

SU(N) lattice gauge theories with physics-informed neural networks

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We present an application of physics-informed neural networks (PINNs) to the study of SU(N_c) lattice gauge theories. Our method enables the learning of eigenfunctions and eigenvalues at arbitrary gauge couplings, smoothly moving from the analytically known strong-coupling regime toward weaker couplings. By encoding the Schrödinger equation and the symmetries of the eigenstates directly into the loss function, the network performs an unsupervised exploration of the spectrum. We validate the approach on the single-plaquette U(1) and SU(2) pure-gauge theories, showing that the PINNs successfully reproduce the hierarchy of energy levels and their corresponding wave functions.

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I. INTRODUCTION

The lattice formulation allows the study of strongly interacting quantum field theories from the first principles of the theory [1,2]. In this formalism, Monte Carlo (MC) techniques are able to approximate the path integral, so that one can extract physical observables from correlation functions [3]. However, despite their successes, MC techniques suffer from fundamental limitations, such as the impossibility to simulate real-time dynamics, the sign problem [4], topological freezing [5,6] and critical slowing down [7,8].

The above limitations are absent if we resort to the Hamiltonian formulation, which works directly at the level of the Schrödinger equations [9]. In recent years this approach has seen a revived interest through quantum computing (QC) [10] and tensor networks (TNs) [11], which work by truncating the infinite-dimensional Hilbert space and extrapolating the result to the infinite-truncation limit. While these techniques remain promising to mitigate Hilbert space size scaling cost, several present applications are still limited to a moderate number of lattice degrees of freedom.

In this paper we propose and explore a novel approach based on physics-informed neural networks (PINNs) [12], applied to the solution of the eigenvalue equation for SU(N_c) lattice gauge theories. We use machine learning to build models that represent the wave functions of the

lattice Hamiltonian, and in the learning process we also learn their corresponding eigenvalues. The result is a prediction of the ladder of energies and eigenstates of the theory, for ranges of the coupling where their analytic expression is not known. In this work we show that it is possible to achieve this goal by using *adiabatic PINNs*: we start from the strong-coupling regime, where we are able to write the eigenstates analytically, and move progressively to the weak-coupling regime (see Sec. III for more details).

For the training of PINNs we sample points in the function domain and penalize, through the loss function, the violation of specific integral and differential constraints. In our case these are the eigenvalue equation, the symmetries of the wave function and its normalization. This feature allows to solve the time-independent Schrödinger equation at nontrivial couplings, without the need of a validation set from the target eigenfunction [13]. Moreover, PINNs do not impose an explicit truncation of the Hilbert space. The accuracy of the result is dictated by the quality of the sampled configurations and choice of the loss function.

In this work we develop the general method for SU(N_c) gauge theories. In order to demonstrate and benchmark the approach, we reproduce the known analytic results for pure-gauge U(1) and SU(2) lattice gauge theories, in the limit of a single plaquette system [14,15].

The paper is structured as follows. In Sec. II we recall some theoretical background. Section III describes our adiabatic PINN method and in Sec. IV we show our results for the single-plaquette system. Finally, in Sec. V we draw our conclusions and discuss future developments. In order to improve the readability of the main sections, we have collected some more technical details in the Appendices. In Appendix A we recall the formulation of the SU(N_c) lattice Hamiltonian, and in Appendix B we describe the gauge-fixing procedure.

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II. THEORETICAL BACKGROUND

In quantum mechanics [9], solving a theory requires to fully identify the physical states by their symmetries and solving the time-independent (i.e., eigenvalue) Schrödinger equation

$$H|\vec{\alpha}, E\rangle = E|\vec{\alpha}, E\rangle. \quad (2.1)$$

Here H is the Hamiltonian, E is the energy and $\vec{\alpha}$ is the set of all the other quantum numbers dictated by the eigenvalues of the symmetries operators. At this point the time-dependent Schrödinger equation dictates how the states evolve in time.

Except for a few examples [16], solving analytically the eigenvalue equation is in general not possible, requiring the use of numerical tools. An example is the case of strongly interacting $SU(N_c)$ gauge theories [17]. On the lattice [18,19], in the wave function formalism, the eigenvalue equation becomes a partial differential equation (PDE) coupling neighboring degrees of freedom. For instance, in a pure-gauge theory it reads [cf. Eq. (A4)]¹:

$$\left[\frac{g^2}{2} \sum_{\vec{x}} \sum_{\mu=1}^{d-1} \sum_{a=1}^{N_g} (L_a)_\mu^2(\vec{x}) - \frac{2}{g^2} \sum_{\vec{x}} \sum_{\mu=1, \nu < \mu}^{d-1} \text{ReTr}[\mathcal{U}_{\mu\nu}(\vec{x})] \right] \psi(\mathcal{U}) = E\psi(\mathcal{U}), \quad (2.2)$$

where $\psi(\mathcal{U}) = \langle \mathcal{U} | \psi \rangle$ is the wave function of the whole configuration of gauge links. The individual links $\mathcal{U}_\mu(\vec{x})$ are elements of the gauge group $SU(N_c)$, and can be parametrized in terms of N_g angles $(\theta^a)_\mu(\vec{x})$, where N_g is the number of generators of the Lie algebra (see Sec. A). Since, for each $\vec{x}$ and μ , the L_a are differential operators in the angles θ^a , Eq. (2.2) is in fact a PDE in the variables $(\theta^a)_\mu(\vec{x})$.

