Title: Physical footprints of intrinsic sign problems

Speakers: Zohar Ringel

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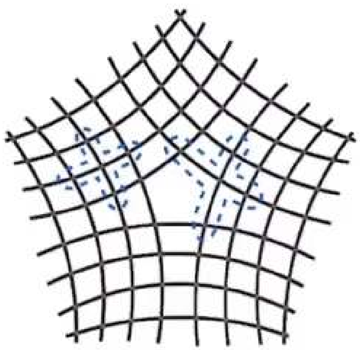
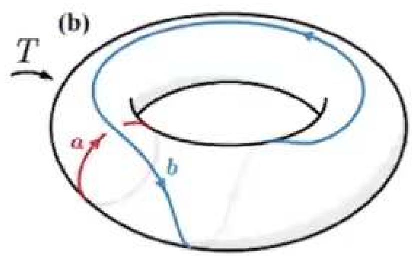
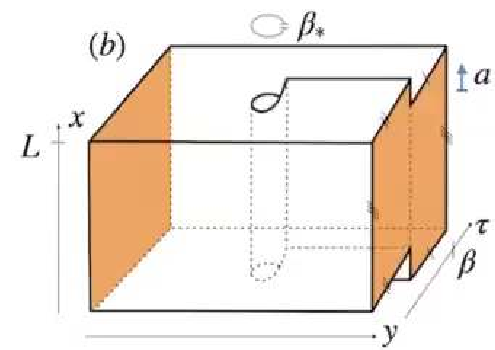
Abstract: The sign problem is a widespread numerical hurdle preventing us from simulating the equilibrium behaviour of many interesting models, most notably the Hubbard model. Research aimed at solving the sign problem, via various clever manipulations, has been thriving for a long time with various recent exciting results. The complementary question, of whether some phases of matter forbid the existence of any sign-free microscopic model, has received attention only recently. In this talk, Iâ€™ll review recent progress and discuss a novel and quite general criteria we obtained for when a topological quantum field theory has no sign-free microscopic model. Iâ€™ll also point out relations to sign problems in frustrated magnets and to the notion of quantum supremacy.

Physical footprints of intrinsic sign problems







Z.R and D. Kovrizhin Science Advances (2017)
O. Golan, A. Smith, Z.R. Arxiv (2020)
A. Smith, O. Golan, Z.R. Arxiv (2020)

Z. Ringel, Perimeter 2020

Omri Golan (Weizmann)

Adam Smith (TUM)

Dmitry Kovrizhin (Cergy-Pontoise)

Outline

1. Quantum Monte Carlo, Intrinsic Sign Problems, Motivations
2. A differential geometry angle on sign problems.
3. The full exchange statistics criterion.
4. Frustrated magnets.
5. Outlook

Path integral Quantum Monte Carlo

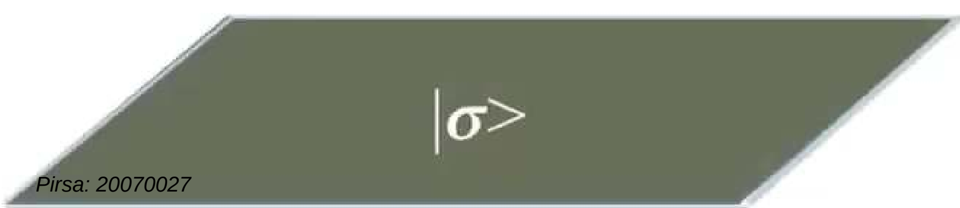
Quantum to Classical mapping

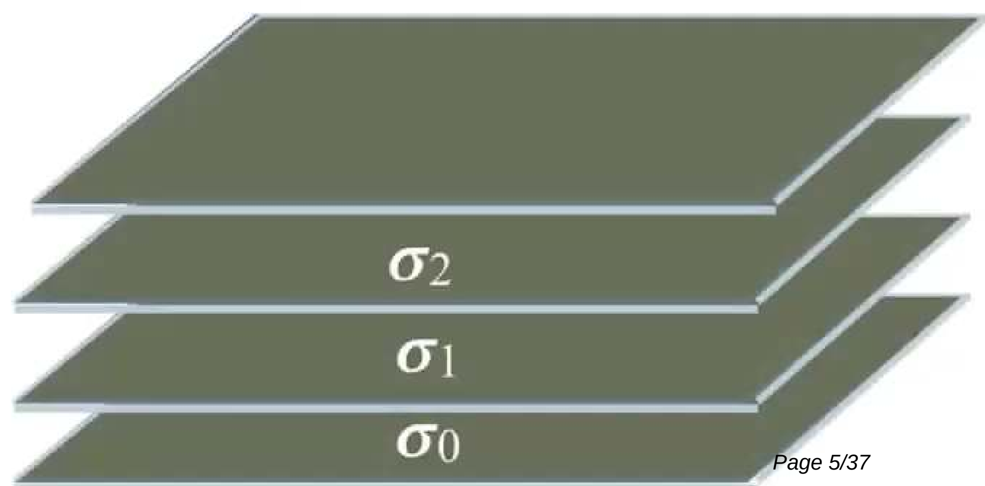
$$Z = Tr[e^{-\beta H}] = Tr[\Pi_{t=0}^{m} e^{-\Delta\tau H}] = Tr[\Pi_{t=0}^{m} e^{-\Delta\tau (K+V)}]$$

$$\underset{\Delta\tau \to 0}{=} \sum_{\sigma_1,\sigma_2,\ldots,\sigma_{2m}} \Pi_t \langle \sigma_{2t} | e^{-\Delta\tau K} | \sigma_{2t+1} \rangle \langle \sigma_{2t+1} | e^{-\Delta\tau V}] | \sigma_{2t+2} \rangle$$

“Classical” (d+1)-dim

Quantum d-dim





What is an intrinsic sign problem (Bosons)?

$$\langle \sigma_t | e^{-\Delta\tau h_r} | \sigma_{t+1} \rangle = \langle \sigma_t | (1 - \Delta\tau h_r) | \sigma_{t+1} \rangle$$

$[h_r]_{i \neq j} \leq 0$?

no → Energies complex

yes → Energies real → Stat. Mech. Problem

Energies complex → Exist *local* S, such that $[S h_r S^{-1}]_{i \neq j} \leq 0$?

yes → Stat. Mech. Problem

no → Exist such *local* S for diff model in the same phase

yes → Stat. Mech. Problem

no → Hard sign pr

Stat. Mech. Problem → Efficient Monte Carlo

Why is that a problem ?

