Geometric complexity in quantum matter: Intrinsic sign problems in topological phases

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Outline

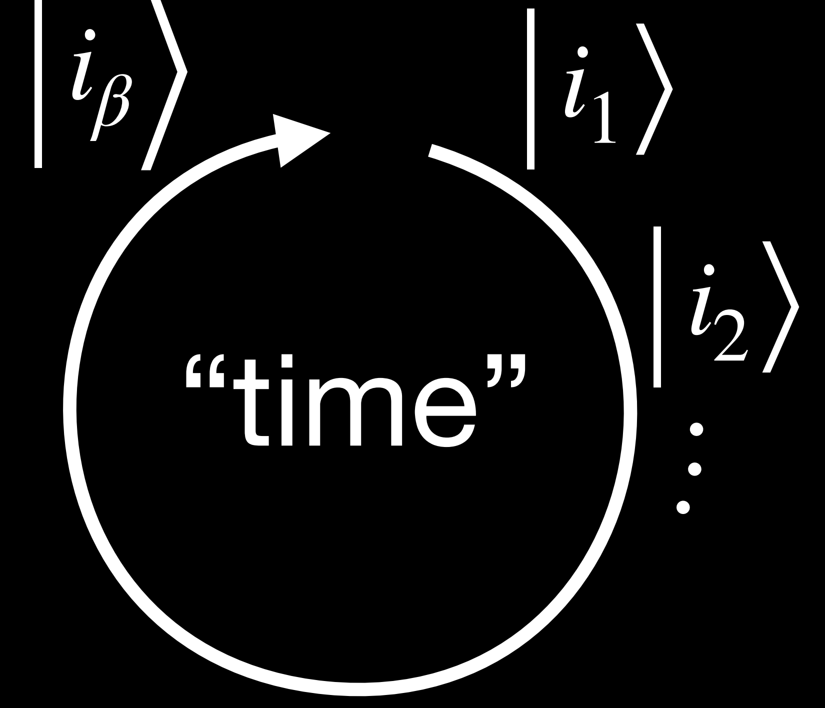
- Into: Quantum Monte Carlo and the sign-problem. (4s)
- Intrinsic sign problems: overview of existing & new results. (6s)
- Intrinsic sign problems in chiral topological matter: precise results & sketch of derivations. (7s)
- Beyond chiral matter: precise results & sketch of derivations. (1s)
- Summary & outlook. (1s)

Intro: QMC and sign-problem

QMC and sign-problem

Monte Carlo (MC): Approximate $\langle O \rangle = \sum_{\phi} O(\phi) p(\phi) \approx \frac{1}{M} \sum_{i=1}^{M} O\left(\phi_i\right)$, where ϕ_i are sampled w.r.t p.

Claim to fame: Generically $M = \text{poly}\,(N)$ where N = system size, though $\{\phi\} = \exp(N)$.



Quantum Monte Carlo (QMC): Map a quantum system in d-dimensions to a

“classical” system in $d+1$ dimensions, and apply MC: $Z = \text{Tr}\left(e^{-\beta H}\right) = \sum_{\phi} p(\phi)$.

Claim to fame: Classical poly(βN) simulation of quantum systems on exp(N)-dimensional Hilbert spaces.

Sign-problem: The generic obstruction to a quantum-to-classical mapping: $p(\phi) \in \mathbb{C}$.

Sign-problem and complexity

Fool's gold*: Can work with $\left|p\right|$, which generically allows for poly(βN) approximations, but of the wrong system.

Mapping back to the system of interest is generically exp(βN) - another facet of the sign-problem [Troyer-Wiese (2005)].

Curing the sign-problem: Try to change the quantum-to-classical mapping s.t $p \geq 0$.

Example: Change local basis to make the Hamiltonian ***stoquastic***, $H_{ij} \leq 0$. This implies $\left(e^{-\beta H}\right)_{ij} \geq 0$, and so $p \geq 0$ in a variety of quantum-to-classical mappings.

Complexity theory: From a number of perspectives, a general poly(βN) curing algorithm is not believed to exist [Bravyi et al (2008), Hastings (2016), Marvian-Lidar-Hen (2018), Klassen-Terhal (2019),…].

Sign-problem and physics

In many-body physics we mostly care about **phases of matter and transitions**, so **sign-free representatives suffice**.

QMC is alive because many **interesting sign-free representatives are discovered**:
He-4 Ceperley (1995), Magnetism & topological phases Kaul-Melko-Sandvik (2013), Quantum critical metals Berg et al (2018), **Fermions:** Determinantal-QMC and **Design principles (H won't be stoquastic)** Wei (2018), Li-Yao (2019)…

Nevertheless, long standing **open problems in many-fermion systems** continue to defy solution:

High-Tc / Hubbard model, Nuclear matter / Lattice QCD, FQH $5/2$ / Coulomb Hamiltonian,…

Intrinsic sign-problems Hastings (2016), Ringel-Kovrizhin (2017)**:**

Are there phases of matter which do not admit a sign-free representative?

Are there physical properties that can not be exhibited by sign-free models?

Intrinsic sign-problems: overview of existing and new results

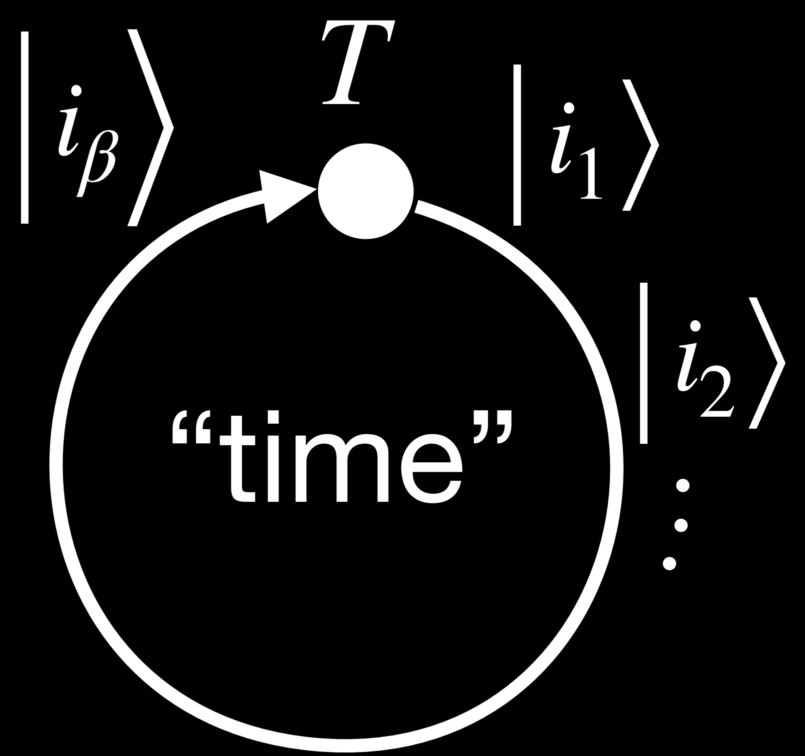
Intrinsic sign-problem from geometry: essence

Topological phases of matter, that are characterized by ‘geometric twists’, are natural candidates!

Q: Why topological phases?

