From topological θ vacua to asymptotic freedom:
Qubit models, sign problems, and anomalies

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- From qubits to QFT
- Qubit regularization of toy-models of QCD
  - UV: asymptotic freedom
  - IR: θ vacua
- Symmetries and anomalies
  - What do anomalies say about constructing new lattice/qubit regularizations?
- Summary

Quantum field theory is important...

The framework of QFT

- underpins the standard model of particle physics – electroweak theory, QCD
- explains long distance behavior of condensed matter systems: critical phenomenon, topological phases,...

...But it is hard!

Despite the enormous importance of precise quantitative computations in QFT, our general tools are lacking

- Perturbation theory
  - Great for weakly coupled theories such as QED
  - Fails for strongly coupled theories such as QCD at low energies
- Lattice Monte Carlo
  - Great for static quantities (like hadron spectrum in QCD) when the sign problem can be solved
  - Insufficient for studying out-of-equilibrium physics, such as realtime dynamics (such as hadronization in QCD); or sectors of high particle number density (such as neutron star cores); or even for static quantities in the presence of a **sign problem**
- With quantum computing at scale, we might solve some of the issues which plague classical lattice calculations

“Digitization” of QFTs for quantum computers

- Traditional lattice regularization for bosons = ∞-dim local Hilbert space. Implied by the bosonic commutation relations

$$[\phi_x, \pi_y] = i\delta_{x,y} \tag{1}$$

- But digital quantum computers need a **finite dimensional** local Hilbert space
- Need to truncate the Hilbert space somehow...
- Several approaches towards finding a “digitization”
  - Field-space digitization [Jordan, Lee, Preskill, 2011, ...]
  - Loop-string hadrons [Raychoudhary et al, 2020, ...]
  - Single-particle digization [Barata et al, 2020, ...]
  - Tensor networks [Meurice, 2020, ...]
  - Discrete subgroups for gauge theories [Lamm et al, ...]
  - D-theory, quantum-link models [Brower et al, 2004, ...]
  - ...

"Digitization"

- Most approaches to digitization: truncate the Hilbert space (to n qubits), then reproduce the traditional lattice Hamiltonian by taking $n \to \infty$, and then take the continuum limit like in traditional lattice models

$$\text{Digitized model} \xrightarrow{n \to \infty} \text{Traditional lattice model} \xrightarrow{a \to 0} \text{continuum QFT} \tag{2}$$

- Is it necessary to do this 2-step procedure? No!

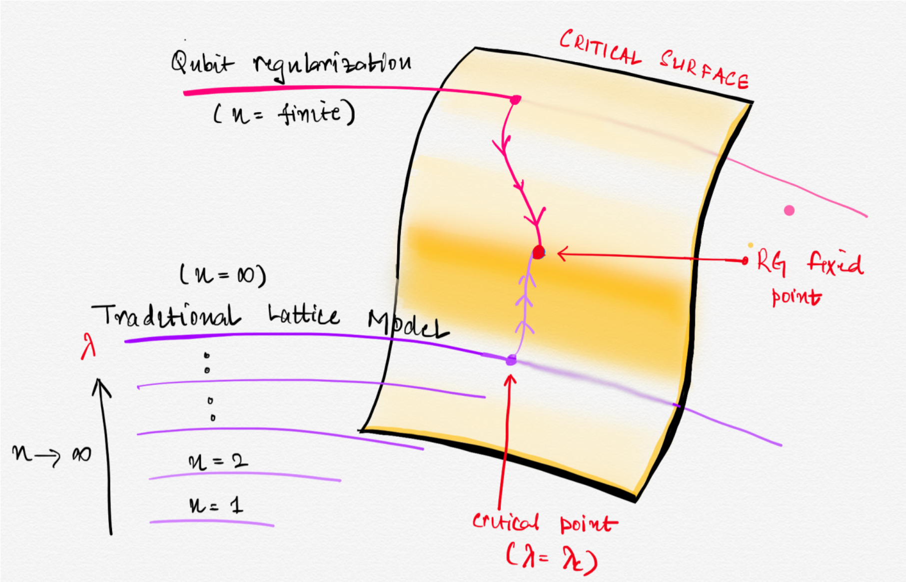
“Digitization”

- **Wilson’s insight: QFT = Second-order phase transitions**
- Even with finite n (#qubits per lattice site) one can obtain continuum limits of field theories

Qubit regularization of field theories

- Continuum limit: tune to a second-order critical point of a quantum lattice Hamiltonian
- This defines a procedure to obtain a continuum QFT
- **Qubit regularization:**
  a quantum lattice Hamiltonian acting on a finite-dimensional local Hilbert space (kept fixed) which reproduces a desired QFT in the vicinity of a quantum critical point.

