Quantum simulation of asymptotically free theories and θ terms

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Nuclear and particle physics on a quantum computer: where do we stand now?
ECT* Trento

Towards quantum advantage for QCD

- We need a clear path towards quantum advantage for high-energy and nuclear physics

Long-term Goal: Quantum Simulation of Lattice QCD

- How can we make progress towards this path?

Short term Goal: Quantum Simulation of QCD-like theories in lower dimensions with a clear path towards QCD

- Two of the most important features of QCD are **asymptotic freedom** and a **topological θ term**
- I would like to discuss quantum simulation of a theory which exhibits both these features
  - This serves as a prototypical roadmap for quantum simulation of QCD.

Bottom line

Proposal:

- Design a spin/qubit model which exactly reproduces an asymptotically-free QFT in the continuum limit
- Perform quantum simulation of the spin system

A toy model of QCD

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

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

  with $\vec{n} \in \mathbb{R}^3$ and $|\vec{n}| = 1$.
- g is classically dimensionless coupling

- *for condensed-matter physicists*
  $\Longrightarrow$ natural in the study of antiferromagnets, topological phases, ...
- *for high-energy physicists*
  $\Longrightarrow$ toy model for QCD, asymptotic freedom, dynamical mass generation, dimensional transmutation, θ-vacua

(3+1)d SU(N) Yang-Mills vs. (1+1)d $O(3)$

$SU(N)$ 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:

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

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

$$S = -\frac{1}{g^2} \sum_{\langle xy \rangle} \vec{n}_x . \vec{n}_y \tag{3}$$

- 2d $O(3)$ NLSM is the continuum QFT which emerges in the $g \to 0$ limit of the lattice model
- Can also write a Kogut-Susskind Hamiltonian for this model
- *Completely analogous to QCD*

“Digitization” and “qubit regularization”

“Digitization” of QFTs for quantum computers

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

$$[\phi_x, \pi_y] = i\delta_{x,y} \tag{4}$$

- 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, ...]
    - Discrete subgroups for gauge theories [Lamm et al, ...]
    - D-theory, quantum-link models [Brower et al, 2004, ...]
    - (see Jesse’s talk as well for more!)
    - . . .

“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

$$\text{Digitized model} \xrightarrow{n\to\infty} \text{Traditional lattice model} \xrightarrow{a\to 0} \text{continuum QFT} \tag{5}$$

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

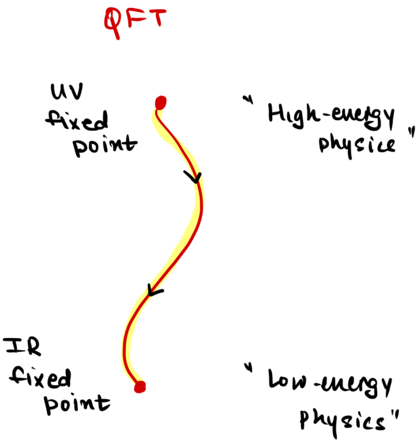
“Digitization”

- **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

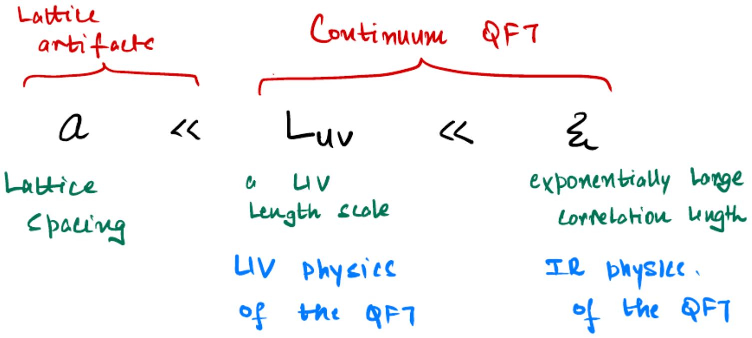
- Continuum limit: tune to a second-order critical point of a quantum lattice Hamiltonian
- This defines a procedure to obtain a continuum QFT
- **Qubit regularization:**
  a quantum lattice Hamiltonian acting on a finite-dimensional local Hilbert space (kept fixed) which reproduces a desired QFT in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