A: Characterized by complex phases in ‘twisted partition functions’:

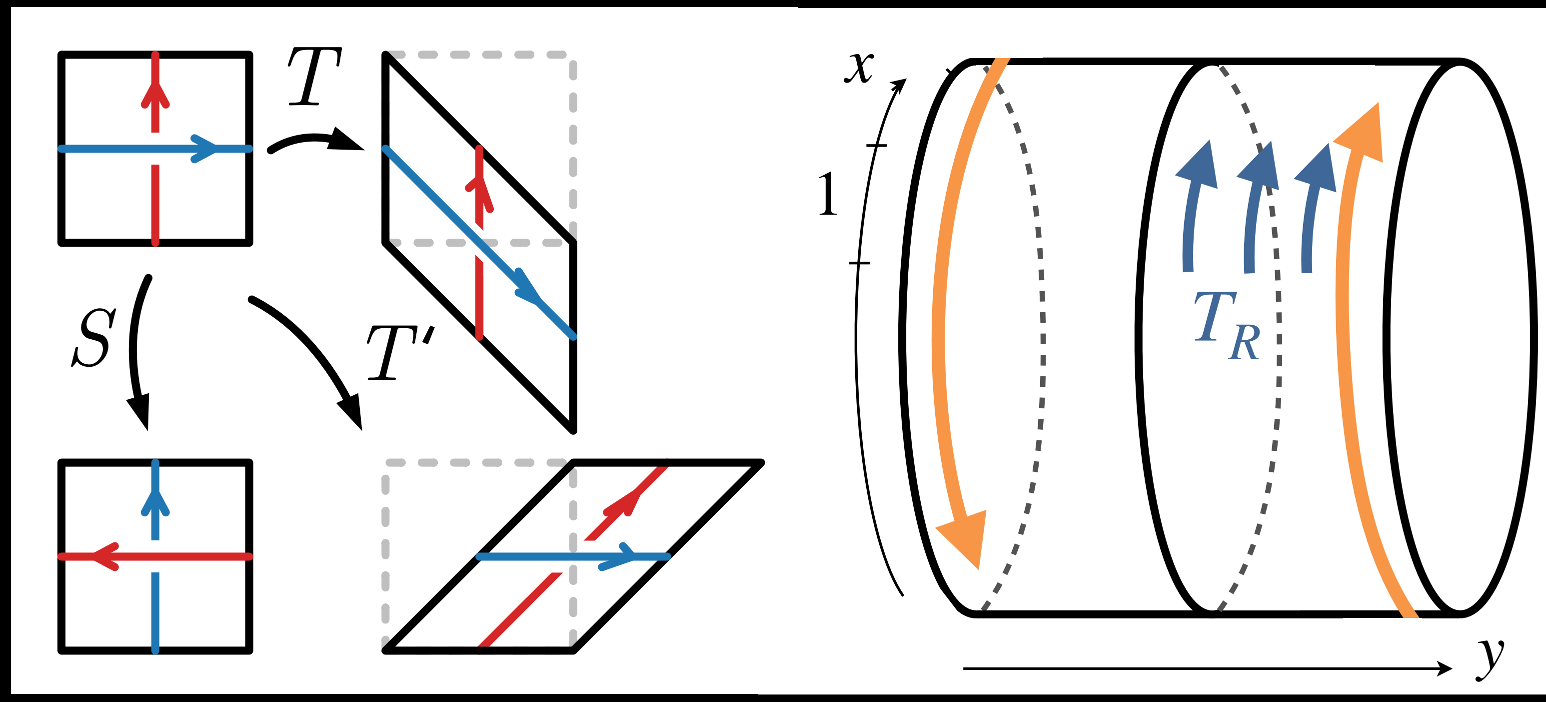
$$\tilde{Z} := \mathrm{Tr}(Te^{-\beta H}) = e^{iS_{topo}+\cdots}, \qquad (\beta \to \infty)\,.$$



Q: Why geometric twists ($T =$ permutation of lattice sites)?

A: These can be implemented without introducing signs:

$$Z = \sum_\phi \underbrace{p(\phi)}_{\geq 0} \quad \Rightarrow \quad \tilde{Z} = \sum_\phi \underbrace{\tilde{p}(\phi)}_{\geq 0} > 0.$$



So, intrinsic sign-problem: $S_{topo} \neq 0 \quad \Rightarrow \quad p(\phi) \ngeq 0.$

Smith-OG-Ringel (2020), OG-Smith-Ringel (2020)

Intrinsic sign-problems: overview

Previous work:

1. No stoquastic, commuting projector, representative for ‘doubled semion’ phase, Hastings (2016).
2. No stoquastic, translationally invariant, representative for bosonic chiral topological phases Ringel-Kovrizhin (2017).

These works:

i. Generalize (1) to ‘most’ bosonic, abelian, non-chiral, topological phases (details to follow). Smith-OG-Ringel (2020).

ii. Obtain a variant of (2), and generalize to fermions (Determinantal-QMC):

An intrinsic sign-problem exists if $\exp\left(2\pi i c/24\right) \notin \left\{\theta_a\right\}$***.*** OG-Smith-Ringel (2020).

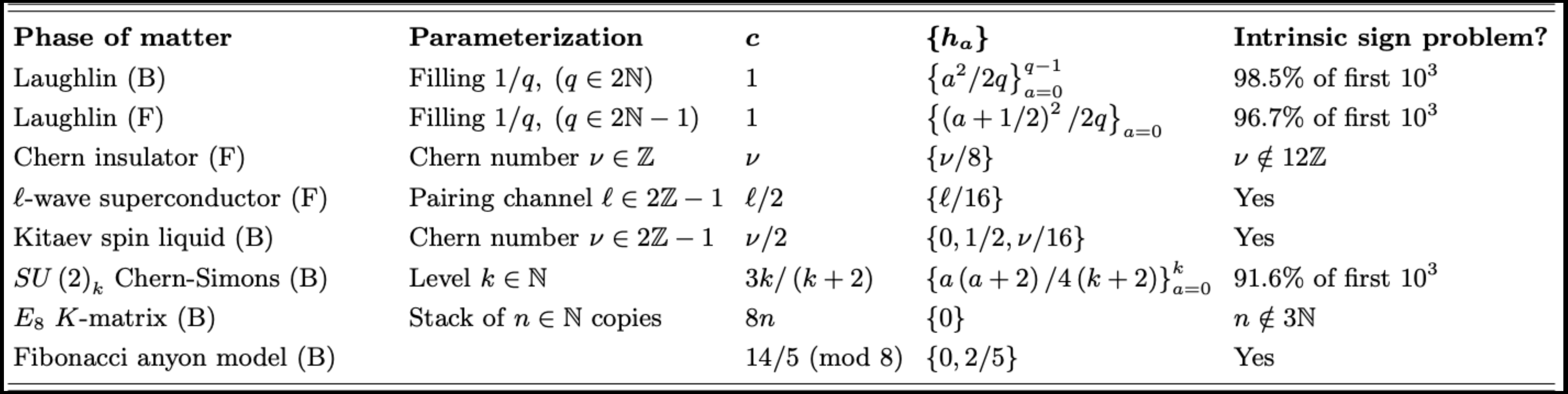
Chiral central charge

Topological spins of anyons

iii. Conjecture a unification & generalization of i.+ii.

