Diagonalizing the Kogut-Susskind Hamiltonian with Physics-Informed Neural Networks

Simone Romiti, David Müller

University of Bern, Switzerland

Lattice 2026

Summary

Wavefunction ansatz

- Neural networks represent $\psi[\mathcal{U}]$ directly
- Gauge symmetry imposed at the level of the network architecture
- The solution is found imposing the fulfillment of the Schrödinger equation

Summary

Wavefunction ansatz

- Neural networks represent $\psi[\mathcal{U}]$ directly
- Gauge symmetry imposed at the level of the network architecture
- The solution is found imposing the fulfillment of the Schrödinger equation

Target: renormalization flow

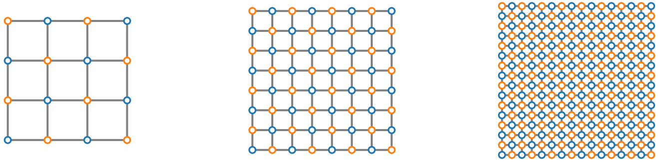
- Training moves along $1/g : 0 \to \infty$
- network adapts to $H(g)$ without explicit Hilbert-space truncation

Simone Romiti. "SU(N) lattice gauge theories with physics-informed neural networks". In: *Phys. Rev. D* 113 (2026), p. 054511. DOI: 10.1103/mb67-9rkf

- Demonstrated for U(1) and SU(2), single plaquette

Table of contents

Lattice gauge theories

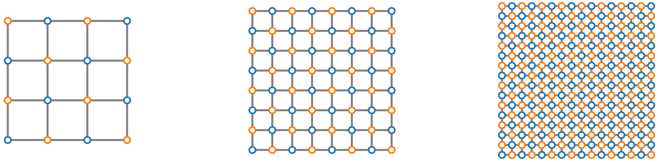


Expectation values (continuum limit)

$$Z_T = \mathrm{Tr}\left[e^{-HT}\right] = \int \mathcal{D}\phi \, e^{-S_E[\phi]}$$

$$\langle O \rangle = \frac{1}{Z_T} \mathrm{Tr}\left[e^{-HT} O\right] = \int \mathcal{D}\phi \, O[\phi] \, \frac{e^{-S_T[\phi]}}{Z_T}$$

Lattice gauge theories



Expectation values (continuum limit)

$$Z_T = \mathrm{Tr}\left[e^{-HT}\right] = \int \mathcal{D}\phi\, e^{-S_E[\phi]}$$

$$\langle O \rangle = \frac{1}{Z_T}\,\mathrm{Tr}\left[e^{-HT} O\right] = \int \mathcal{D}\phi\, O[\phi]\, \frac{e^{-S_T[\phi]}}{Z_T}$$

Physical predictions by extrapolation

Multiple simulations at different lattice spacings a and volumes V,

- **Infinite volume**: $V \to \infty$ (increase N_s)
- **Continuum limit**: $a \to 0$ (renormalization flow)

Lagrangian VS Hamiltonian

Lagrangian	**Hamiltonian**
Path integral + Monte Carlo	Hilbert space + Schrödinger equation
Importance sampling $\rightarrow$ effective Hilbert space	Hilbert-space truncation $\rightarrow$ effective Hilbert space
Wick rotation $\rightarrow$ analytic continuation	No sampling $\rightarrow$ no MC limitations
MC limitations: sign problem, critical slowing down, topological freezing	Main challenge: infinite-dimensional Hilbert space

Lagrangian VS Hamiltonian

Lagrangian	**Hamiltonian**
Path integral + Monte Carlo	Hilbert space + Schrödinger equation
Importance sampling → effective Hilbert space	Hilbert-space truncation → effective Hilbert space
Wick rotation → analytic continuation	No sampling → no MC limitations
MC limitations: sign problem, critical slowing down, topological freezing	Main challenge: infinite-dimensional Hilbert space

Finite-difference methods (QC, TN)

- Choose a fixed basis at strong coupling
- Basis is rigid: adequate only in a region of the coupling
- Truncation becomes inadequate toward the continuum $g \to 0$

