Fermionic partial transpose and non-local order parameters for SPT phases of fermions

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Main Ref:
KS-Shapourian-Gomi-Ryu, arXiv:1710.01886
Related refs:
Shapourian-KS-Ryu, arXiv:1607.03896
KS-Ryu, arXiv:1607.06504
KS-Shapourian-Ryu, arXiv:1609.05970
Shapourian-KS-Ryu, 1611.07536

## Take-home message

- Transpose $\sim$ time-reversal (TR) transformation for the imaginary time path-integral.

$$
\left(\mathcal{O}_{n} \ldots \mathcal{O}_{2} \mathcal{O}_{1}\right)^{t r}=\mathcal{O}_{1}^{t r} \mathcal{O}_{2}^{t r} \cdots \mathcal{O}_{n}^{t r}
$$

- The partial transpose enable us to simulate the partition function over some non-orientable manifolds in the operator formalism.


Real projective plane


Klein bottle

- We proposed a new partial transpose for fermions such that it simulates the partition function over pin manifolds.

$$
A^{t r_{1}}=\sum_{k_{1}, k_{2}, k_{1}+k_{2} \in \mathrm{even}} A_{p_{1} \cdots p_{k_{1}}, q_{1} \cdots q_{k_{2}}} i^{k_{1}} \underbrace{a_{p_{1}} \cdots a_{p_{k_{1}}}}_{I_{1}} \underbrace{b_{q_{1}} \cdots b_{q_{k_{2}}}}_{I_{2}}
$$

## Motivation

- How to detect symmetry protected topological (SPT) phases ( $\sim$ gapped phases without ground state degeneracy)
- The classification of symmetry-protected topological phases $\sim$ the classification of $U(1)$-valued topological pattition functions [Kapustin, Freed-Hopkins, ‥]

Euclidian spacetime manifold


Excited states

Characterizes SPT phases

## Motivation

- In SPT phases with time-reversal (TR) symmetry, the spacetime manifold $M$ to detect nontrivial SPT phases is sometimes nonorientable.
$\checkmark$ Ex: Haldane chain phase, topological insulator/superconductor, $\cdots$
- The partition function over a suitable non-orientable manifold is the "order parameter" of SPT phases.
- Ex: $(1+1)$ d bosonic SPT phases with TR sym.
$\checkmark$ "Order parameter" = real projective plane RP²

$$
\begin{aligned}
& e^{i S_{\mathrm{top}}(M)}=e^{i \pi \nu \int_{M} w_{2}(T M)}, \quad(\nu=0,1) \\
& \quad \Rightarrow e^{i S_{\mathrm{top}}\left(R P^{2}\right)}=(-1)^{\nu}
\end{aligned}
$$

$\checkmark$ If the partition function over $\mathrm{RP}^{2}$ is negative, the theory is in nontrivial SPT phases.

## Motivation

- Non-orientable manifold???
- In cond-mat, we have only
$\checkmark$ Hamiltonian $H$ or the ground state $|\psi\rangle$, and
$\checkmark$ TR operator $T$.
- How to make non-orientable manifold from a set of a ground state wave function and a TR operator?

- An answer is to use the partial transpose.


## TRS $\leftrightarrow$ Transpose

## TRS $\leftrightarrow$ Transpose

- Given a TR operator, how to get the transpose?
- Let's consider the expectation value of the TR operator.

$$
\langle\psi| T|\psi\rangle
$$

- This is ill-defined, because T is anti-linear.
- However, the amplitude is well-defined.
- Some calculation:

$$
\begin{aligned}
|\langle\psi| T| \psi\rangle\left.\right|^{2} & =\langle\psi| U|\psi\rangle^{*}\left\langle\left.\psi\right|^{*} U^{\dagger} \mid \psi\right\rangle \\
& =\operatorname{tr}\left[|\psi\rangle\langle\psi| U|\psi\rangle^{*}\left\langle\left.\psi\right|^{*} U^{\dagger}\right]\right. \\
& =\operatorname{tr}\left[\rho U \rho_{*}^{*} U^{\dagger}\right] \\
& =\operatorname{tr}\left[\rho U \rho_{*}^{t r} U^{\dagger}\right],
\end{aligned} \quad \text { Complex conjugate } \quad \text { Transpose in the operator algebra }
$$