Regularization from a Wilsonian RG perspective



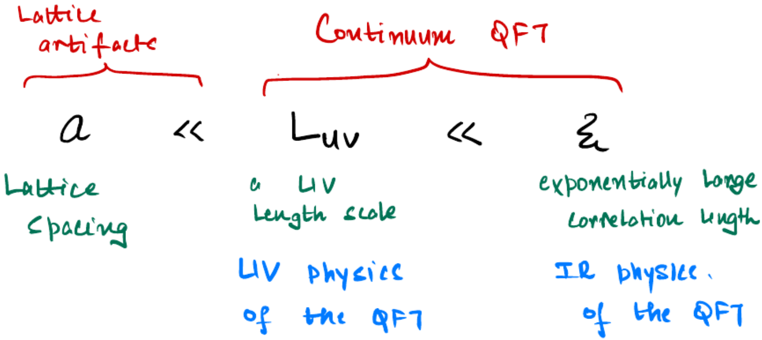
Qubit regularization of QCD

- For some QFTs, it is quite easy to construct such “qubit” models.
- For example, the Ising model famously reproduces the ϕ^4 theory in $d = 3, 4$ dimensions
- However, it is not obvious that *all* QFTs can be obtained in this way
- Question:

  Can we recover all features of QCD from models of qubits?

  - asymptotic freedom
  - topological θ term

The challenge of asymptotic freedom



- To get the continuum limit, we need to recover both the IR physics and the UV physics

A toy model of QCD

- **$O(3)$ nonlinear sigma model in 1+1 dimensions**
- Continuum action

$$S[\vec{n}(x)] = \frac{1}{2g^2} \int d^2x \, \partial_\mu \vec{n} \cdot \partial^\mu \vec{n} \tag{3}$$

  with $\vec{n} \in \mathbb{R}^3$ and $|\vec{n}| = 1$.
- toy model for QCD: asymptotic freedom, dynamical mass generation, dimensional transmutation, θ-vacua

QCD vs. (1+1)d $O(3)$

QCD/$SU(N)$-YM

- $3+1$-dimensional
- Local gauge symmetry
- Asymptotically free
- Dimensional transmutation
- Nonperturbative mass gap
- Nontrivial topology, θ-term

$O(3)$ NLσM

- $1+1$-dimensional
- Global $O(3)$ symmetry
- Asymptotically free
- Dimensional transmutation
- Nonperturbative mass gap
- Nontrivial topology, θ-term

Traditional lattice regularization

- $O(3)$ **nonlinear sigma model in 1+1 dimensions**
- Lattice regulated action:

$$S = \frac{1}{2g^2} \int d^2x \, \partial_\mu \vec{n} \cdot \partial^\mu \vec{n} \tag{4}$$

$$\Big\downarrow \text{ Naïve discretization}$$

$$S = -\frac{1}{g^2} \sum_{\langle xy \rangle} \vec{n}_x . \vec{n}_y \tag{5}$$

- 2d $O(3)$ NLSM is the continuum QFT which emerges in the $g \to 0$ limit of the lattice model

Qubit Regularization of the
$O(3)$ NLSM with a θ term

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From Asymptotic Freedom to θ Vacua: Qubit Embeddings of the O(3) Nonlinear σ Model

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$O(3)$ NLSM at arbitrary θ

- So far, we have talked about the $O(3)$ NLSM at $\theta = 0$.
- Just like QCD, the $O(3)$ NLSM allows for a topological θ term

$$S_\theta[\vec{\phi}] = \frac{1}{g^2} \int d^2x (\partial_\mu \vec{\phi})^2 + i\theta Q[\vec{\phi}] \tag{6}$$

where

$$Q[\vec{\phi}] = \frac{1}{8\pi} \int d^2x \, \varepsilon_{\mu\nu} \, \vec{\phi} \cdot (\partial^\mu \vec{\phi}) \times (\partial^\nu \vec{\phi}) \tag{7}$$

is the *topological* theta term.