Without signs

$$\langle O \rangle_E = \frac{\sum_{conf} O_{conf} e^{-E_{conf}}}{\sum_{conf} e^{-E_{conf}}} = N^{-1} \sum_{n=1}^{N} O_{conf[n]} + O\left(\sqrt{var[O]/N}\right)$$

With signs

$$\langle O \rangle_{E+i\Phi} = \frac{\sum_{conf} O_{conf} e^{-E_{conf}+i\Phi_{conf}}}{\sum_{conf} e^{-E_{conf}+i\Phi_{conf}}} = \frac{\langle O e^{i\Phi} \rangle_E}{\langle e^{i\Phi} \rangle_E}$$

Exponentially small in Volume

Chandrasekharan, Wiese (1999)

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Sign problem severity =
rate of exponential decay with Volume

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Chandrasekharan, Wiese (1999)

Intrinsic sign problem for Fermions (I)

Path integrals for Fermions include Grassman variables which are inherently sign-full

To circumvent the Grassmans numerically, one integrates over them

$$Z = \int D\phi D\psi e^{-S_\phi - S_{\psi,\phi}}$$
$$= \int D\phi e^{-S_\phi} \mathrm{Det}\left(D_\phi\right)$$

Various locally verifiable criteria, known as “de-sign” principals, can be used to ensure that the resulting determinant is non-negative.

One of the basic ones is time-reversal-symmetry, but there are many more…

Done

Intrinsic sign problem for Fermions (II)

For Bosons an Intrinsic Sign Problem can be phrased as:

"*None of the Hamiltonians in this phase of matter are stoquastic*"

For Fermions we define an Intrinsic Sign Problem as:

"*None of the Hamiltonians in this phase of matter obey any of the known design principals*"

, A. Smith, Z.R. Arxiv (2020)

Prevalence of Intrinsic Sign Problems

Phase of matter	Hard Sign Problem
Fermi-Liquid	No
Ferromagnets/Antiferromagnets	No
Superconductors/Superfliuds	No
Magnetically assisted Superconductivity	No
Topological insulators	In most cases No
Spin-liquids and bosonic SPTs	In many cases No
Quantum Hall effect	No if $k_{xy} = 0$
Hubbard model and QCD	(Yes)
Frustrate	[illegible]

Some analytical viewpoints

- Doubled Semion lattice gauge theory with commuting projectors has a sign problem [Hastings 2015]
- Complexity arguments : QMA > StoqMA

Motivating questions:

Are there phases of matter whose partition function admits no local probabilistic description?

Are there physically measurable effects which imply Intrinsic Sign Problems?

Are there phases of matter in which a generic Hamiltonian instance is computationally hard?

Can we in principal, using available computational technology, simulate with fair precision the phenomena we currently see in nature?

The simulation argument

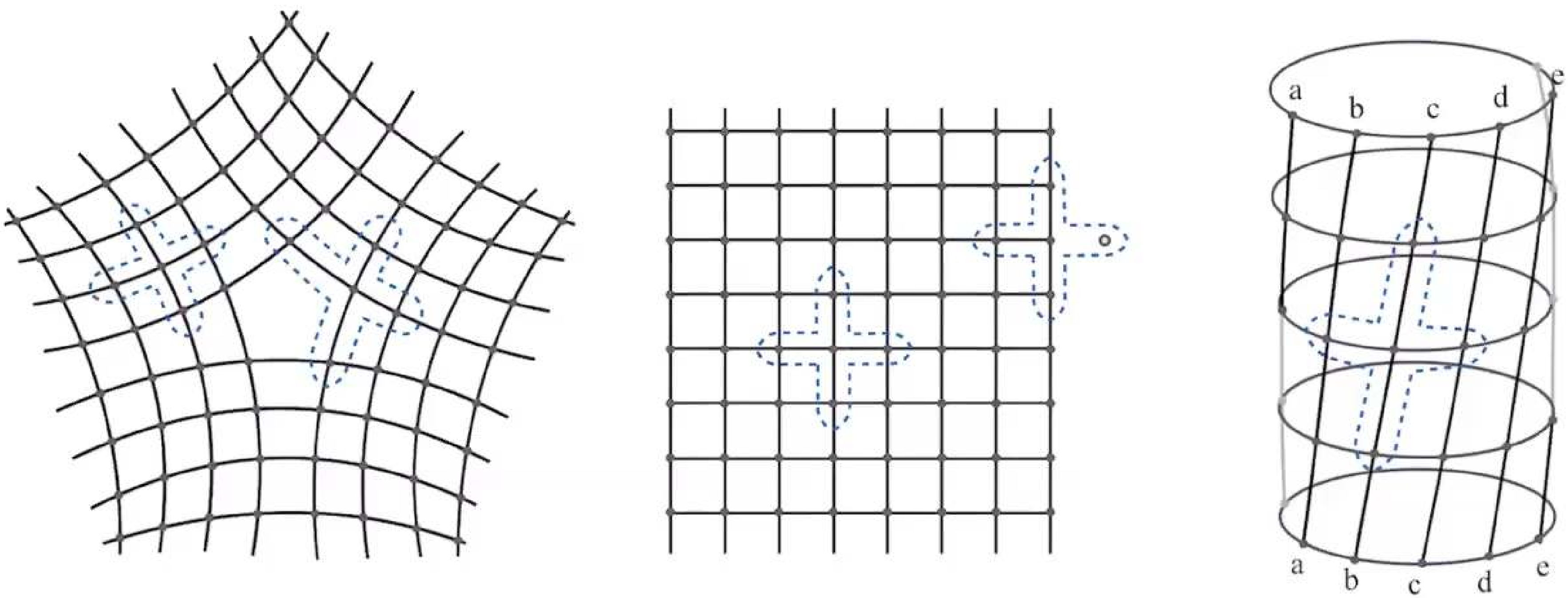
One thing that later generations might do with their super-powerful computers is run detailed simulations of their forebears or of people like their forebears. Because their computers would be so powerful, they could run a great many such simulations. Suppose that these simulated people are conscious (as they would be if the simulations were sufficiently fine-grained and if a certain quite widely accepted position in the philosophy of mind is correct). Then it could be the case that the vast majority of minds like ours do not belong to the original race but rather to people simulated by the advanced descendants of an original race.