- Here, $\rho=|\psi\rangle\langle\psi|$ and $U$ is the unitary part of the TR operator, i.e. $T=$ $U K$ with $K$ the complex conjugate.
- We used the Hermiticity $\rho^{\dagger}=\rho$.
- In this way, a TR operator $T$ induces a sort of the transpose in the operator algebra.

$$
T=U K \quad \Rightarrow \quad U \rho^{\operatorname{tr}} U^{\dagger}
$$

- The transpose is understood as the time-reversal transformation in the imaginary time path-integral.

$$
\left(\mathcal{O}_{n} \ldots \mathcal{O}_{2} \mathcal{O}_{1}\right)^{t r}=\mathcal{O}_{1}^{t r} \mathcal{O}_{2}^{t r} \cdots \mathcal{O}_{n}^{t r}
$$



- Therefore, it is expected that the transpose can be used to "simulate" non-orientable manifolds.
- Advantage: the transpose operation is linear, so it can be applied to a subsystem of the real space.
$\Rightarrow$ Partial transpose


## Partial transpose and non-orientable manifolds in bosonic systems

## Bosonic transpose

- In bosonic (spin) systems, the operator algebra is the matrix algebra.
- The transpose is the matric transpose

$$
(|i\rangle\langle j|)^{t r}=|j\rangle\langle i|
$$

- Given operator

$$
A=\sum_{i, j} A_{i, j}|i\rangle\langle j|,
$$

the transposed operator is given by

$$
A^{t r}=\sum_{i, j} A_{i, j}|j\rangle\langle i|
$$

## Bosonic partial transpose

- Divide the Hilbert space into two parts.

$$
I_{1}
$$

$$
I_{2}
$$

- Given a operator:

$$
A=\sum_{i j, k l} A_{i j, k l}\left|i \in I_{1}, j \in I_{2}\right\rangle\left\langle k \in I_{1}, l \in I_{2}\right|
$$

- The partial transpose on the subsystem $I_{1}$ is defined as the matrix transpose on $I$.

$$
A^{t r_{1}}=\sum_{i j, k l} A_{i j, k l}\left|k \in I_{1}, j \in I_{2}\right\rangle\left\langle i \in I_{1}, l \in I_{2}\right|
$$

# An application: the non-local order parameter for the Haldane chain phase 

- A model Hamiltonian: $(1+1)$ d antiferromagnetic Heisenberg model

$$
H=\sum_{j} \boldsymbol{S}_{j} \cdot \boldsymbol{S}_{j+1}
$$

- TR symmetry $T=\bigotimes_{j} e^{i \pi S_{j}^{y}} K$
- The classification of SPT phases is known to be $Z_{2}$.
- For the $S=1$ spin system, the ground state is nontrivial SPT phase. (the Haldane chain).
- The $Z_{2}$ "order parameter" is the partition function on RP2 (real projective plane).
- Let's construct the $Z_{2}$ "order parameter" in the operator formalism.
- The rule of this game is:
$\checkmark$ Input data
- Pure state (ground state) $|\psi\rangle$
- TR operator $T=\bigotimes_{j} e^{i \pi S_{j}^{y}} K$
$\checkmark$ Out put $=Z_{2}$ order parameter
- Pollmann and Turner discovered that the $Z_{2}$ order parameter is the "partial transpose" on two adjacent intervals. [Pollmann-Turner '12]
$I_{1}$
$I_{2}$
- The partial transpose on two adjacent intervals. [Pollmann-Turner '12]

$$
Z_{P T}:=\operatorname{tr}\left[\rho_{I_{1} \cup I_{2}}\left(\prod_{j \in I_{1}} e^{i \pi S_{j}^{y}}\right)\left(\rho_{I_{1} \cup I_{2}}\right)^{\operatorname{tr}_{1}}\left(\prod_{j \in I_{1}} e^{-i \pi S_{j}^{y}}\right)\right]
$$