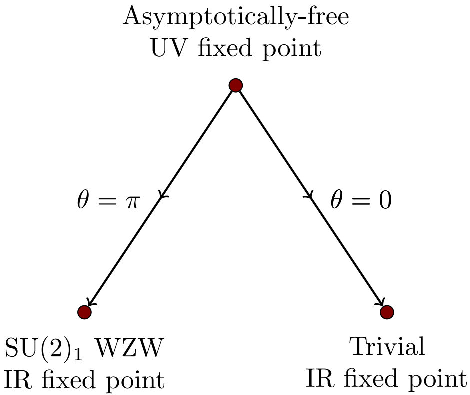
In nature, $\theta < 10^{-10} \implies$ **Strong CP problem**

Physics of θ

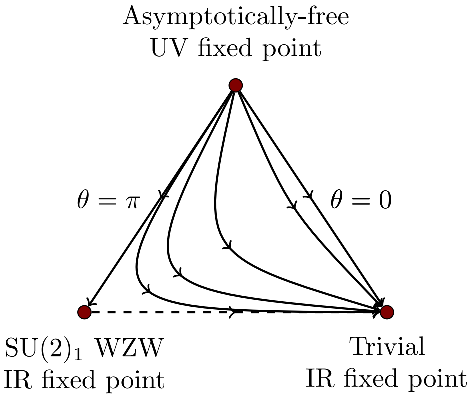
$$S_\theta[\vec{\phi}] = S_0 + i\theta Q[\vec{\phi}]$$

- The physics of θ is totally non-pertubative
- θ does not show up in perturbation theory $\implies$ UV physics unchanged.
  - S_θ is an *asymptotically free* theory for all θ with a non-pertubatively generated energy scale.
- What about the IR physics?
  - θ non-perturbatively changes IR physics
  - At $\theta = \pi$, the low-energy physics is completely different from $\theta = 0$!
  - It is, in fact, massless in the IR $\implies$ flows to the $\mathrm{SU}(2)_1$ WZW CFT.
- What happens at arbitrary θ?

RG flow


Asymptotically-free
UV fixed point
$\theta = \pi$
$\theta = 0$
$SU(2)_1$ WZW
IR fixed point
Trivial
IR fixed point

RG flow


Asymptotically-free
UV fixed point
$\theta = \pi$
$\theta = 0$
$SU(2)_1$ WZW
IR fixed point
Trivial
IR fixed point

The theory at $\theta \neq 0, \pi$

- $\theta = 0, \pi$ points are very special due to their integrability [Zamolodchikov et al, 1978; 1992] and we have a very good understanding.
- At $\theta \neq 0, \pi$ the situation is not so clear.
- Many attempts to understand the behavior of the theory, but questions still remain...

The problem with θ

- It has been argued that the topological charge has ultraviolet divergences for the $O(3)$ model and is not a physical quantity [Schwab, 1982; Luscher, 1982; Blatter et al, 1996].
- If so, it might happen that θ is an irrelevant parameter (for $\theta \neq \pi$) and simply renormalizes to zero.
- Other studies, by studying the theory about $\theta = \pi$ WZW point, have argued that that in fact there is a critical θ_c below which the theory renormalizes to zero, but is nontrivial for $\theta \geq \theta_c$ [Controzzi, Mussardo, 2003; Venuti et al 2005].
- **Question: Is there a continuum QFT S_θ for each value of θ?**
- If these concerns can not be sorted out for the 2d $O(3)$ NLSM, the case of QCD is even harder...

Lattice formulation

- In the conventional approach, θ introduces a severe sign problem (imaginary coefficient in Euclidean time)
- [Bögli, Niedermayer, Pepe, Wiese, 2011] studied the θ-vacua using non-standard ("topological") actions:
  - In their approach the sign problem is "mild" for smaller lattices.
  - Concluded that S_θ is unique for each θ.
- It would be good to have a completely sign-problem free way of studying θ vacua.

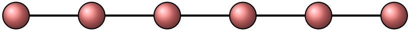
Qubit regularization

Is there a "qubit regularization" of this model?

- We need to obtain
  - UV physics (asymptotic freedom)
  - IR physics (θ-vacua)

Haldane Conjecture

- In 1981, Haldane surprised both condensed matter and high-energy communities
- Consider the antiferromagnetic spin-S Heisenberg chain



$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} \tag{8}$$

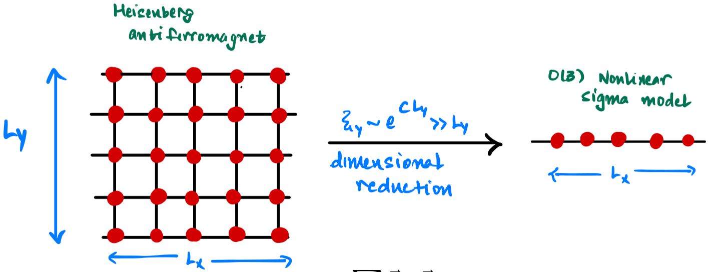
- Haldane Conjecture

$$\text{Spin-}S \text{ chain} \leftrightarrow \text{O(3) sigma model at } \theta = 2\pi S \tag{9}$$

S=1/2 chain	$\theta = \pi$ NLSM	massless
S=1 chain	$\theta = 0$ NLSM	massive

- How do we take the continuum limit (asymptotic freedom)?

