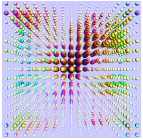
Numerical methods in lattice field theory beyond the standard model

David Schaich (University of Liverpool)

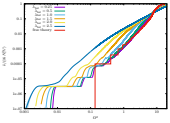
Numerical Methods in Theoretical Physics

Asia Pacific Center for Theoretical Physics, Pohang, 13 July 2023

Overview and plan

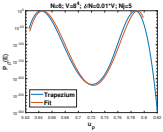


Broader applications of lattice field theory
motivate novel numerical methods

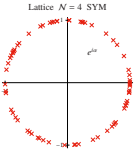


Lattice motivation and foundations

Near-conformal composite Higgs
[arXiv:2007.01810, arXiv:2102.06775, arXiv:2305.03665]



Composite dark matter and gravitational waves
[arXiv:2112.11868, arXiv:2212.09199, arXiv:2303.01149]



Lattice supersymmetry and spontaneous susy breaking
[arXiv:2112.07651, arXiv:2208.03580, arXiv:2301.02230]

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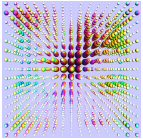

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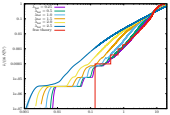

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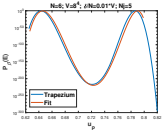

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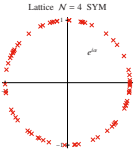
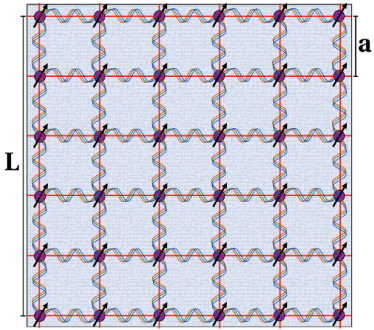


Interaction encouraged — complete coverage unnecessary

Lattice regularization of quantum field theories

Formally $\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\Phi \;\; \mathcal{O}(\Phi) \;\; e^{-S[\Phi]}$

Regularize by formulating theory in finite, discrete, euclidean space-time
↖ Gauge invariant, non-perturbative, d-dimensional



P. Vranas LLNL

Spacing between lattice sites ("a")
$\longrightarrow$ UV cutoff scale $1/a$

Remove cutoff: $a \to 0 \quad (L/a \to \infty)$

Discrete $\longrightarrow$ continuous symmetries ✓

Numerical lattice field theory calculations

High-performance computing $\longrightarrow$ evaluate up to $\sim$billion-dimensional integrals
(Dirac operator as $\sim 10^9 \times 10^9$ matrix)

Results to be shown, and work in progress, require state-of-the-art resources

Many thanks to USQCD–DOE, DiRAC–STFC–UKRI, and computing centres!

Lassen @Livermore

USQCD @Fermilab

DiRAC @Cambridge

Barkla @UoL

Numerical lattice field theory calculations




Importance sampling Monte Carlo

Standard algorithms sample field configurations with probability $\frac{1}{\mathcal{Z}} e^{-S[\Phi]}$

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\Phi \;\; \mathcal{O}(\Phi) \;\; e^{-S[\Phi]} \longrightarrow \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}(\Phi_i) \;\; \text{with stat. uncertainty} \propto \frac{1}{\sqrt{N}}$$

Novel methods being developed and explored

Application: Composite Higgs sectors

Large Hadron Collider priority

Study fundamental nature of Higgs boson

Composite Higgs sector
can stabilize electroweak scale

New strong dynamics must differ from QCD

—Flavour-changing neutral currents
—Electroweak precision observables
—SM-like Higgs boson with $M \approx 0.5 v_{\mathrm{EW}}$

Challenge: Near-conformal dynamics for composite Higgs

New strong dynamics must differ from QCD

—Flavour-changing neutral currents
—Electroweak precision observables
—SM-like Higgs boson with $M \approx 0.5 v_{\mathrm{EW}}$

Near-conformal dynamics
can help with all three issues

Near-conformality $\longrightarrow$ natural scale separation, novel IR dynamics

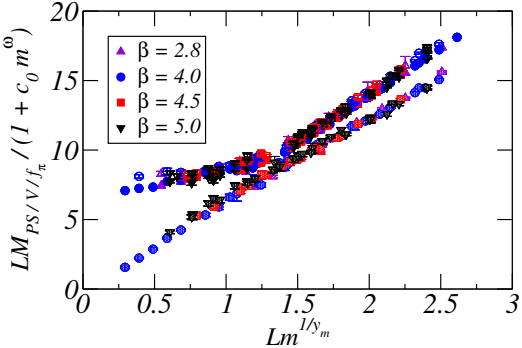
Conformality broken by finite volume and non-zero lattice spacing

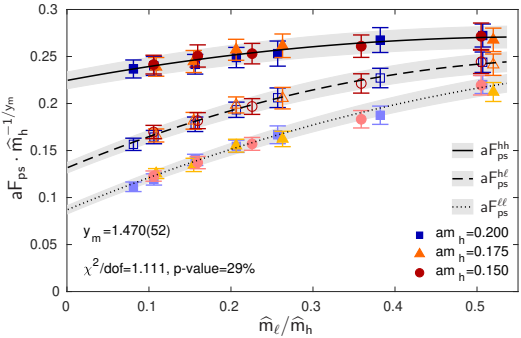
Anomalous dimensions

Pheno prefers large anomalous dimensions $\gamma_{\mathcal{O}} = -\frac{\mathrm{d}\log Z_{\mathcal{O}}(\mu)}{\mathrm{d}\log\mu}$