Examples: Intrinsic sign-problems from $e^{2\pi ic/24} \notin \{\theta_a\}$

$\theta_a = e^{2\pi ih_a}$



Phase of matter	**Parameterization**	c	$\{h_a\}$	**Intrinsic sign problem?**
Laughlin (B)	Filling $1/q,\ (q \in 2\mathbb{N})$	1	$\{a^2/2q\}_{a=0}^{q-1}$	98.5% of first 10^3
Laughlin (F)	Filling $1/q,\ (q \in 2\mathbb{N}-1)$	1	$\left\{(a+1/2)^2/2q\right\}_{a=0}$	96.7% of first 10^3
Chern insulator (F)	Chern number $\nu \in \mathbb{Z}$	ν	$\{\nu/8\}$	$\nu \notin 12\mathbb{Z}$
ℓ-wave superconductor (F)	Pairing channel $\ell \in 2\mathbb{Z}-1$	$\ell/2$	$\{\ell/16\}$	Yes
Kitaev spin liquid (B)	Chern number $\nu \in 2\mathbb{Z}-1$	$\nu/2$	$\{0, 1/2, \nu/16\}$	Yes
$SU(2)_k$ Chern-Simons (B)	Level $k \in \mathbb{N}$	$3k/(k+2)$	$\{a(a+2)/4(k+2)\}_{a=0}^{k}$	91.6% of first 10^3
E_8 K-matrix (B)	Stack of $n \in \mathbb{N}$ copies	$8n$	$\{0\}$	$n \notin 3\mathbb{N}$
Fibonacci anyon model (B)		$14/5 \pmod 8$	$\{0, 2/5\}$	Yes

\+ three Pfaffian candidates for filling $5/2$.

'Most' chiral topological phases are intrinsically sign-problematic: fermionic / bosonic, abelian / non-abelian, SPT / topologically ordered.

Keep in mind Laughlin 1/3: $\{h_a\} = \left\{\frac{1}{24}, \frac{3}{8}, \frac{1}{24}\right\}$ and $c = 1$, so $e^{2\pi ic/24} \in \{\theta_a\}$.

Many phases which are universal for topological quantum computation, are also intrinsically sign-problematic ($SU(2)_{k\neq 1,2,4}$ and Fibonacci), supporting the paradigm of 'quantum advantage' or 'supremacy'.

OG-Smith-Ringel (2020)

Beyond chiral matter

For bosonic, abelian, non-chiral phases, we have:

An intrinsic sign-problem exists if $Spec(\mathbf{T}) = \{\theta_a\}$ is not a disjoint union of complete sets of roots of unity*. Smith-OG-Ringel (2020)

* $Spec(\mathbf{T}) \neq \cup_k R_{n_k}$, where $R_{n_k} = \{e^{2\pi i m/n_k}\}_{m=1}^{n_k}$ are the n_kth roots of unity.

Examples: Toric code is stoquastic, and accordingly $Spec(\mathbf{T}) = \{1,1,1,-1\} = R_1 \cup R_1 \cup R_2$. Doubled semion is intrinsically sign-problematic, since $Spec(\mathbf{T}) = \{1,i,-i,1\}$. Similar picture for $\mathbb{Z}_N$ string-nets.

A conjecture for all phases described by TQFT unifies both results:

An intrinsic sign-problem exists if $Spec(\mathbf{T}) = \{\theta_a e^{-2\pi i c/24}\}$ is not a disjoint union of complete sets of roots of unity.

The criterion $e^{2\pi i c/24} \notin \{\theta_a\}$ can be written as $1 \notin Spec(\mathbf{T})$, and the conjecture raises the table percentages to 100%, including Lauhglin 1/3.

Complexity and physics

The intrinsic sign-problem is a statement of complexity, phrased in terms of physical observables:

- Chiral central charge c:
  - Boundary thermal Hall conductance, measured in quantum Hall and spin systems. [Jezouin et al (2013), Banerjee et al (2016, 2018), Kasahara et al (2018).]
  - Angular momentum at conical defects, observed in an optical realization of integer quantum Hall states on a cone. [Schine et al (2018).]
  - Bulk Hall viscosity at finite wave-vector / curved background. [Abanov-Gromov (2014), Klevtsov-Wiegmann (2015), Bradlyn-Read (2015), OG-Hoyos-Moroz (2019).]
- Topological spins $\{\theta_a\}$: determine the exchange statistics of anyons, measured in interferometry and 'collision' experiments. [Nakamura et al (2020), Bartolomei et al (2020).]
- Important for this talk: c and $\{\theta_a\}$ enter the boundary momentum density.

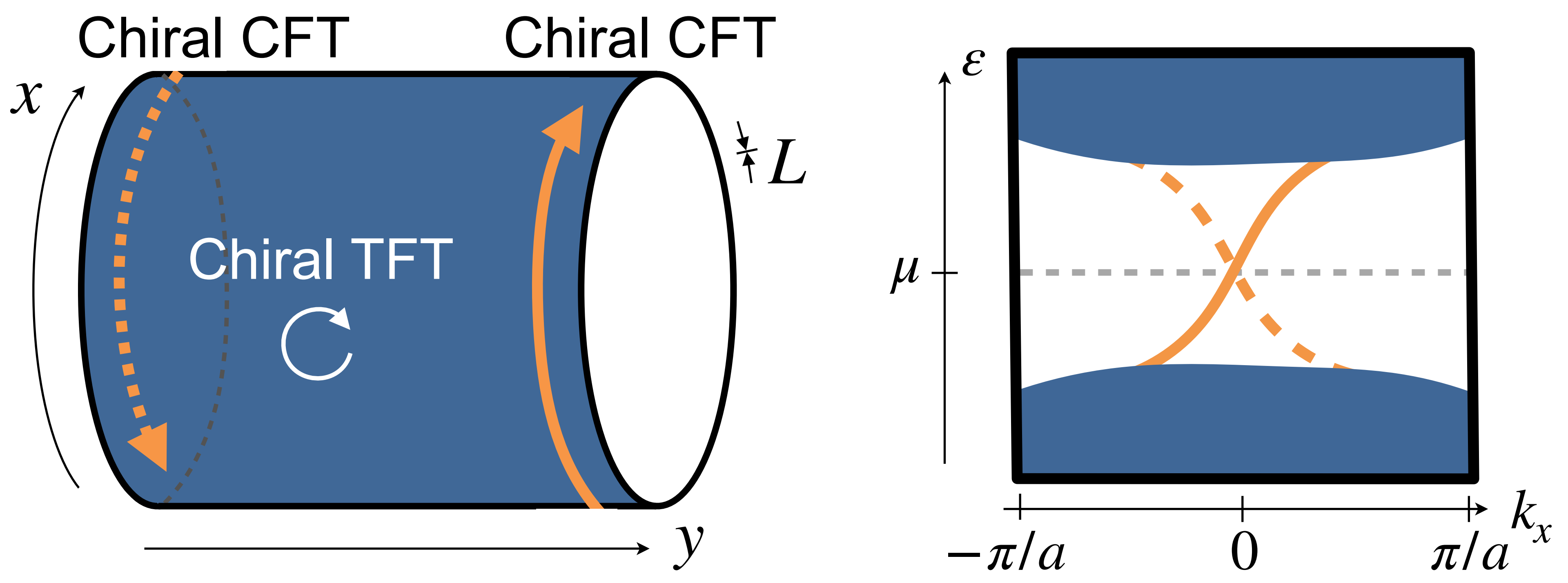
Results and sketch of derivations for:

An intrinsic sign-problem exists if $e^{2\pi ic/24} \notin \{\theta_a\}$**.**

OG-Smith-Ringel (2020)

Physics of chiral topological matter

Low energy description of chiral topological matter: chiral topological field theory in bulk, chiral conformal field theory on boundary.