Asymptotic Freedom



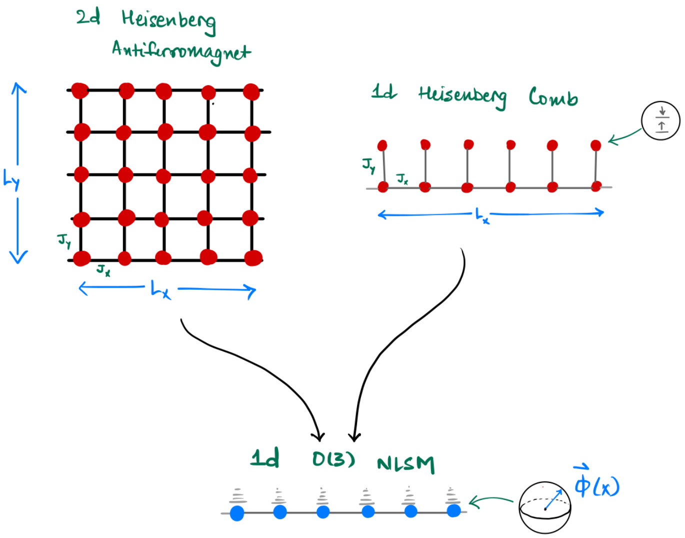
- A lattice regularization must reproduce the physics of all scales
- Otherwise, it is just a "low-energy EFT"

The challenge of asymptotic freedom

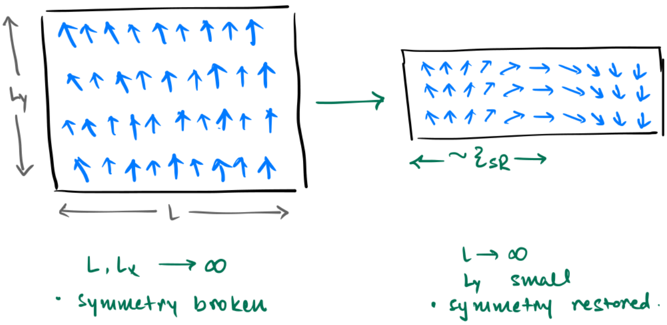


- To get the continuum limit, we need to recover both the IR physics and the UV physics
- I will show two methods to obtain the UV physics from qubit models

Two qubit models for asymptotic freedom

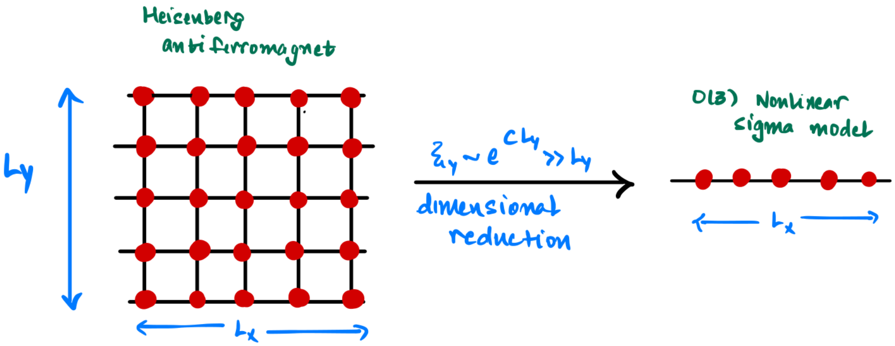


UV: asymptotic freedom from dimensional reduction



- Start with a 2+1d lattice. Make L, L_y large $\implies$ Symmetry breaking $SO(3) \to SO(2)$, massless goldstone modes
- What happens as make L_y small? $SO(3)$ symmetry cannot be broken. System orders at length scales ξ_{SR} (*symmetry restoration scale*). Goldstone modes pick up a mass $\sim \xi_{\text{SR}}^{-1}$
- Asymptotic freedom in 1+1d theory ensures that $\xi_{\text{SR}} \sim e^{\# L_y} \gg L_y$. Therefore, the system is effectively (1+1)d.

UV: asymptotic freedom from dimensional reduction



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

- The continuous fields $\vec{n}$ arise from collective Goldstone mode excitations of the spin-1/2 variables $\vec{S}_i$
- Dimensional reduction back to (1+1)-d theory! [Chandrasekharan, Wiese, 1997]
- Also has been generalized to QCD using quantum link models [Brower et al, 1999]

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

$$\frac{\xi(\beta, 2L)}{\xi(\beta, L)} \equiv F\left(\xi(\beta, L)/L\right) \tag{6}$$