Nick Bostrom

$$f_{sims} = \frac{f_{post} f_{interested} N}{f_{post} f_{interested} N + 1}$$

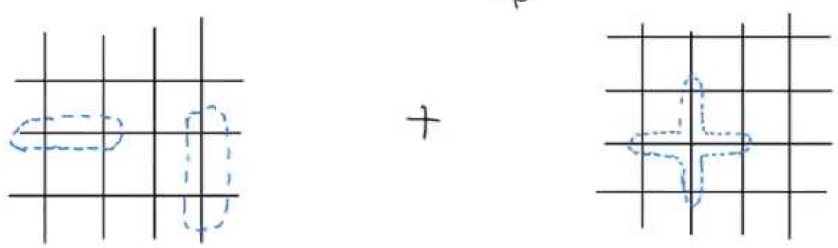
A geometric viewpoint on Sign Problems

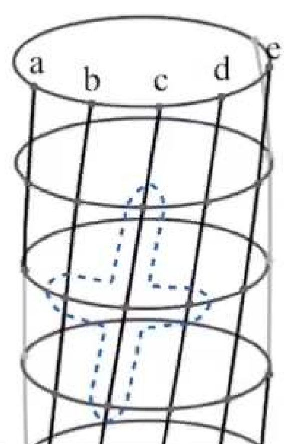
Lattice defects and twists as metric manipulations



Local Hamiltonians can be placed on interesting metrics

$$\mathcal{H} = \sum_{\langle ij \rangle} a_{ij} b_i^{\dagger} b_j + \sum_{\substack{ijkl \\ \in S'}} c_{ijkl} b_i^{\dagger} b_j^{\dagger} b_k b_l + \ldots$$





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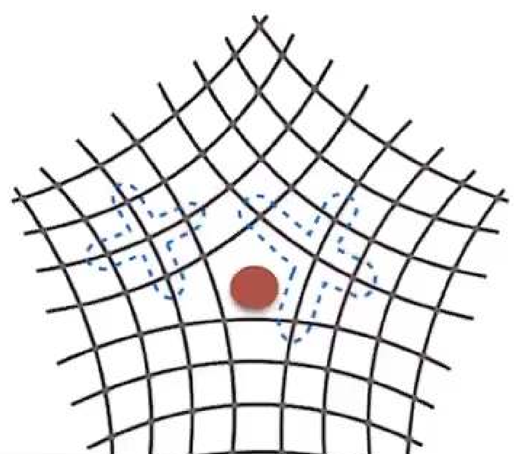

- Some arbitrariness…

Local Hamiltonians can be placed on interesting metrics

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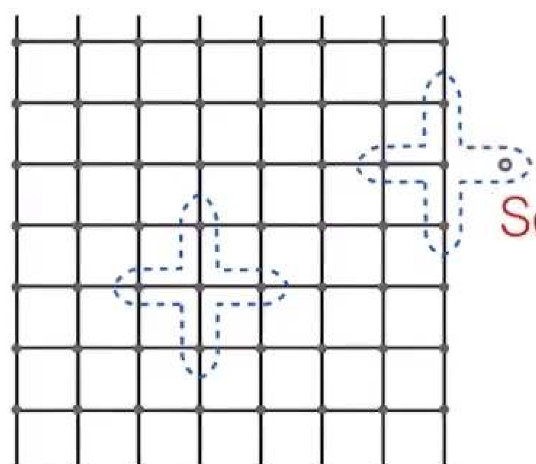


Some arbitrariness…

Changing the metric (morally) leaves the Hamiltonian sign-free

- Since de-sign principal and stoquasicity are local, they often remain valid after the lattice twists needed for metric changes.

- Establishing this requires careful treatment of all the arbitrariness issues.

- From a field-theory perspective, such lattice defects introduce, apart from the desirable changes to the metric, various superfluous operators whose irrelevance needs to be argued for.

A strategy for establishing Intrinsic Sign Problems

Z is **Sign-Free**

Sign-free
Changes to the metric
$\xrightarrow{\pi_{SF}}$

$Z^{(\pi_{SF})}$ is also **Sign-Free**

In various circumstances

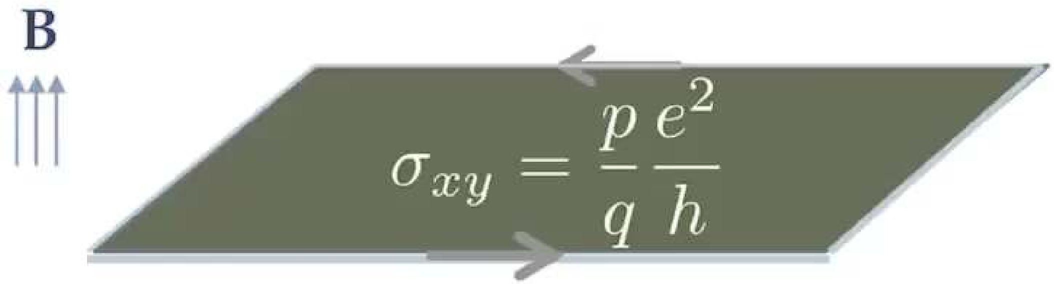
$$Z^{(\pi_{SF})} = e^{i\pi\eta_{\pi_{SF}}} Z$$