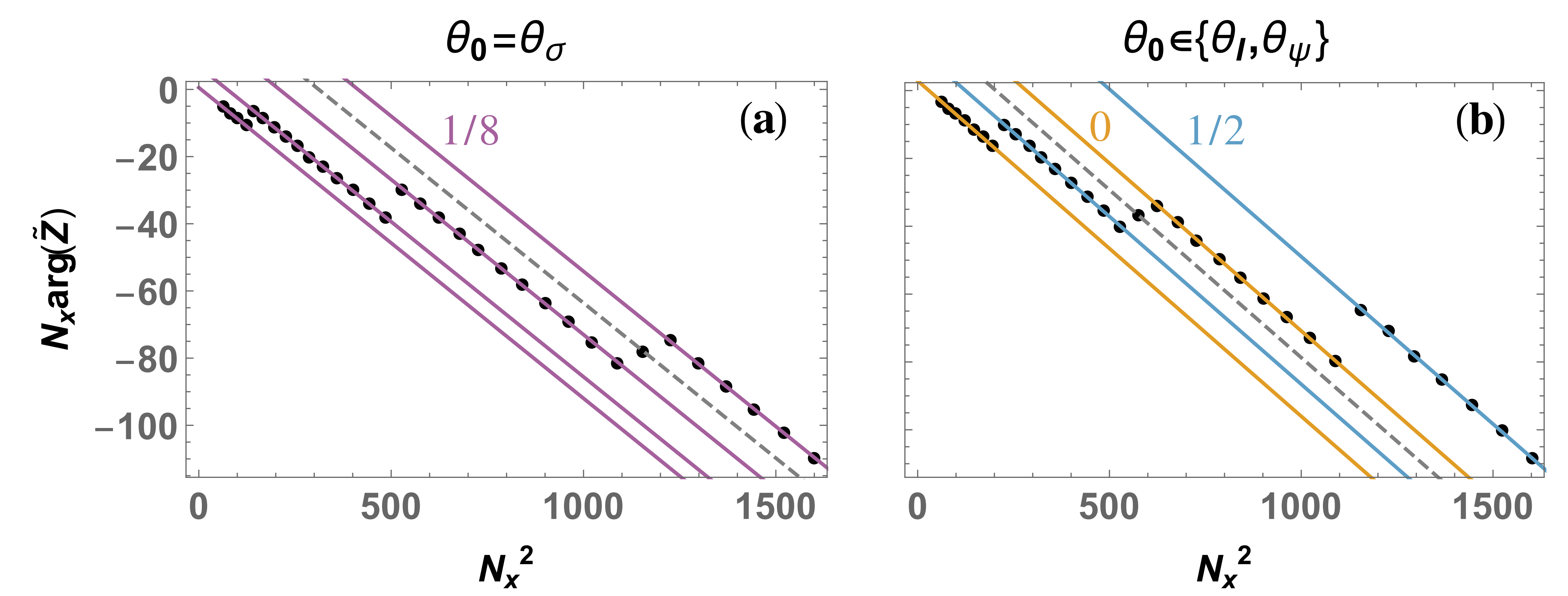
Boundary energy current: $J_E(T) = J_E(0) + 2\pi T^2 c/24$, experimentally observed. Banerjee et al (2018), Kasahara et al (2018).

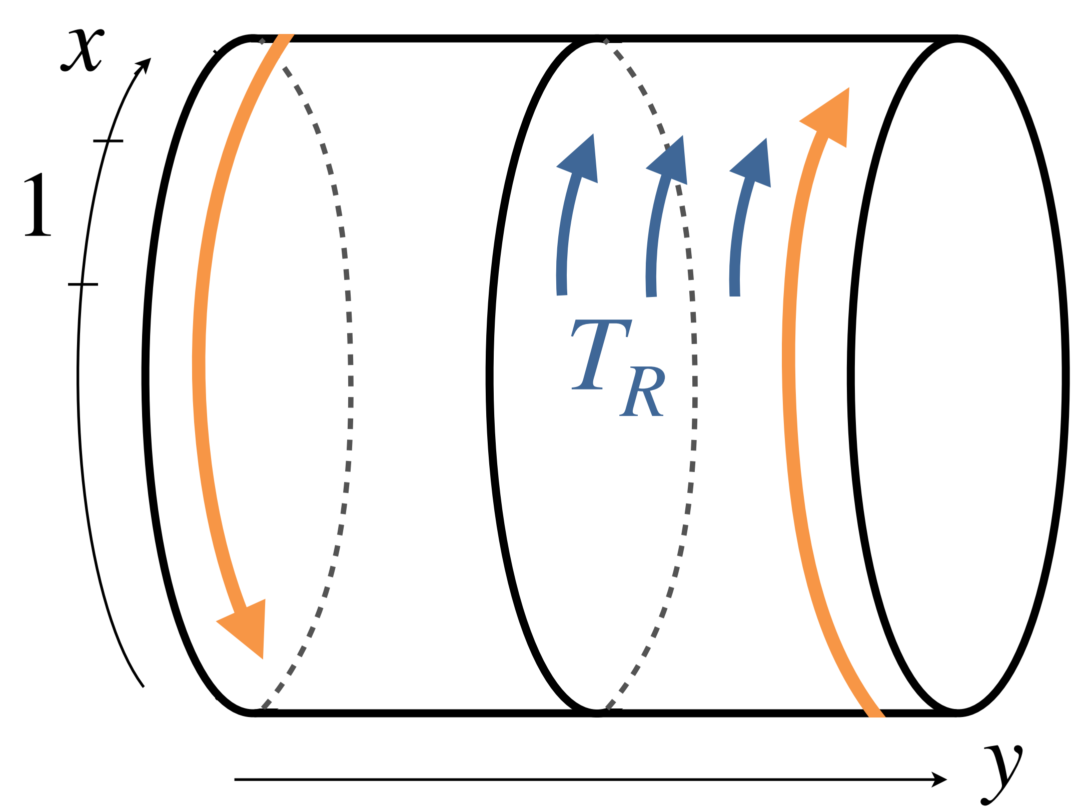
Boundary momentum density:

$$p(L) = p(\infty) + 2\pi L^{-2}\left(h_0 - c/24\right), \text{ where } e^{2\pi i h_0} = \theta_0 \in \{\theta_a\}.$$