Scaling of traditional composite spectrum $\longrightarrow$ γ_m

but corrections to scaling hard to control

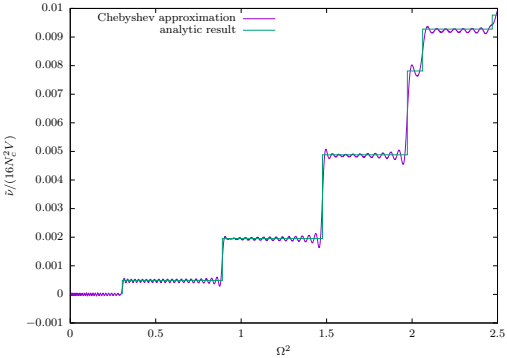




Novel method: Fermion operator eigenspectrum

Newer approach extracts γ_m from eigenvalue mode number of $D^\dagger D$

$$\nu(\Omega^2) = \int_0^{\Omega^2} \rho(\omega^2)\, d\omega^2 \propto \left(\Omega^2\right)^{2/(1+\gamma_m)} \qquad \rho(\omega^2) = \frac{1}{V}\sum_k \left\langle \delta(\omega^2 - \lambda_k^2)\right\rangle$$



Stochastic Chebyshev expansion covers full spectral range

[Fodor et al., arXiv:1605.08091]

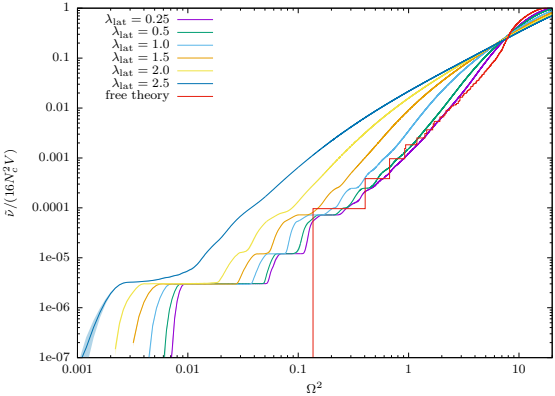
$$\rho_r(x) \approx \sum_{n=0}^{P} \frac{2-\delta_{n0}}{\pi\sqrt{1-x^2}} c_n T_n(x)$$

Testing with lattice $\mathcal{N} = 4$ SYM

arXiv:2102.06775

Continuum $\mathcal{N} = 4$ SYM known conformal theory with $\gamma_m = 0$

$\longrightarrow$ test finite-volume and discretization artifacts



Even free theory shows lattice effects

Power law varies with scale Ω^2

$\longrightarrow$ scale-dependent effective $\gamma_{\rm eff}(\Omega^2)$

Extract by fitting in windows $[\Omega^2, \Omega^2 + \ell]$

with fixed $\ell \in [0.03, 1]$

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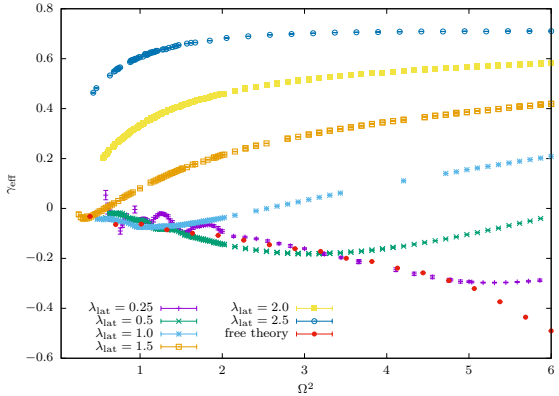


Even free theory shows lattice effects

Scale-dependent effective $\gamma_{\rm eff}(\Omega^2)$ converges to true $\gamma_m = 0$ in IR, $\Omega^2 \ll 1$

Stronger couplings $\longrightarrow$ larger artifacts

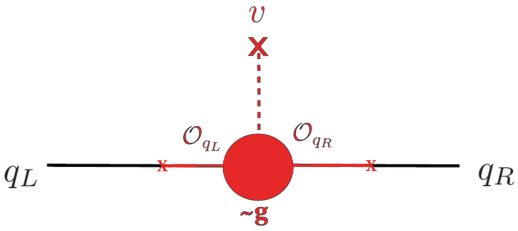
Aside: Anomalous dimensions for partial compositeness

Fermion masses set by anom. dim.
of composite partner operators

$$\mathcal{L} \supset \lambda \overline{q} \mathcal{O}_q + \text{h.c.}$$

$$\longrightarrow m_q \sim v_{\text{EW}} \left(\frac{\text{TeV}}{\Lambda_{UV}} \right)^{4-2\gamma_q}$$

SU(3) gauge theories
$\mathcal{O}_q \sim \psi\psi\psi \sim$ baryons with $[\mathcal{O}_q] = \frac{9}{2} - \gamma_q$



Large mass hierarchy $\longleftrightarrow$ $\mathcal{O}(1)$ anomalous dimensions

$\Lambda_{UV} = 10^{10}$ TeV $\longrightarrow$ $m_q \sim \mathcal{O}(\text{MeV})$ from $\gamma_q \approx 1.75$; $\mathcal{O}(\text{GeV})$ from $\gamma_q \approx 1.9$

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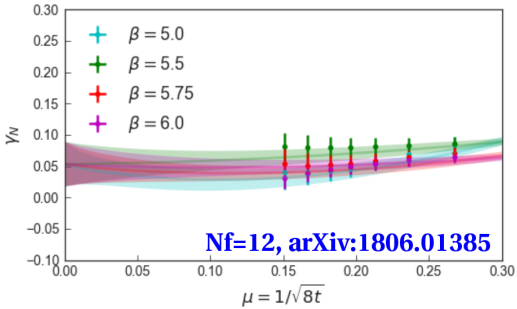


