3+1d SU(3) θ-term with Neural Network Quantum States

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The QCD θ-term

$$\mathscr{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \bar{\theta}\frac{g^2}{32\pi^2}F_{\mu\nu}\tilde{F}^{\mu\nu} + \bar{\psi}(i\gamma^\mu D_\mu - m)\psi\,.$$

- Strong CP-puzzle: why $\bar{\theta} \leq 10^{-10}$?

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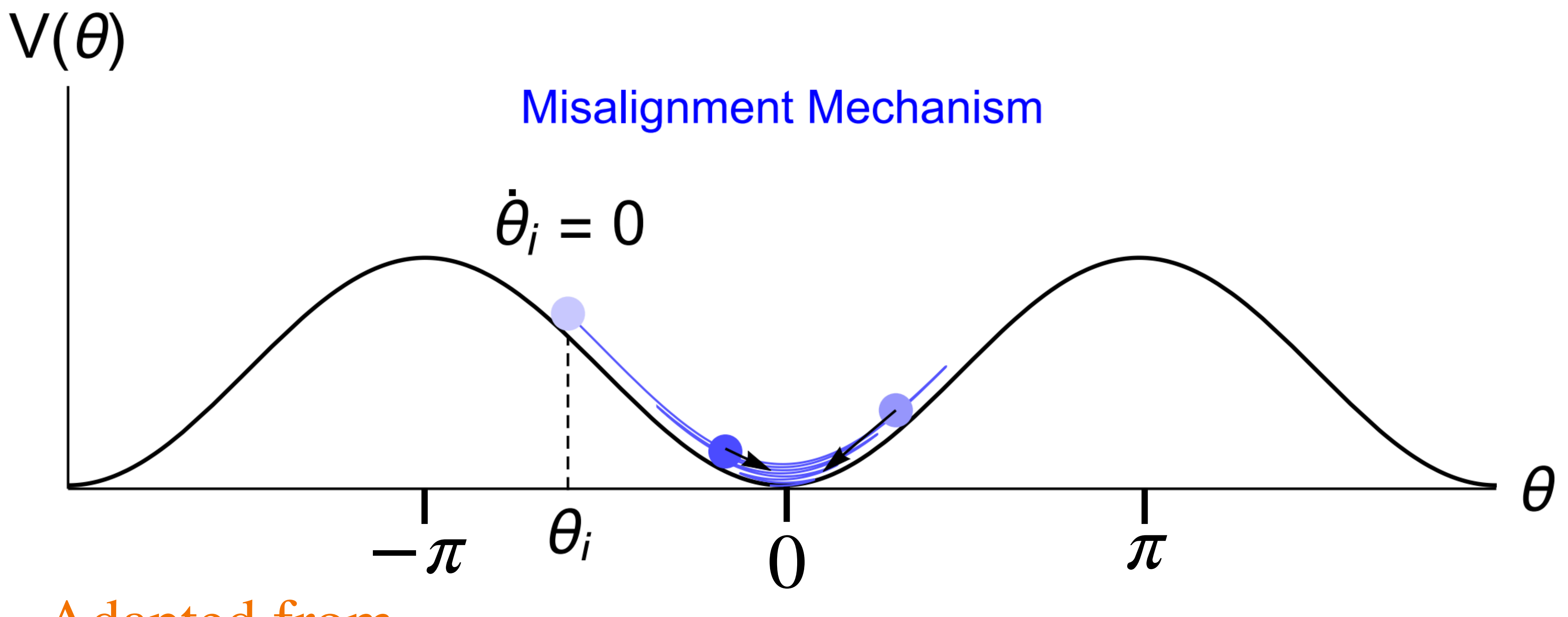
- One proposed solution is axions. Energy density as a function of θ is important for QCD-axion phenomenology.

[Wilczek, PRL 40] [Weinberg, PRL 40]



Adapted from
[Co, Hall, Harigaya et al, PRL 124]

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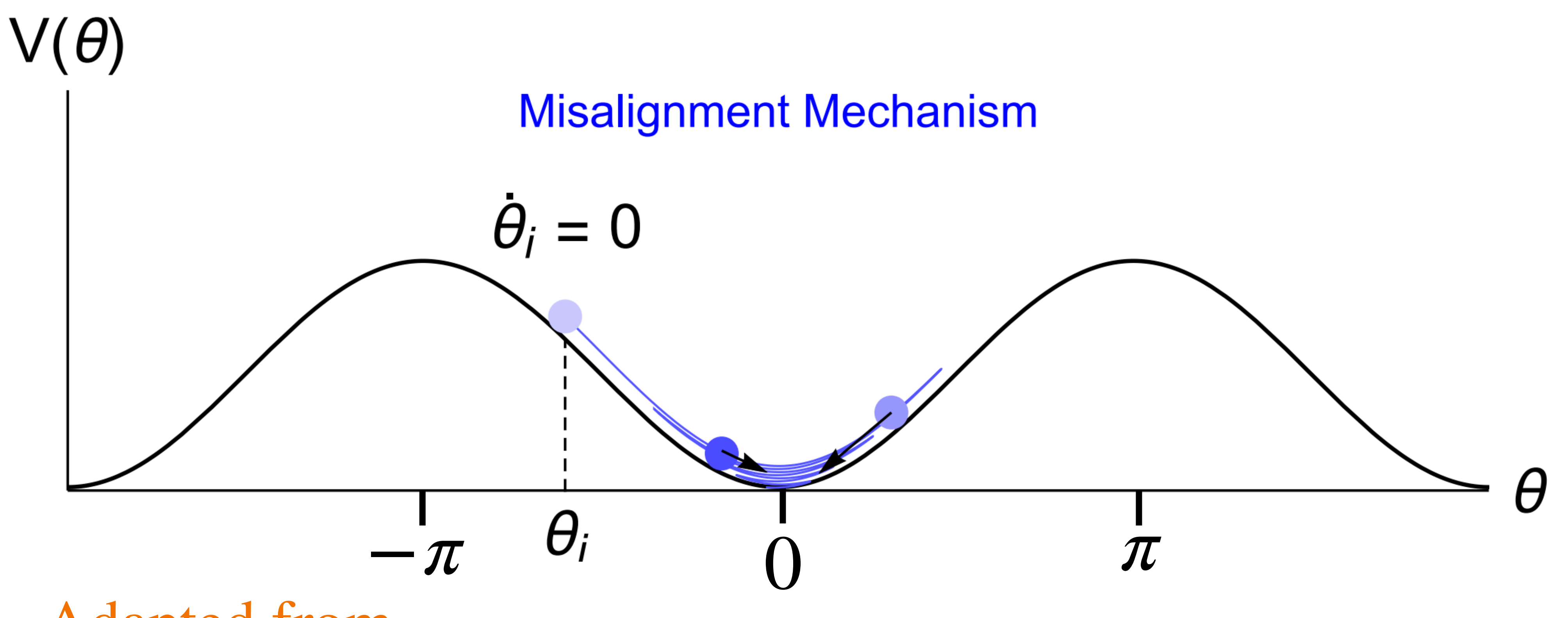
- Including the θ-term into the Euclidean path integral results in a sign problem

$$S = \frac{-1}{g^2}\sum_{\vec{n},\mu,\nu}\mathrm{Tr}(U_{\vec{n},\mu\nu}) + \frac{i\theta}{32\pi^2}\sum_{\vec{n},\mu\nu\rho\sigma}\epsilon_{\mu\nu\rho\sigma}\mathrm{Tr}\left(U_{\vec{n},\mu\nu}U_{\vec{n},\rho\sigma}\right)$$