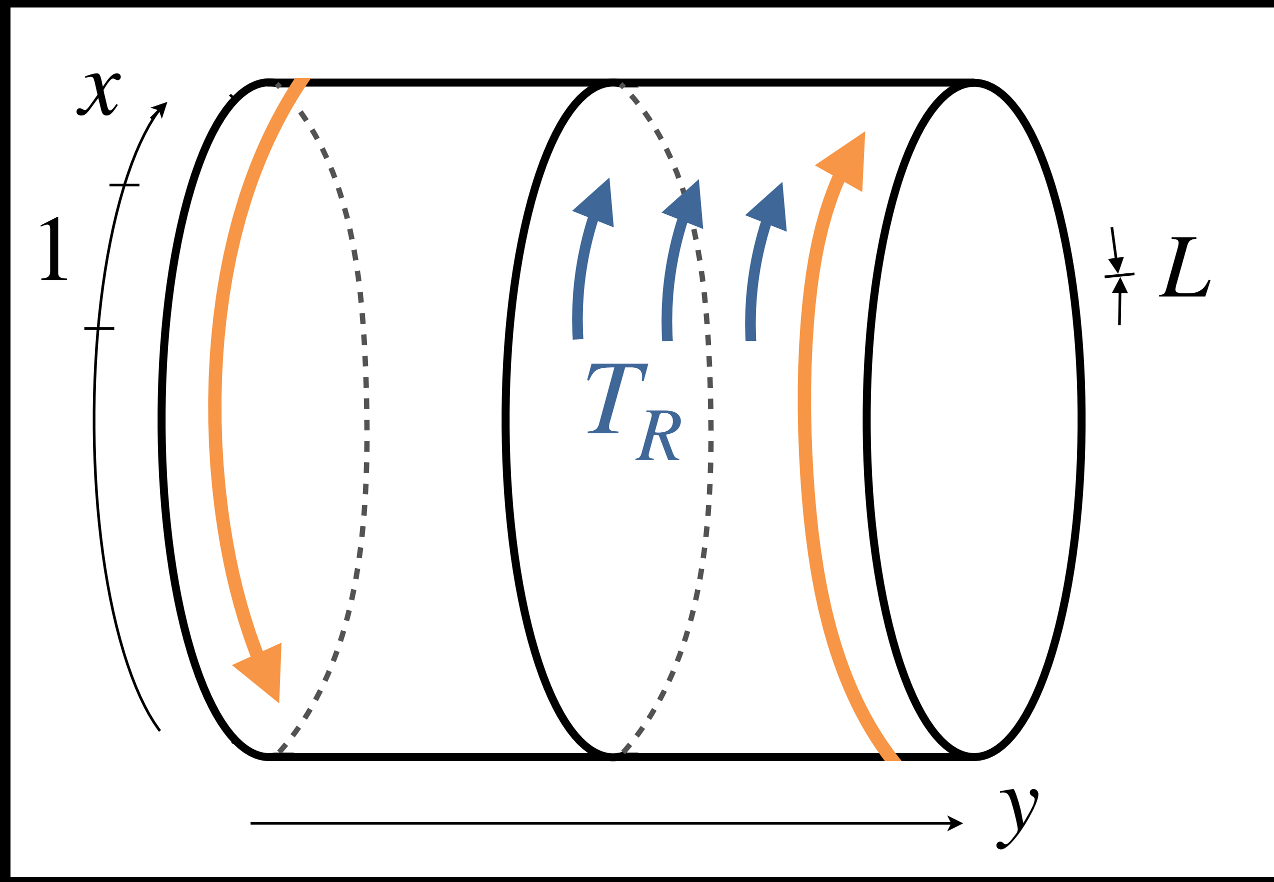
Can be extracted from lattice models using 'momentum polarization' Tu-Zhang-Qi (2013), Zaletel-Mong-Pollman (2013)**:**

$$\tilde{Z} := \mathrm{Tr}(T_R e^{-\beta H}), \qquad \arg(Z) = \alpha L + 2\pi L^{-1}(h_0 - c/24), \qquad (\beta^{-1} \ll L^{-1}).$$





Excluding stoquastic Hamiltonians for bosonic chiral topological matter



Momentum polarization:

$$\tilde{Z} := \mathrm{Tr}(T_R e^{-\beta H}), \qquad \arg(\tilde{Z}) = \alpha L + 2\pi L^{-1}(h_0 - c/24), \qquad (\beta^{-1} \ll L^{-1}).$$

Two facts: (i) If $H' = UHU^\dagger$ is stoquastic, then $T_R e^{-\beta H'}$ has positive entries.

(ii) If U is a local finite-depth circuit, then H' in same phase as H, so $c' = c$, $\{\theta'_a\} = \{\theta_a\}$.

As a result, we have for $\tilde{Z}' := \mathrm{Tr}(T_R e^{-\beta H'})$: $\quad 0 \overset{\text{(i)}}{=} \arg(\tilde{Z}')^L/2\pi \overset{\text{(ii)}}{=} (\alpha'/2\pi)L^2 + h_0 - c/24.$

Taking $L \to \infty$ shows $\alpha'/2\pi \in \mathbb{Q}$, and therefore $e^{2\pi i c/24} = e^{2\pi i h_0} \in \{\theta_a\}$.

Result 1: ***If a local bosonic Hamiltonian is both locally stoquastic and in a chiral topological phase, then $e^{2\pi i c/24} \in \{\theta_a\}$.***

OG-Smith-Ringel (2020)

Excluding sign-free DQMC for chiral topological matter

DQMC: $Z = \int D\phi D\psi e^{-S_\phi - S_{\psi,\phi}} \longleftarrow S_{\psi,\phi} = \int d\tau \overline{\psi} D_\phi \psi$

Result 1F: ***If a local fermion-boson Hamiltonian, which is in a chiral topological phase of matter, admits a*** $\underbrace{\textit{locally sign-free DQMC}}_{???}$ ***simulation, then*** $e^{2\pi i c/24} \in \{\theta_a\}$**.**

OG-Smith-Ringel (2020)

Excluding sign-free DQMC for chiral topological matter

DQMC: $$Z = \int D\phi \underbrace{e^{-S_\phi} Det\left(I + U_\phi\right)}_{p(\phi)} \longleftarrow U_\phi = \mathscr{T} e^{-\int_0^\beta h_{\phi(\tau)} d\tau}$$

Origin of sign-problem: time-dependence and non-Hermiticity of $h_{\phi(\tau)}$. [Exclude τ-independent ϕ. e.g Nasu-Yoshitake-Motome (2017)]

Design principle (loose): An on-site, homogeneous, multiplicative algebraic condition on U_ϕ, manifestly obeyed for all ϕ, which implies $Det(I + U_\phi) \geq 0$. Additionally, $S_\phi \in \mathbb{R}$ manifestly for all ϕ.

Example: Time-reversal. $\mathrm{T} = I_X \otimes \mathrm{t}$ anti-unitary, $\mathrm{T}^2 = -I$, and $[\mathrm{T}, U_\phi] = 0$. Wu-Zhang (2005)

Locally sign-free DQMC: Exists local unitary U, such that $H' = UHU^\dagger$ has a DQMC representation, which obeys a design principle (c.f 'locally stoquastic').

Result 1F: ***If a local fermion-boson Hamiltonian, which is in a chiral topological phase of matter, admits a locally sign-free DQMC simulation, then*** $e^{2\pi i c/24} \in \{\theta_a\}$**.**

$$\underbrace{\text{locally sign-free DQMC}}_{???}$$

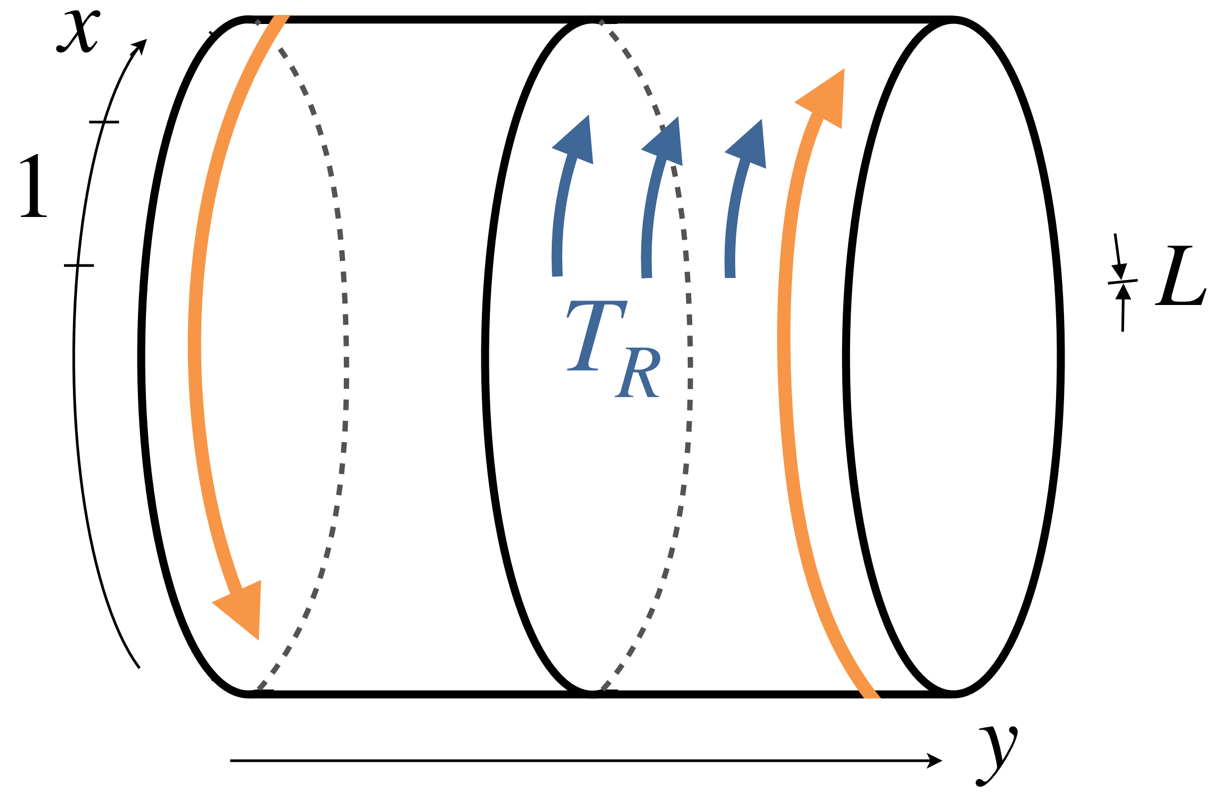
OG-Smith-Ringel (2020)