- Using the MPS, one can prove that the $\mathrm{U}(1)$ phase of $Z_{P T}$ is quantized if intervals are large enough compared to the correlation length.

$$
Z_{P T} /\left|Z_{P T}\right| \rightarrow \pm 1, \quad\left|I_{1}\right|,\left|I_{2}\right| \gg \xi
$$

- The Pollmann-Turner invariant $Z_{P T}$ is topologically equivalent to the partition function over RP². [KS-Ryu, '16]

$$
Z:=\operatorname{tr}\left[\rho_{I_{1} \cup I_{2}}\left(\prod_{j \in I_{1}} e^{i \pi S_{j}^{y}}\right)\left(\rho_{I_{1} \cup I_{2}}\right)^{t r_{1}}\left(\prod_{j \in I_{1}} e^{-i \pi S_{j}^{y}}\right)\right]
$$



- In the same way, the partial transpose for disjoint two intervals is topologically equivalent to the Klein bottle partition function. [Calabrese-Cardy-Tonni '12]




## Partial transpose and non-orientable manifolds in <br> fermionic systems

## Transpose in the fermionic operator algebra

- Every operator can be expanded by Majorana fermions

$$
\begin{aligned}
& A=\sum_{k=1}^{2 N} \sum_{p_{1}<p_{2} \cdots<p_{k}} A_{p_{1} \cdots p_{k}} c_{p_{1}} \cdots c_{p_{k}} \\
& c_{j}^{\dagger}=c_{j}, \quad\left\{c_{j}, c_{k}\right\}=2 \delta_{j k} .
\end{aligned}
$$

- Operator algebra = the algebra generated by the Majorana fermions (Clifford algebra).
- The transpose (linear anti-automorphism) would be defined as reversing the order of Majorana fermions.

$$
\begin{aligned}
& \left(c_{p_{1}} c_{p_{2}} \cdots c_{p_{k}}\right)^{t r}:=c_{p_{k}} \cdots c_{p_{2}} c_{p_{1}} \\
& (\alpha A+\beta B)^{t r}=\alpha A^{t r}+\beta B^{t r}, \quad(A B)^{t r}=B^{t r} A^{t r}
\end{aligned}
$$

- This transpose is "canonical" in the sense that the transpose is compatible with the basis change

$$
\begin{aligned}
V c_{j} V^{\dagger} & =\left[\mathcal{O}_{V}\right]_{j k} c_{k}, \quad \mathcal{O}_{V} \in O(2 N) \\
A & \xrightarrow{V} V A V^{\dagger} \\
t r \downarrow & \circlearrowleft \\
& \operatorname{tr} \downarrow \\
A^{t r} & \xrightarrow{V} V A^{t r} V^{\dagger}
\end{aligned}
$$

- We got the full transpose for fermions.
- A remark: we did not use a TR transformation to define the transpose of fermions. This can be compared with the transpose of bosons where there is no canonical transpose in the absence of a TR transformation.


## Fermionic transpose and Grassmannian

- Does the fermionic transpose give the TR transformation in the imaginary time path-integral?
- Yes. Let us consider a simple TR transformation for complex fermions $f_{j}$ as

$$
T f_{j}^{\dagger} T^{-1}=f_{j}^{\dagger}, \quad T|v a c\rangle=|v a c\rangle .
$$

- The unitary part of the TR transformation $T$ is found to be the particle-hole transformation

$$
C_{T} f_{j}^{\dagger} C_{T}^{-1}=f_{j}, \quad C_{T}|v a c\rangle=|f u l l\rangle .
$$

- The transpose operation corresponding to the TR transformation $T$ is

$$
A \mapsto C_{T} A^{t r} C_{T}^{\dagger}
$$

- For coherent state basis

$$
\left|\left\{\xi_{j}\right\}\right\rangle=e^{-\sum_{j} \xi_{j} f_{j}^{\dagger}}|v a c\rangle
$$

the transpose with the particle-hole transformation reads

$$
C_{T}\left(\left|\left\{\xi_{j}\right\}\right\rangle\left\langle\left\{\chi_{j}\right\}\right|\right)^{t r} C_{T}^{\dagger}=\left|\left\{i \chi_{j}\right\}\right\rangle\left\langle\left\{i \xi_{j}\right\}\right| .
$$

- This is the desired TR transformation for the path-integral.
- Therefore, the partial transpose in fermions is expected to be used to simulate the real projective plane and the Klein bottle, as in the cases of bosons.