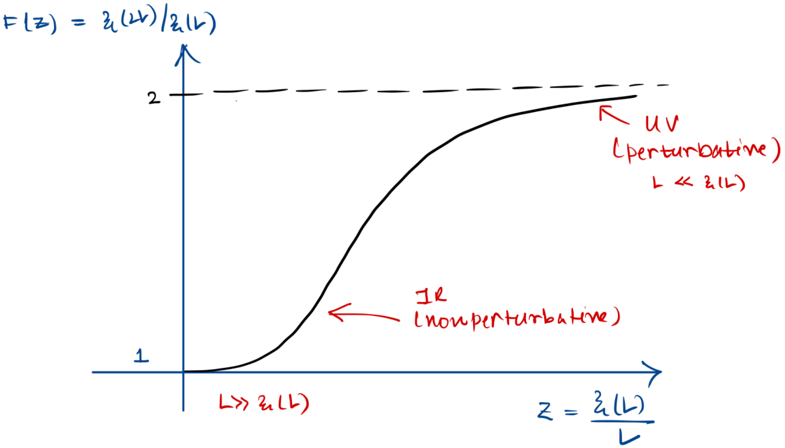
where β is a bare coupling and $z = \xi(\beta, L)/L$ is the renormalized coupling

- $\xi(\beta, L)$ is a definition of finite-volume correlation length: the “second-moment” correlation length

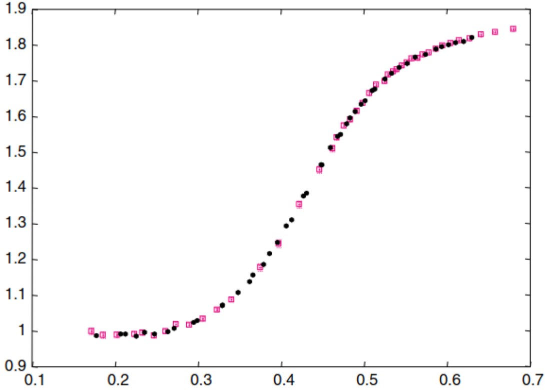
$$\xi(L) = \frac{\sqrt{\tilde{G}(0)/\tilde{G}(2\pi/L) - 1}}{2\sin(\pi/L)} \tag{7}$$

- Easy to measure

Step scaling function: qualitative behavior



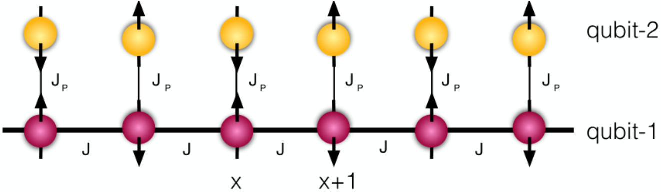
$$z = \xi(L)/L, \quad F(z) = \xi(2L)/\xi(L) \tag{8}$$



- Comparison between step-scaling curves of D-theory with the standard lattice action
- [Beard, Pepe, Riederer, U.-J. Wiese (PRL 94, 010603 (2005))]

A two-qubit regularization of asymptotic freedom

- In another work [1], we showed that a two-qubit regularization of asymptotic freedom can also be obtained
- “Heisenberg Comb”



- Hamiltonian

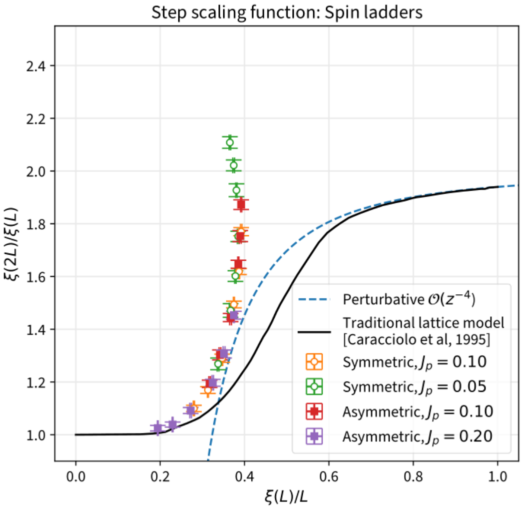
$$H = \sum_i \quad J_p\, H_{(i,1),(i,2)} + J\, H_{(i,1),(i+1,1)} \tag{9}$$

- Set $J_2 = 0,\ J_p = 1$. Continuum limit: $J \to \infty$.
- **Note that there is no extra dimension here!**

