia=Verstraete=Wolf=Cirac

- Total Hilbert space:

$$
\mathcal{H}_{\text {total }}^{(L)}=\bigotimes_{x=1}^{L} \mathcal{H}_{x}, \quad \mathcal{H}_{x}=\mathbb{C}^{N} .
$$

- A pure state $|\psi\rangle \in \mathcal{H}_{\text {total }}^{(L)}$ is specified by the wave function

$$
|\psi\rangle=\sum_{i_{1}, \ldots, i_{L}} \psi\left(i_{1}, \ldots, i_{L}\right)\left|i_{1} \cdots i_{L}\right\rangle .
$$

- The MPS representation is a way to write the wave function $\psi\left(i_{1}, \ldots, i_{L}\right)$ in the following form:

$$
\psi\left(i_{1}, \ldots, i_{L}\right)=\operatorname{tr}\left[A^{[1] i_{1}} \cdots A^{[L] i_{L}}\right] .
$$

Here, $\left\{A^{[x] i_{x}}\right\}_{x=1}^{N}$ is set of $D_{j} \times D_{j+1}$ matrices.

- An MPS representation is given by successive singular value decompositions from left to right.


## Translational invariant MPS Perez-Garcia=Verstraete=Wolf=Cirac

- Let $\hat{T}_{r}$ be the translation operator

$$
\hat{T}_{r}\left|i_{1} \cdots i_{L}\right\rangle=\left|i_{2} \cdots i_{L} i_{1}\right\rangle .
$$

- Fact. Translation invariant state $\hat{T}_{r}|\psi\rangle=|\psi\rangle$ has a translational invariant MPS representation

$$
|\psi\rangle=\left|\left\{A^{i}\right\}_{i}\right\rangle_{L}:=\sum_{i_{1}, \ldots, i_{L}} \operatorname{tr}\left[A^{i_{1}} \cdots A^{i_{L}}\right]\left|i_{1} \cdots i_{L}\right\rangle .
$$

- In the rest of this talk, I focus only on translational invariant states and MPSs.
- ( $D$-MPS) A $D$-MPS is the set of $D \times D$ matrices

$$
\left\{A^{i}\right\}_{i=1}^{N}, \quad A^{i} \in \operatorname{Mat}_{D \times D}(\mathbb{C})
$$

$D$ is called the bond dimension.

## Injective MPS Perez-Garcia=Verstraete=Wolf=Cirac

- D-MPS may be a cat state, a superposition of macroscopically different states.
- To remove such MPSs, we impose "injectivity" on MPS:
- (Transfer matrix) We introduce the transfer matrix $T \in \operatorname{End}\left(\operatorname{Mat}_{D \times D}(\mathbb{C})\right.$ ) by

$$
T(X):=\sum_{i=1}^{N} A^{i} X A^{i \dagger}
$$

- (Injectivity) $D$-MPS is injective iff
(i) The largest eigenvalue $\lambda_{0}$ of $T$ in magnitude $|\lambda|$ is unique, and its eigenspace is non-degenerate.
(ii) The corresponding eigenvector $X$ is positive $X>0$.
- $T$ is completely positive $\rightarrow \lambda_{0}>0$ (positive real number).
- If $D$-MPS is injective, the correlation function decays exponentially.

$$
\left\langle\hat{O}_{x} \hat{O}_{y}^{\prime}\right\rangle-\left\langle\hat{O}_{x}\right\rangle\left\langle\hat{O}_{y}^{\prime}\right\rangle \sim e^{-|x-y| / \xi}, \quad \xi=-1 / \log \left(\left|\lambda_{1}\right| /\left|\lambda_{0}\right|\right),
$$

where $\lambda_{1}$ is the second largest eigenvalue in magnitude.
$\rightarrow$ "invertible" state.