UV: Asymptotic Freedom from D-theory



$$H = J \sum_{ij} \vec{S}_i \cdot \vec{S}_j \tag{10}$$

- For large L_Y, spontaneous symmetry breaking: $O(3) \to O(2)$
- The continuous fields $\vec{\phi}$ arise from collective Goldstone mode excitations of the spin-1/2 variables $\vec{S}_i$
- Study the limit: $1 \ll L_Y \lesssim L_X$
  - Asymptotic freedom of the $O(3)$ model guarantees exponential convergence in L_Y
- Dimensional reduction back to (1+1)-d theory! [Chandrasekharan, Wiese, 1997; Brower et al, 1999]

UV and IR

- D-theory provides a recipe to get the UV physics of asymptotically free theories
- But what about IR? Can we generate a θ term in the IR?

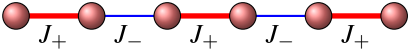
IR: θ term in spin chains

- In terms of the spin variables, it can be shown using bosonization [Affleck, 1988]

$$a^{-1}\vec{S}_n = \vec{J}_L + \vec{J}_R + i(-1)^n c(\mathrm{Tr}\, g)\vec{\sigma}. \tag{11}$$

- Note that "charge conjugation" $g \mapsto -g$ maps to translation by one unit $S_n \mapsto S_{n+1}$
- Therefore, to generate a θ term, we must break this translation-by-one symmetry.
- For example, we can stagger the couplings on even and odd sites

$$J_\pm = J(1 \pm \gamma). \tag{12}$$



- For this case, [Haldane, Affleck]

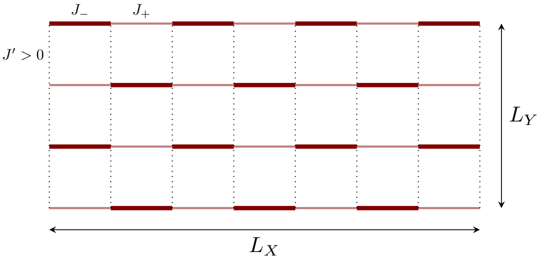
$$\theta = 2\pi S(1+\gamma). \tag{13}$$

- Can be generalized to spin ladders [Sierra, 1996; Sierra et al, 1997]

Taking the continuum limit with θ term

- We can finally put the two pieces of the puzzle together
  - UV = Asymptotic freedom $\implies$ Dimensional reduction
  - IR = topological θ term $\implies$ C breaking using staggered couplings
- Therefore, we can now take the *continuum limit* of these models at non-trivial θ!

θ-term with D-theory



- *Proposal: Continuum limit of the $O(3)$ NLSM with θ term obtained in the $L_X \gg L_Y \gg 1$ limit*
- Analysis of spin ladders [1] suggests, for $J_\pm = J(1 \pm \gamma)$,

$$\theta \approx 2\pi S L_Y (1 + c\gamma) \implies |\theta - \pi| = c\pi\gamma L_Y \text{ (odd } L_y) \tag{14}$$

- **A gift:** *no sign problem!* So we can actually numerically check this.

[1] Sierra 1995; Martin-Delgado, Shankar, Sierra 1996

Probing the continuum limit for asymptotically free theories

- To probe the universal behavior of the continuum limit, we can use the **step scaling function** as a convenient tool [Luscher, Weisz, Wolff, 1991]
- Put the asymptotically free theory in a box of size L (natural length scale)
- Define a dimensionless renormalized coupling $\bar{g}^2(L)$
  - For example, we can choose $\bar{g}^2(L) = M(L)L$, where $M(L)$ is the finite-volume mass gap
- All dimensionless observables depend only on the renormalized coupling $\bar{g}^2(L)$.