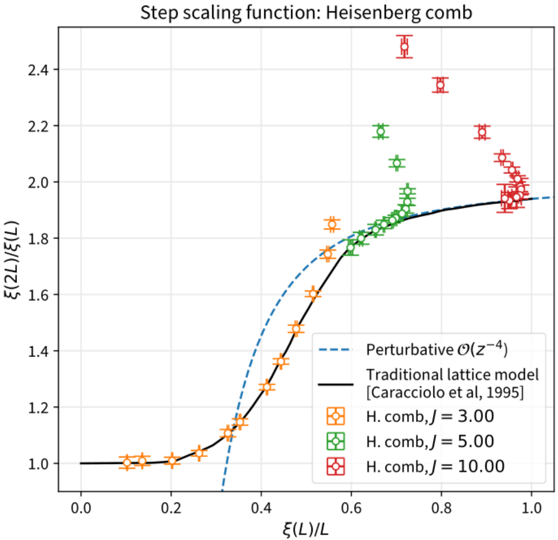
[1] PRL 126, 172001 (2021) [Bhattacharya, Buser, Chandrasekharan, Gupta, HS]

Results: Spin ladders

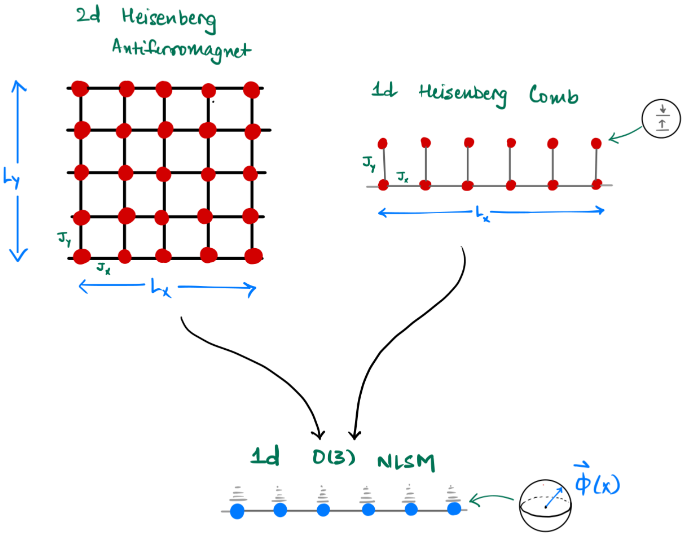
- Two weakly coupled chains
  - Symmetric ladder: $J_1 = J_2 \gg J_p$
  - Asymmetric ladder: $J_1 \gg J_2 \gg J_p$
- Again, the spin ladders describe the low-energy physics correctly [Shelton, Narseyan, Tsvelik, 1996]
- But not the UV physics



Results: Heisenberg comb



O(3) NLSM from qubits (*Codesign*)



O(3) NLSM from qubits (*Codesign*)

- **Universality** $\implies$ Different microscopic descriptions can give the same continuum QFT!
- The continuum QFT of the $O(3)$ NLSM can be obtained from a spin-1/2 system
  - Only $O(3)$-symmetric nearest-neighbor Heisenberg interactions needed
  - There are at least two known ways to regulate the $O(3)$ NLSM using spin-1/2 microscopic degrees of freedom
  - **Natural for Rydberg systems!**
- Similar ideas can be used to simulate other field theories

Topological θ terms with qubits

$O(3)$ NLSM at arbitrary θ

- Just like QCD, the $O(3)$ NLSM allows for a topological θ term

$$S_\theta[\vec{\phi}] = \frac{1}{g^2} \int d^2x (\partial_\mu \vec{\phi})^2 + i\theta Q[\vec{\phi}] \tag{10}$$

where

$$Q[\vec{\phi}] = \frac{1}{8\pi} \int d^2x \, \varepsilon_{\mu\nu} \, \vec{\phi} \cdot (\partial^\mu \vec{\phi}) \times (\partial^\nu \vec{\phi}) \tag{11}$$

is the *topological* theta term.

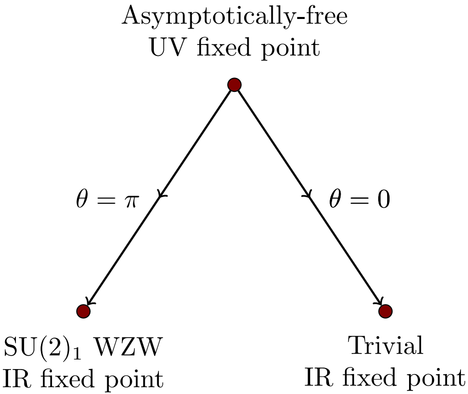
In nature, $\theta < 10^{-10} \implies$ **Strong CP problem**