## Fermionic partial transpose

[KS-Shapourian-Gomi-Ryu, 1710.01886, cf. Shapourian-KS-Ryu, 1607.03896;

Shapourian-Ryu, 1804.08637]

- What is the partial transpose for fermions?
- Introduce two subsystems of degrees of freedom.

$$
a_{1}, a_{2}, \ldots \quad b_{1}, b_{2}, \ldots
$$

$$
A=\sum_{k_{1}, k_{2}}^{I_{1}} A_{p_{1} \cdots p_{k_{1}}, q_{1} \cdots q_{k_{2}}} \underbrace{a_{p_{1}} \cdots a_{p_{k_{1}}}}_{I_{1}} \underbrace{b_{q_{1}} \cdots b_{q_{k_{2}}}}_{I_{2}}
$$

- We want to define the partial transpose " $A^{t r_{1} \text { " }}$ on the subsystem $I_{1}$.
- It is natural to impose the following three good properties on the partial transpose :

1. Preserve the identity:

$$
(\mathrm{Id})^{t r_{1}}=\mathrm{Id}
$$

2. The successive partial transposes on $I_{1}$ and $I_{2}$ goes back to the full transpose:

$$
\left(A^{t r_{1}}\right)^{t r_{2}}=A^{t r}
$$

3. The partial transpose is compatible with the basis changes preserving subsysems $I_{1} \cup I_{2}$.

$$
\begin{aligned}
& \left(V A V^{\dagger}\right)^{t r_{1}}=V A^{t r_{1}} V^{\dagger} \\
& V a_{j} V^{\dagger}=\left[\mathcal{O}_{I_{1}}\right]_{j k} a_{k}, \quad V b_{j} V^{\dagger}=\left[\mathcal{O}_{I_{2}}\right]_{j k} b_{k}
\end{aligned}
$$

- For generic operators there is no solution that meets the above three conditions.
- For operators preserving the total fermion parity (like the density matrix)

$$
A=\sum_{k_{1}, k_{2}, k_{1}+k_{2} \in \text { even }} A_{p_{1} \cdots p_{k_{1}}, q_{1} \cdots q_{k_{2}}} \underbrace{a_{p_{1}} \cdots a_{p_{k_{1}}}}_{I_{1}} \underbrace{b_{q_{1}} \cdots b_{q_{k_{2}}}}_{I_{2}},
$$

there is the unique solution.

- The partial transpose for the subsystem $I_{1}$ is the scalar multiplication by $i^{k_{1}}$ which depends on the number of the Majorana fermions in the subspace $I_{1}$.

$$
A^{t r_{1}}=\sum_{k_{1}, k_{2}, k_{1}+k_{2} \in \mathrm{even}} A_{p_{1} \cdots p_{k_{1}}, q_{1} \cdots q_{k_{2}}} i^{k_{1}} \underbrace{a_{p_{1}} \cdots a_{p_{k_{1}}}}_{I_{1}} \underbrace{b_{q_{1}} \cdots b_{q_{k_{2}}}}_{I_{2}}
$$

Shapourian-KS-Ryu, 1607.03896.; KS-Shapourian-Gomi-Ryu, 1710.01886.