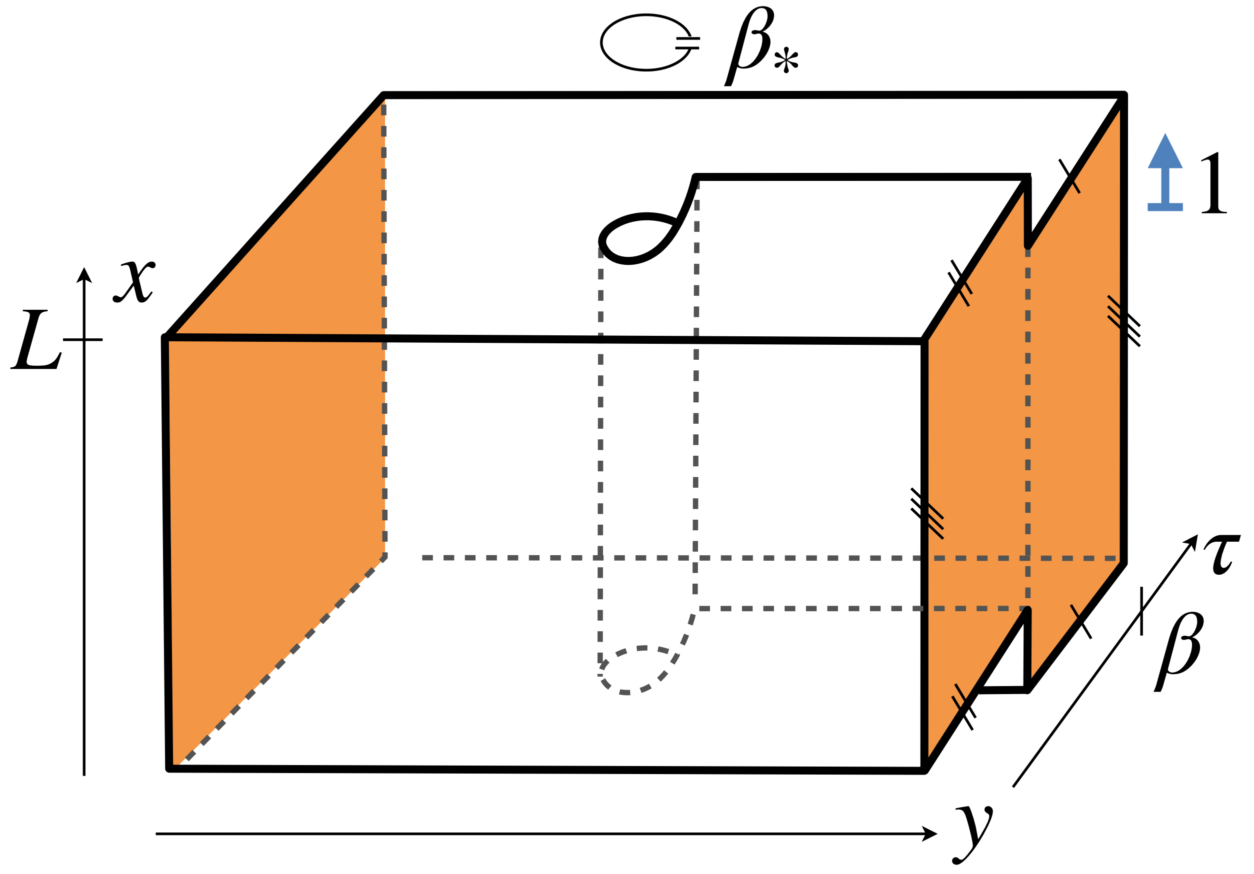
Excluding sign-free DQMC for chiral topological matter

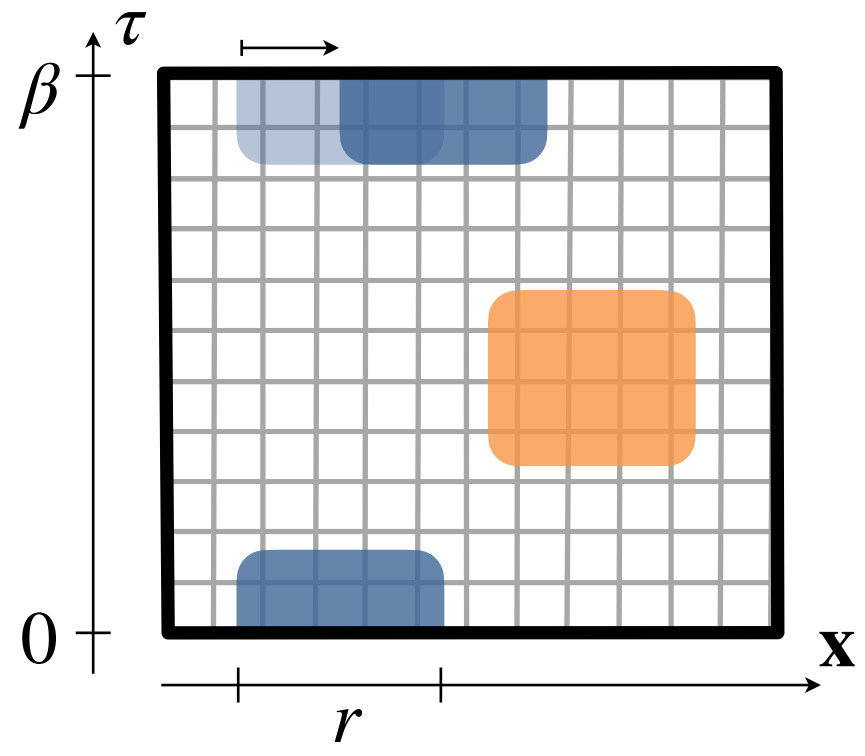
Sign-free implementation of 'momentum polarization' $\tilde{Z}' = \mathrm{Tr}(T_R e^{-\beta H'})$:

$$Z' = \int D\phi \underbrace{e^{-S_\phi} Det\left(I + U_\phi\right)}_{p \geq 0} \quad \mapsto \quad \tilde{Z}' = \int D\phi \underbrace{e^{-\tilde{S}_\phi} Det\left(I + T_R U_\phi\right)}_{\tilde{p} \geq 0} .$$

Example: Time-reversal $\mathsf{T} = I_X \otimes \mathsf{t}$. Clearly $[\mathsf{T}, T_R] = 0$.