New method extracts anomalous dimensions from gradient flow

$\longrightarrow$ ratios of flowed operators $\propto t^{\gamma_{\mathcal{O}}/2}$

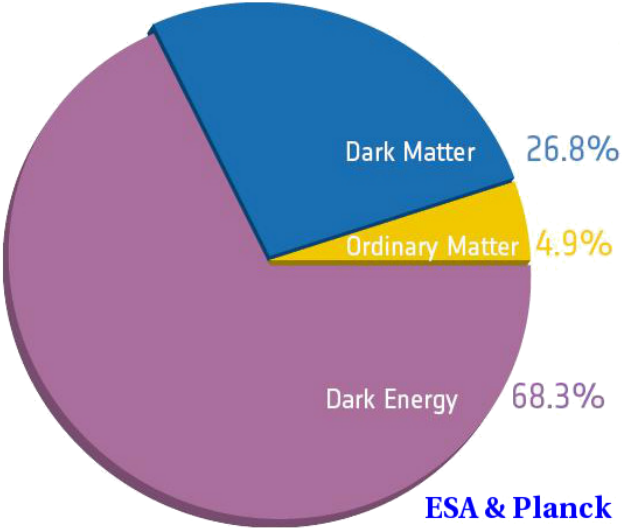
[Carosso–Hasenfratz–Neil, arXiv:1806.01385]

Application: Composite dark matter

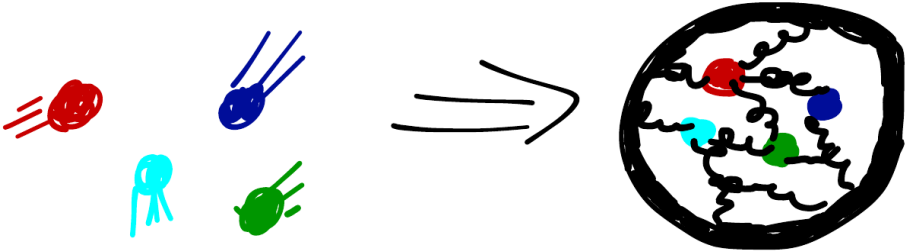
Abundant gravitational evidence for dark matter (details unknown)

$$\frac{\Omega_{\text{dark}}}{\Omega_{\text{ordinary}}} \approx 5 \quad \ldots \text{not } 10^5 \text{ or } 10^{-5}$$

Explained by non-gravitational interactions in the early universe



Composite dark-sector phase transition



Early universe

Deconfined charged fermions $\longrightarrow$ explain relic density

Present day

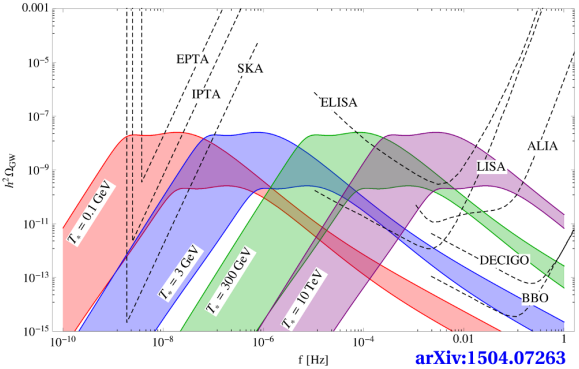
Confined neutral ‘dark baryons’ $\longrightarrow$ no experimental detections

Challenge: Gravitational waves from early-universe transition

First-order transition $\longrightarrow$ stochastic background of gravitational waves

Lattice analyses of transition
predict features of spectrum

Initial targets:
- Latent heat
- Surface tension



arXiv:1504.07263

Challenge: Super-critical slowing down at first-order transition;
difficult to tunnel between coexisting phases

Novel method: Density of states

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\Phi \;\; \mathcal{O}(\Phi) \;\; e^{-S[\Phi]} \longrightarrow \frac{1}{\mathcal{Z}} \int \mathrm{d}E \;\; \mathcal{O}(E) \;\; \rho(E) \;\; e^{-\beta E}$$

'LLR' adaptation of Landau–Wang algorithm [Langfeld et al., arXiv:1509.08391]

$\longrightarrow$ continuous density of states $\rho(E)$ with exponential error suppression

1) Divide E into many small intervals $[E_i - \delta/2,\; E_i + \delta/2]$

2) Find $a(E_i)$ for which $\displaystyle \frac{1}{\mathcal{N}_i} \int_{E_i-\delta/2}^{E_i+\delta/2} \mathrm{d}E \;\; (E - E_i) \;\; \rho(E) \;\; e^{-aE} = 0$

using iterative Robbins–Monro algorithm with importance sampling for each a_n

3) $\rho(E)\; e^{-aE} \sim$ const. in interval $\longrightarrow$ reconstruct $\rho(E)$ from $a(E_i) = \left.\dfrac{\mathrm{d}\log\rho}{\mathrm{d}E}\right|_{E=E_i}$