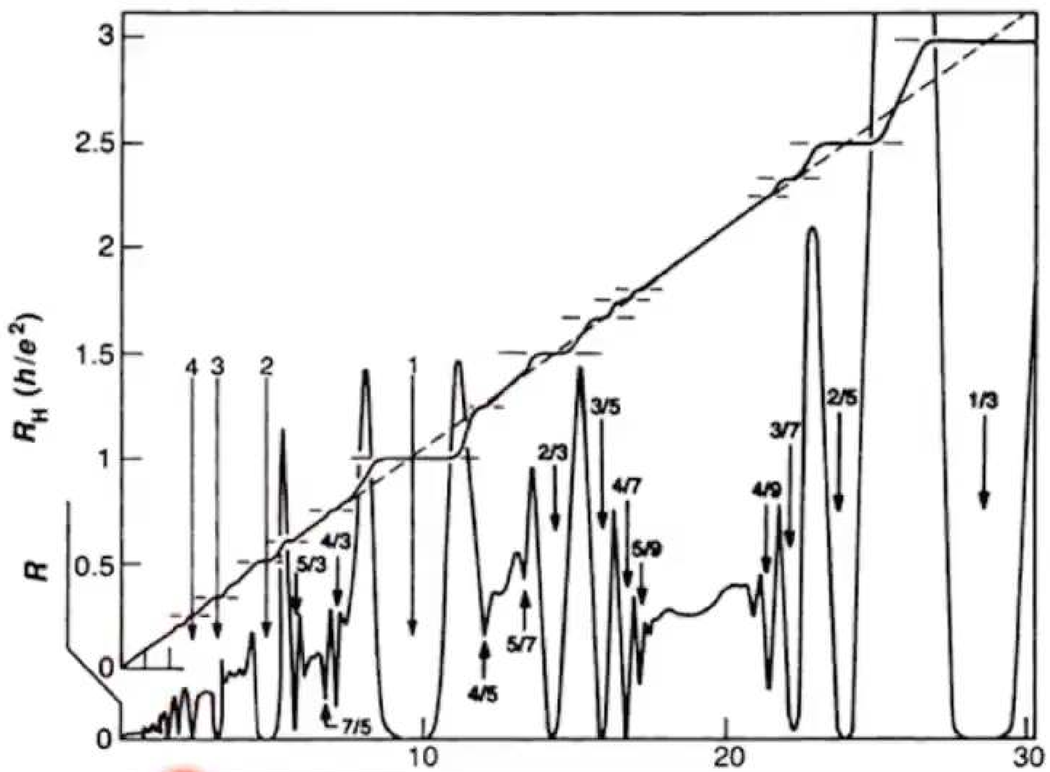
Contradiction !

But what ge ... $e^{i\pi\eta_{\pi_{SF}}} \neq 1$?

Intrinsic Sign Problems in the QHEs

Quantum Hall effects

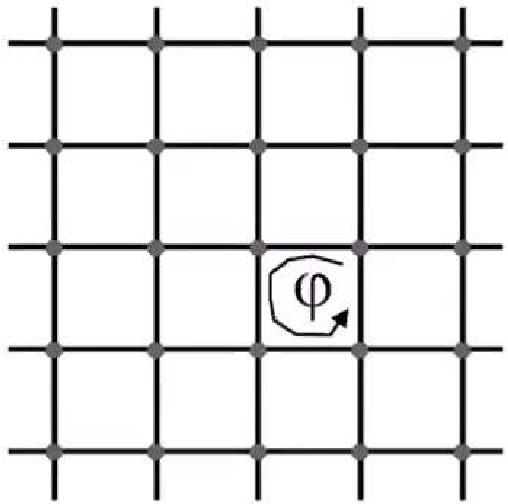




The Nobel Prize in Phy

Not all QHE have a sign problem !

$\sigma_{xy} = 2e^2/h$



$\varphi = 3/7$
bosons

Moller, Cooper (2009)
Geraedts, Motrunich (2013)
Bondesan, ZR (2016)

