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

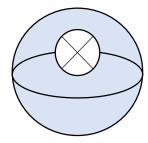
Shapourian-KS-Ryu, 1611.07536

Take-home message

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

$$(\mathcal{O}_n \dots \mathcal{O}_2 \mathcal{O}_1)^{tr} = \mathcal{O}_1^{tr} \mathcal{O}_2^{tr} \dots \mathcal{O}_n^{tr}$$

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



Real projective plane



Klein bottle

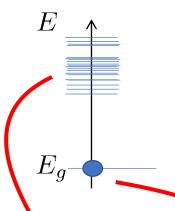
 We proposed a new partial transpose for fermions such that it simulates the partition function over pin manifolds.

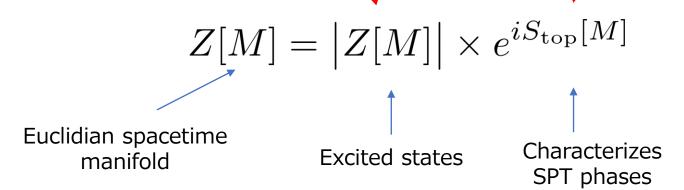
$$A^{tr_1} = \sum_{k_1, k_2, k_1 + k_2 \in \text{even}} A_{p_1 \dots p_{k_1}, q_1 \dots q_{k_2}} i^{k_1} a_{p_1} \dots a_{p_{k_1}} b_{q_1} \dots b_{q_{k_2}}$$

$$I_1 \qquad I_2$$

Motivation

How to detect symmetry protected topological (SPT) phases (\sim gapped phases without ground state degeneracy)





Motivation

- In SPT phases with time-reversal (TR) symmetry, the spacetime manifold M to detect nontrivial SPT phases is sometimes nonorientable.
 - ✓ Ex: Haldane chain phase, topological insulator/superconductor,…
- 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.
 - ✓ "Order parameter" = real projective plane RP²

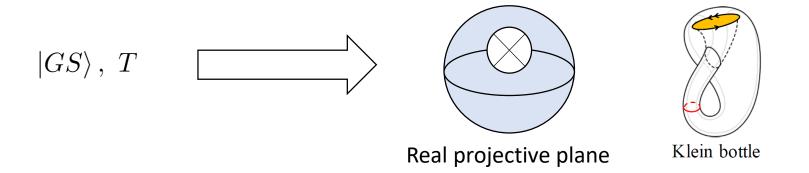
$$e^{iS_{\text{top}}(M)} = e^{i\pi\nu \int_M w_2(TM)}, \quad (\nu = 0, 1)$$

 $\Rightarrow e^{iS_{\text{top}}(RP^2)} = (-1)^{\nu}.$

✓ If the partition function over RP² 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.

 $\mathsf{TRS} \leftrightarrow \mathsf{Transpose}$

TRS ↔ 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:

$$\begin{split} |\left\langle \psi | T | \psi \right\rangle|^2 &= \left\langle \psi | \, U \, | \psi \right\rangle^* \left\langle \psi |^* \, U^\dagger \, | \psi \right\rangle \\ &= \mathrm{tr}[|\psi\rangle \left\langle \psi | \, U \, | \psi \right\rangle^* \left\langle \psi |^* \, U^\dagger \right] \\ &= \mathrm{tr}[\rho U \rho^* U^\dagger] \\ &= \mathrm{tr}[\rho U \rho^{tr} U^\dagger], \end{split}$$
 Complex conjugate
$$&= \mathrm{tr}[\rho U \rho^{tr} U^\dagger], \end{split}$$
 Transpose in the operator algebra

- Here, $\rho = |\psi\rangle\langle\psi|$ and U is the unitary part of the TR operator, i.e. T = UK 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.

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

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

$$(\mathcal{O}_n \dots \mathcal{O}_2 \mathcal{O}_1)^{tr} = \mathcal{O}_1^{tr} \mathcal{O}_2^{tr} \dots \mathcal{O}_n^{tr}$$