Testing with large-N bulk transition

arXiv:2303.01149

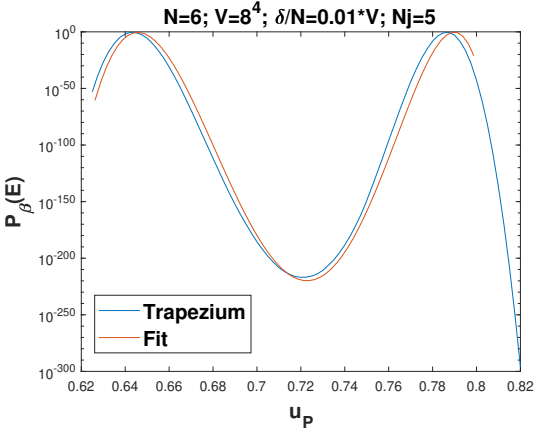
Lattice SU(N) Yang–Mills has strong first-order 'bulk' transition for $N \geq 5$
(not feature of continuum theory)

Ongoing work by Felix Springer

$N = 4, 5, 6, 8;$ $\quad P_\beta = \rho(E) \;\; e^{-\beta E}$

Distance between peaks
$\longrightarrow$ latent heat

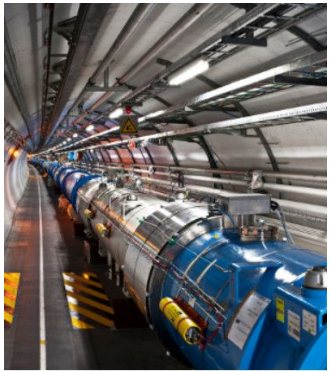
Volume dependence of valley
$\longrightarrow$ surface tension



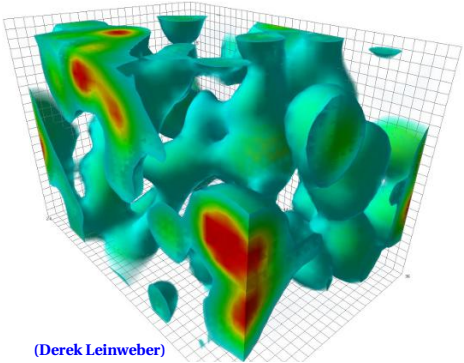
Application: Lattice supersymmetry

Lattice field theory promises first-principles predictions
for strongly coupled supersymmetric QFTs

BSM

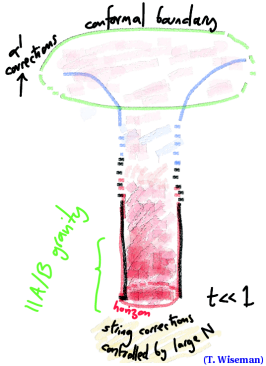


QFT



(Derek Leinweber)

Holography



(T. Wiseman)

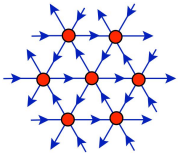
Challenge 1: Explicit supersymmetry breaking

Supersymmetry is a space-time symmetry, $(\mathrm{I} = 1, \cdots, \mathcal{N})$

adding spinor generators Q^{I}_{α} and $\overline{Q}^{\mathrm{I}}_{\dot{\alpha}}$ to translations, rotations, boosts

$\left\{ Q^{\mathrm{I}}_{\alpha}, \overline{Q}^{\mathrm{J}}_{\dot{\alpha}} \right\} = 2\delta^{\mathrm{IJ}} \sigma^{\mu}_{\alpha\dot{\alpha}} P_{\mu}$ broken in discrete lattice space-time

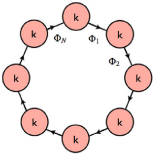
$\longrightarrow$ relevant susy-violating operators



Last year:

Preserve susy sub-algebra in discrete space-time

$\Longrightarrow$ correct continuum limit with little or no fine tuning



Challenge 2: Sign problems

Importance sampling becomes more complicated when action S complex
or we consider real-time dynamics

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\Phi \;\; \mathcal{O}(\Phi) \;\; e^{-S[\Phi]} \longrightarrow \frac{1}{\mathcal{Z}} \int \mathcal{D}\Phi \;\; \mathcal{O}(\Phi) \;\; e^{iS[\Phi]}$$

Arranging $\frac{1}{\mathcal{Z}} \int \mathcal{D}\Phi \;\; \mathcal{O} \;\; e^{iS} = \frac{\int \mathcal{D}\Phi \;\; \mathcal{O} \; \frac{e^{iS}}{e^{-|S|}} \;\; e^{-|S|}}{\int \mathcal{D}\Phi \; \frac{e^{iS}}{e^{-|S|}} \;\; e^{-|S|}} = \frac{\left\langle \mathcal{O} \; \frac{e^{iS}}{e^{-|S|}} \right\rangle_{||}}{\left\langle \frac{e^{iS}}{e^{-|S|}} \right\rangle_{||}}$

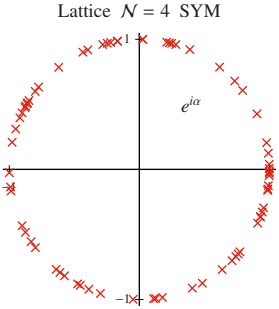
Sign problem: $\langle \mathrm{sign} \rangle_{||} = \left\langle \frac{e^{iS}}{e^{-|S|}} \right\rangle_{||} \to 0$ exponentially quickly

Sign problem examples

$$\frac{e^{-S}}{e^{-|S|}} \text{ is pure phase}$$

for lattice $\mathcal{N} = 4$ supersymmetric Yang–Mills

Averages to zero when using periodic BCs



Spontaneous supersymmetry breaking

Requires vanishing **Witten index**

$$\mathcal{W} = \mathrm{Tr}\left[(-1)^F e^{-iHt}\right] = \mathrm{Tr}_B\left[e^{-iHt}\right] - \mathrm{Tr}_F\left[e^{-iHt}\right] \propto \langle \mathrm{sign} \rangle_{||}$$

$\langle \mathrm{sign} \rangle_{||} = 0 \longrightarrow$ maximally bad sign problem