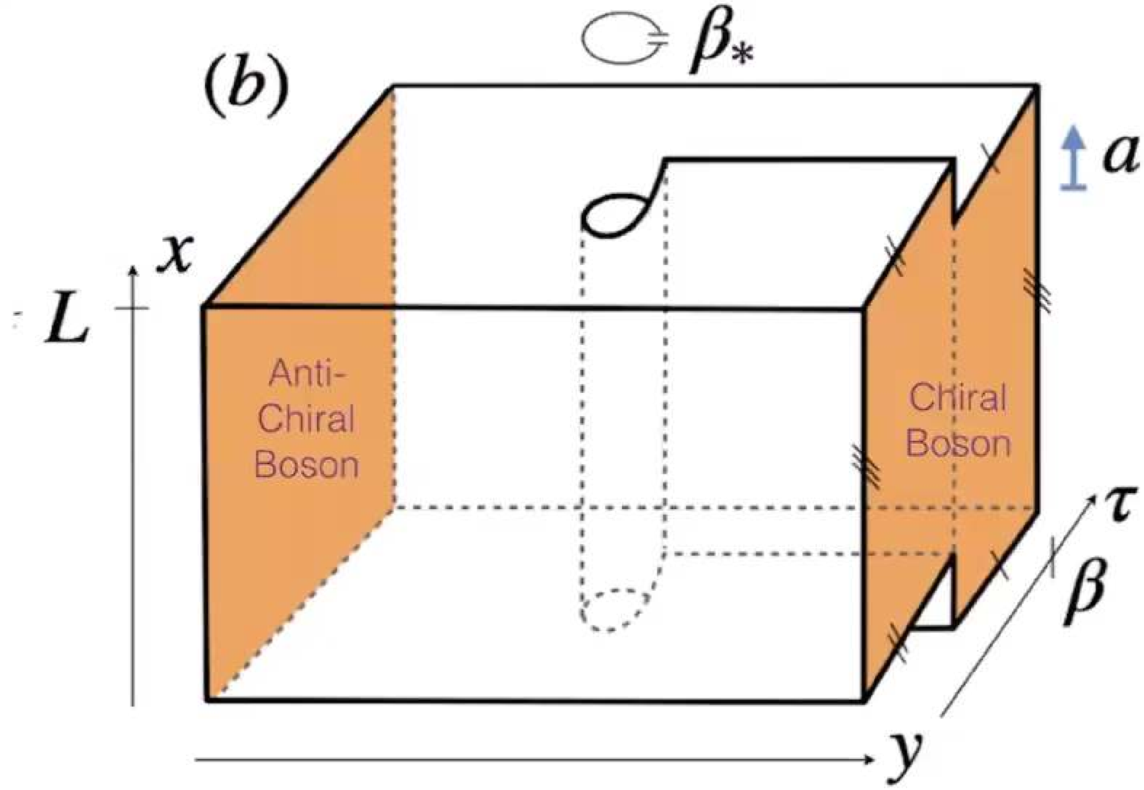
<u>They exhibit :</u>

1. Quantized σ_{xy}
2. U(1)-charge anomaly on edges

<u>They do not exhibit:</u>

1. **Thermal Hall conductance**
2. Ability to perform universal quantum computation

π_{SF} For QHE



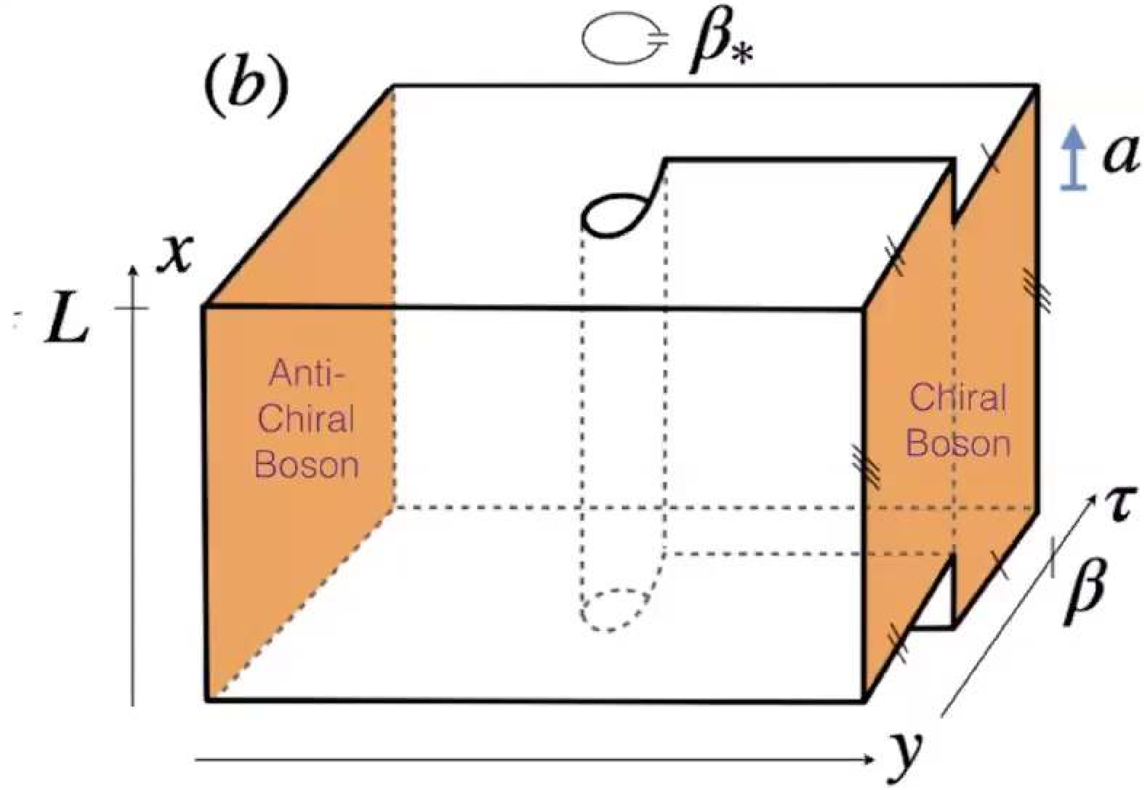
Can be interpreted as translation of only the right side of the system (Momentum Polarization)

* Gravtitional anomaly

$$\tilde{Z} = Z \exp\left[\alpha N_x + \frac{2\pi i}{N_x}\left(h_0 - \frac{c^{*}}{24}\right) + o\left(N_x^{-1}\right)\right] = Z\, e^{i\pi\eta_\pi}$$

One can show

π_{SF} For QHE



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One can show this cannot be real for all N_x

Our results on the Fractional Hall effect

TABLE I. Examples of intrinsic sign problems based on the criterion $e^{2\pi ic/24} \notin \{\theta_a\}$, in terms of the chiral central charge c and the topological spins $\theta_a = e^{2\pi i h_a}$. The number of spins h_a is equal to the dimension of the ground state subspace on the torus. We mark bosonic/fermionic phases by (B/F). The quantum Hall Laughlin phases corresond to $U(1)_q$ Chern-Simons theories. The ℓ-wave superconductor is chiral, e.g $p+ip$ for $\ell=1$, and spinless. Data for the spinfull case is identical to that of the Chern insulator, with $-\ell$ odd (even) in place of ν, for triplet (singlet) pairing. The modulo 8 ambiguity in the central charge of the Fibonacci anyon model corresponds to the stacking of a given realization with copies of the E_8 K-matrix phase. Data for the three quantum Hall Pfaffian phases is given at the minimal filling 1/2. The physical filling 5/2 is obtained by stacking with a $\nu=2$ Chern insulator, and an intrinsic sign problem appears in this case as well.