Table of contents

Wavefunctions on the lattice

State vector

$$|\psi\rangle = \int \mathcal{D}U \; \psi(\mathcal{U})\, |\mathcal{U}\rangle \,, \qquad \psi(\mathcal{U}) = \langle \mathcal{U} | \psi \rangle$$

Inner product & expectation

$$\langle \phi | \, O \, | \psi \rangle = \int \mathcal{D}U \; \phi^*(\mathcal{U})\, O(\mathcal{U})\, \psi(\mathcal{U})$$

$$\langle \psi | \, O \, | \psi \rangle = \int \mathcal{D}U \; |\psi(\mathcal{U})|^2\, O(\mathcal{U})$$

No sign problem

$|\psi|^2 \geq 0 \implies$ importance sampling directly from the wavefunction

Diagonalization of the Hamiltonian

Hamiltonian approach

$$H |n, \alpha\rangle = E_{n,\alpha} |n, \alpha\rangle$$

$E_{n,\alpha}$ and $\psi_{n,\alpha}$ are **direct outputs**

If you have the E_n and you can sample *d.o.f.*s from the ψ_n, you can compute the expectation values.

Diagonalization of the Hamiltonian

Hamiltonian approach

$$H\,|n,\alpha\rangle = E_{n,\alpha}\,|n,\alpha\rangle$$

$E_{n,\alpha}$ and $\psi_{n,\alpha}$ are **direct outputs**

If you have the E_n and you can sample *d.o.f.*s from the ψ_n, you can compute the expectation values.

Contrast with MC

$$C(t) = \sum_n |\,\langle\Omega|O|n\rangle\,|^2 e^{-E_n t}$$

- Features extracted *a posteriori* from t dependence $\implies$ signal-to-noise ratio
- Sign problem for imaginary actions

Table of contents

Kogut-Susskind Hamiltonian

Hamiltonian

$$\boxed{H_{\mathrm{KS}} = \underbrace{\frac{g^2}{2}\sum_{\vec{x},\mu,a}(L_a)^2_\mu(\vec{x})}_{H_E} \underbrace{-\frac{1}{g^2}\sum_{\vec{x},\mu>\nu}\mathrm{Tr}\left[U_{\mu\nu}+U^\dagger_{\mu\nu}\right](\vec{x})}_{H_B}}$$

H_E: chromoelectric term, H_B: chromomagnetic term

Analogy

- N interacting particles (one per link)
- Plaquette term $\leftrightarrow$ many-body potential
- $H_{\mathrm{KS}} \xrightarrow{a\to 0} \int d^3x\,(\vec{E}^2+\vec{B}^2)/2$

Canonical momenta

Left and right generators

Left and right gauge transformations for a single link are independent.

$$(L_a)_\mu \psi(\mathcal{U}) = -i\frac{d}{d\omega}\psi(e^{-i\omega\tau_a}\mathcal{U}_\mu)\Big|_{\omega=0}, \qquad (R_a)_\mu \psi(\mathcal{U}) = -i\frac{d}{d\omega}\psi(\mathcal{U}_\mu e^{i\omega\tau_a})\Big|_{\omega=0}$$

Canonical momenta

Left and right generators

Left and right gauge transformations for a single link are independent.

$$(L_a)_\mu \psi(\mathcal{U}) = -i \frac{d}{d\omega} \psi(e^{-i\omega\tau_a} \mathcal{U}_\mu) \Big|_{\omega=0}, \qquad (R_a)_\mu \psi(\mathcal{U}) = -i \frac{d}{d\omega} \psi(\mathcal{U}_\mu e^{i\omega\tau_a}) \Big|_{\omega=0}$$

Gauge invariance is not automatic:

Gauss's law

$$G_a(\vec{x}) = \sum_\mu (L_a)_\mu(\vec{x}) + (R_a)_\mu(\vec{x} - \hat{\mu}), \qquad G_a \left|\psi\right\rangle_{\text{phys}} = 0$$