Novel method: Quantum computing

In principle evade exponential classical computing costs

Change perspective

Path integral $\longrightarrow$ continuous-time hamiltonian H on spatial lattice

Generic targets:

Find ground state $|\Omega\rangle \longrightarrow$ test spontaneous symmetry breaking

Real-time evolution $|\Psi(t)\rangle = e^{-iHt}\,|\Psi(0)\rangle \sim \left(\exp\left[-iH\delta_T\right]\right)^{N_T} |\Psi(0)\rangle$

(1+1)-dimensional Wess–Zumino model

arXiv:2301.02230

Supersymmetric $H \longleftrightarrow$ matched boson / fermion d.o.f. at each lattice site:

$$H = \sum_n \left[\frac{p_n^2}{2} + \frac{1}{2}\left(\frac{\phi_{n+1} - \phi_{n-1}}{2}\right)^2 + \frac{1}{2}[W(\phi_n)]^2 + W(\phi_n)\frac{\phi_{n+1} - \phi_{n-1}}{2} \right.$$
$$\left. + (-1)^n W'(\phi_n)\left(\chi_n^\dagger \chi_n - \frac{1}{2}\right) + \frac{1}{2}\left(\chi_n^\dagger \chi_{n+1} + \chi_{n+1}^\dagger \chi_n\right)\right]$$

Prepotential $W(\phi)$ ensures supersymmetric interactions

$W \propto \phi \longrightarrow$ free theory $\longrightarrow$ expect supersymmetric $|\Omega\rangle$

$W \propto \phi^2 \longrightarrow$ expect dynamical supersymmetry breaking

Wess–Zumino set up for quantum computing

Lattice $\longrightarrow$ finite number of d.o.f.

Need to map bosons and fermions to finite number of qubits

Fermions — Jordan–Wigner transformation $\longrightarrow$ one qubit per site

Bosons — retain lowest $\Lambda = 2^B$ harmonic oscillator modes

binary encoding $\longrightarrow$ B qubits per site

Different treatment breaks supersymmetry, recovered as $\Lambda \to \infty$

Ongoing work by Chris Culver focuses on exploratory development & testing

$\longrightarrow$ Qiskit simulator for rapid turnaround

[github.com/chrisculver/WessZumino]

Variational quantum eigensolver (VQE)

'Hybrid' quantum–classical algorithm

Quantum circuit implements wave-function ansatz $|\Psi(\theta_i)\rangle$ with tunable params

Loss function measurements $\longrightarrow$ classical optimizer adjusts θ_i

$\nwarrow$ shallow circuit $\longrightarrow$ less sensitive to noise / errors

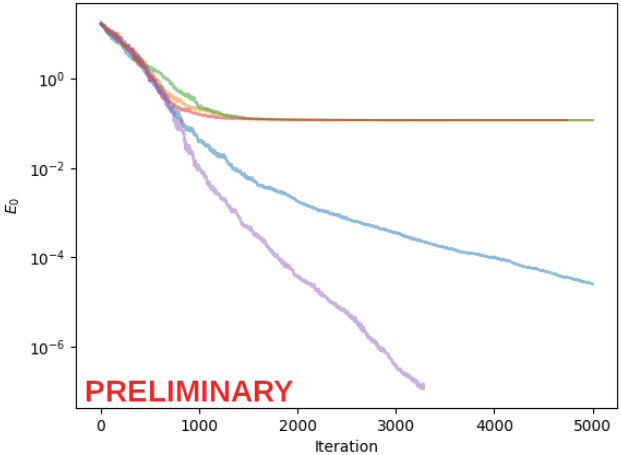
Energy as loss function $\longrightarrow$ approximate ground state

Apply to Wess–Zumino model

Spontaneous supersymmetry breaking $\longleftrightarrow$ non-zero ground-state energy

Wess–Zumino VQE

$W = \phi$ with $\Lambda = 16$ and 2 lattice sites



Even free theory
doesn't always converge

For interacting cases,
easier to converge to non-zero E
harder to decide whether $E \to 0$

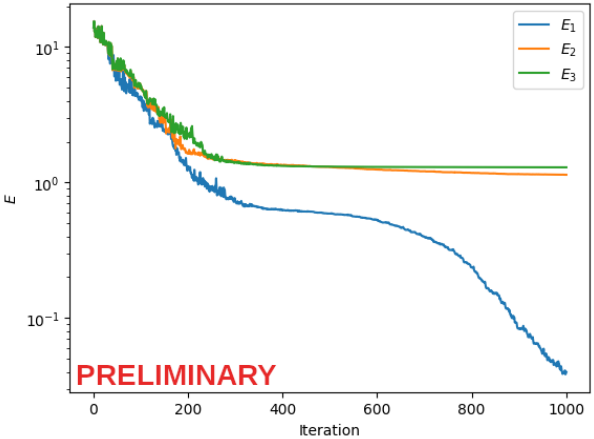
Variational quantum deflation (VQD)

Supersymmetry
$\longrightarrow$ all nonzero-energy states paired

Idea: Find three smallest energies, check pairing

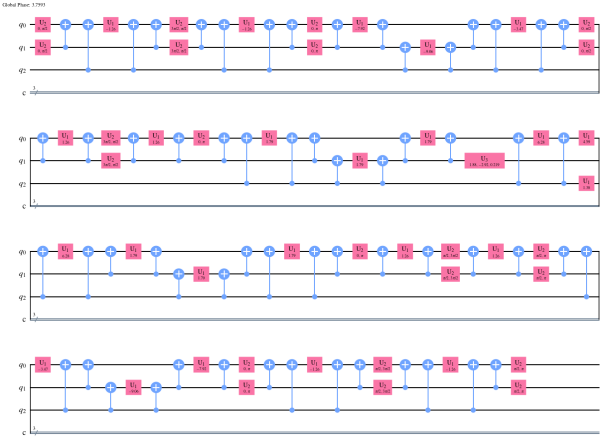
Use VQD algorithm
[Higgott–Wang–Brierley, arXiv:1805.08138]

$W = \phi$ with $\Lambda = 16$ and 2 lattice sites



Real-time evolution

For now, need far too many gates for reasonable $\Lambda \gtrsim \mathcal{O}(10)$



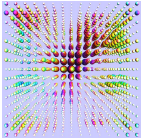
Here $\Lambda = 4$ on single site

$\longrightarrow$ supersymmetric quantum mech.