# An application: the non-local order parameter for 1d superconductors with TR symmetry 

- A model Hamiltonian: (1+1)d p-wave superconductor (Kitaev chain)

- TR symmetry $T f_{j}^{\dagger} T^{-1}=f_{j}^{\dagger}, \quad T|v a c\rangle=|v a c\rangle$.
- The classification of SPT phases is known to be $Z_{8}$. [Fidkowski-Kitaev '10]
- The $Z_{8}$ "order parameter" is the partition function on RP2 (real projective plane). $\quad \Omega_{2}^{\text {Pin- }_{-}}(p t)=\mathbb{Z}_{8}$
- The $Z_{8}$ order parameter in operator formalism is the partial transpose on adjacent two intervals

$$
Z=\operatorname{tr}_{I_{1} \cup I_{2}}\left[\rho_{I_{1} \cup I_{2}} C_{T}^{I_{1}} \rho_{I_{1} \cup I_{2}}^{t_{1}}\left[C_{T}^{\left.I_{1}\right]^{\dagger}}\right]\right.
$$



- Numerical calculation [arXiv:1607.03896]

$$
\begin{gathered}
H=-t \sum_{j}\left[f_{j}^{\dagger} f_{j}-\Delta f_{j+1}^{\dagger} f_{j}^{\dagger}+h . c .\right]-\mu \sum_{j} f_{j}^{\dagger} f_{j} \\
Z=\operatorname{tr}_{I_{1} \cup I_{2}}\left[\rho_{I_{1} \cup I_{2}} C_{T}^{I_{1}} \rho_{I_{1} \cup I_{2}}^{t r_{1}}\left[C_{T}^{I_{1}}\right]^{\dagger}\right]
\end{gathered}
$$


$\Delta$ is fixed to be $\Delta=t$.

## Manybody $Z_{2}$ Kane-Mele invariant

- $\quad(2+1) d$ topological insulator (TR symmetry with Kramers)
- The generating manifold is the Klein bottle $\times \mathrm{S}^{1}$ with a unit magnetic flux. [Witten '16]
- Combine two technics:
$\checkmark$ Disjoint partial transpose -> Klein bottle

$\checkmark$ Twist operator -> a unit magnetic flux

$$
\begin{aligned}
& \rho_{R_{1} \cup R_{3}}^{ \pm}:=\operatorname{Tr}_{\overline{R_{1} \cup R_{3}}}\left[e^{ \pm \sum_{(x, y) \in R_{2}} \frac{2 \pi i y}{L_{y}} \hat{n}(x, y)}|G S\rangle\langle G S|\right], \\
& Z:=\operatorname{Tr}_{R_{1} \cup R_{3}}\left[\rho_{R_{1} \cup R_{3}}^{+} C_{T}^{I_{1}}\left[\rho_{R_{1} \cup R_{3}}^{-}\right]^{t r_{1}}\left[C_{T}^{I_{1}}\right]^{\dagger}\right]
\end{aligned}
$$

## Manybody $Z_{2}$ Kane-Mele invariant

- Numerical calculation for a free fermion model

$$
Z:=\operatorname{Tr}_{R_{1} \cup R_{3}}\left[\rho_{R_{1} \cup R_{3}}^{+} C_{T}^{I_{1}}\left[\rho_{R_{1} \cup R_{3}}^{-}\right]^{\operatorname{tr}_{1}}\left[C_{T}^{I_{1}}\right]^{\dagger}\right]
$$



## Take-home message

- Transpose $\sim$ time-reversal (TR) transformation for the imaginary time path-integral.

$$
\left(\mathcal{O}_{n} \ldots \mathcal{O}_{2} \mathcal{O}_{1}\right)^{t r}=\mathcal{O}_{1}^{t r} \mathcal{O}_{2}^{t r} \cdots \mathcal{O}_{n}^{t r}
$$

- The partial transpose enable us to simulate the partition function over non-orientable manifolds in the operator formalism.

- Developed the partial transpose for fermions in the operator formalism

$$
A^{t r_{1}}=\sum_{k_{1}, k_{2}, k_{1}+k_{2} \in \mathrm{even}} A_{p_{1} \cdots p_{k_{1}}, q_{1} \cdots q_{k_{2}}} i^{k_{1}} \underbrace{a_{p_{1}} \cdots a_{p_{k_{1}}}}_{I_{1}} \underbrace{b_{q_{1}} \cdots b_{q_{k_{2}}}}_{I_{2}}
$$