$$\uparrow_{\mathcal{O}_n} \qquad \qquad \downarrow_{\mathcal{O}_2} \qquad \qquad \downarrow_{\mathcal{O}_1^{tr}} \qquad \qquad \downarrow_{\mathcal{O}_2^{tr} \\ \mathcal{O}_1^{tr}} \qquad \qquad \downarrow_{\mathcal{O}_1^{tr}} \qquad \qquad \downarrow_{\mathcal{O}_2^{tr} \\ \mathcal{O}_1^{tr}} \qquad \qquad \downarrow_{\mathcal{O}_2^{tr} \\ \mathcal{O}_1^{tr} \qquad \qquad \downarrow_{\mathcal{O}_2^{tr} \\ \mathcal{O}_1^{tr}} \qquad \qquad \downarrow_{\mathcal{O}_2^{tr} \\ \mathcal{O}_1^{tr} \qquad \qquad \downarrow_{\mathcal{O}_2^{tr} \\ \mathcal{O}_1^{tr}} \qquad \qquad \downarrow_{\mathcal{O}_2^{tr} \\ \mathcal{O}_1^{tr} \qquad \qquad \downarrow_{\mathcal{O}_2^{tr} \\ \mathcal{O}_1^{tr}} \qquad \qquad \downarrow_{\mathcal{O}_2^{tr} \\ \mathcal{O}_1^{tr}} \qquad \qquad \downarrow_{\mathcal{O}_2^{tr} \\ \mathcal{O}_1^{tr} \qquad \qquad \downarrow_$$

- 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.
 - ⇒ 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

$$(|i\rangle\langle j|)^{tr} = |j\rangle\langle i|$$
.

Given operator

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

the transposed operator is given by

$$A^{tr} = \sum_{i,j} A_{i,j} |\mathbf{j}\rangle \langle \mathbf{i}|.$$

Bosonic partial transpose

Divide the Hilbert space into two parts.

 I_1 I_2

Given a operator:

$$A = \sum_{ij,kl} A_{ij,kl} | i \in I_1, j \in I_2 \rangle \langle k \in I_1, l \in I_2 |$$

• The partial transpose on the subsystem I_1 is defined as the matrix transpose on I_1 .

$$A^{tr_1} = \sum_{ij,kl} A_{ij,kl} | \mathbf{k} \in I_1, j \in I_2 \rangle \langle \mathbf{i} \in I_1, l \in I_2 |$$

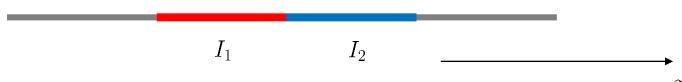
An application: the non-local order parameter for the Haldane chain phase

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

$$H = \sum_j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}.$$

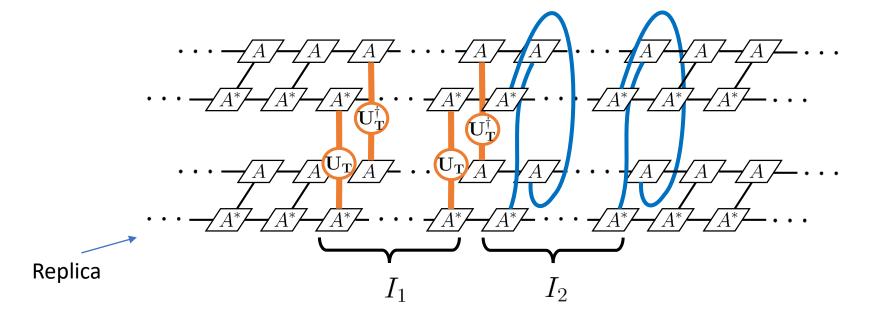
- TR symmetry $T = \bigotimes_{i} e^{i\pi S_{j}^{y}} K$
- The classification of SPT phases is known to be Z_2 .
- For the S=1 spin system, the ground state is nontrivial SPT phase. (the Haldane chain).
- The Z_2 "order parameter" is the partition function on RP² (real projective plane).

- Let's construct the Z_2 "order parameter" in the operator formalism.
- The rule of this game is:
 - ✓ Input data
 - Pure state (ground state) $|\psi\rangle$
 - TR operator $T = \bigotimes_{j} e^{i\pi S_{j}^{y}} K$
 - ✓ 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]



• The partial transpose on two adjacent intervals. [Pollmann-Turner '12]

$$Z_{PT} := \operatorname{tr} \left[\rho_{I_1 \cup I_2} \left(\prod_{j \in I_1} e^{i\pi S_j^y} \right) \left(\rho_{I_1 \cup I_2} \right)^{tr_1} \left(\prod_{j \in I_1} e^{-i\pi S_j^y} \right) \right]$$

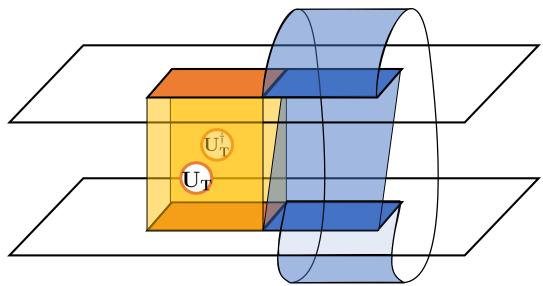


• Using the MPS, one can prove that the U(1) phase of Z_{PT} is quantized if intervals are large enough compared to the correlation length.