Step scaling function

- We will look at the universal function $F(z)$ defined by

$$\frac{\xi(\beta, 2L)}{\xi(\beta, L)} \equiv F\left(\xi(\beta, L)/L\right) \tag{15}$$

  where β is a bare coupling and $z = \xi(\beta, L)/L$ is the renormalized coupling
- $\xi(\beta, L)$ is a definition of finite-volume correlation length: the "second-moment" correlation length

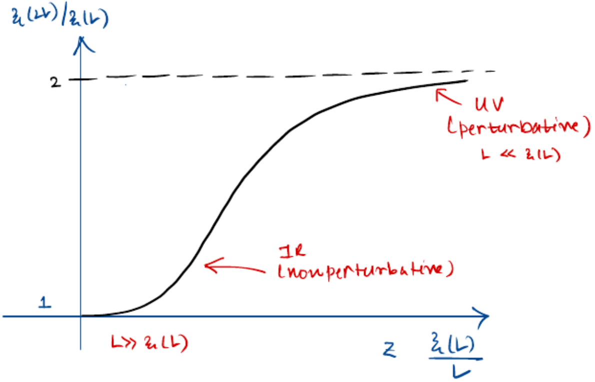
$$\xi(L) = \frac{\sqrt{\tilde{G}(0)/\tilde{G}(2\pi/L) - 1}}{2\sin(\pi/L)} \tag{16}$$

- Easy to measure

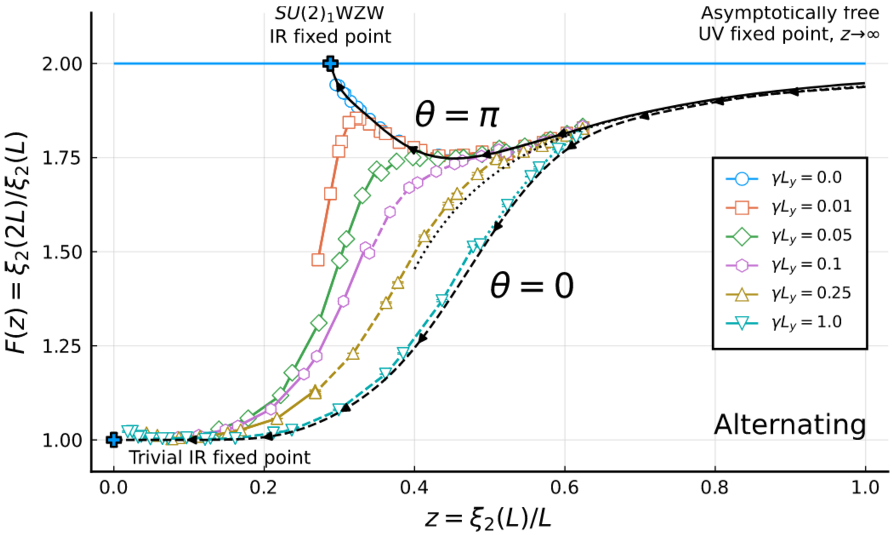
Step scaling function: qualitative behavior

$$z = \xi(L)/L$$
$$F(z) = \xi(2L)/\xi(L)$$

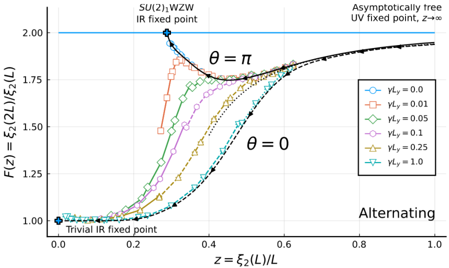
- IR physics: $z \to 0$
- UV physics: $z \to \infty$

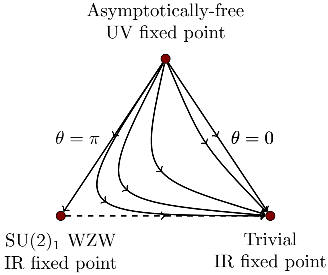


Step-scaling function and the RG flow



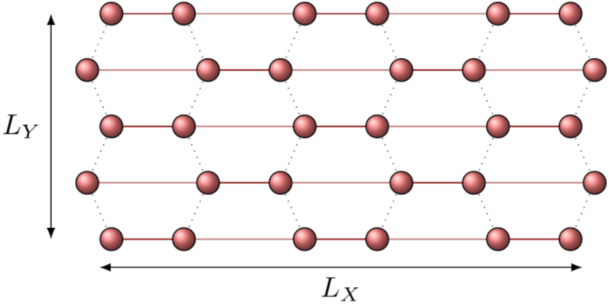
Step-scaling function and the RG flow





The step-scaling curves mimic the expected RG flow diagram beautifully!