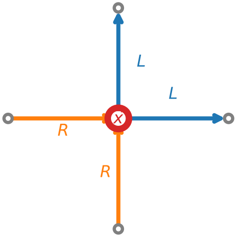


Table of contents

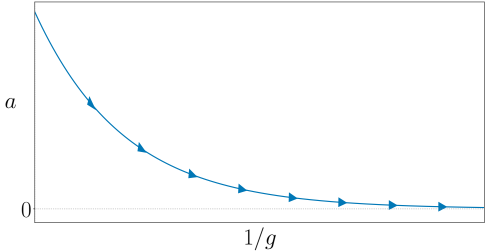
Finding the ansatz for $\psi[\mathcal{U}]$

L-CNN[2] + MLP ansatz

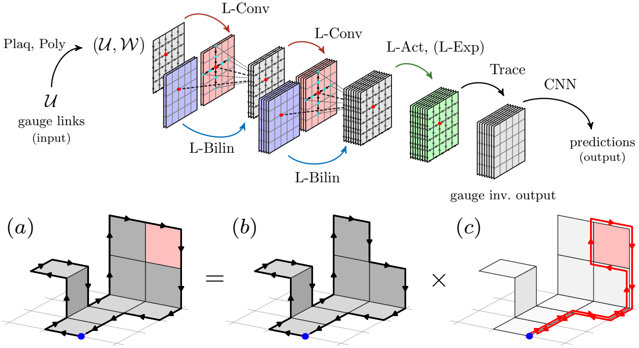
- Built from **gauge-covariant** layers
- **Automatic gauge invariance**, i.e. Gauss law by construction
- Gauge-invariant trace + MLP $\rightarrow$ scalar $\psi[\mathcal{U}] \in \mathbb{C}$

$$\hat{H} = \hat{H}(g)$$

- Learn ψ_n, E_n from Schrödinger equation
- Evolve along RG flow $1/g : 0 \rightarrow \infty$



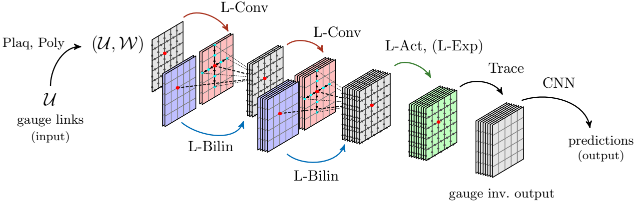
L-CNN + MLP



Three layers[3]

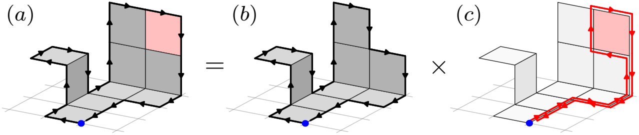
1. **L-Conv**:
   $W' = \sum_{\mu,k} \omega_{\mu k} \, U_\mu \, W \, U_\mu^\dagger$
2. **L-Bilin**: $W'' = \sum_{ij} \alpha_{ij} \, W'_i \, W'_j$
3. **L-Act**: $W''' = f(\mathrm{Tr}\, W'') \, W''$

L-CNN + MLP



Three layers[3]

1. **L-Conv**:
   $W' = \sum_{\mu,k} \omega_{\mu k}\, U_\mu\, W\, U_\mu^\dagger$
2. **L-Bilin**: $W'' = \sum_{ij} \alpha_{ij}\, W_i'\, W_j'$
3. **L-Act**: $W''' = f(\mathrm{Tr}\, W'')\, W''$



$U_\mu \longrightarrow$ L-CNN $\longrightarrow$ Tr $\longrightarrow$ MLP $\longrightarrow$ ψ

$$\psi(U) = \mathrm{MLP}\big(\mathrm{Tr}[W''']\big) \in \mathbb{C} \implies G_a(\vec{x})\, \psi = 0 \text{ by construction}$$

Table of contents

Physics-Informed Neural Networks (PINNs)

Key idea (example)

Neural network $f_\theta(x)$ solves the minimizes the violation of the Cauchy problem

$$\begin{cases} \dfrac{df}{dx} = -xf, \\ f(0) = 1 \end{cases} \implies \mathcal{L} = \sum_i \left| \frac{df_\theta}{dx_i} + x_i f_\theta(x_i) \right|^2 + |f_\theta(0) - 1|^2$$

Unsupervised learning

We sample points in the **domain** of the function, we don't need to know a priori the solution.