## Canonical form Perez-Garcia=Verstraete=Wolf=Cirac

- (Canonical form) A $D$-MPS is in the canonical form when

$$
\sum_{i=1}^{N} A^{i} A^{i \dagger}=1_{D} \quad \text { and } \quad \sum_{i=1}^{N} A^{i \dagger} \Lambda^{2} A^{i}=\Lambda^{2}
$$

hold, where $\Lambda$ is a positive-definite diagonal matrix whose entries are the Schmidt eigenvalues and satisfy $\operatorname{tr}\left[\Lambda^{2}\right]=1$.

- This is a normalization condition for MPSs.
- Remark. Injective $D$-MPS can be in the canonical form:

$$
\begin{aligned}
& \sum_{i=1}^{N} A^{i} X A^{i \dagger}=\lambda_{0} X \quad \Rightarrow \quad \sum_{i=1}^{N}\left(\frac{1}{\sqrt{\lambda_{0}}} X^{-1 / 2} A^{i} X^{1 / 2}\right)\left(\frac{1}{\sqrt{\lambda_{0}}} X^{-1 / 2} A^{i} X^{1 / 2}\right)^{\dagger}=1_{D} \\
& \sum_{i=1}^{N} A^{i \dagger} Y_{0} A^{i}=Y_{0}, Y_{0}=U^{\dagger} \Lambda^{2} U \quad \Rightarrow \quad \sum_{i=1}^{N}\left(U A^{i \dagger} U^{\dagger}\right) \Lambda^{2}\left(U^{\dagger} A^{i} U\right)^{\dagger}=\Lambda^{2}
\end{aligned}
$$

- In the rest of my talk, I assume $D$-MPSs are injective and in the canonical form.


## Gauge structure of MPS Perez-Garcia=Verstraete=Wolf=Cirac

- Theorem. (Fundamental theorem of MPS.) For two $D$-MPSs $\left\{A_{0}^{i}\right\}_{i=1}^{N},\left\{A_{1}^{i}\right\}_{i=1}^{N}$ with the matrices of the Schmidt eigenvalues $\Lambda_{0}$ and $\Lambda_{1}$, if ${ }^{\exists} L>c D^{4}(c=O(1))$ and ${ }^{\exists} e^{i \alpha} \in U(1)$ s.t. $\left|\left\{A_{0}^{i}\right\}_{i}\right\rangle_{L}=e^{i \alpha}\left|\left\{A_{1}^{i}\right\}_{i}\right\rangle_{L}$, then ${ }^{\exists 1} e^{i \theta_{01}} \in U(1)$ and ${ }^{\exists} V_{01} \in U(D)$ s.t.

$$
A_{0}^{i}=e^{i \theta_{01}} V_{01} A_{1}^{i} V_{01}^{\dagger}, \quad i=1, \ldots N, \quad \text { and } \quad V_{01} \Lambda_{1}=\Lambda_{0} V_{01} .
$$

Here, $V_{01}$ is unique up to $U(1)$ phases.

- The matrix $V_{01}$ is unique as an element of the projective unitary group

$$
P U(D)=U(D) /\left(V_{01} \sim e^{i \beta} V_{01}\right) .
$$

- Thus, a family of $D$-MPS over a parameter space $\mathcal{M}$ is a $U(1) \times P U(D)$ bundle over $\mathcal{M}$.
- Remark. $U(1)$ part is from 0-dim nature because we are considering translational invariant MPSs.


## Charastristic class of $P U(D)$ bundle Grothendieck 66

- Let's consider a $D$-MPS bundle over $\mathcal{M}$.
- Let $\left\{U_{\alpha}\right\}_{\alpha}$ be a good cover of $\mathcal{M}$. ${ }^{1}$
- On two patch intersections $U_{\alpha \beta}=U_{\alpha} \cap U_{\beta}$, we have transition functions $\left(e^{i \theta_{\alpha \beta}(x)}, V_{\alpha \beta}(x)\right)$ by

$$
A_{\beta}^{i}(x)=e^{i \theta_{\alpha \beta}(x)} V_{\alpha \beta}^{\dagger}(x) A_{\alpha}^{i}(x) V_{\alpha \beta}(x) .
$$