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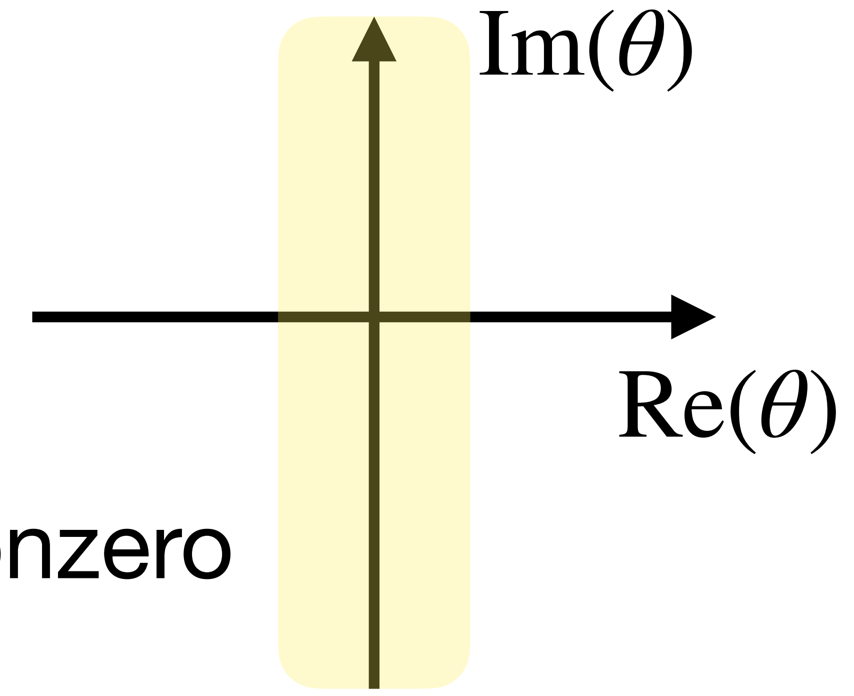
- Attempts to recover finite-θ physics nonperturbatively can all be considered expansions around $\mathrm{Re}(\theta) = 0$.

  [Bonanno et al, JHEP 05(2024)]
  [Hirasawa et al, JHEP 05(2025)]
  [Del Debbio et al, J. Phys. Conf. Ser. 110]
  and many others



- Can we do direct calculations at nonzero $\mathrm{Re}(\theta)$?

Hamiltonian formulation of Yang Mills + θ-term

$$S = \frac{-1}{g^2}\sum_{\vec{n},\mu,\nu}\mathrm{Tr}(U_{\vec{n},\mu\nu}) + \frac{i\theta}{32\pi^2}\sum_{\vec{n},\mu\nu\rho\sigma}\epsilon_{\mu\nu\rho\sigma}\mathrm{Tr}\left(U_{\vec{n},\mu\nu}U_{\vec{n},\rho\sigma}\right)$$

Transfer Matrix

[Angus Kan, Lena Funcke et al, PRD 104]

$$\langle U|H|\psi\rangle = \frac{-1}{a_s g^2}\sum_{\vec{n},ij}\mathrm{Tr}(U_{\vec{n},ij})\psi(U) + \frac{-g^2}{2a_s}\sum_{A,\vec{n},i}\partial^2_{A,\vec{n},i}\psi(e^{i\epsilon^A T^A}U) +$$

$$\frac{-2g^2\theta}{16\pi^2 a_s}\sum_{\vec{n},i}\epsilon_{ijk}\partial_A\psi(e^{i\epsilon_{B,\vec{n},i}T_B}U)\mathrm{Tr}(T^A U_{\vec{n},jk})$$

$$\frac{-4g^2\theta^2}{512\pi^4 a_s}\sum_{\vec{n}}\left[\mathrm{Tr}(T^A\epsilon_{ijk}U_{\vec{n},jk})\mathrm{Tr}(T^A\epsilon_{ij'k'}U_{\vec{n},j'k'})\right]\psi(U)$$

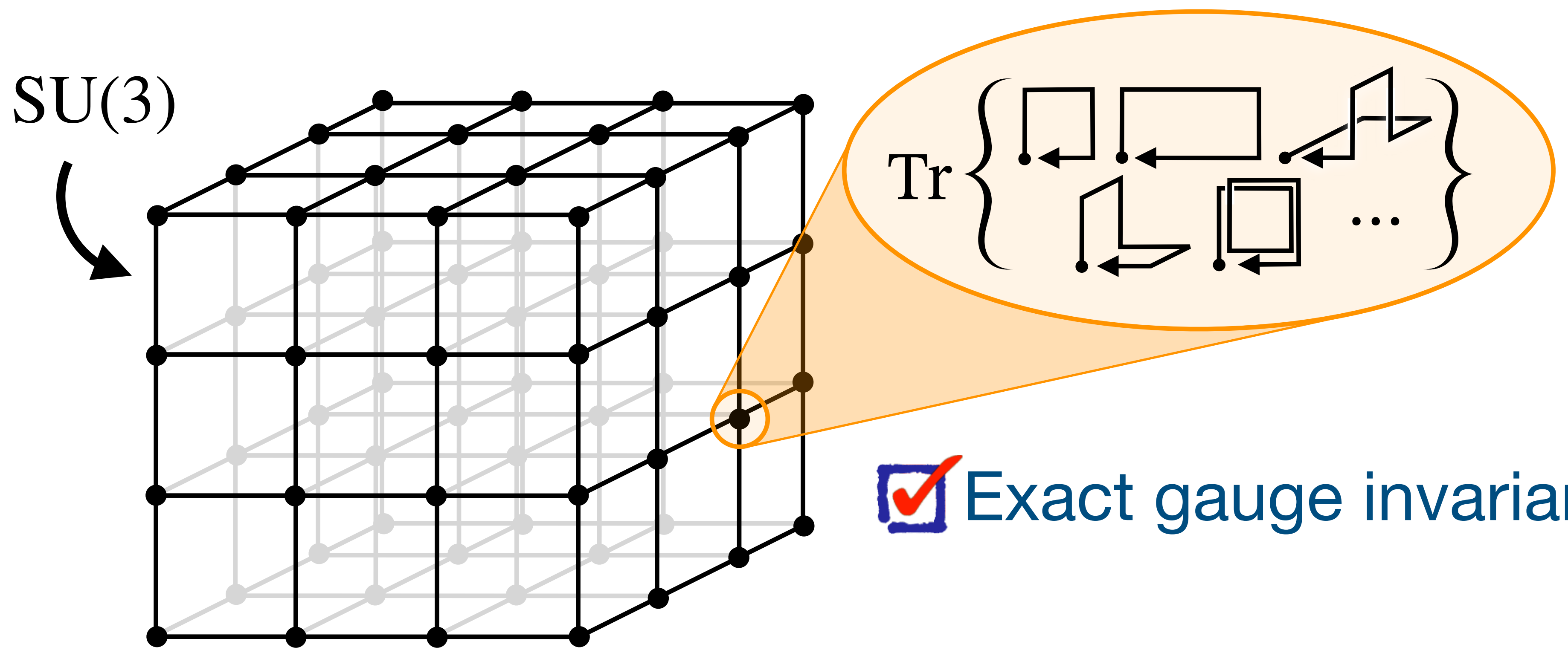
- Critical difficulty: the Hilbert space is infinite dimensional.