Interpolation property

- Solution quality depends on where points are sampled
- Network interpolates between the configurations used in training

PINNs for the Schrödinger equation

Eigenvalue problem

Network represents ψ:

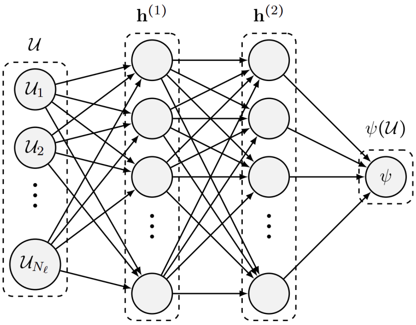
$$\boxed{H\psi = E\psi}$$

E learned as an additional parameter

Normalization (bound states)

$$\boxed{\int \mathcal{D}U \, |\psi|^2 = 1}$$

Condition for confined hadrons



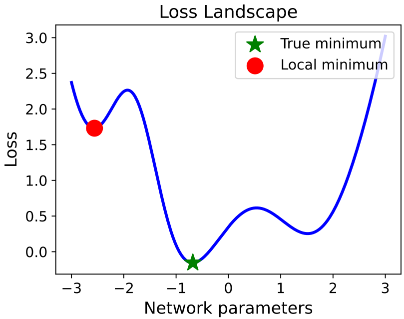
$$\theta^{(t+1)} = \theta^{(t)} - \eta \, \nabla_\theta \mathcal{L}(\theta)$$

$\theta = \{\text{weights}, E\}$ tuned via gradient descent

Table of contents

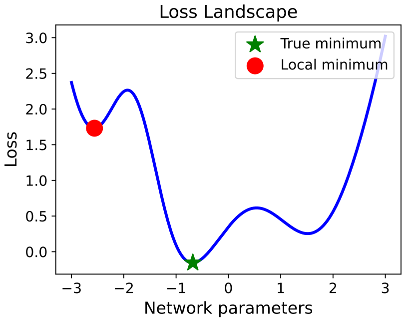
Loss function: minimization challenges

The loss function is in general hard to minimize...



Loss function: minimization challenges

The loss function is in general hard to minimize...

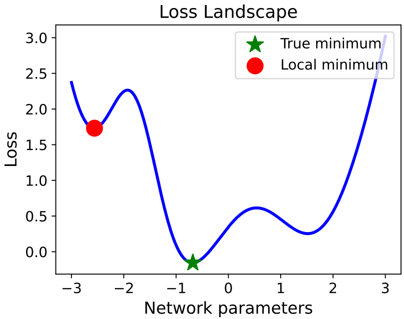


How do we formulate the problem?

- We do not want to accidentally end up in the minimum corresponding to another eigenstate
- We want to access different eigenstates, not just the ground state (cf. variational methods)
- Once we train at some coupling, how do we move to another coupling?

Loss function: minimization challenges

The loss function is in general hard to minimize...



How do we formulate the problem?

- We do not want to accidentally end up in the minimum corresponding to another eigenstate
- We want to access different eigenstates, not just the ground state (cf. variational methods)
- Once we train at some coupling, how do we move to another coupling?

Solution: adiabatic flow

Start at $1/g = 0$ where eigenstates are known analytically; slowly vary g to track the state along the RG flow

Evolving eigenstates from $1/g$

Strong-coupling eigenstates ϕ_n

$$\phi_0[\mathcal{U}] = 1, \qquad \phi_n[\mathcal{U}] = \text{known analytically}$$

Neural-network eigenstates

$$\psi_n(g)[\mathcal{U}] = \mathrm{NN}[\mathcal{U}], \qquad \psi_n(\infty) = \phi_n$$

At finite g, $\psi_n(g)$ is the same physical state deformed by the RG flow; the NN learns the deformation.