- Over $x \in U_{\alpha \beta \gamma}=U_{\alpha} \cap U_{\beta} \cap U_{\gamma}$, consider two deformations ( $x \in U_{\alpha \beta \gamma}$ is omitted)

$$
A_{\gamma}^{i}=e^{i \theta_{\alpha \gamma}} V_{\alpha \gamma}^{\dagger} A_{\alpha}^{i} V_{\alpha \gamma}, \quad A_{\gamma}^{i}=e^{i \theta_{\beta \gamma}} V_{\beta \gamma}^{\dagger} A_{\beta}^{i} V_{\beta \gamma}=e^{i \theta_{\beta \gamma}} e^{i \theta_{\alpha \beta}} V_{\beta \gamma}^{\dagger} V_{\alpha \beta}^{\dagger} A_{\alpha}^{i} V_{\alpha \beta} V_{\beta \gamma},
$$

and using the uniqueness of $V_{\alpha \gamma}$, we have the 1-cocycle condition for $\left\{V_{\alpha \beta}\right\}_{\alpha \beta}$ :

$$
V_{\alpha \beta}(x) V_{\beta \gamma}(x)=e^{i \phi_{\alpha \beta \gamma}(x)} V_{\alpha \gamma}(x), \quad{ }^{\exists} e^{i \phi_{\alpha \beta \gamma}(x)} \in U(1), \quad x \in U_{\alpha \beta \gamma} .
$$

- The formula Ohyama=Ryu, 2304.05356.:

$$
e^{i \phi_{\alpha \beta \gamma}(x)}=\operatorname{tr}\left[\Lambda_{\alpha}^{2}(x) V_{\alpha \beta}(x) V_{\beta \gamma}(x) V_{\gamma \alpha}(x)\right] .
$$

[^0]
## cont.

- There is a consistency condition on $e^{i \phi_{\alpha \beta \gamma}(x)} . V_{\alpha \beta}\left(V_{\beta \gamma} V_{\gamma \delta}\right)=\left(V_{\alpha \beta} V_{\beta \gamma}\right) V_{\gamma \delta}$ gives us

$$
e^{i \phi_{\alpha \beta \delta}(x)} e^{i \phi_{\beta \gamma \delta}(x)}=e^{i \phi_{\alpha \beta \gamma}(x)} e^{i \phi_{\alpha \gamma \delta}(x)}, \quad x \in U_{\alpha \beta \gamma \delta},
$$

meaning that $e^{i \phi_{\alpha \beta \gamma}(x)}$ is a 2-cocycle in $\check{Z}^{2}(\mathcal{M}, U(1))$.

- The change of $\mathrm{U}(1)$ phase $V_{\alpha \beta}(x) \mapsto V_{\alpha \beta}(x) e^{i \xi_{\alpha \beta}(x)}$ leads the equivalence relation by the 2-coboundary $e^{i \phi} \sim e^{i \phi} \delta e^{i \xi}$. Thus, $\left[e^{i \phi_{\alpha \beta \gamma}(x)}\right] \in \check{H}^{2}(\mathcal{M}, \underline{U(1)})$.
- Take a lift $\mathbb{R} / 2 \pi \mathbb{Z} \ni \phi_{\alpha \beta \gamma}(x) \rightarrow \tilde{\phi}_{\alpha \beta \gamma}(x) \in \mathbb{R}$, we have a $\mathbb{Z}$-valued 3-cocycle

$$
c=\frac{1}{2 \pi} \delta \tilde{\phi} \in \check{Z}^{3}(\mathcal{M}, \mathbb{Z})
$$

and its equivalence class (from choices of lifts) is the characteristic class (Dixmier-Douady class) of $P U(D)$-bundle

$$
[c] \in \check{H}^{3}(\mathcal{M}, \mathbb{Z})
$$

## cont.

- However, $[c]$ never represents a free part of $\check{H}^{3}(\mathcal{M}, \mathbb{Z})$.
- This is because we can choose $V_{\alpha \beta}(x)$ to be a $S U(D)$ matrix by using the $U(1)$ phase freedom. In doing so, the 2-cocycle $e^{i \phi_{\alpha \beta \gamma}(x)}$ is quantized to a $\mathbb{Z}_{D}$-value