Physics of θ

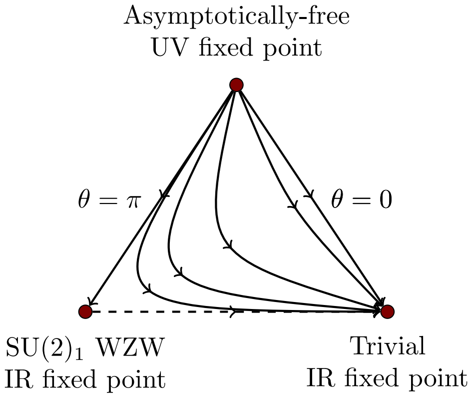
$$S_\theta[\vec{\phi}] = S_0 + i\theta Q[\vec{\phi}]$$

- 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 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
$\theta = \pi$
$\theta = 0$
$\mathrm{SU}(2)_1$ WZW
IR fixed point
Trivial
IR fixed point

Lattice formulation

- In the conventional approach, θ introduces a severe sign problem in the naive formulation (imaginary coefficient in Euclidean spacetime)

$$S_\theta[\vec{\phi}] = \frac{1}{g^2} \int d^2x (\partial_\mu \vec{\phi})^2 + i\theta Q[\vec{\phi}] \tag{12}$$

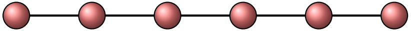
- Actually, the $\theta = \pi$ sign problem can in fact be solved using a meron cluster algorithm [Bietenholz, A. Pochinsky, U.-J. Wiese 1996]
- Bögli, Niedermayer, Pepe, Wiese (2011) studied the θ-vacua using non-standard ("topological") actions:
    - In their approach the sign problem is "mild" for 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.
- Qubits?

UV and IR

- We have a recipe to get the UV physics of asymptotically free theories from a qubit model
- But what about IR? Can we generate a θ term in the IR?

Haldane Conjecture

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



$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} \tag{13}$$

- Haldane Conjecture: at **low energies**

$$\text{Spin-}S \text{ chain} \leftrightarrow \text{O(3) sigma model at } \theta = 2\pi S \tag{14}$$

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

IR: θ term in spin chains

- $\theta \neq 0, \pi$ breaks charge conjugation symmetry $C : \vec{n} \to -\vec{n}$ since $C : i\theta Q \to -i\theta Q$.
- In terms of the spin variables, it can be shown using bosonization [Affleck, 1988]

$$a^{-1}\vec{S}_n = \vec{J}_L + \vec{J}_R + i(-1)^n c(\mathrm{Tr}\, g)\vec{\sigma}. \quad (15)$$

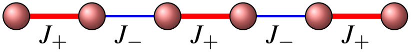
- Note that "charge conjugation" $g \mapsto -g$ maps to translation by one unit $S_n \mapsto S_{n+1}$.
- Manifestation of the antiferromagnetic nature of the spin chain

- Therefore, to generate a θ term in the spin system, we must break this translation-by-one symmetry.

IR: θ term in spin chains

- Therefore, to generate a θ term in the spin system, we must break this translation-by-one symmetry.
- For example, we can stagger the couplings on even and odd bonds

$$J_{\pm} = J(1 \pm \gamma). \tag{16}$$



- For this case, [Haldane, Affleck]

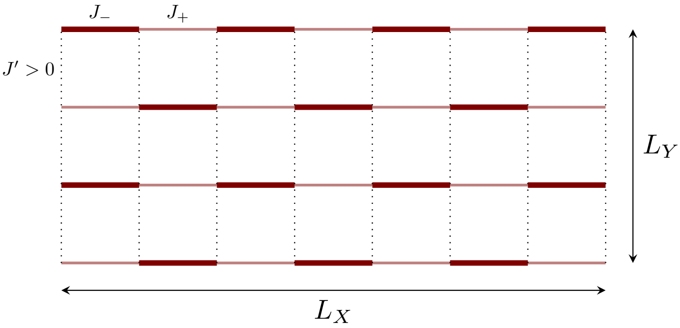
$$\theta = 2\pi S(1 + \gamma). \tag{17}$$

- 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! [Casper, HS (Phys.Rev.Lett. 129 (2022) 2, 022003)]