Why this matters

- Without analytic ϕ_n: "just" a variational method
- With ϕ_n: pick any sector at $1/g = 0$, track it along $g : \infty \to 0$
- *Note*: no crossing because of von Neumann-Wigner theorem.

Solution: adiabatic learning

Adiabatic evolution

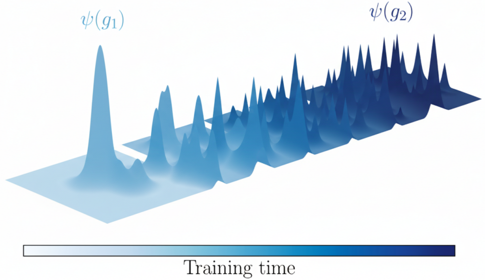
If at $t = 0$ we start from an eigenstate $|n_0\rangle$ ($c_m(0) = \delta_{mn_0}$), and vary $g(t)$:

$$|\psi(t)\rangle = \sum_i c_i(t)\,|n(t)\rangle$$

$$\dot{c}_n + i\dot{\theta}_{\text{tot}} c_n = \sum_{m \neq n} \frac{\langle n|\dot{H}|m\rangle}{E_n - E_m} c_m$$

Adiabatic theorem

Small $\dot{H} \implies$ stays in instantaneous eigenstate



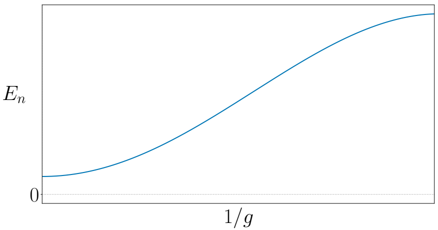
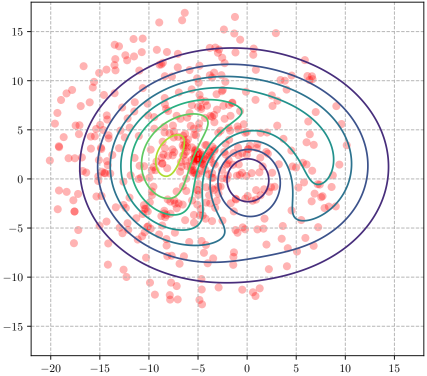


Table of contents

Loss at Strong Coupling ($1/g \to 0$)



Supervised training

$$\boxed{\mathcal{L}^{(1/g \to 0)} = \frac{1}{N_{\mathrm{pt}}} \sum_{i=1}^{N_{\mathrm{pt}}} \left| \psi(\mathcal{U}_i) - \phi_n(\mathcal{U}_i) \right|^2}$$

Points sampled via Langevin dynamics of ϕ_n

ϕ_n is an eigenstate: $H_E \phi_n = E_n^{1/g=0} \phi_n$

Loss at Finite Coupling $(1/g \neq 0)$

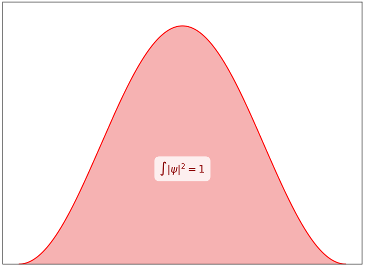
Total Loss

$$\mathcal{L} = \omega_{\mathrm{PDE}} \mathcal{L}_{\mathrm{PDE}} + \omega_{\mathrm{norm}} \mathcal{L}_{\mathrm{norm}}$$