On quantum simulators

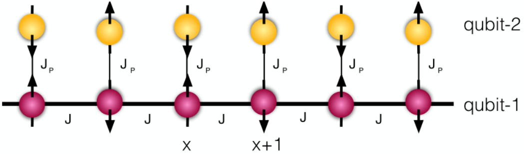


- On Rydberg systems with native Ising-type interactions, we can use Floquet engineering techniques to implement Heisenberg interactions [2]

[2] arXiv: 2207.09438 [Ciavarella, Caspar, HS, Savage, Lougovski, 2022]

A two-qubit regularization

- In another work [3], we showed that a two-qubit regularization of asymptotic freedom can also be obtained
- "Heisenberg Comb"



- Hamiltonian

$$H = \sum_i \quad J_p \, H_{(i,1),(i,2)} + J \, H_{(i,1),(i+1,1)} \tag{17}$$

- Set $J_2 = 0, \; J_p = 1$. Continuum limit: $J \to \infty$.

[3] PRL 126, 172001 (2021) [Bhattacharya, Buser, Chandrasekharan, Gupta, HS]

Summary

- The 2d $O(3)$ NLSM allows for a θ term, just like QCD.
- However, physics of θ is non-perturbative and therefore hard to study – both
  - analytically (no small parameter, non-integrable),
  - and on the lattice (sign problem)
- We constructed a qubit regularization of the $O(3)$ NLSM with a θ term
  - Completely **solves the sign problem** present in conventional approaches for the θ term, for the first time.
  - Allowed us to take the **continuum limit** and demonstrate **asymptotic freedom** for various θ
  - Step-scaling curves give a quantitative instantiation of the RG flow
  - **Very natural for quantum simulators** with qubit degrees of freedom
- Opens up many paths forward...
  - systematic understanding of the RG flow as a function of θ, comparison with analytical results from instanton calculations, ...

- We saw that there is a lattice regularization of the θ term where θ appears as the staggering of couplings

$$\text{Staggering } \gamma \longleftrightarrow \theta \text{ term} \tag{18}$$

- But: why does such a regularization exist? Did we simply get lucky?
- Is there a way to systematically explore this space of lattice regularizations?

- An interesting perspective comes from symmetries and **anomalies**

Lattice regularizations of θ vacua: Anomalies and qubit models

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[arXiv: 2209.12630]

Symmetries and Anomalies

- It is clear that symmetries play a huge role in constructing lattice regulators.
  - It is ideal if the lattice regulator explicitly preserves a symmetry of the continuum theory
- However, some symmetries have a subtle structure, which we call an **anomaly**

't Hooft Anomalies

- The word *anomaly* has many meanings..
- For us, anomaly = **'t Hooft anomaly**

"'t Hooft Anomaly"

G is a genuine global symmetry of the theory, but it cannot be gauged.

"Mixed anomaly"

G_1, G_2 are genuine global symmetries. They can be gauged individually, but gauging one breaks the other.

Classic example of a mixed ’t Hooft anomaly

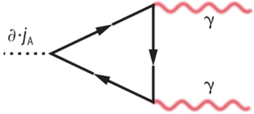
$U(1) \times U(1)_A$ for a free Dirac fermion

- A *free* Dirac fermion has exact global (vector) $U(1)$ and (chiral) $U(1)_A$ symmetries

$$\psi \xmapsto{U(1)} e^{i\theta}\psi \tag{19}$$

$$\psi \xmapsto{U(1)_A} e^{i\theta\gamma_5}\psi \tag{20}$$

- However, *if you gauge $U(1)$, then you lose $U(1)_A$!*



- In other words, $U(1)$ and $U(1)_A$ cannot be gauged simultaneously.

A mixed anomaly in the sigma models

- At $\theta = 0, \pi$, the $O(3)$ model has exact global SO(3) and charge conjugation C symmetries

$$\vec{\phi} \xmapsto{SO(3)} e^{i\theta\hat{n}\cdot\vec{J}}\vec{\phi} \tag{21}$$

$$\vec{\phi} \xmapsto{C} -\vec{\phi} \tag{22}$$

$$\tag{23}$$

- This is a mixed anomaly at $\theta = \pi$ between SO(3) and C[4]
- If you gauge SO(3), then you lose C!

$$\langle\mathcal{O}\rangle \xmapsto{C} e^{i\,\text{Anomaly}}\langle\mathcal{O}\rangle \tag{24}$$

[4] [Gaiotto, Kapustin, Komargodski, Seiberg, 2017]

Anomalies and lattice regularizations?