- Recent studies have considered a Hamiltonian approach for nonabelian gauge theories, using Quantum Computers:

At this conference:

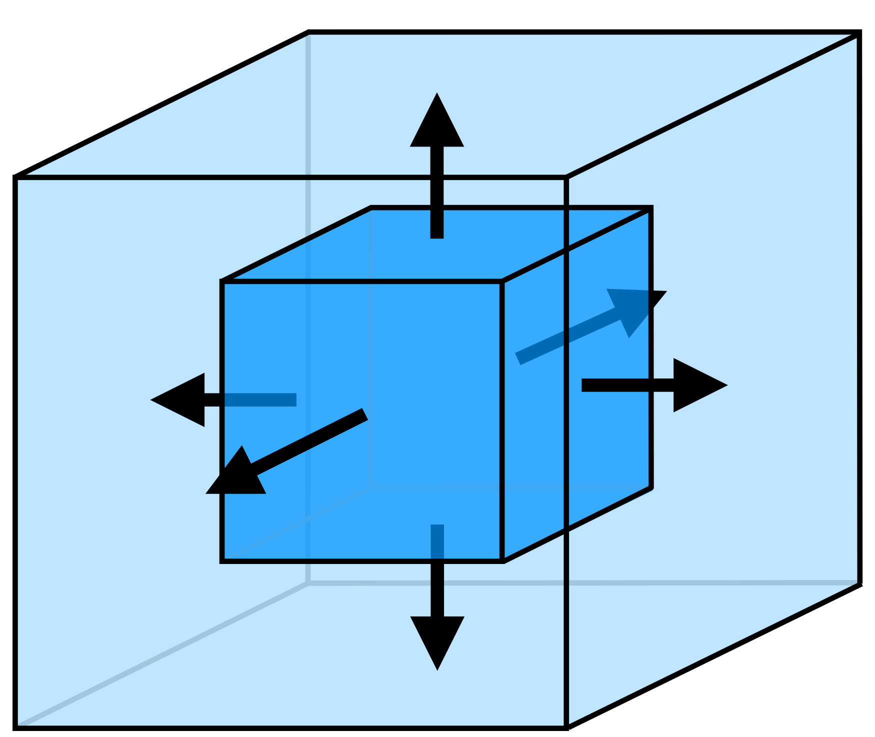
- Lena Funcke: Simulating (3+1)D SU(2) Hamiltonian lattice gauge theory with a topological -term
- Emil Otis Rosanowski: A Path to Quantum Simulations of (3+1)D U(1) Gauge Theory with a Topological -Term
- Luis Hidalgo: Quantum Simulations of Lattice QCD in the Representation Basis