$$
e^{i \phi_{\alpha \beta \gamma(x)}} \in \mathbb{Z}_{D}=\left\{\left.e^{\frac{2 \pi i p}{D}} \right\rvert\, p=0, \ldots, D-1\right\}
$$

resulting in

$$
D \times[c]=0 \in \check{H}^{3}(\mathcal{M}, \mathbb{Z})
$$

- Therefore, $D$-MPS bundle can provide only the $D$-torsion part of $H^{3}(\mathcal{M}, \mathbb{Z})$,

$$
\left\{x \in H^{3}(\mathcal{M}, \mathbb{Z}) \mid D x=0\right\} .
$$

- cf. See Ohyama=Terashima=KS for an explicit construction of MPS when $\mathcal{M}=\mathbb{R} P^{2} \times S^{1}$ and $\mathcal{M}=L(3,1) \times S^{1}$.


## Is constant bond dimension $D$ physically reasonable?

- No.
- The bond dimension $D$ is just a parameter to represent a true gapped state $|\psi\rangle$ with an MPS $|\mathrm{MPS}\rangle$ with an error $\langle\psi \mid \mathrm{MPS}\rangle=1-\epsilon$.
- Even in the class of MPSs with finite bond dimensions (like AKLT state), it is easy to make a continuous path from different bond dimensions:

$$
|\psi(t)\rangle=(1-t)|D-\mathrm{MPS}\rangle+t\left|D^{\prime}-\mathrm{MPS}\right\rangle .
$$

- It is natural to think of a family of MPS over $\mathcal{M}$ whose bond dimension $D_{x}$ is also a function over $\mathcal{M}$.
- In this talk, the interest is a lattice formulation of the higher Berry phase. We introduce a triangulation $|\mathcal{M}|$ of $\mathcal{M}$.
- Input: a set of $D_{p}$-MPSs over the vertices $p$ of $|\mathcal{M}|$.


## What is the "measure" of the space of MPSs?

- How to estimate the distance between two MPSs?
- For the purpose of making the higher Berry phase, a measure may be given by the spectrum of the mixed transfer matrix.
- For physically different $D_{0}$-MPS $\left\{A_{0}^{i}\right\}_{i=1}^{N}$ and $D_{1}$-MPS $\left\{A_{1}^{i}\right\}_{i=1}^{N}$, we define the mixed transfer matrix $T_{01} \in \operatorname{End}\left(\operatorname{Mat}_{D_{0} \times D_{1}}(\mathbb{C})\right)$ by

$$
T_{01}(X):=\sum_{i=1}^{N} A_{0}^{i} X A_{1}^{i \dagger}
$$

- If two MPSs are physically "close" to each other, the spectrum of $T_{01}$ should resemble the spectra of transfer matrices for each.

$$
T_{00}(X)=\sum_{i=1}^{N} A_{0}^{i} X A_{0}^{i \dagger}, \quad T_{11}(X)=\sum_{i=1}^{N} A_{1}^{i} X A_{1}^{i \dagger} .
$$

- In particular, the largest eigenvalue $\lambda_{01}$ of $T_{01}$ in magnitude $|\lambda|$ is unique, its eigenspace is non-degenerate, $\left|\lambda_{01}\right| \sim 1$, and there is a finite gap $|\lambda|<\left|\lambda_{01}\right|-|\delta \lambda|$ for $\lambda \neq \lambda_{01}$.


## "Overlap matrix" $V_{01}$

- Let $V_{01}$ be the eigenvector with $\lambda=\lambda_{01}$ of the mixed transfer matrix $T_{01}$, namely,

$$
\sum_{i=1}^{N} A_{0}^{i} V_{01} A_{1}^{i \dagger}=\lambda_{01} V_{01}, \quad V_{01} \in \operatorname{Mat}_{D_{0} \times D_{1}}(\mathbb{C})
$$

- We can fix $V_{10}=V_{01}^{\dagger}$.
- The matrix $V_{01}$ plays the role of the inner product $\left\langle\psi\left(x_{j}\right) \mid \psi\left(x_{j+1}\right)\right\rangle$ in the discrete Berry phase formula in 0-dim.
- cf. $V_{01}$ is nothing but the transition function when $\left\{A_{0}^{i}\right\}_{i}$ and $\left\{A_{1}^{i}\right\}_{i}$ represent the same physical state.
- There are two types of gauge transformation of $V_{01}$ :
(i) $V_{01} \rightarrow W_{0} V_{01} W_{1}^{\dagger}$.