θ-term with D-theory



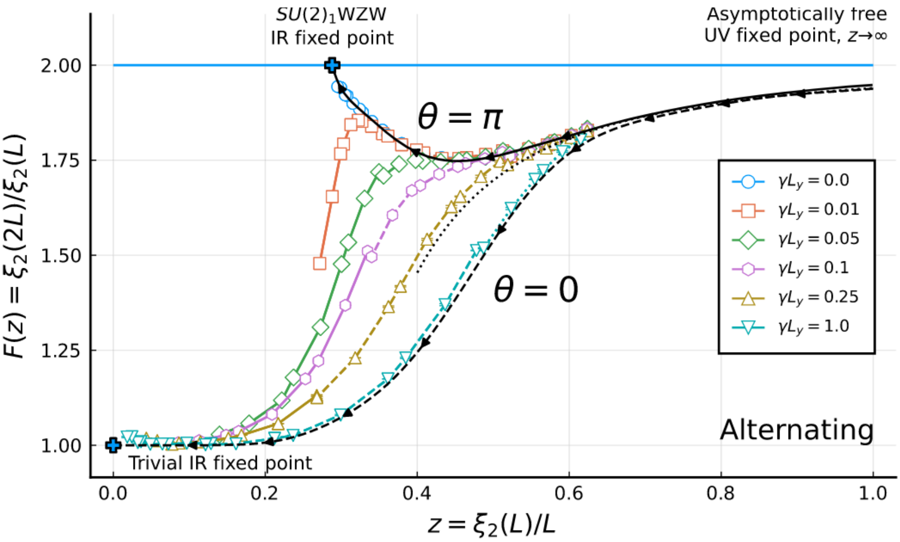
- *Proposal: Continuum limit of the $O(3)$ NLSM with θ term obtained in the $L_X \gg L_Y \gg 1$ limit*
- Analysis of spin ladders [2] suggests, for $J_\pm = J(1 \pm \gamma)$,

$$\theta \approx 2\pi S L_Y (1 + c\gamma) \implies |\theta - \pi| = c\pi\gamma L_Y \text{ (odd } L_y) \tag{18}$$

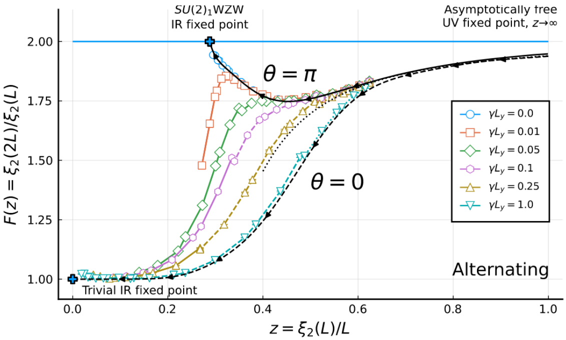
- **A gift:** *no sign problem!* So we can actually numerically check this.

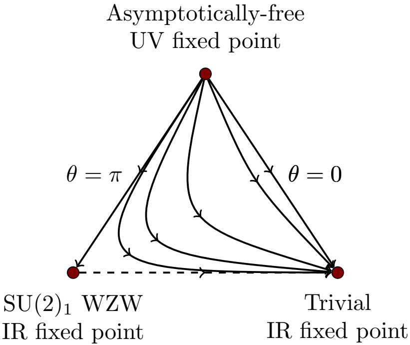
[2]Sierra 1995; Martin-Delgado, Shankar, Sierra 1996

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!

[Casper, HS (Phys.Rev.Lett. 129 (2022) 2, 022003)]

Summary (so far)

- 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 and on the lattice (sign problem)
- We constructed a lattice regularization using "qubits" for 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**

Anomalies and Qubit Models of Topological θ terms

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

$$\text{Staggering } \gamma \longleftrightarrow \theta \text{ term} \tag{19}$$

- 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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[Phys.Rev.D 107 (2023) 1, 014507]

Anomalies and Lattice Regularizations of θ theta vacua

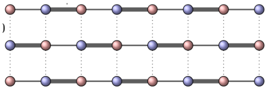
Anomaly

Lattice

symmetric, local, same d

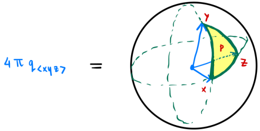
Offsite symmetry

- "qubit regularization"
- Staggered couplings
- No sign problem!
- Natural for quantum computers (finite-dimensional local Hilbert spaces)