Result 1F: ***If a local fermion-boson Hamiltonian, which is in a chiral topological phase of matter, admits a locally sign-free DQMC simulation, then*** $e^{2\pi i c/24} \in \{\theta_a\}$.

OG-Smith-Ringel (2020)

Spontaneous chirality

Assume H is spontaneously-chiral: P (reflection) and T (time-reversal) symmetric, but $P \times T \to PT$ spontaneously (e.g chiral superconductors).

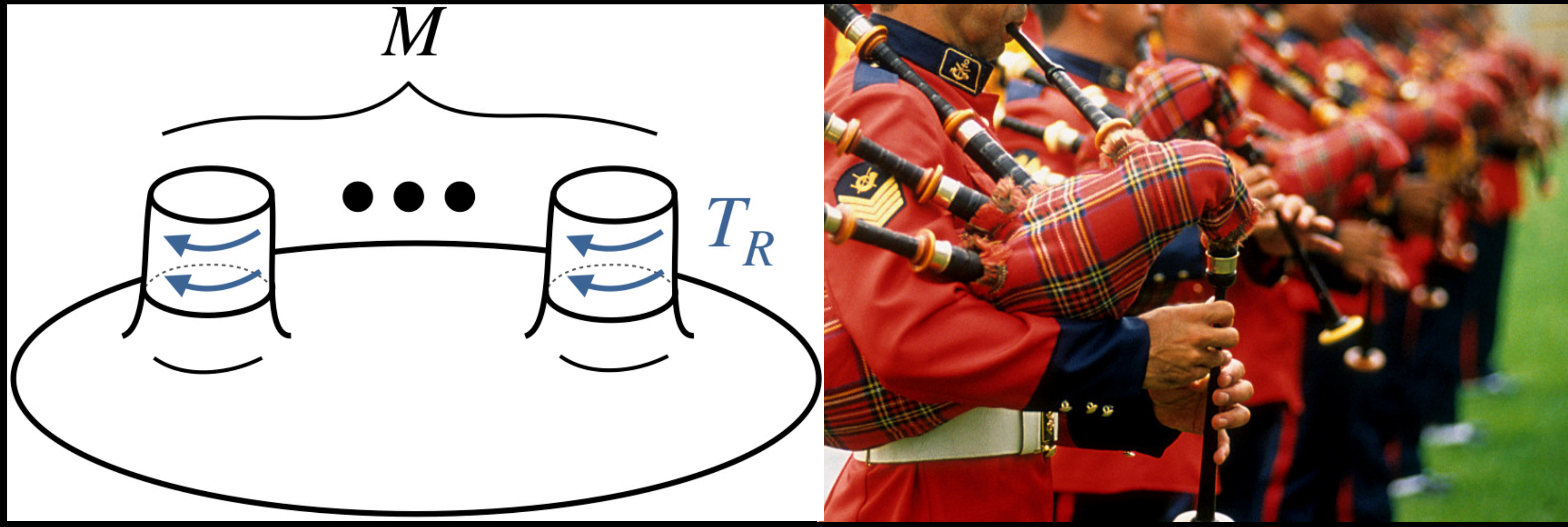
Ground states: $e^{-\beta H}/Z = W\left(\rho_+ + \rho_-\right) W^\dagger/2,$ for $\Delta E \ll \beta^{-1} \ll L^{-1},$

where $\rho_\pm = \left| \pm \right\rangle \left\langle \pm \right|$, $W =$ finite-depth circuit, $\Delta E = \exp(-L)$, think of Ising.

Previously: $Z' := \mathrm{Tr}(T_R e^{-\beta H'})$, and $\arg(Z') = \alpha' L + 2\pi L^{-1}(h_0 - c/24)$.

Here: $0 < Z' \propto \cos\left[\alpha' L + 2\pi L^{-1}(h_0 - c/24)\right]$. Need spontaneous analog of taking powers:

Result 2 (2F): ***If a local bosonic (fermionic) Hamiltonian is both locally stoquastic (admits locally sign-free DQMC) and in a spontaneously-chiral topological phase, then*** $e^{2\pi i c/24} \in \{\theta_a\}$**.**



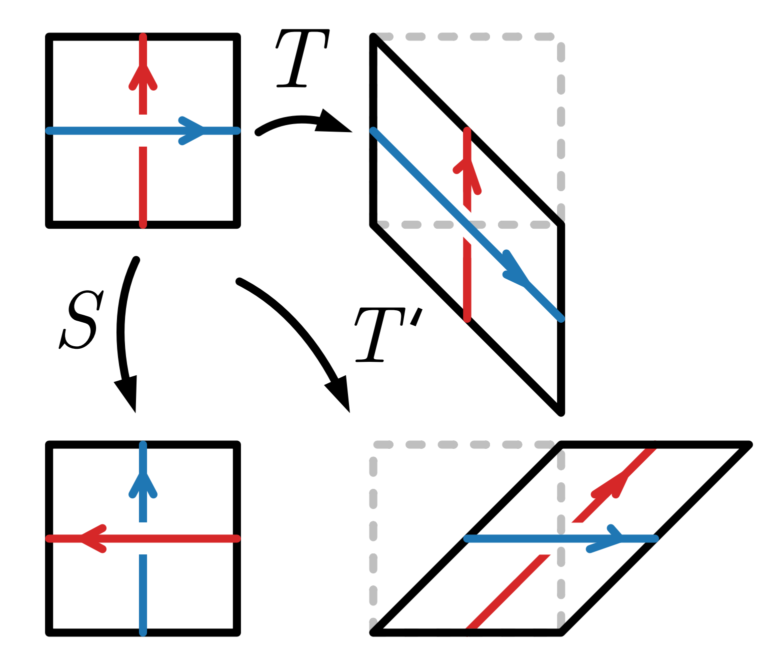
‘Bagpipes construction’

OG-Smith-Ringel (2020)

Beyond chiral matter

Universal wave-function overlap: $\langle i \left| \mathbf{T}_m \right| j\rangle = e^{-\alpha_{\mathbf{T}}A+o\left(A^{-1}\right)}\mathbf{T}_{ij}$, where $Spec(\mathbf{T}) = \{\theta_a e^{-2\pi i c/24}\}$.

Moradi-Wen (2015)



Define $Z_{\mathbf{T}} := \mathrm{Tr}\left(\mathbf{T}_m e^{-\beta H}\right) = Ze^{-\alpha_{\mathbf{T}}A+o\left(A^{-1}\right)}\mathrm{Tr}\left(\mathbf{T}\right), \qquad (\beta^{-1} \ll E_g)$.

Repeat previous logic: $e^{-2\pi i c/24}\sum \theta_a = \mathrm{Tr}\left(\mathbf{T}\right) \geq 0$. Not enough (e.g doubled semion)…

Refine by means of Frobenius-Perron: $\mathbf{T}_{ij} \geq 0$, in some basis.

Since $\mathbf{T}^\dagger\mathbf{T} = I$, for some perm σ: $\mathbf{T}_{ij} = \delta_{i,\sigma(j)}$.

Conjecture: ***If a local bosonic Hamiltonian is both locally stoquastic and in a topological phase, then*** $Spec\left(\mathbf{T}\right) = \cup_k R_{n_k} =$ ***roots of unity.***

Established by other means for non-chiral bosonic abelian phases.

Smith-OG-Ringel (2020)

Summary & outlook

(spontaneously-) Chiral topological matter: *Intrinsic sign-problem if* $e^{2\pi i c/24} \notin \{\theta_a\}$.