Phase of matter	Parameterization	c	$\{h_a\}$	Intrinsic sign problem?
Laughlin (B) [36]	Filling $1/q$, $(q \in 2\mathbb{N})$	1	$\{a^2/2q\}_{a=0}^{q-1}$	In 98.5% of first 10^3
Laughlin (F) [36]	Filling $1/q$, $(q \in 2\mathbb{N}-1)$	1	$\{(a+1/2)^2/2q\}_{a=0}^{q-1}$	In 96.7% of first 10^3
Chern insulator (F) [App.B]	Chern number $\nu \in \mathbb{Z}$	ν	$\{\nu/8\}$	For $\nu \notin 12\mathbb{Z}$
ℓ-wave superconductor (F) [61]	Pairing channel $\ell \in 2\mathbb{Z}-1$	$-\ell/2$	$\{-\ell/16\}$	Yes
Kitaev spin liquid (B) [46]	Chern number $\nu \in 2\mathbb{Z}-1$	$\nu/2$	$\{0, 1/2, \nu/16\}$	Yes
$SU(2)_k$ Chern-Simons (B) [68]	Level $k \in \mathbb{N}$	$3k/(k+2)$	$\{a(a+2)/4(k+2)\}_{a=0}^{k}$	In 91.6% of first 10^3
E_8 K-matrix (B) [69]	Stack of $n \in \mathbb{N}$ copies	$8n$	$\{0\}$	For $n \notin 3\mathbb{N}$
Fibonacci anyon model (B) [68]		14/5 (mod 8)	$\{0, 2/5\}$	Yes
Pfaffian (F) [70]		3/2	$\{0, 1/2, 1/4, 3/4, 1/8, 5/8\}$	Yes
PH-Pfaffian (F) [70]		1/2	$\{0, 0, 1/2, 1/2, 1/4, 3/4\}$	Yes
Anti-Pfaffian (F) [70]		$-1/2$	$\{0, 1/2, 1/4, 3/4, 3/8, 7/8\}$	Yes

O. Golan, A. Smith, Z.R. Arxiv (2020)

Intrinsic Sign Problems in non-chiral TQFTs

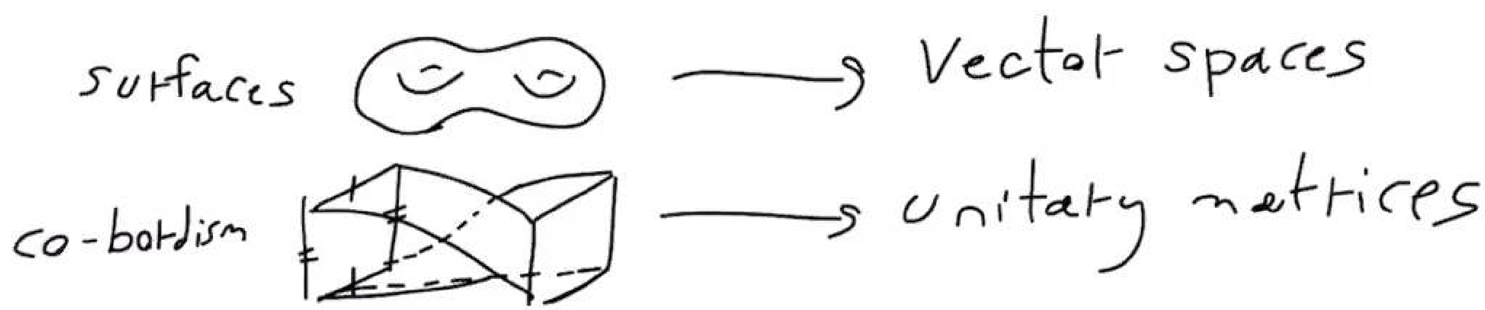
, O. Golan, Z.R. Arxiv (2020)

Topological Quantum Field Theories

Examples: Toric Code, Doubled Semion Model, String-Net models

Definition I: A field theory which is metric independent (e.g. Chern-Simons)