[arXiv:2112.07651]

Smarter Trotterization & transpilation should help

Recap: An exciting time for lattice BSM numerical methods



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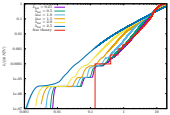
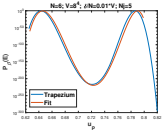
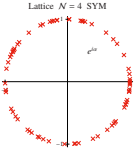


Eigenspectrum and gradient flow methods
$\longrightarrow$ anomalous dimensions for near-conformal composite Higgs



Density of states methods avoid super-critical slowing down
at first-order transitions producing gravitational waves



Quantum computing can avoid sign problems
to explore spontaneous supersymmetry breaking

Thanks for your attention! Any further questions?

Collaborators on highlighted work

Georg Bergner, Chris Culver, Angel Sherletov, Felix Springer

Lattice Strong Dynamics Collaboration (esp. James Ingoldby, Oliver Witzel)

Funding and computing resources

UK Research and Innovation

LIVERPOOL THEORETICAL PHYSICS

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

USQCD

Backup: Lattice Strong Dynamics Collaboration

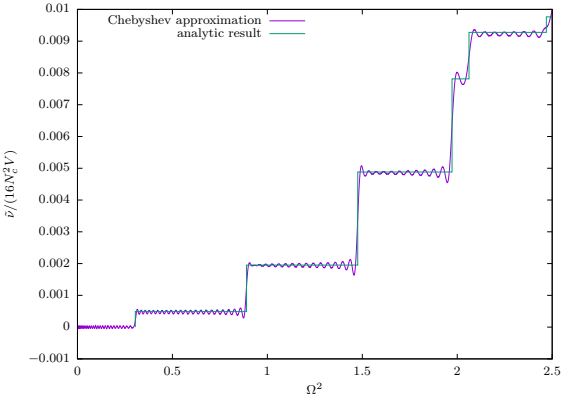
Argonne	Xiao-Yong Jin, James Osborn
Bern	Andy Gasbarro
Boston	Venkitesh Ayyar, Rich Brower, Evan Owen, Claudio Rebbi
Colorado	Anna Hasenfratz, Ethan Neil, Curtis Peterson
UC Davis	Joseph Kiskis
Fermilab	George Fleming
Livermore	Pavlos Vranas
Liverpool	Chris Culver, DS, Felix Springer
Nvidia	Evan Weinberg
Oregon	Graham Kribs
Quantinuum	Enrico Rinaldi
Siegen	Oliver Witzel
Trieste	James Ingoldby
Yale	Thomas Appelquist, Kimmy Cushman

Exploring the range of possible phenomena in strongly coupled field theories

Backup: Chebyshev expansion for mode number

Stochastically estimate Chebyshev expansion $\rho_r(x) \approx \sum_{n=0}^{P} \frac{2-\delta_{n0}}{\pi\sqrt{1-x^2}} c_n T_n(x)$

[Fodor et al., arXiv:1605.08091]



⟵ Example $\mathcal{N}=4$ SYM mode number for U(2) 8^4 free theory, $P=1000$

$5000 \leq P \leq 10000$ for U(2), U(3), U(4) volumes up to 16^4

Checked vs. direct eigensolver and stochastic projection

Backup: Options for fermion mass generation

"Extended technicolor"

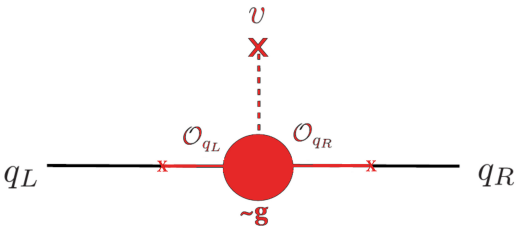
$$\frac{\bar{q}q\bar{\psi}\psi}{\Lambda_{UV}^2} \longrightarrow m_q \sim v_{\rm EW}\left(\frac{\rm TeV}{\Lambda_{UV}}\right)^{2-\gamma_m} \qquad \text{vs.} \qquad \text{flavour-changing NCs} \sim \frac{\bar{q}q\bar{q}q}{\Lambda_{UV}^2}$$

Partial compositeness

Linear mixing with composite partners

$$\mathcal{L} \supset \lambda \bar{q}\mathcal{O}_q + \text{h.c.}$$

$$\longrightarrow m_q \sim v_{\rm EW}\left(\frac{\rm TeV}{\Lambda_{UV}}\right)^{4-2\gamma_q}$$



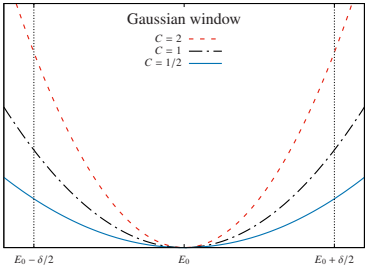
$\Lambda_{UV} = 10^{10}$ TeV $\longrightarrow$ $m_q \sim \mathcal{O}(\text{MeV})$ from $\gamma_q \approx 1.75$; $\mathcal{O}(\text{GeV})$ from $\gamma_q \approx 1.9$