Neural Network Quantum States for Gauge Theories



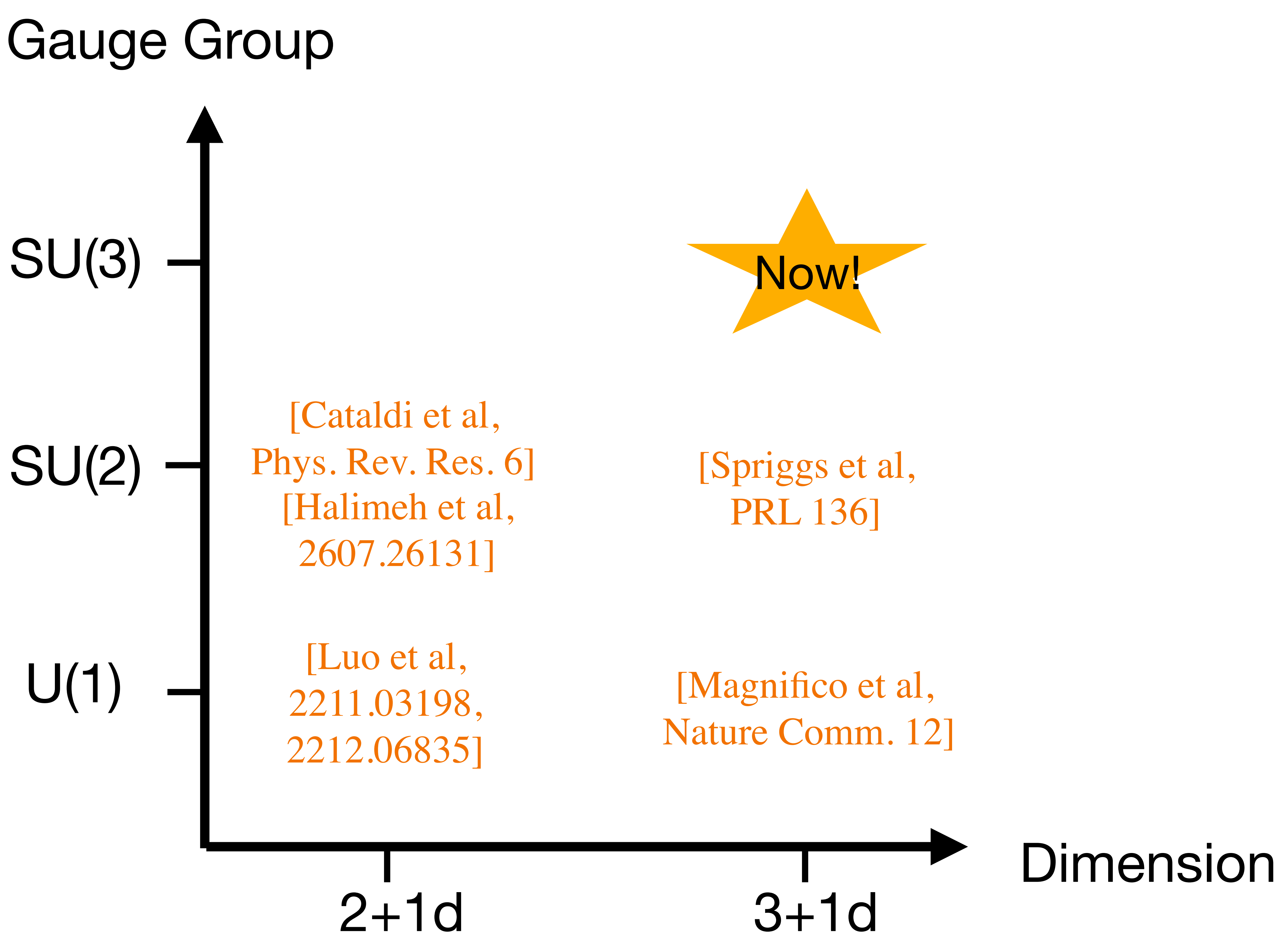
☑ Exact gauge invariance

Scalar field of gauge-invariant information



☑ Exact translation invariance, easy transfer learning

$\psi(U)$



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Variational Principles

- Evaluating the expectation value of any state gives an upper bound on the ground state energy.

$$E_\alpha := \langle \psi_\alpha | \hat{H} | \psi_\alpha \rangle \geq E_0$$

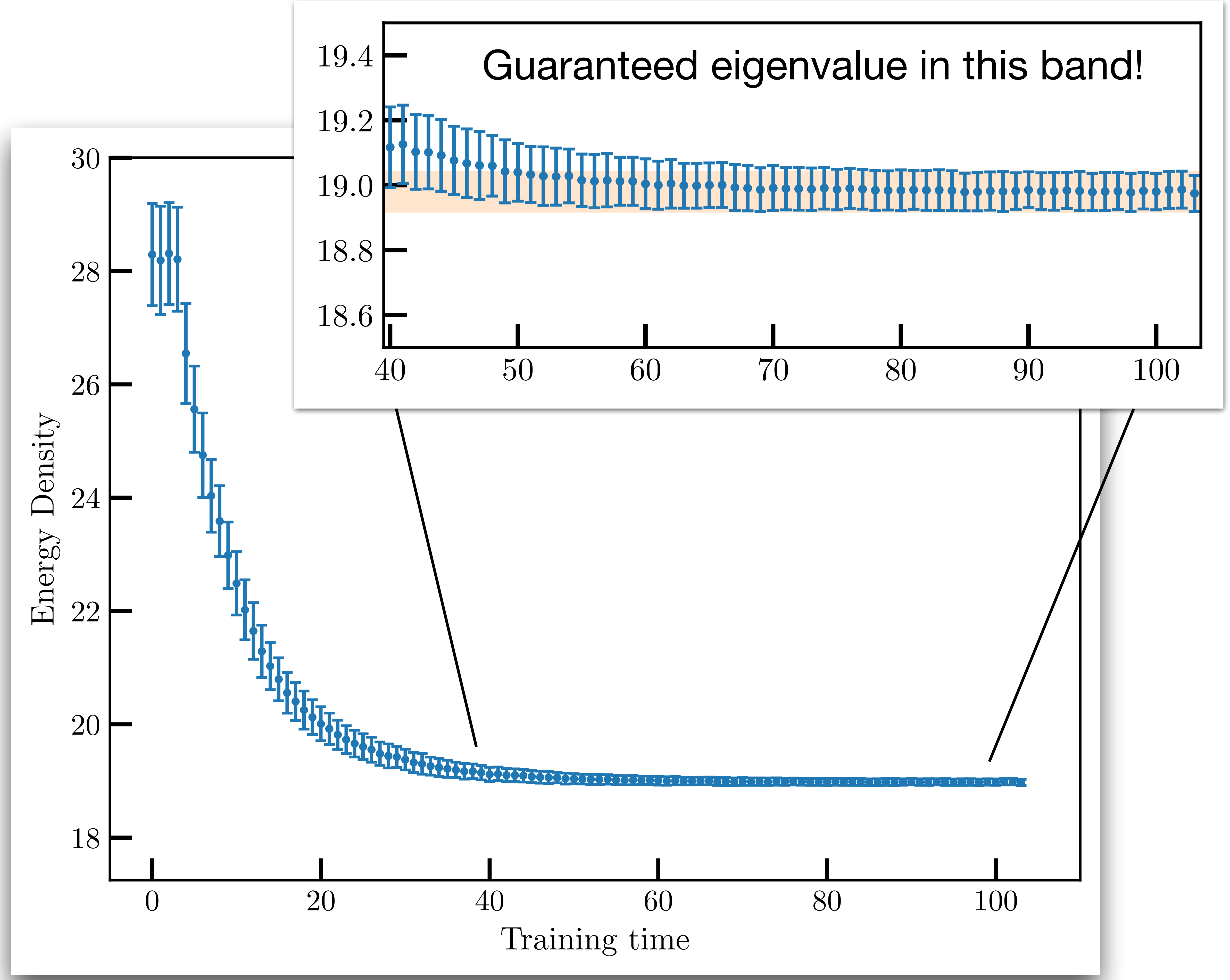
- By an application of Chebyshev's inequality, there is guaranteed to be an eigenvector of $\hat{H}$ contained in the two-sided bound:

$$[E_\alpha - \sigma_\alpha, E_\alpha + \sigma_\alpha]$$

$$\sigma_\alpha^2 := \langle \psi_\alpha | \hat{H}^2 | \psi_\alpha \rangle - (\langle \psi_\alpha | \hat{H} | \psi_\alpha \rangle)^2$$

(The "first residual bound" discussed in [M. Wagman, PRL 134] and elsewhere, thanks Rob for pointing this connection out)

- As variance decreases, variational state approaches exact eigenstate.