Individual terms

$$\mathcal{L}_{\mathrm{PDE}} = \frac{1}{N_{\mathrm{pt}}} \sum_i |(H - E)\psi(\mathcal{U}_i)|^2$$

$$\mathcal{L}_{\mathrm{norm}} = \left(1 - \sqrt{\int d\mathcal{U}\, |\psi(\mathcal{U})|^2}\right)^2$$



$$\int d\mathcal{U}\, |\psi(\mathcal{U})|^2 \approx \frac{1}{N_{\mathrm{pt}}} \sum_i \frac{|\psi(\mathcal{U}_i)|^2}{q(\mathcal{U}_i)}$$

Monte Carlo estimate

$\mathcal{U}_i \sim q(\mathcal{U})$ (reference distribution)

Sampling from $|\psi|^2$ via Langevin dynamics

Stochastic flow

$$dx_t = g_t(x)\,dt + \frac{\sigma^2}{2}\nabla\log(\sigma^2 p_t(x))\,dt + \sigma\,dW$$

$g_t(x) = 0 \implies$ Langevin dynamics $\implies$ convergence to $p_\infty(x)$.

Sampling from $|\psi|^2$ via Langevin dynamics

Stochastic flow

$$dx_t = g_t(x)\,dt + \frac{\sigma^2}{2}\nabla \log(\sigma^2 p_t(x))\,dt + \sigma\,dW$$

$g_t(x) = 0 \implies$ Langevin dynamics $\implies$ convergence to $p_\infty(x)$.

Langevin dynamics on SU(N)

$$U \to e^{i\theta^a \tau_a} U$$

$$\theta^a = -\varepsilon\,\nabla_a \log p(U) + \sqrt{2\varepsilon}\,\eta^a$$

Sampling from $|\psi|^2$

$$\boxed{\theta^a = -\varepsilon\,L_a[\log|\psi|^2] + \sqrt{2\varepsilon}\,\eta^a}$$

Stationary solution: $p_\infty(U) \propto |\psi(U)|^2$

Sampling from $|\psi|^2$ via Langevin dynamics

Stochastic flow

$$dx_t = g_t(x)\,dt + \frac{\sigma^2}{2}\nabla \log(\sigma^2 p_t(x))\,dt + \sigma\,dW$$

$g_t(x) = 0 \implies$ Langevin dynamics $\implies$ convergence to $p_\infty(x)$.

Langevin dynamics on SU(N)

$$U \to e^{i\theta^a \tau_a} U$$

$$\theta^a = -\varepsilon\,\nabla_a \log p(U) + \sqrt{2\varepsilon}\,\eta^a$$

Sampling from $|\psi|^2$

$$\boxed{\theta^a = -\varepsilon\, L_a[\log|\psi|^2] + \sqrt{2\varepsilon}\,\eta^a}$$

Stationary solution: $p_\infty(U) \propto |\psi(U)|^2$

Normalization at the next coupling

$$\int d\mathcal{U}\,|\psi_{g_{i+1}}|^2 \;=\; \left\langle \frac{|\psi_{g_{i+1}}(\mathcal{U})|^2}{|\psi_{g_i}(\mathcal{U})|^2} \right\rangle_{|\psi_{g_i}|^2}$$

Table of contents

U(1): single plaquette

$$\mathcal{U} = e^{i\phi}, \qquad L = -R = i\frac{\partial}{\partial\phi}.$$

Hamiltonian

$$H = -\frac{g^2}{2}\sum_k \frac{\partial^2}{\partial\phi_k^2} - \frac{2}{g^2}\sum_{\Box}\cos\phi_{\Box}.$$

Schrödinger equation after gauge fixing

$$\left(-2g^2\frac{d^2}{d\omega^2} - \frac{2}{g^2}\cos\omega\right)\psi(\omega) = E\psi(\omega).$$

U(1): single plaquette

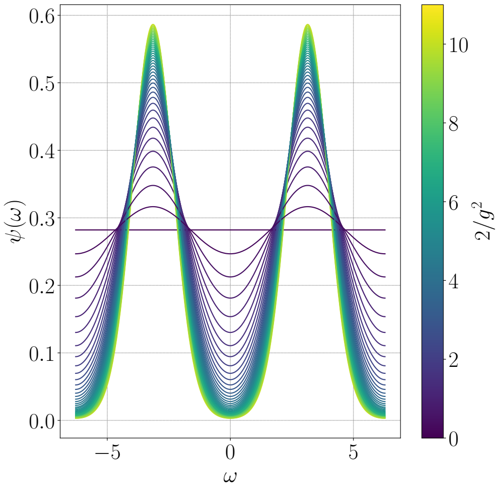
$$\mathcal{U} = e^{i\phi}, \qquad L = -R = i\frac{\partial}{\partial \phi}.$$