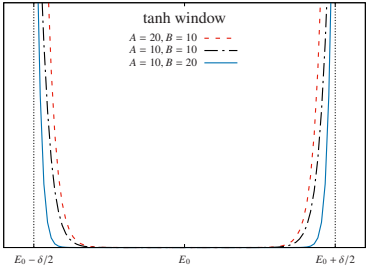
Backup: Importance sampling for density of states

Robbins–Monro algorithm: $$a_{n+1} = a_n + \frac{\langle\langle E - E_i \rangle\rangle_n}{\sigma^2(n+1)}$$

Restricted expect. value: $$\langle\langle E - E_i \rangle\rangle_n = \frac{1}{\mathcal{N}_{i;n}} \int \mathcal{D}\Phi \;\; (E - E_i) \;\; \Theta(E_i, \delta) \;\; e^{-a_n S}$$

Restriction can be hard cut-off (for OR/heatbath) or diff'able potential (for HMC)





Backup: Breakdown of Leibniz rule on the lattice

$\left\{Q_\alpha, \overline{Q}_{\dot\alpha}\right\} = 2\sigma^\mu_{\alpha\dot\alpha} P_\mu = 2i\sigma^\mu_{\alpha\dot\alpha}\partial_\mu$ is problematic

$\Longrightarrow$ try finite difference $\partial\phi(x) \longrightarrow \Delta\phi(x) = \frac{1}{a}\left[\phi(x+a) - \phi(x)\right]$

Crucial difference between ∂ and Δ

$$\Delta\left[\phi\eta\right] = a^{-1}\left[\phi(x+a)\eta(x+a) - \phi(x)\eta(x)\right]$$
$$= \left[\Delta\phi\right]\eta + \phi\Delta\eta + a\left[\Delta\phi\right]\Delta\eta$$

Full supersymmetry requires Leibniz rule $\partial\left[\phi\eta\right] = \left[\partial\phi\right]\eta + \phi\partial\eta$

only recoverd in $a \to 0$ continuum limit for any local finite difference

Backup: Breakdown of Leibniz rule on the lattice

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only recoverd in $a \to 0$ continuum limit for any local finite difference

Supersymmetry vs. locality 'no-go' theorems

by Kato–Sakamoto–So [arXiv:0803.3121] and Bergner [arXiv:0909.4791]

Complicated constructions to balance locality vs. supersymmetry

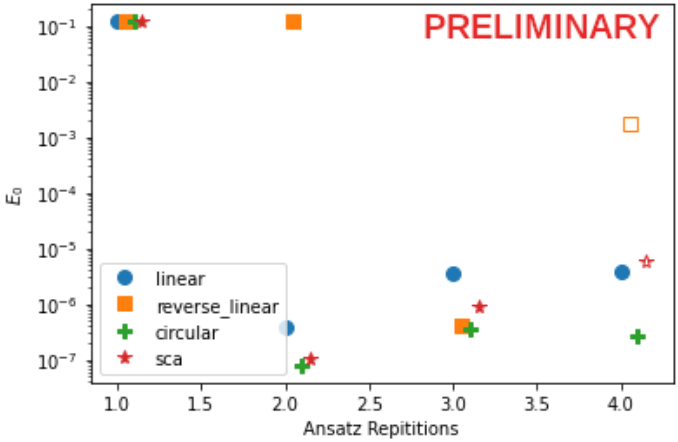
Non-ultralocal product operator $\longrightarrow$ lattice Leibniz rule but not gauge invariance

D'Adda–Kawamoto–Saito, arXiv:1706.02615

Cyclic Leibniz rule $\longrightarrow$ partial lattice supersymmetry but only (0+1)d QM so far

Kadoh–Kamei–So, arXiv:1904.09275

Backup: Ansatz testing for Wess–Zumino VQE



Test four different ways of entangling qubits

More repetitions $\longrightarrow$ more params to optimize

In principle more expressive

In practice harder to converge

Backup: Supersymmetric quantum mechanics

arXiv:2112.07651

Reduce to single spatial site:

$$\hat{H}_{\mathrm{SQM}} = \frac{1}{2}\left[\hat{p}^2 + [W(\hat{q})]^2 - W'(\hat{q})\left(\hat{b}^\dagger\hat{b} - \hat{b}\hat{b}^\dagger\right)\right].$$

Spontaneous supersymmetry breaking no longer dynamical

$\longrightarrow$ determined by prepotential

Harmonic oscillator $W_{\mathrm{HO}} = m\hat{q} \longrightarrow$ expect (free) supersymmetric $|\Omega\rangle$

Anharmonic oscillator $W_{\mathrm{AHO}} = m\hat{q} + g\hat{q}^3 \longrightarrow$ expect supersymmetric $|\Omega\rangle$

Double-well $W_{\mathrm{DW}} = m\hat{q} + g\left(\hat{q}^2 + \mu^2\right) \longrightarrow$ expect spont. susy breaking