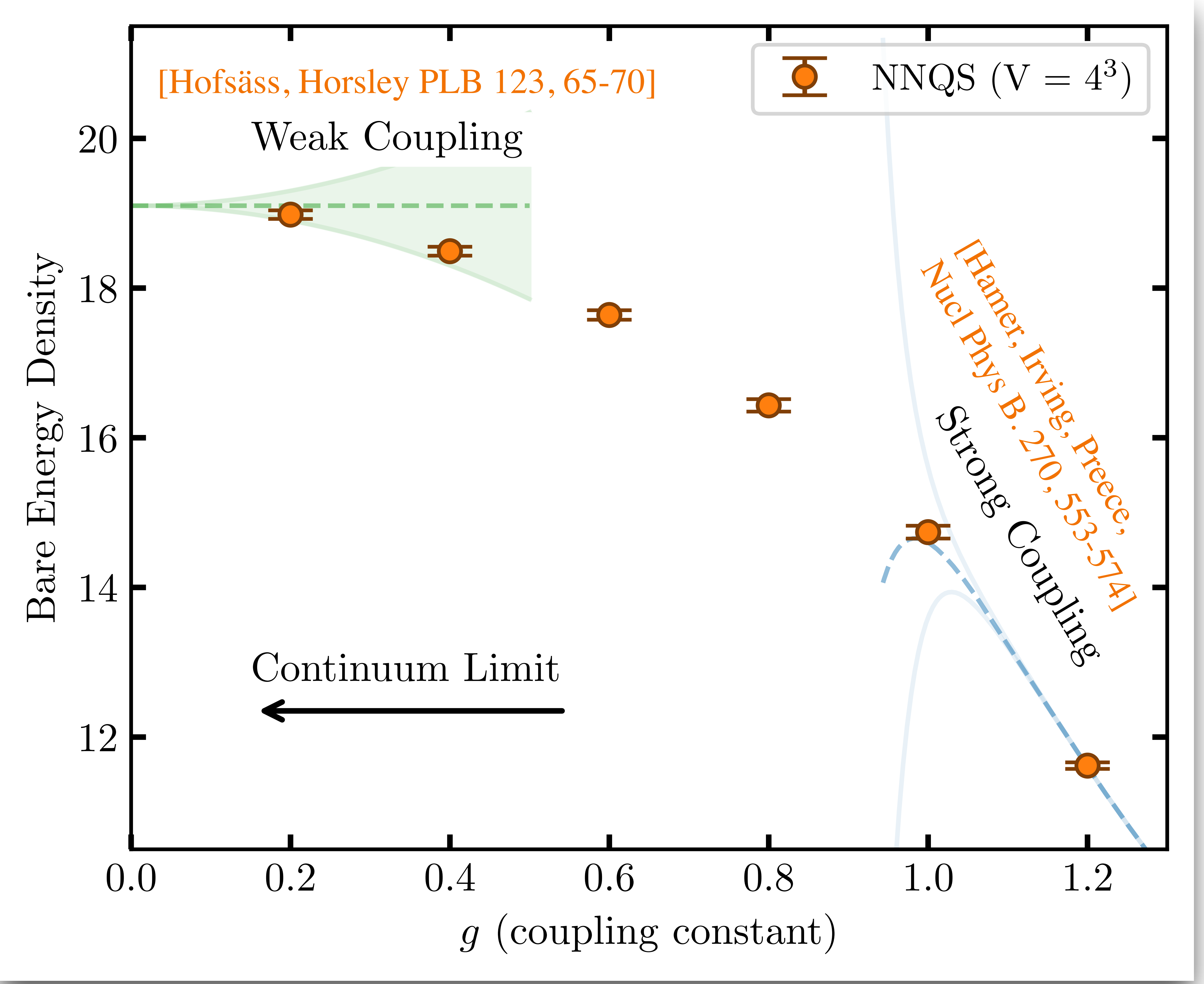


3+1d SU(3) Kogut Susskind ground states

(1840 parameters)

NEW It works!

- At strong coupling, the wave function is close to haar-uniform. (easy)
- Weak coupling result is the zero-point-energy for the gauge boson degrees of freedom. This is *not* a delta function on unity plaquettes.
- Variance can be driven down by adding universal gauge-equivariant layers (universal smearing), or increasing readout.