Hamiltonian

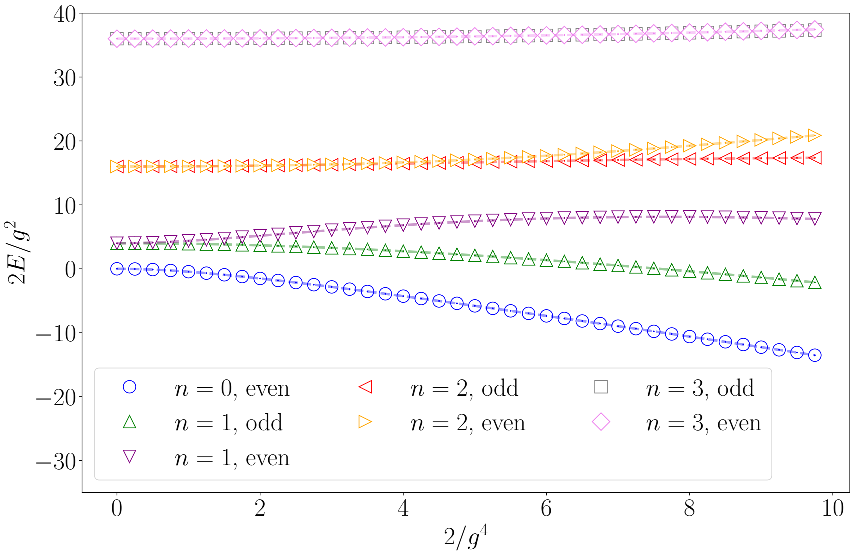
$$H = -\frac{g^2}{2}\sum_k \frac{\partial^2}{\partial \phi_k^2} - \frac{2}{g^2}\sum_{\square} \cos\phi_{\square}.$$

Schrödinger equation after gauge fixing

$$\left(-2g^2\frac{d^2}{d\omega^2} - \frac{2}{g^2}\cos\omega\right)\psi(\omega) = E\psi(\omega).$$



U(1) spectrum: PINNs VS exact results



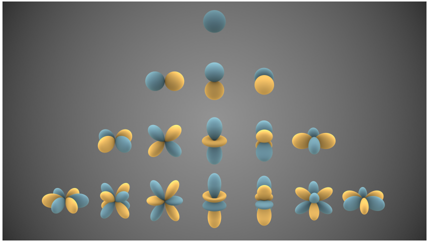
SU(2): single plaquette

Gauge link

$$\mathcal{U}(\omega,\theta,\phi) = \begin{pmatrix} \cos\frac{\omega}{2} - i\sin\frac{\omega}{2}\cos\theta & -i\sin\frac{\omega}{2}\sin\theta\, e^{-i\phi} \\ -i\sin\frac{\omega}{2}\sin\theta\, e^{i\phi} & \cos\frac{\omega}{2} + i\sin\frac{\omega}{2}\cos\theta \end{pmatrix}$$

Hamiltonian

$$H = 2g^2\left[\frac{\mathbb{L}^2}{4\sin^2\frac{\omega}{2}} - \frac{\partial^2}{\partial\omega^2} - \cot\frac{\omega}{2}\frac{\partial}{\partial\omega}\right] - \frac{4}{g^2}\cos\frac{\omega}{2}.$$