- We are interested in constructing new lattice regularizations
- The presence of an 't Hooft anomaly for G must be reflected by a lattice regularization.

Gauging a symmetry on the lattice

- Assume a lattice regulator, with
  - same spacetime dimensionality
  - exact symmetry on the lattice
  - locality
  - symmetry implemented **“onsite”**
- Onsite $\implies$ we can gauge it on the lattice by introducing link variables
- But if there is an anomaly, there must be some obstruction to this procedure!

QFT Lore

“There are no anomalies on the lattice”

- Example: attempts to put chiral fermions on the lattice result in doublers [Nielsen, Ninomiya]

Obstructions to gauging on the lattice

- A way in which it is impossible to gauge a symmetry is that the symmetry is **not** onsite
  - Well appreciated in cond-mat [5]
- If the symmetry is offsite, there is no obvious way to gauge it on the lattice
- Indeed, in the spin-chain regularization, the charge conjugation symmetry was offsite

$$C : \vec{S}_i \mapsto \vec{S}_{i+1} \tag{25}$$

- The spin-1/2 chain naturally realizes the $\theta = \pi$ model, which has a $\mathrm{SO}(3) \times \mathrm{C}$ anomaly
- Now, we see that the offsite-ness of the symmetry was no accident – it is *almost* forced by the anomaly!

[5] For example: Jian, Bi, Xu (2018); Cho, Hsieh, Ruy (2017)

Obstructions to gauging on the lattice

- But what if we *insist* that an anomalous symmetry is onsite on the lattice?
- Consider the **standard lattice action** at $\theta = 0$

$$S_0 = -\frac{1}{g^2} \sum_{\langle xy \rangle} \vec{n}_x \cdot \vec{n}_y \tag{26}$$

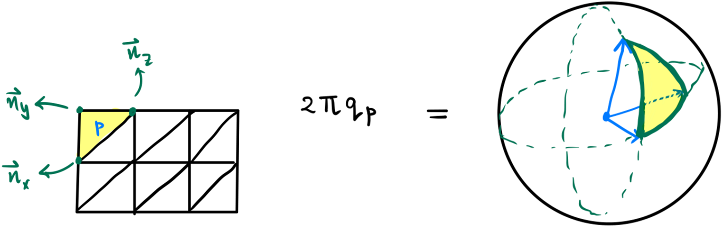
- Both SO(3) and C are **onsite**
- Indeed, a topological θ term on the lattice was defined by [Berg, Lüscher, 1981] which maintains this property

A topological definition of the θ term on the lattice

- Topological θ term on the lattice [Berg, Lüscher, 1981]

$$S[\vec{n}] = S_0[\vec{n}] + i\theta Q[\vec{n}] \tag{27}$$

$$Q[\vec{n}] = \sum_{\langle xyz \rangle} q_{\langle xyz \rangle} \tag{28}$$



Obstruction?

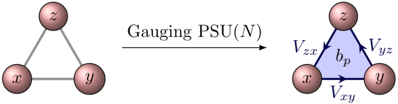
- So if the symmetry is both exact and onsite on the lattice, where is the obstruction? What prevents us from gauging it on the lattice?
- In [arXiv: 2209.12630, Nguyen, HS] we find that this rather well-known lattice model **explicitly** reproduces the exact anomaly on the lattice!

How to detect the anomaly?

SO(3) $\times$ C anomaly

- We turn on a background gauge field (A, B) for the SO(3) symmetry and then perform a C transformation

$$Z \xmapsto{\text{Gauging PSU}(N)} \tilde{Z}[A, B] \tag{29}$$



- We then check whether Z is invariant under C.

$$\text{C}: \begin{cases} \tilde{Z}[A, B, \theta = 0] \mapsto \tilde{Z}[A, B, \theta = 0], \\ \tilde{Z}[A, B, \theta = \pi] \mapsto \tilde{Z}[A, B, \theta = \pi] \underbrace{e^{-ik \int B}}_{\text{anomaly}} \end{cases} \tag{30}$$

- Analogy: Chiral anomaly $\Longrightarrow$ we turn on background field for $U(1)$ and find that the partition function is not invariant under $U(1)_\chi$

"~~No~~ anomalies on the lattice"

- The lore "no anomalies on the lattice" is incomplete!
- Indeed there can be anomalies on the lattice
- Other examples of anomalies on the lattice: Kahler-Dirac fermions [Catterall, 2022], Ginsparg-Wilson realization of chiral fermions[6] [Lüscher, Neuberger, Kaplan, ...]