Definition II: An associated between

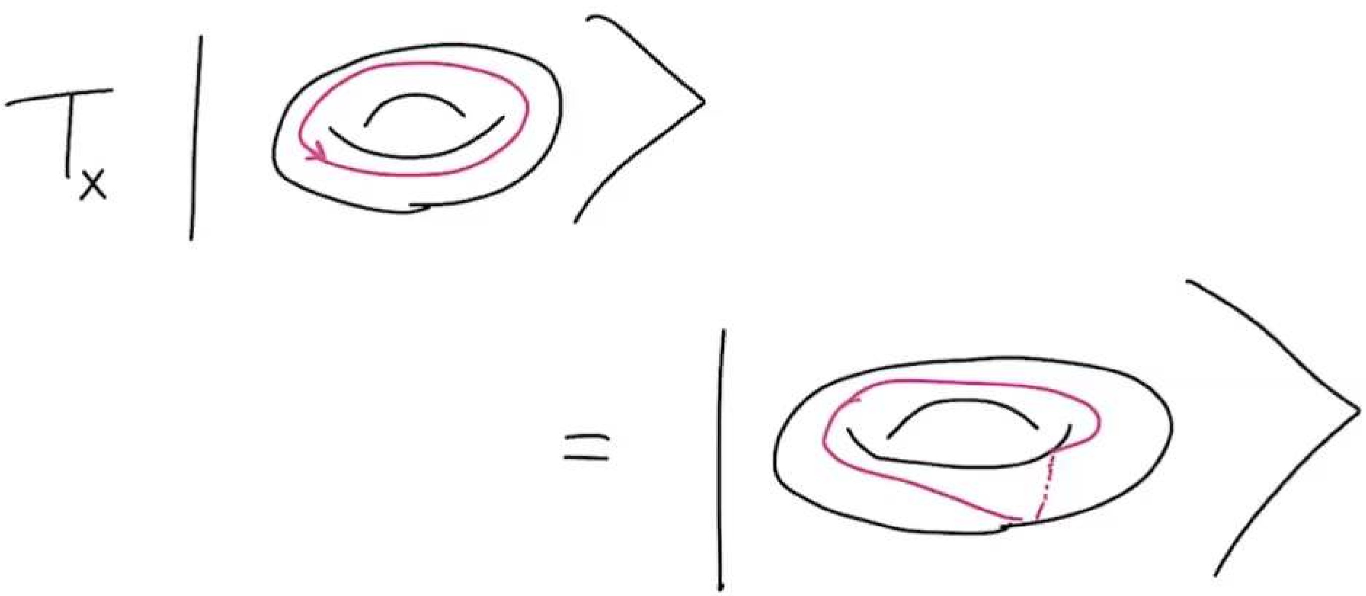


Non-Chiral: No gravitational anomaly on boundaries, Admits a commuting projectors lattice description

The T matrix

A TQFT on a torus has several ground states.

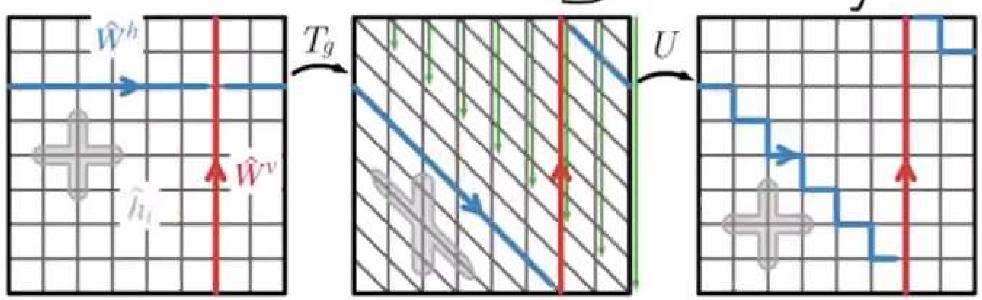
The T matrix gives the overlap between pairs of ground states after a Dehn-twist of the torus.



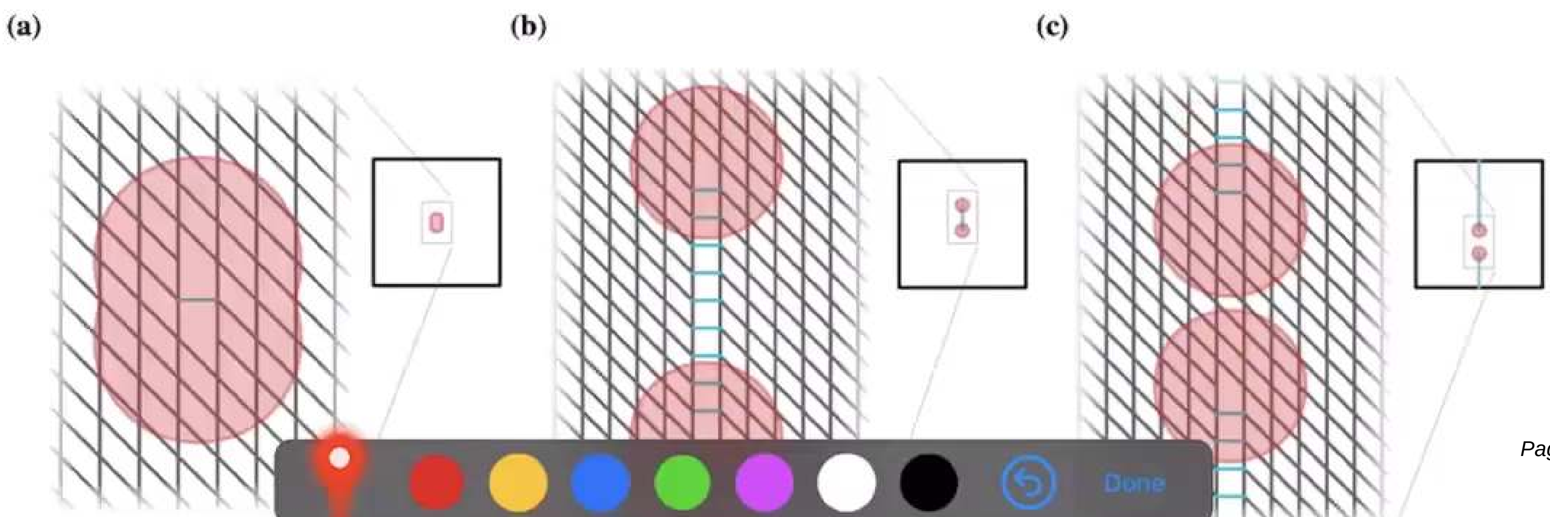
Sign-Free implementation the T-matrix in a lattice Hamiltonian

$T = U\,T_g$ $\quad$ T_g permutation of lattice sites

U reordering of bonds



How we implement U



The exchange statistics criterion

Consider Bosons.

Ground state degeneracy and stoquasticity imply all ground states are positive.

The Dehn-twist implementation is also positive.

The T-matrix on the basis in which the ground-state are positive is element-wise non-negative.

An element-wise non-negative unitary matrix is a permutation matrix.

A permutation matrix has eigenvalues which form full sets of roots of identity.

The Spectrum of the T-matrix, which gives the exchange statistics, must consist of full sets of roots of identity.