SU(2) after gauge fixing

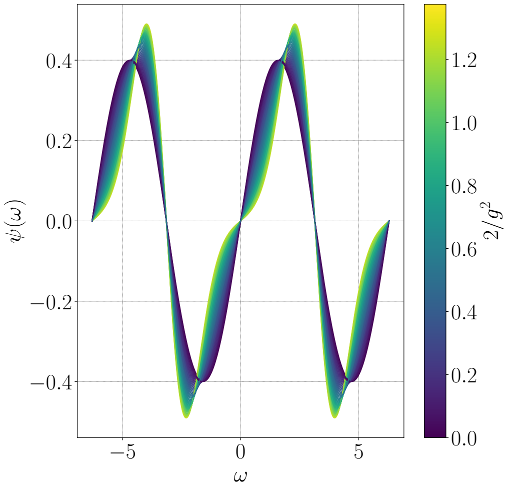
Gauss's law

$G_a^2 = \mathbb{L}^2$

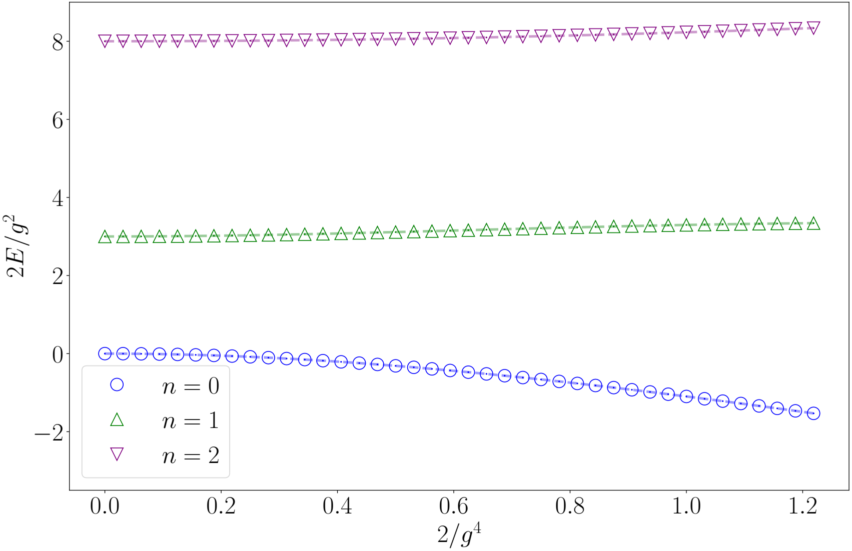
Gauge-invariant sector

$$\psi = Y_0^0(\theta,\phi)\,\frac{u(\omega)}{\sin(\omega/2)}$$

$$\left[-\frac{d^2}{d\omega^2} - \frac{1}{4} - \frac{2}{g^4}\cos\frac{\omega}{2}\right]u = \frac{E}{2g^2}u$$



SU(2) spectrum: PINNs VS exact results



Conclusion

Achievements

- PINNs can solve lattice gauge Schrödinger equation
- **L-CNN** $\implies$ gauge invariance by construction, no Gauss penalty
- Adiabatic training follows the RG flow $g : \infty \to 0$
- U(1) and SU(2) single-plaquette: exact agreement

Outlook

SU(3), larger volumes, fermions, real-time dynamics

Thank you for your attention!

Bibliography I

[1] Simone Romiti. "SU(N) lattice gauge theories with physics-informed neural networks". In: *Phys. Rev. D* 113 (2026), p. 054511. DOI: 10.1103/mb67-9rkf (cit. on pp. 2, 3).

[2] Kieran Holland, Andreas Ipp, David I. Müller, and Urs Wenger. "Machine learning a fixed point action for SU(3) gauge theory with a gauge equivariant convolutional neural network". In: *Phys. Rev. D* 110.7 (2024), p. 074502. DOI: 10.1103/PhysRevD.110.074502. arXiv: 2401.06481 [hep-lat] (cit. on p. 18).

[3] Matteo Favoni, Andreas Ipp, David I. Müller, and Daniel Schuh. "Lattice Gauge Equivariant Convolutional Neural Networks". In: (Dec. 2020). arXiv: 2012.12901 [hep-lat] (cit. on pp. 19, 20).