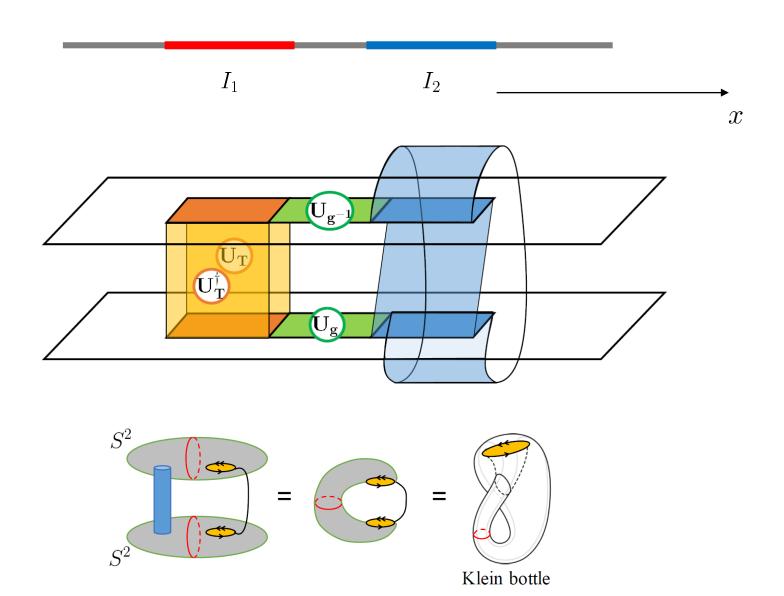
$$Z_{PT}/|Z_{PT}| \to \pm 1, \qquad |I_1|, |I_2| \gg \xi.$$

• The Pollmann-Turner invariant Z_{PT} is topologically equivalent to the partition function over RP². [KS-Ryu, '16]

$$Z := \operatorname{tr} \left[\rho_{I_1 \cup I_2} \left(\prod_{j \in I_1} e^{i\pi S_j^y} \right) \left(\rho_{I_1 \cup I_2} \right)^{tr_1} \left(\prod_{j \in I_1} e^{-i\pi S_j^y} \right) \right]$$



• 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 fermionic systems

Transpose in the fermionic operator algebra

Every operator can be expanded by Majorana fermions

$$A = \sum_{k=1}^{2N} \sum_{p_1 < p_2 \dots < p_k} A_{p_1 \dots p_k} c_{p_1} \dots c_{p_k},$$

$$c_j^{\dagger} = c_j, \quad \{c_j, c_k\} = 2\delta_{jk}.$$

- 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.

$$(c_{p_1}c_{p_2}\cdots c_{p_k})^{tr} := c_{p_k}\cdots c_{p_2}c_{p_1}$$
$$(\alpha A + \beta B)^{tr} = \alpha A^{tr} + \beta B^{tr}, \quad (AB)^{tr} = B^{tr}A^{tr}.$$

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

$$Vc_{j}V^{\dagger} = [\mathcal{O}_{V}]_{jk}c_{k}, \quad \mathcal{O}_{V} \in O(2N).$$

$$A \xrightarrow{V} VAV^{\dagger}$$

$$tr \downarrow \qquad \circlearrowleft \qquad tr \downarrow$$

$$A^{tr} \xrightarrow{V} VA^{tr}V^{\dagger}$$

- 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

$$Tf_j^{\dagger}T^{-1} = f_j^{\dagger}, \qquad T|vac\rangle = |vac\rangle.$$

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

$$C_T f_j^{\dagger} C_T^{-1} = f_j, \qquad C_T |vac\rangle = |full\rangle.$$

ullet The transpose operation corresponding to the TR transformation T is

$$A \mapsto C_T A^{tr} C_T^{\dagger}$$

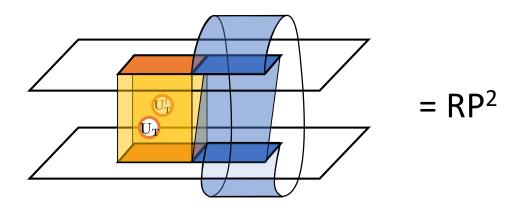
For coherent state basis

$$|\{\xi_j\}\rangle = e^{-\sum_j \xi_j f_j^{\dagger}} |vac\rangle,$$

the transpose with the particle-hole transformation reads

$$C_T \left(\left| \{ \xi_j \} \right\rangle \left\langle \{ \chi_j \} \right| \right)^{tr} C_T^{\dagger} = \left| \{ i \chi_j \} \right\rangle \left\langle \{ i \xi_j \} \right|.$$