[6] for a modified chiral symmetry

Anomalies and Lattice Regularizations of θ theta vacua

Anomaly

Lattice

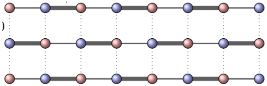
symmetric, local, same d

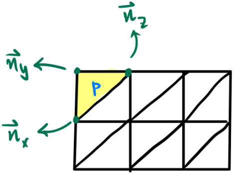
Offsite symmetry

- Qubit regularization
- Staggered couplings
- No sign problem!
- Natural for quantum computers

Exact anomaly

- Berg–Lüscher θ term
- Manifestly topological
- Sign problems
- Infinite-dimensional Hilbert space





Guidance from anomalies

- These arguments seem general. Do all models with mixed 't Hooft anomalies have such a dichotomy of lattice regularizations?
- We were able to generalize the O(3) constructions to a wider class of 2d asymptotically free theories, called the **Grassmannian nonlinear sigma models**.
- Here, instead of unit vectors on $\mathbb{R}^3$, the fields P live on

$$P_x \in \mathsf{Gr}_k(N) = \frac{U(N)}{U(N-k) \times U(k)} \tag{31}$$

with the action

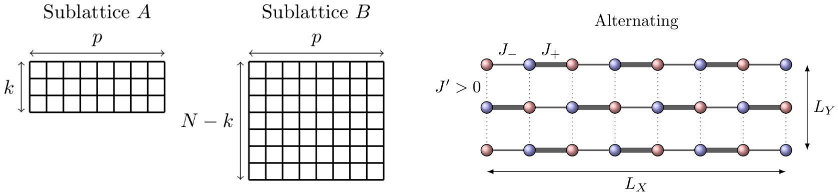
$$S = \frac{1}{g^2} \int d^2x \, \mathrm{Tr}(\partial_\mu P)^2 + \frac{\theta}{4\pi} \int d^2x \, \epsilon^{\mu\nu} \, \mathrm{Tr} \, P \, \partial_\mu P \, \partial_\nu P \tag{32}$$

- These $\mathsf{Gr}_k(N)$ models also have an anomaly at $\theta = \pi$ (N) between PSU(N) and C for (N, k)=(even, odd)[7].

[7] for other cases, we have a more subtle scenario called "global inconsistency"

Lattice regularization for Grassmannian models

- Qubit regularization
  - Now, we have $SU(N)$ spins at each site in certain conjugate representations[8]



  - Again, we can argue that a continuum limit at a fixed θ arises in the $L_y \to \infty$ limit if you keep γL_y fixed.
- Conventional regularization
  - The geometric Berg–Lüscher construction can also be generalized

[8] [Read, Sachdev, 1989]

Summary

- In the quest to find new regulators with unique advantages for quantum and classical simulation, anomalies can be a strong guide.
- The importance of anomalies been long appreciated for chiral fermions on the lattice.
- For the $O(3)$ model (and Grassmannian $\mathrm{Gr}_k(N)$ models), we saw a dichotomy of regularizations: qubit and conventional, which reflect how the $\mathrm{SO}(3) \times \mathrm{C}$ anomaly manifests.
- They have quite different advantages! Which one is useful depends on the hardware and the question.
- There are very suggestive parallels with 4d nonabelian gauge theories
  - Indeed, pure $SU(N)$ Yang-Mills has a very similar anomaly at $\theta = \pi$, between time reversal and $\mathbb{Z}_N$ center symmetry [9]
  - What does this say for lattice/qubit regularizations of QCD?

[9] [Gaiotto et al, 2017]

Conclusions

- "Qubit" regularization: continuum limit of a desired QFT with a finite-dim local Hilbert space.
- Such regularizations seem very natural for quantum computers, unlike traditional lattice regularizations
- Question: **Can the Standard Model be obtained in such a way?**
- We have demonstrated that a qubit regularization of the $O(3)$ NLSM with arbitrary θ can be constructed
  - solved a sign problem along the way
- Lattice regularizations where anomalies are manifested differently seem to have quite different properties. What does this imply for lattice QCD?
  - We found that anomalies can indeed be present on the lattice, invalidating an old lore in QFT. Implications?
- The space of such non-traditional formulations of lattice QFTs is quite rich and important for near-term quantum computers
- Developing new tools for simulations of Standard Model, occasionally finding new perspectives on old problems

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Thank you for listening!