...n, O. Golan, Z.R. Arxiv (2020)

The exchange statistics criterion - Examples

Doubled Semion Model

$$T = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Intrinsic Sign Problem (Consistent with Hastings)

Toric-Code

$$T = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

No Intrinsic Sign Problem (Stoquastic Hamiltonians are known)

FQHE

$$T_{aa} = \theta_a e^{-2\pi i c/24}$$

Intrinsic Sign Problem (Consistent with previous FQHE argument)

The exchange statistics criterion - Examples

Doubled Semion Model

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Intrinsic Sign Problem (Consistent with Hastings)

Toric-Code

$$T = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

No Intrinsic Sign Problem (Stoquastic Hamiltonians are known)

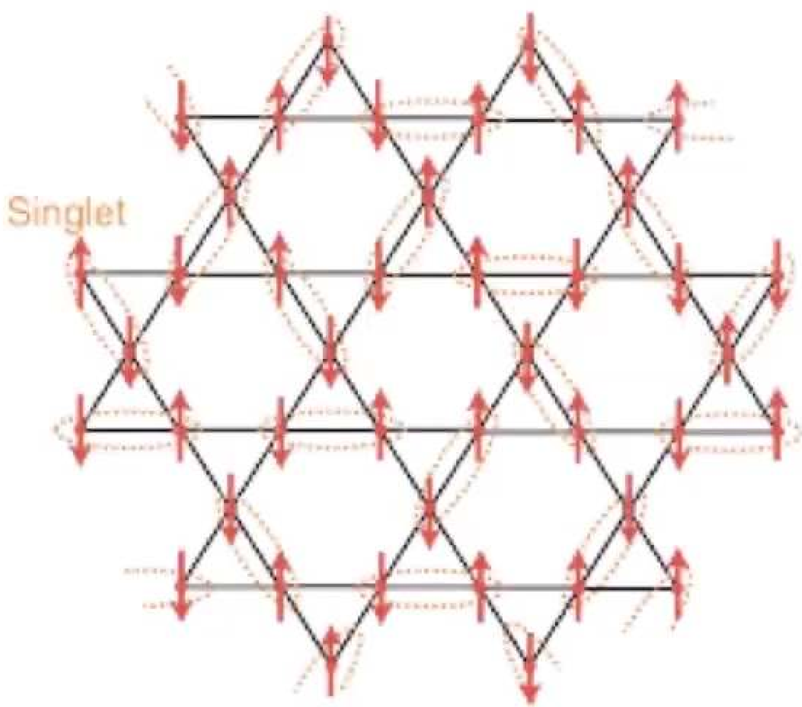
FQHE

$e^{i2\pi h_a}$

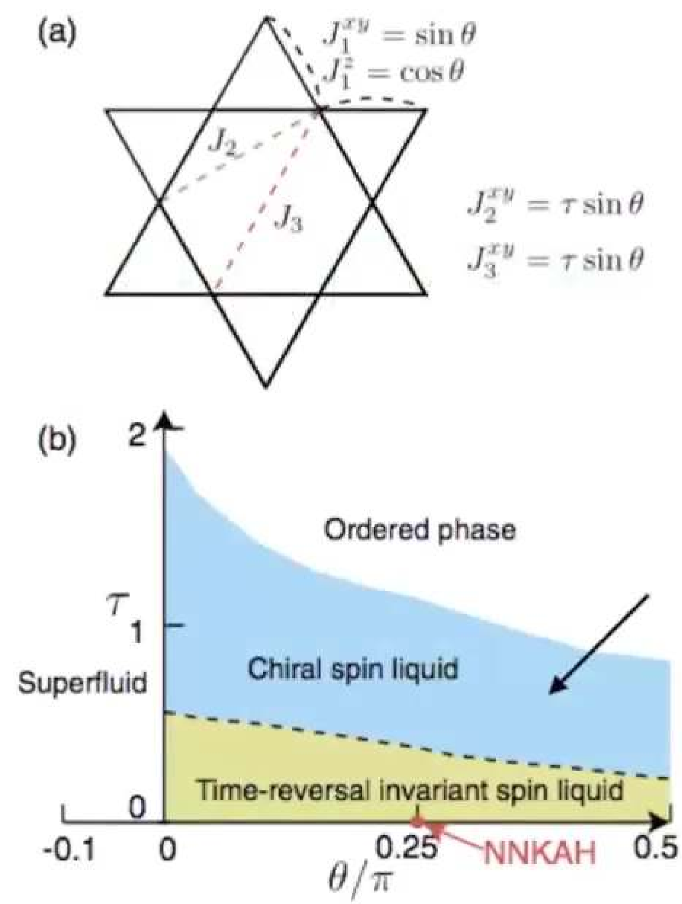
$$T_{aa} = \theta_a e^{-2\pi i c/24}$$

Intrinsic Sign Problem (Consistent with previous FQHE argument)

Kagome Anti-Ferromagnet



$$H = \sum_{ij} J \vec{S}_i \cdot \vec{S}_j$$



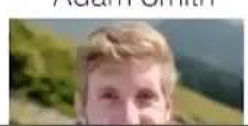
and Yan Chen (2015)

Outlook

- **Classifying sign problems** - Can all intrinsic sign problems be linked with quantum geometrical twists? For instance the repulsive Hubbard model??
- **Sign-problem detection** - Given a ground state, can we numerically infer an intrinsic sign-problem (at a lower computational cost than required for solving it)?
- **Quantum Supremacy** - Given we can engineer models in the doubled-semion phase in the lab, would that be considered as proof for quantum supremacy.
- **Sign oracles** - if we had a device which can efficiently sample from the doubled-semion partition function, can we use it to sample from other TQFT partition functions.
- **Sign Problem severity** - Not all sign problems are equally bad, can we say something about the severity of Intrinsic Sign Problem (Decay of $\langle e^{i\Phi} \rangle_E$)?

Omri Golan

Adam Smith



Dmitry Kovrizhin