Backup: Supersymmetric quantum mechanics

arXiv:2112.07651

Ground-state energies from VQE

Free theory clearly converges to zero energy

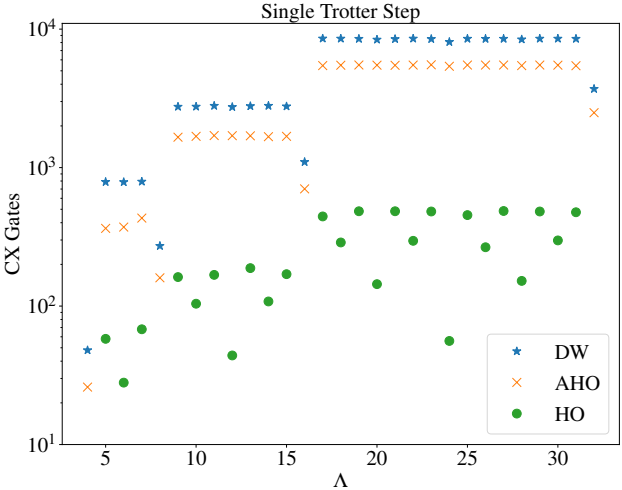
More params $\longrightarrow$ harder to converge, especially for anharmonic oscillator W_{AHO}

Clear non-zero energy (spont. susy breaking) for double-well W_{DW}

Λ	HO	VQE	AHO	VQE	DW	VQE
2	0	5.34e-10	9.38e-01	9.38e-01	1.08e+00	1.08e+00
4	0	1.07e-09	1.27e-01	1.27e-01	9.15e-01	9.15e-01
8	0	4.06e-09	2.93e-02	2.93e-02	8.93e-01	8.93e-01
16	0	1.13e-08	1.83e-03	6.02e-02	8.92e-01	8.94e-01
32	0	4.81e-08	1.83e-05	6.63e-01	8.92e-01	8.95e-01

Backup: Supersymmetric quantum mechanics

arXiv:2112.07651



Count number of entangling gates
for single Trotter step
(default Qiskit transpilation)

Big improvements when $\Lambda = 2^B$
(note log scale)

Backup: Quiver superQCD from twisted SYM

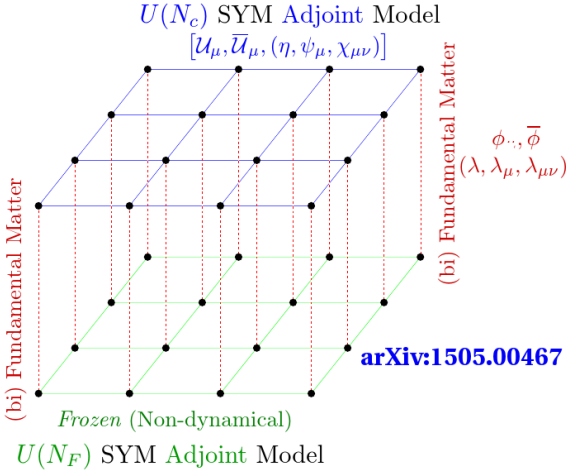
2-slice lattice SYM
with U(N) $\times$ U(F) gauge group

Adj. fields on each slice

Bi-fundamental in between

Decouple U(F) slice

$\longrightarrow$ U(N) SQCD in ($d-1$) dims.
with F fund. hypermultiplets



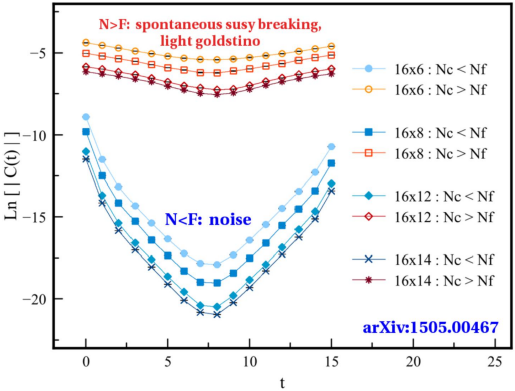
Ongoing work by Angel Sherletov: Dynamical susy breaking in 2d superQCD

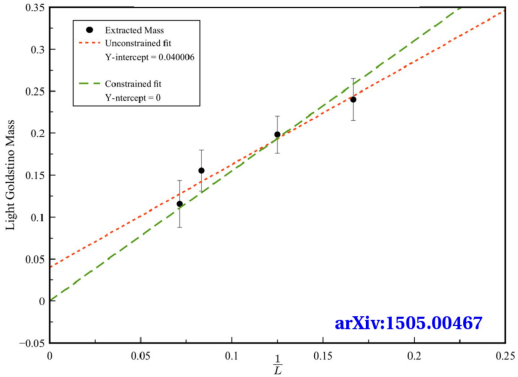
Backup: Dynamical susy breaking in 2d lattice superQCD

U(N) superQCD with F fundamental hypermultiplets

Observe spontaneous susy breaking only for $N > F$, as expected

Catterall–Veernala, arXiv:1505.00467





Backup: More on dynamical susy breaking

Spontaneous susy breaking means $\langle \Omega | H | \Omega \rangle > 0$ or equivalently $\langle \mathcal{Q}\mathcal{O} \rangle \neq 0$

Twisted superQCD auxiliary field e.o.m. $\longleftrightarrow$ Fayet–Iliopoulos D-term potential

$$d = \overline{\mathcal{D}}_a \mathcal{U}_a + \sum_{i=1}^{F} \phi_i \overline{\phi}_i - r\mathbb{I}_N \qquad \longleftrightarrow \qquad \mathrm{Tr}\left[\left(\sum_i \phi_i \overline{\phi}_i - r\mathbb{I}_N\right)^2\right] \in H$$

Have $F \times N$ scalar vevs to zero out $N \times N$ matrix

$\longrightarrow N > F$ suggests susy breaking, $\langle \Omega | H | \Omega \rangle > 0 \longleftrightarrow \langle \mathcal{Q}\eta \rangle = \langle d \rangle \neq 0$