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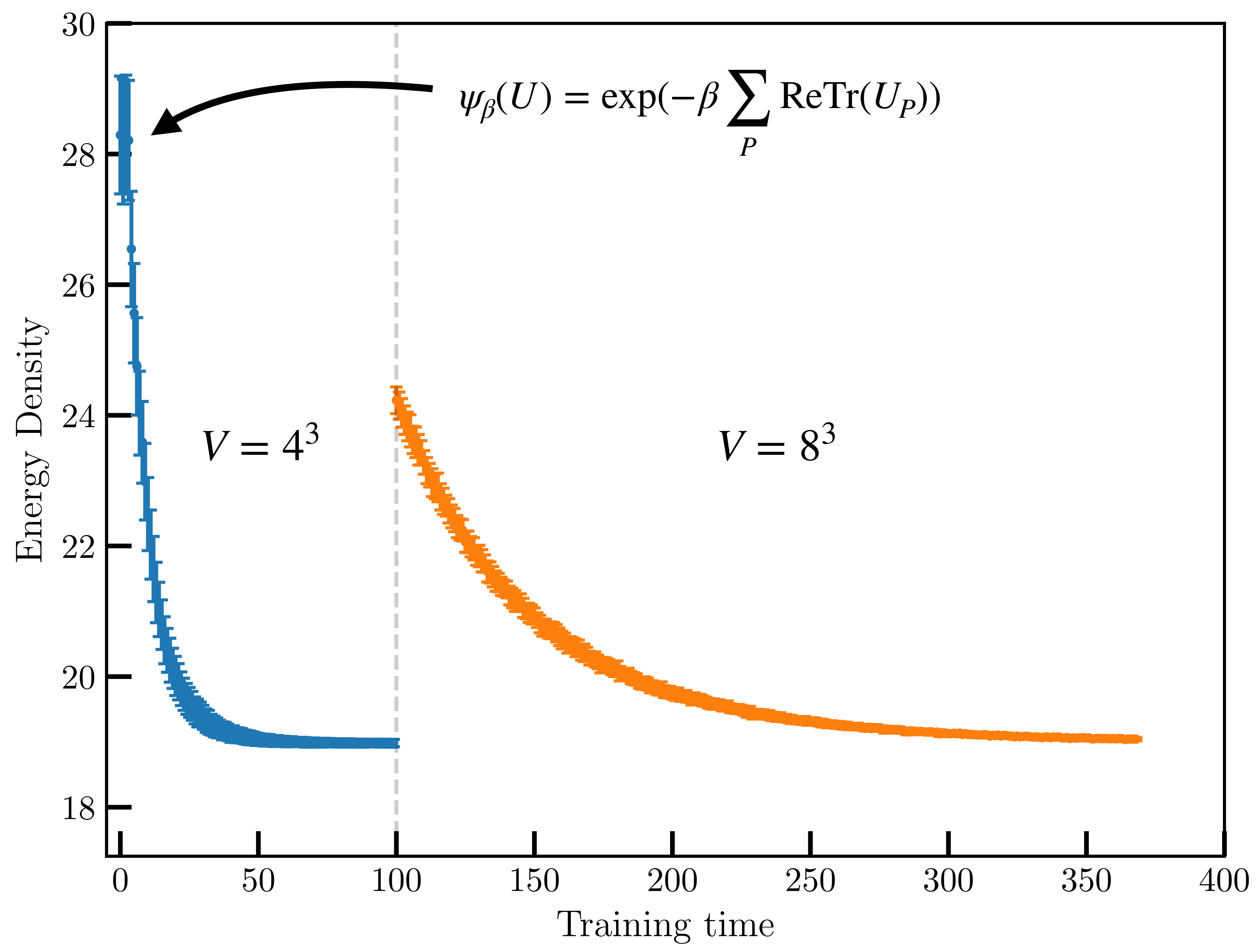
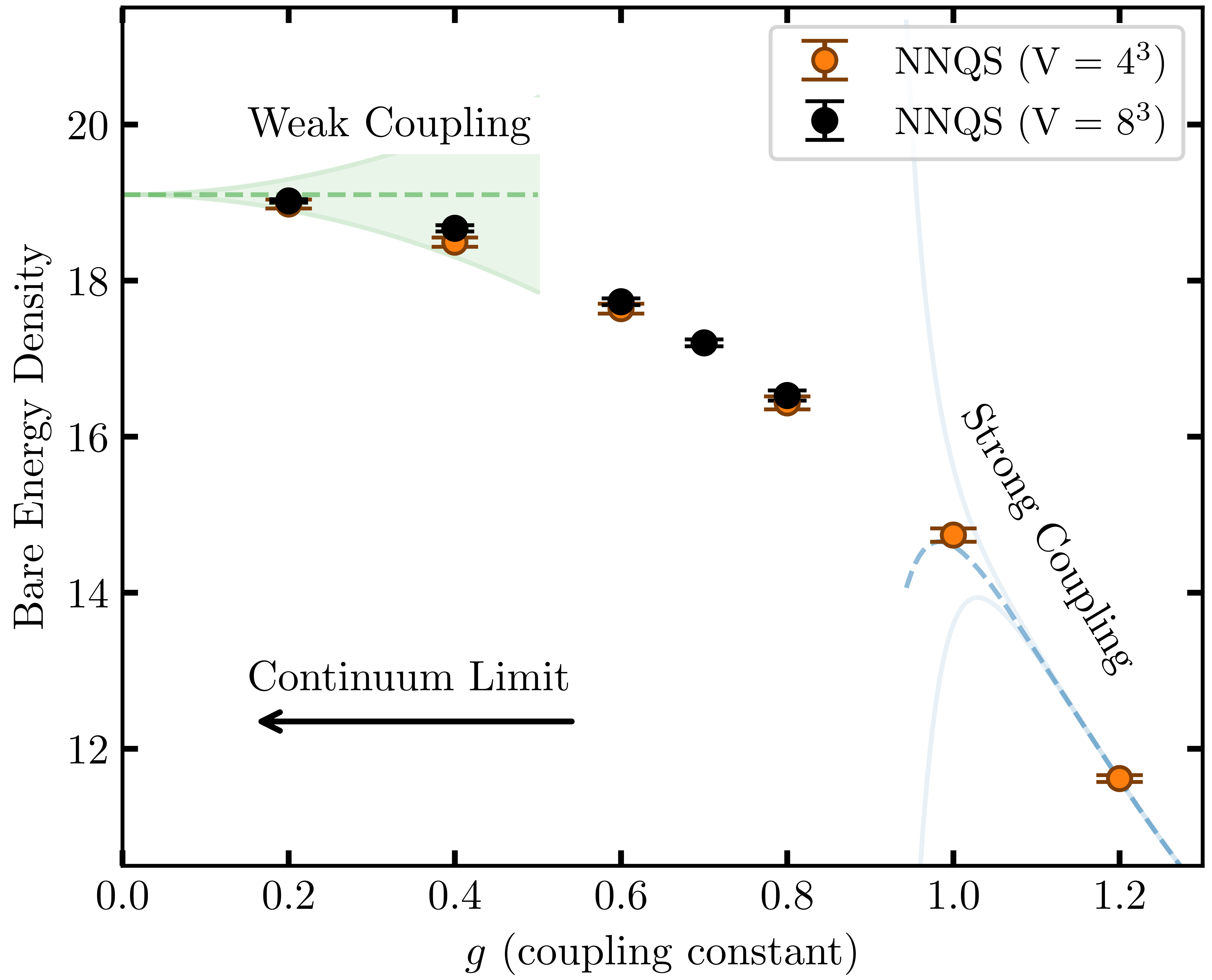
Transfer learning to $V = 8^3$





Scale setting

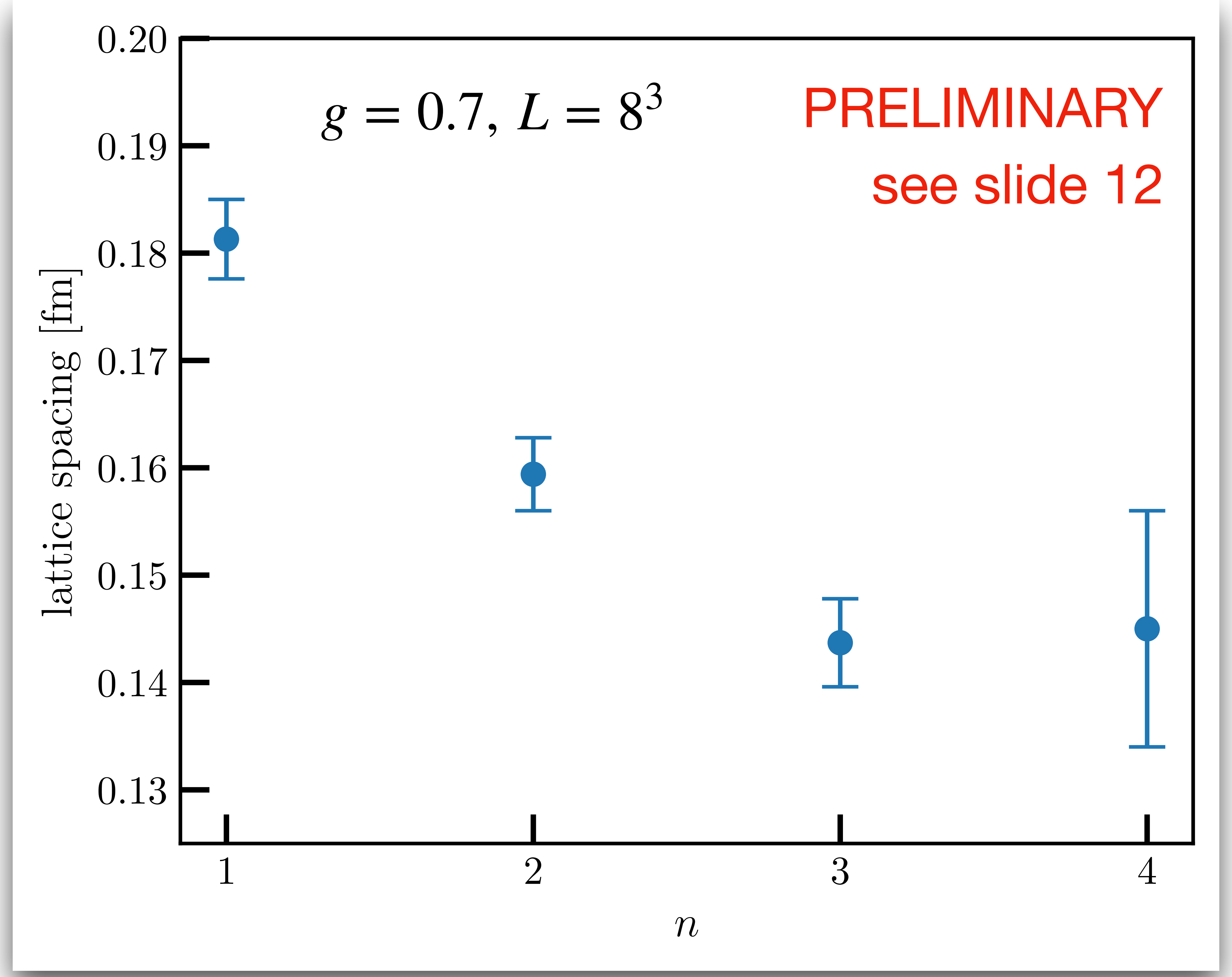
- Scale setting can be performed in various ways, the simplest being to measure the string tension via the Creutz ratios:

$$\frac{\langle\psi|\mathcal{O}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\int \mathrm{d}U \ \langle\psi|U\rangle\langle U|\psi\rangle \frac{\langle U|\mathcal{O}|\psi\rangle}{\langle U|\psi\rangle}}{\int \mathrm{d}U \ \langle\psi|U\rangle\langle U|\psi\rangle}$$

$$\chi(I,J) = -\ln\left[\frac{W(I,J)\,W(I-1,J-1)}{W(I,J-1)\,W(I-1,J)}\right]. \qquad a = \sqrt{\frac{\chi(n+1,n+1)}{\sigma}}$$

- Alternatively, can measure glue-ball masses [WIP]
- Alternatively, can scaleset anisotropic Lattice-QCD ensembles, and extrapolate to the Hamiltonian limit.

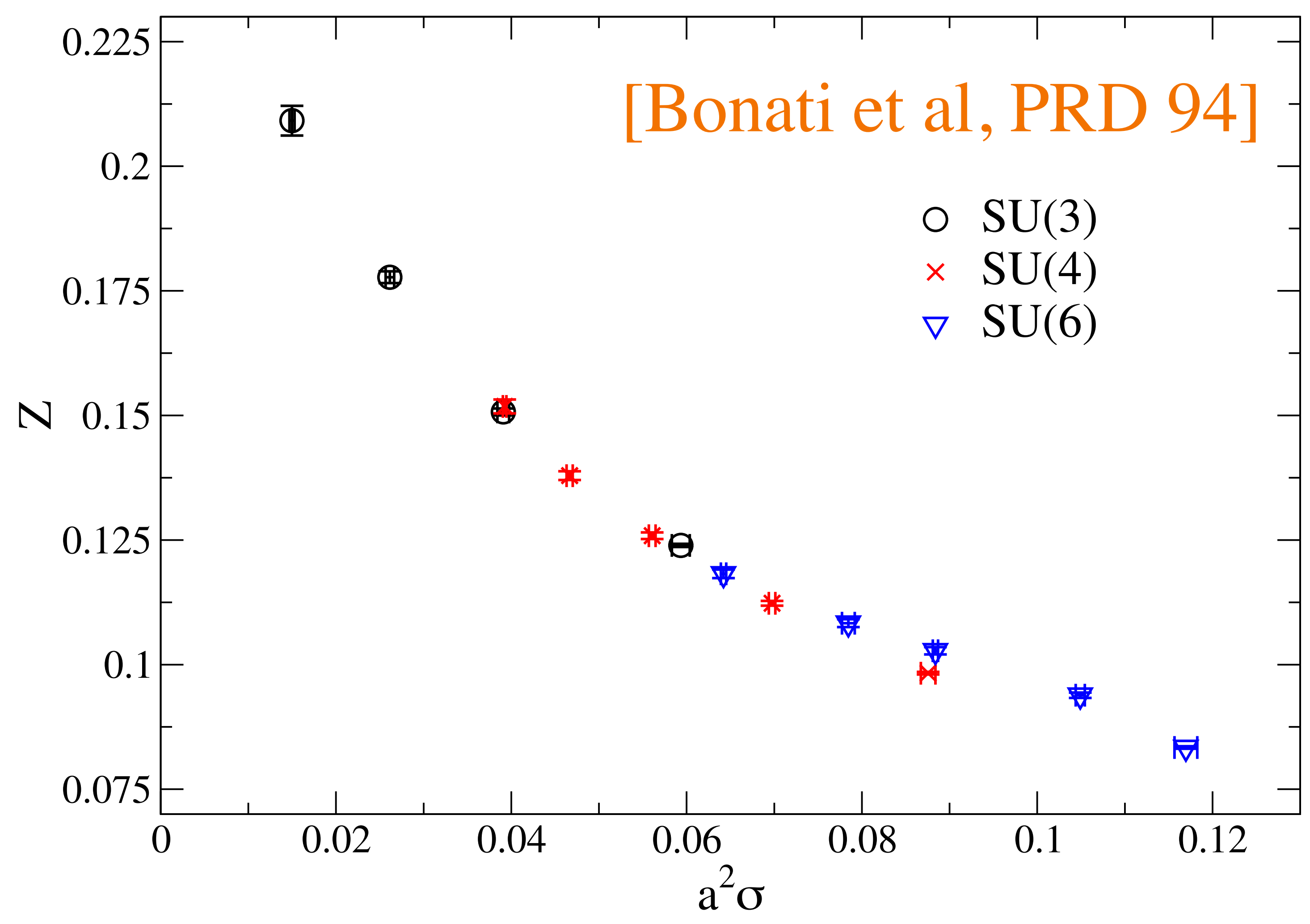
[Groß et al, Eur. Phys. J. C 85] for 2+1d U(1) matching