Exact anomaly

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



Guidance from anomalies: CP(N-1) models and more

- These arguments seem general. Do all models with mixed ’t Hooft anomalies have such a dichotomy of lattice regularizations?
- Can generalize the O(3) constructions to a wider class of 2d asymptotically free theories, called the Grassmannian nonlinear sigma model.
- Here, instead of S^2, the fields P live on

$$P_x \in \mathsf{Gr}_k(N) = \frac{U(N)}{U(N-k) \times U(k)} \tag{20}$$

with the action

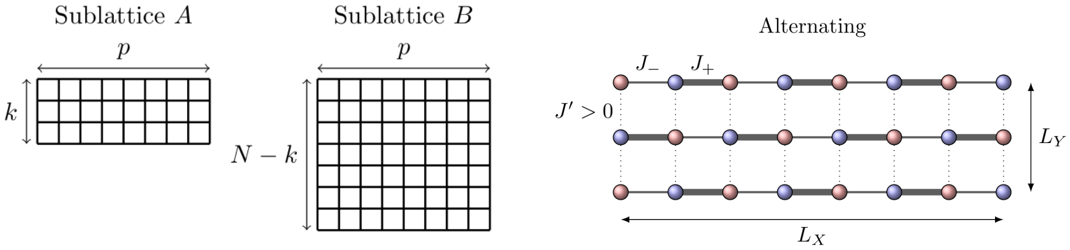
$$S = \frac{1}{g^2} \int d^2x \, \mathrm{Tr}(\partial_\mu P)^2 + \frac{\theta}{4\pi} \int d^2x \, \epsilon^{\mu\nu} \, \mathrm{Tr} \, P \, \partial_\mu P \, \partial_\nu P \tag{21}$$

- These $\mathsf{Gr}_k(N)$ models also have an anomaly at $\theta = \pi$ between PSU(N) and C for (N, k)=(even, odd)[3].

[3] 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[4]

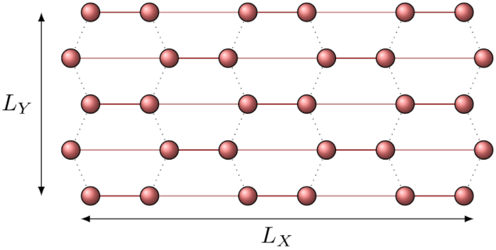


  - Again, we can argue that a continuum limit at a fixed θ arises in the $L_y \to \infty$ limit if you keep γL_y fixed.

[4] [Read, Sachdev, 1989]

Analog Quantum Simulation on Rydberg Systems

On quantum simulators



PHYSICAL REVIEW A **107**, 042404 (2023)

Preparation for quantum simulation of the (1 + 1)-dimensional O(3) nonlinear σ model using cold atoms

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- On Rydberg systems with native Ising-type interactions, we can use Floquet engineering techniques to implement Heisenberg interactions
- Based on recent works with Anthony Ciavarella, Stephan Caspar, Martin Savage, Pavel Lougovski [2207.09438] [Phys.Rev.A 107 (2023) 4, 042404] [Quantum 7 (2023) 970]

On Rydberg Atoms

- We have a 2d array of atoms with native Ising-like interactions
- We need Heisenberg $\vec{S} \cdot \vec{S}$ interactions

$$H = \sum_i \frac{1}{2}\Omega(t)\hat{X}_i + \sum_i \Delta_i(t)\hat{n}_i + \sum_{i<j} C_6 \frac{\hat{n}_i\hat{n}_j}{r_{ij}^2} \tag{22}$$

$$\downarrow$$

$$H = \sum \frac{(-1)^{x_1+y_1+x_2+y_2}}{a_x^2(x_1 - x_2)^2 + a_y^2(y_1 - y_2^2)} \vec{S}_{x_1,y_1} \cdot \vec{S}_{x_2,y_2} \tag{23}$$

- This can be done via “Floquet engeering” with *constant* drive fields! [“Floquet Engineering Heisenberg from Ising Using Constant Drive Fields for Quantum Simulation” Ciavarella, Caspar, HS, Savage, Lougovski, arXiv:2207.09438]

Heisenberg from Ising

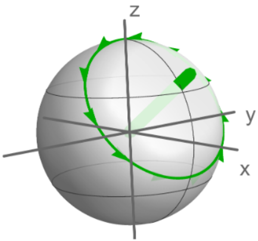
- Starting with an Ising-like interaction, fix $\vec{\Omega} = \Omega(\cos\theta, 0, \sin\theta)$ and take $\Omega/J \gg 1$

$$H^{\text{Ising}} = \sum_{ij} J_{ij} Z_i Z_j + \frac{1}{2} \sum_i \vec{\Omega} \cdot \vec{\sigma}_i \tag{24}$$

$\downarrow$ Average over time period $\tau = 2\pi/\Omega$

$$U_F = T \exp\left\{ -i \int_0^{2\pi/\Omega} dt' \, H_I^{\text{Ising}}(t') \right\} \tag{25}$$

$$= U_B^\dagger \exp\left\{ -i \frac{2\pi}{\Omega} \left(H_1 + O(\Omega^{-1}) \right) \right\} U_B \tag{26}$$