Bosons: *no locally stoquastic Hamiltonians.*
Fermions: *no locally sign-free DQMC.*

Beyond chiral matter: *intrinsic sign problem if* $\{e^{-2\pi i c/24}\theta_a\} \neq \cup R_{n_k}$.

Final example: fermionic vs bosonic descriptions of Kitaev spin liquids**.**

Outlook: Many open questions, here are a few:

- Complexity of chiral topological matter: non-local commuting projectors Son-Alicea (2018), non-local Projected Entangled Pair States Wahl-Tu-Schuch-Cirac (2014). Overcoming intrinsic sign problems in chiral topological matter via non-locality?
- State of the art DMRG of U-V model doesn't exclude chiral d-wave Kantian-Dolfi-Troyer-Giamarchi (2019). Does this explain the lack of a sign-free representation?
- Easing intrinsic sign-problems? $\langle \text{sign} \rangle = \sum p / \sum |p| \sim e^{-\Delta\beta N}$ Hangleiter-Roth-Nagaj-Eisert (2019).
- Additional sign problems in topo matter? SPT: Ellison-Kato-Liu-Hsieh (2020), Any c: Kim-Shi-Kato-Albert (2021).
- Other dimensions? Phases not gapped, not topological, or both?

State of the art design principles

Contraction semi-groups and Majorana time-reversals Li-Jiang-Yao (2016), Wei et al (2016), Wei (2017):

If: $$\mathsf{J}_1 h_\phi - h_\phi^* \mathsf{J}_1 = 0, \qquad i(\mathsf{J}_2 h_\phi - h_\phi^* \mathsf{J}_2) \geq 0,$$

where h_ϕ is anti-symmetric (free Majorana operator), and $\mathsf{J}_1, \mathsf{J}_2$ are real, orthogonal, and obey $\mathsf{J}_1^T = \pm \mathsf{J}_1$, $\mathsf{J}_2^T = - \mathsf{J}_2$, $\{\mathsf{J}_1, \mathsf{J}_2\} = 0$, then $Det(I + U_\phi) \geq 0$.

Mathematical structure: in terms of Majorana time reversal $\mathsf{T}_1 = \mathsf{J}_1 K$, $\mathsf{T}_1^2 = \pm I$, and Hermitian metric $\eta_2 = i\mathsf{J}_2$, $\eta_2^2 = I$, which are compatible: $[\mathsf{T}_1, \eta_2] = 0$, get $[\mathsf{T}_1, h_\phi] = 0$, $\eta_2 h_\phi + h_\phi^\dagger \eta_2 \geq 0$, or

$$[\mathsf{T}_1, U_\phi] = 0, \quad \eta_2 - U_\phi^\dagger \eta_2 U_\phi \geq 0.$$

These imply $Det(I + U_\phi) \in \mathbb{R}$, and $1 \notin Spec(U_\phi)$. Therefore $Det(I + U_\phi) \in \mathbb{R} - \{0\}$. Adding continuity in U_ϕ and using $U_\phi = I$, gives the result.

Applications: time reversal invariant spinfull fermions, with pairing terms,…

State of the art design principles

Split orthogonal group Wang et al (2015):

A time reversal $\tilde{\mathsf{T}}^2 = I$, and Hermitian metric $\tilde{\eta}$ with signature Diag $\left(I_n, -I_n\right)$, which are compatible: $[\tilde{\mathsf{T}}, \tilde{\eta}] = 0$, such that get $[\tilde{\mathsf{T}}, h_\phi] = 0, \quad \tilde{\eta} h_\phi + h_\phi^\dagger \tilde{\eta} = 0$, or

$$[\tilde{\mathsf{T}}, U_\phi] = 0, \qquad \tilde{\eta} - U_\phi^\dagger \tilde{\eta} U_\phi = 0,$$

Imply that $Det(I + U_\phi) \in \mathbb{R}$, and its sign is fixed by the connected component of U_ϕ in $O(n, n)$.

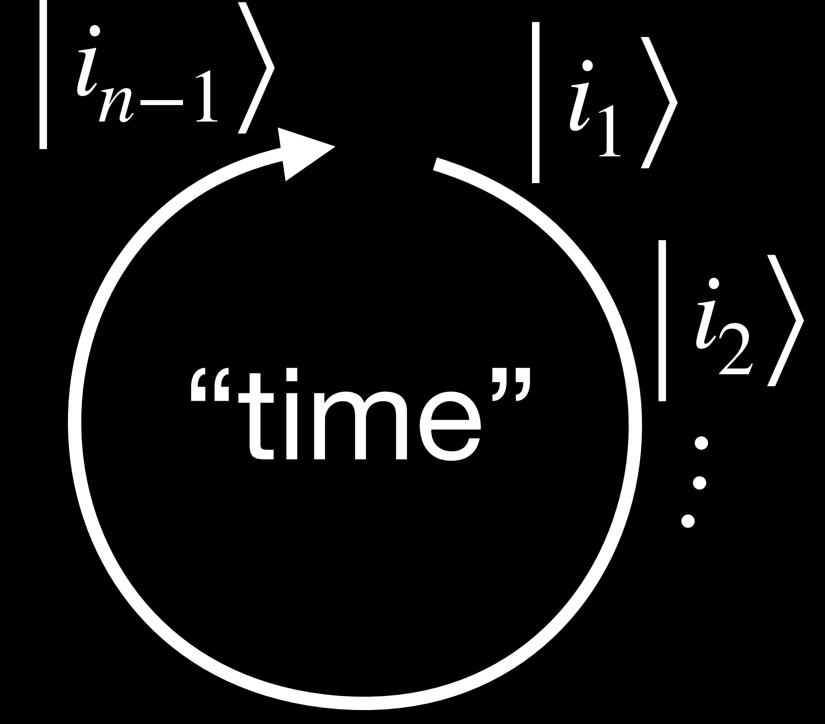
Applications: spineless fermions, particle number conserving, half filling, bipartite lattices.

Example:
World-line mapping and stoquastic Hamiltonians

World-line method:

$$Z = \mathbf{Tr}\left(e^{-\beta H}\right) = \sum_{k=0}^{\infty} \frac{\beta^k}{k!} \mathbf{Tr}\left(-H\right)^k = \sum_{k=0}^{\infty} \sum_{\{i_n\}} \frac{\beta^k}{k!} \prod_{n=1}^{k} \left(-H\right)_{i_n, i_{n+1}}$$

$$= \sum_{\phi} p\left(\phi\right)$$



Stoquastic Hamiltonians: $H_{i,j} \leq 0 \quad \Rightarrow \quad p(\phi) \geq 0.$

Sign-problem and complexity

- A general poly(βN) algorithm to compute $\langle$sign$\rangle$ (probably) doesn't exist: it would imply a solution to Barahona's classical Ising problem, which is NP-complete, leading to P=NP Troyer-Wiese (2005).

- Deciding whether a stoquastic basis exists can be NP-complete Marvian-Lidar-Hen (2018), Klassen-Terhal (2019). Therefore, a general poly(βN) curing algorithm (probably) doesn't exist.

- The problem LH-MIN (approximating ground state energies) is (probably) easier if restricted to stoquastic H's (contained in AM, rather than QMA-complete) Bravyi et al (2008). This implies that a local stoquastic basis cannot exist for all H's Hastings (2016).

- Adiabatic quantum computation with stoquastic H's is (probably) non-universal (can only solve problems is PostBPP, rather than BQP) Bravyi et al (2008). This implies that a local stoquastic basis cannot exist for all H's.

PT symmetry and DQMC