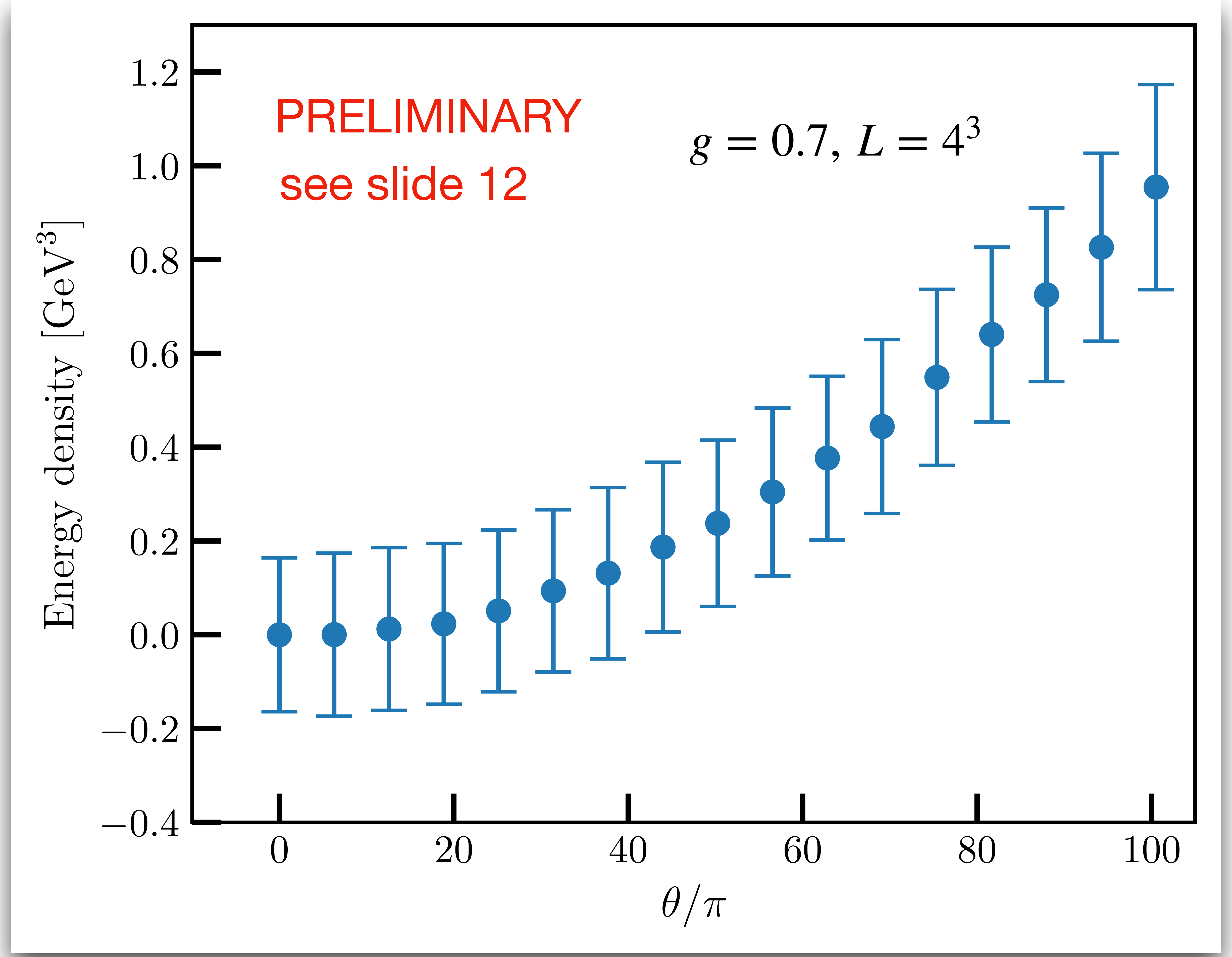
θ-dependence of the vacuum

- Note! The bare topological charge undergoes a multiplicative renormalization!

  [M. Campostrini et al, *Nucl.Phys.B* 329 (1990) 683-697]



- Physical results (and 2π-periodicity) are only recovered in the infinite volume, and continuum limits.



The path towards systematic control

Scale setting:

- 1st path: At fixed g, infinite volume, zero variance extrapolations of a scale setting scheme e.g. in [Sorella, PRB 64]
- 2nd path: Anisotropic limit of Lattice-QCD calculations [Groß et al, Eur. Phys. J. C 85] for 2+1d U(1) matching

Renormalization of the θ-term:

- 1st path: Stick with the bare current, because taking the continuum limit causes $\lim_{a\to 0} Z_\theta \to 1$.
- 2nd path: Flow/smear the Hamiltonian θ-terms, requires some thinking. (Smearing in Lagrangian formulation makes writing a transfer matrix down difficult)
  Alternative: fermionic definition, fixes renormalization (see Lena's talk)
- Lena Funcke: Simulating (3+1)D SU(2) Hamiltonian lattice gauge theory with a topological -term

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The path towards systematic control

Lagrangian Formulation

- Infinite volume, continuum limits
- Excited state control by large Euclidean times, fits
- Renormalization (mostly) done by NPR

Hamiltonian Formulation

- Infinite volume, continuum limits
- Excited states controlled by more expressive NNs, variance extrapolation.
- Unclear! In this work, I present a quantity that is protected

The Future...

The immediate future

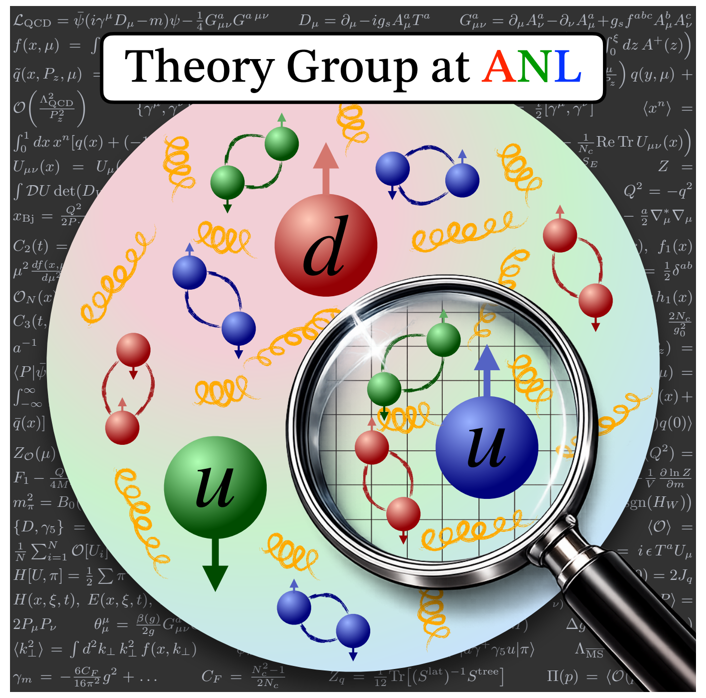
- GFMC can be used as a check (though, expensive at finite θ)
- Glueball spectrum as a function of θ

The future

- Real-time simulation is also possible, either via Time-dependent-variational-principle or otherwise. But it suffers systematic errors.
- Adding fermions is the next step, consider for example the baryon chemical potential.

Thank you to my collaborators,

and thank you for listening!



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