This comes from the gauge transformations of MPSs $A_{n}^{i} \rightarrow e^{i \theta_{n}} W_{n}^{\dagger} A_{n}^{i} W_{n}, n=0,1$.
(ii) $V_{01} \rightarrow z V_{01}$ with $z \in \mathbb{C}^{\times}$.

This is because the eigenvalue equation $T_{01}\left(V_{01}\right)=\lambda_{01} V_{01}$ does not fix the overall $\mathbb{C}$ number of $V_{01}$.

## 2-cocycle and weighting by Schmidt eigenvalues

- Let's construct a gauge invariant quantity from the set of $V_{01} s$ !
- Before we do so, we return to the cases of physically equivalent three MPSs. For physically equivalent three $D$-MPSs $\left\{A_{0}^{i}\right\}_{i},\left\{A_{1}^{i}\right\}_{i},\left\{A_{2}^{i}\right\}_{i}$ with the matrices of Schmidt eigenvalues $\Lambda_{0}, \Lambda_{1}, \Lambda_{2}$, the 2-cocycle $e^{i \phi_{012}}$ is given by

$$
e^{i \phi_{012}}=\operatorname{tr}\left[\Lambda_{0}^{2} V_{01} V_{12} V_{20}\right] .
$$

- This is not symmetric in the labels $0,1,2$. A more symmetric expression that is suitable for physically different MPSs is

$$
e^{i \phi_{012}}=\operatorname{tr}\left[\Lambda_{0}^{\frac{2}{3}} V_{01} \Lambda_{1}^{\frac{2}{3}} V_{12} \Lambda_{2}^{\frac{2}{3}} V_{20}\right] .
$$

- We employ this formula for MPSs, which are physically different but close to each other.


## Higher Berry connection

- For a 2 -simplex $\Delta^{2}=(012)$ of the discretized parameter space $|\mathcal{M}|$, we define a $U(1)$-valued quantity

$$
e^{i \phi_{012}}:=\frac{\operatorname{tr}\left[\Lambda_{0}^{\frac{2}{3}} V_{01} \Lambda_{1}^{\frac{2}{3}} V_{12} \Lambda_{2}^{\frac{2}{3}} V_{20}\right]}{\left|\operatorname{tr}\left[\Lambda_{0}^{\frac{2}{3}} V_{01} \Lambda_{1}^{\frac{2}{3}} V_{12} \Lambda_{2}^{\frac{2}{3}} V_{20}\right]\right|} \in U(1) .
$$

$\rightarrow$ invariant under the 1st gauge (i) $V_{01} \rightarrow W_{0} V_{01} W_{1}^{\dagger}$.


## Higher Berry curvature (flux)

- For a 3-simplex $\Delta^{3}=(0123)$ of $|\mathcal{M}|$, we define the "higher Berry flux"

$$
e^{i F\left(\Delta^{3}\right)}:=e^{i \phi_{123}} e^{-i \phi_{023}} e^{i \phi_{013}} e^{i \phi_{012}} \in U(1) .
$$

$\rightarrow$ invariant under the 2 nd gauge (ii) $V_{01} \rightarrow z V_{01}$ with $z \in \mathbb{C}^{\times}$.


- If the triangulation $|\mathcal{M}|$ is small enough then $e^{i F\left(\Delta^{3}\right)} \sim 1$ so that we can think $F\left(\Delta^{3}\right)$ as an $\mathbb{R}$-valued quantity.