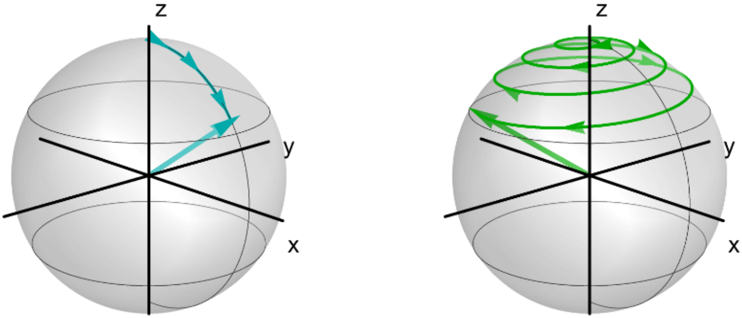


with

$$H_1 = \sum_{ij} J_{ij} \left[\cos(\theta)^2 Z_i Z_j + \frac{1}{2} \sin^2(\theta) \left(X_i X_j + Y_i Y_j \right) \right] \tag{27}$$

- Set $\tan\theta = \sqrt{2}$ to get the XXX Heisenberg model

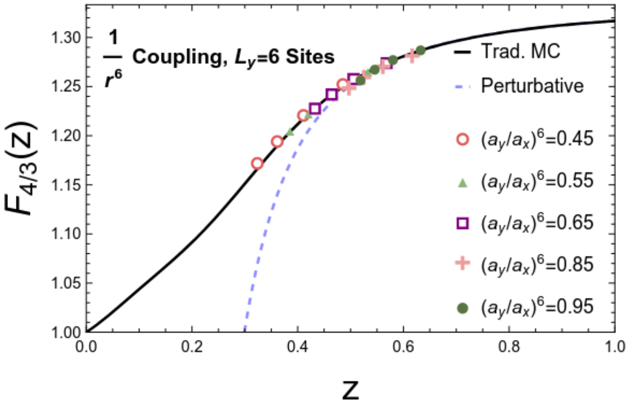
Preparing ground states with "adiabatic spiral"



(a) Laboratory　　(b) Interaction Picture

["State Preparation in the Heisenberg Model through Adiabatic Spiraling" Quantum 7, 970]

Simulations



- SSF in the UV reproduced on simulations for $L_x = 6, 12, 18, 24$ and $L_y = 6$!
- [“Preparation for quantum simulation of the (1+1)-dimensional O(3) nonlinear σ model using cold atoms” Ciavarella, Caspar, HS, Savage | Phys.Rev.A 107 (2023) 4, 042404]

Simulations

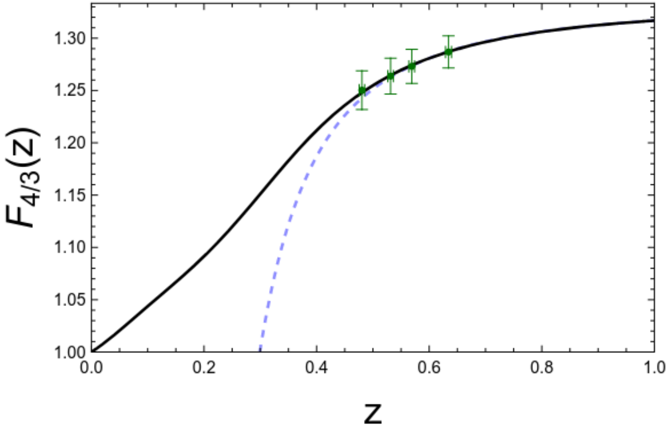


FIG. 5. Results for $F_{4/3}(z)$ computed in a TDVP simulation of a rectangular array of ^{87}Rb atoms assuming 5000 shots are used.

Outlook

- Simple qubit models of the $O(3)$ NLSM with arbitrary θ can be constructed
  - solved a sign problem along the way!
- *Codesign question:* Universality allows for many microscopic descriptions. Hardware decides the best one.
  - Some guidance can come from anomalies
- On cold-atom simulators, such a model is very natural.
  - Heisenberg interactions can be Floquet engineered with constant drive fields!
  - Strong evidence that we can observe asymptotic freedom on near-term cold-atom devices
- Roadmap for quantum simulation of QCD-like theories
  - Goal 1: Match UV physics (step-scaling function). Demonstrate Asymptotic Freedom.
  - Goal 2: Realtime dynamics $\Longleftarrow$ towards quantum advantage!
- The space of such non-traditional formulations of lattice QFTs is quite rich and important for near-term quantum computers!

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