- 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.

$$a_{1}, a_{2}, \dots \qquad b_{1}, b_{2}, \dots$$

$$I_{1} \qquad I_{2}$$

$$A = \sum_{k_{1}, k_{2}} A_{p_{1} \dots p_{k_{1}}, q_{1} \dots q_{k_{2}}} a_{p_{1}} \dots a_{p_{k_{1}}} b_{q_{1}} \dots b_{q_{k_{2}}}$$

$$I_{1} \qquad I_{2}$$

• We want to define the partial transpose " A^{tr_1} " on the subsystem I_1 .

- It is natural to impose the following three good properties on the partial transpose:
 - Preserve the identity:

$$(\mathrm{Id})^{tr_1} = \mathrm{Id}$$

2. The successive partial transposes on I_1 and I_2 goes back to the full transpose:

$$(A^{tr_1})^{tr_2} = A^{tr}$$

3. The partial transpose is compatible with the basis changes preserving subsysems $I_1 \cup I_2$.

$$(VAV^{\dagger})^{tr_1} = VA^{tr_1}V^{\dagger},$$

$$Va_iV^{\dagger} = [\mathcal{O}_{I_1}]_{ik}a_k, \quad Vb_iV^{\dagger} = [\mathcal{O}_{I_2}]_{ik}b_k.$$

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

$$A = \sum_{k_1, k_2, k_1 + k_2 \in \text{even}} A_{p_1 \dots p_{k_1}, q_1 \dots q_{k_2}} \underbrace{a_{p_1} \dots a_{p_{k_1}}}_{I_1} \underbrace{b_{q_1} \dots b_{q_{k_2}}}_{I_2},$$

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 .

$$A^{tr_1} = \sum_{k_1, k_2, k_1 + k_2 \in \text{even}} A_{p_1 \dots p_{k_1}, q_1 \dots q_{k_2}} i^{k_1} a_{p_1} \dots a_{p_{k_1}} b_{q_1} \dots b_{q_{k_2}}$$

$$I_1 \qquad I_2$$

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

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

$$H = \sum_{j} \left[-t f_{j+1}^{\dagger} f_{j} + \Delta f_{j+1}^{\dagger} f_{j}^{\dagger} + h.c. \right] - \mu \sum_{j} f_{j}^{\dagger} f_{j}$$

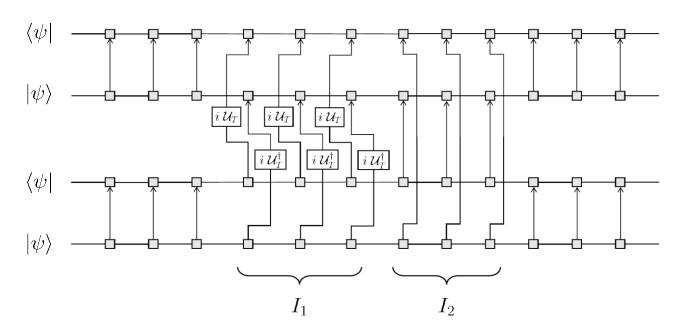
$$f_{j}^{\dagger}, f_{j}$$

$$\vdots$$

- TR symmetry $Tf_i^{\dagger}T^{-1} = f_i^{\dagger}, \qquad T|vac\rangle = |vac\rangle$.
- The classification of SPT phases is known to be \mathbb{Z}_8 . [Fidkowski-Kitaev '10]
- The Z_8 "order parameter" is the partition function on RP² (real projective plane). $\Omega_2^{Pin_-}(pt)=\mathbb{Z}_8$