## Topological invariant (Dixmier-Douady class)

- The sum over all 3 -simplexes of $|\mathcal{M}|$ is manifestly quantized

$$
\nu(|X|)=\frac{1}{2 \pi} \sum_{\Delta^{3} \in|X|} F\left(\Delta^{3}\right) \in \mathbb{Z}
$$

since

$$
e^{2 \pi i \nu(|X|)}=\prod_{\Delta^{3} \in|X|} e^{2 \pi i F\left(\Delta^{3}\right)}=\prod_{\Delta^{3}} e^{i \phi_{123}} e^{-i \phi_{023}} e^{i \phi_{013}} e^{i \phi_{012}}=1
$$

- We expect that $\nu(|X|)$ characterizes the free part of the 3rd cohomology group $H^{3}(\mathcal{M}, \mathbb{Z})$, the topological nature of the parameter family of invertible 1-dim spin systems.


## Model (Xueda Wen, et al. + perturbation)

- Two spin $1 / 2$ dof $\sigma_{l}$ and $\tau_{l}$ for each site.

$$
\begin{aligned}
& H_{0}\left(\alpha \in\left[-\frac{\pi}{4}, \frac{\pi}{4}\right], \boldsymbol{n} \in S^{2}\right) \\
& =\sin (2 \alpha) \sum_{l \in \mathbb{Z}}\left\{\begin{array}{cc}
-\boldsymbol{\sigma}_{j} \cdot \boldsymbol{\tau}_{j} & \left(\alpha \in\left[-\frac{\pi}{4}, 0\right]\right) \\
\boldsymbol{\tau}_{l} \cdot \boldsymbol{\sigma}_{l+1} & \left(\alpha \in\left[0, \frac{\pi}{4}\right]\right)
\end{array}+\cos (2 \alpha) \sum_{l \in \mathbb{Z}}\left(-\boldsymbol{n} \cdot \boldsymbol{\sigma}_{l}+\boldsymbol{n} \cdot \boldsymbol{\tau}_{l}\right) .\right.
\end{aligned}
$$



- This is an array of two spin problems, so easy to solve.
- At $\alpha= \pm \frac{\pi}{4}, \boldsymbol{n}$ disappears, implying that the parameter space is $S^{3}$.
- The bond dimension is $D=1$ for $\alpha \in\left[-\frac{\pi}{4}\right]$ and $D=2$ for $\alpha \in\left[0, \frac{\pi}{4}\right]$.
- This model shows a nontrivial value for the topological invariant introduced by


## cont.

- We add NN and NNN Heisenberg terms to $H_{0}(\alpha, \boldsymbol{n})$.

$$
H(\alpha, \boldsymbol{n})=H_{0}(\alpha, \boldsymbol{n})+J_{1} \sum_{l \in \mathbb{Z}}\left(\boldsymbol{\sigma}_{l} \cdot \boldsymbol{\tau}_{l}+\boldsymbol{\tau}_{l} \cdot \boldsymbol{\sigma}_{l+1}\right)+J_{2} \sum_{l \in \mathbb{Z}}\left(\boldsymbol{\sigma}_{l} \cdot \boldsymbol{\sigma}_{l+1}+\boldsymbol{\tau}_{l} \cdot \boldsymbol{\tau}_{l+1}\right)
$$

- We numerically solve this model by DMRG with TeNPy (Tensor Network Python) package Hauschild=Pollmann.
- In this model, the higher Berry flux is symmetric for the $S^{2}$-direction.



## Numerical results



## cont.



## cont.



## cont.



## Summary

- We studied the geometric structure of the family of MPSs.
- We propose that the eigenvector $V_{01}$ of the mixed transfer matrix $T_{01}$ for physically different but close MPSs resembles the inner product $\left\langle\psi_{0} \mid \psi_{1}\right\rangle$ of two states in 0-dim. We constructed the higher Berry phase and the higher Berry curvature of MPSs.
- We demonstrated that by using DMRG the integrated higher Berry curvature over the 3 -sphere shows the nontrivial topological invariant $\nu(|\mathcal{M}|)=1$.

KS, Heinsdorf, Ohyama, 2305.08109.


[^0]:    ${ }^{1}$ All sets and all non-empty intersections of finitely-many sets are contractible.