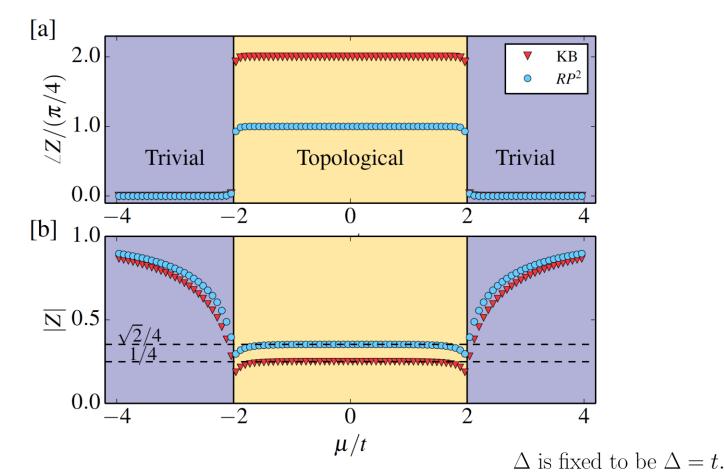
• The Z_8 order parameter in operator formalism is the partial transpose on adjacent two intervals

$$Z = \operatorname{tr}_{I_1 \cup I_2} \left[\rho_{I_1 \cup I_2} C_T^{I_1} \rho_{I_1 \cup I_2}^{tr_1} [C_T^{I_1}]^{\dagger} \right]$$



Numerical calculation [arXiv:1607.03896]

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



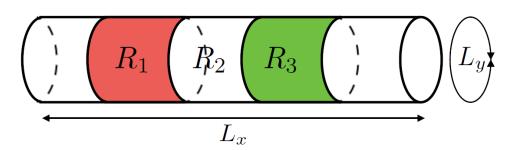
Manybody Z_2 Kane-Mele invariant

- (2+1)d topological insulator (TR symmetry with Kramers)
- The generating manifold is the Klein bottle × S¹ with a unit magnetic flux. [Witten '16]

IQHE for spin up

IQHE for spin down

- Combine two technics:
 - ✓ Disjoint partial transpose -> Klein bottle
 - ✓ Twist operator -> a unit magnetic flux



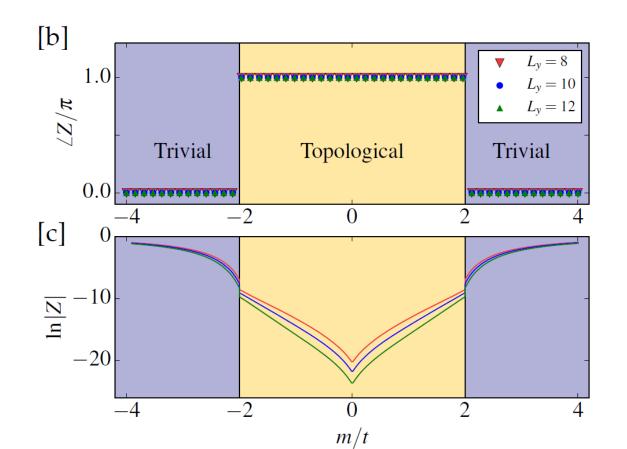
$$\rho_{R_1 \cup R_3}^{\pm} := \operatorname{Tr}_{\overline{R_1 \cup R_3}} \left[e^{\pm \sum_{(x,y) \in R_2} \frac{2\pi i y}{L_y} \hat{n}(x,y)} |GS\rangle \langle GS| \right],$$

$$Z := \operatorname{Tr}_{R_1 \cup R_3} \left[\rho_{R_1 \cup R_3}^+ C_T^{I_1} [\rho_{R_1 \cup R_3}^-]^{tr_1} [C_T^{I_1}]^{\dagger} \right].$$

Manybody Z_2 Kane-Mele invariant

Numerical calculation for a free fermion model

$$Z := \operatorname{Tr}_{R_1 \cup R_3} \left[\rho_{R_1 \cup R_3}^+ C_T^{I_1} [\rho_{R_1 \cup R_3}^-]^{tr_1} [C_T^{I_1}]^{\dagger} \right].$$

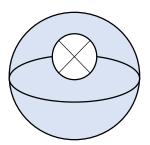


Take-home message

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

$$(\mathcal{O}_n \dots \mathcal{O}_2 \mathcal{O}_1)^{tr} = \mathcal{O}_1^{tr} \mathcal{O}_2^{tr} \dots \mathcal{O}_n^{tr}$$

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



Real projective plane



Klein bottle

Developed the partial transpose for fermions in the operator formalism

$$A^{tr_1} = \sum_{k_1, k_2, k_1 + k_2 \in \text{even}} A_{p_1 \dots p_{k_1}, q_1 \dots q_{k_2}} i^{k_1} a_{p_1} \dots a_{p_{k_1}} b_{q_1} \dots b_{q_{k_2}}$$