The eigenvalue equation does not fully determine the properties of the state. First, the eigenvalue may be degenerate, requiring to specify the other quantum numbers in order to fully determine it. Second, the wave function can be multiplied by an arbitrary constant complex number (phase and normalization). The choice of the phase can be fixed by, e.g., imposing that ψ should be real at given configuration, while the normalization is fixed by imposing the total probability to be 1 [1,9]

$$\int \mathcal{D}\mathcal{U} |\psi(\mathcal{U})|^2 = 1, \quad (2.3)$$

where $\mathcal{D}\mathcal{U}$ is the Haar measure of the gauge group. Finally, the physical states must be gauge-invariant, i.e.,

¹We work in natural units, $\hbar = c = 1$, and measure all quantities in units of the lattice spacing. The sign of the coupling g is immaterial; we adopt the convention $g > 0$ throughout.

$$G_a(\vec{x})\psi(\mathcal{U}) = 0, \quad \forall a, \vec{x}. \quad (2.4)$$

The $G_a(\vec{x})$ are also differential operators in the angles $(\theta^a)_\mu(\vec{x})$, that represent the generators of gauge transformations (see Sec. A).

III. STRATEGY FOR TRAINING THE NEURAL NETWORK

In this section we describe our general strategy to solve the time-independent Schrödinger equation with PINNs. We discuss how to find numerically the dependence of a set of eigenstates (and eigenvalues) as a function of the gauge coupling, moving away *adiabatically* from the strong-coupling limit.

A. Adiabatic training and existence of the solution

Training a network at an arbitrary coupling in order to “just solve” the eigenvalue equation is an ill-posed numerical problem: in general there exist multiple solutions with the same quantum numbers except for the energy. This does not simply make the convergence to the solution very hard, but even if successful it does not inform about where in the spectrum hierarchy one landed. For these reasons, we propose an algorithm defined in terms of the adiabatic approximation theorem of quantum mechanics [9]. According to the theorem, a physical state remains in its instantaneous eigenstate if the Hamiltonian H changes slowly over time and a energy gap with the other states is preserved. On a finite volume, the latter condition is fulfilled because the spectrum is discrete for $SU(N_c)$ theories on a torus [20]. We apply the concept of the adiabatic evolution to an Hamiltonian whose coupling changes over the training time, and interpret the training process from one coupling to the other as a quantum time evolution with a time-dependent Hamiltonian. In this sense, the algorithm presented in this work predicts the coupling dependencies of eigenfunctions and energies of the system, using the strong-coupling limit as a starting point and flowing to larger values of $1/g$.

The adiabatic theorem also guarantees the existence of the solution according to this procedure. In fact, let us assume that we have a perfect model that describes our normalized eigenstate of $H(g_1)$ at some coupling g_1 . We now refine it to become an eigenstate of $H(g_2)$ and by enforcing the normalization condition exactly while training. Since the norm does not change, by definition, the latter condition means that we are evolving the state with a unitary operator. If our model converges to an eigenstate of $H(g_2)$, we have performed a time-evolution of the eigenstate from the couplings g_1 to g_2 . The adiabatic theorem ensures that if we have done it sufficiently slowly we have not moved from the instantaneous eigenstate. In Fig. 1 we show a pictorial representation of this process.

We remark that in the $1/g \rightarrow 0$ limit the wave function of the electric vacuum $|0\rangle_E$ is known analytically: the electric

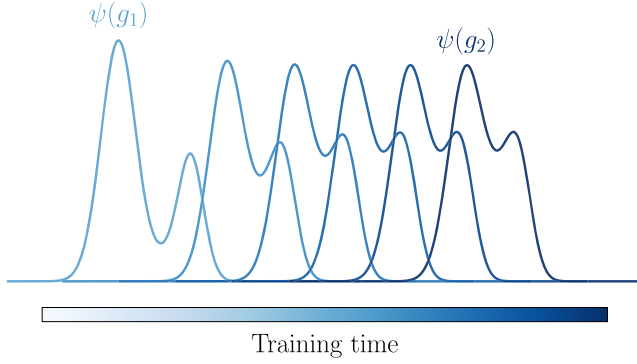


FIG. 1. Pictorial representation of the ideal adiabatic learning described in the text. The normalization of the state and the eigenvalue equation are imposed throughout, while we evolve the coupling smoothly from g_1 to g_2 (from left to right). The eigenfunction $\psi(g_1)$ remains in its instantaneous eigenstate, with final form given by $\psi(g_2)$.

Hamiltonian is a semipositive definite differential operator, so that its vacuum is proportional to the identity function of the gauge links. Moreover, by acting with gauge-invariant loop operators on $|0\rangle_E$ we obtain the expression of the electric eigenstates and an (overcomplete) basis for the Hilbert space of physical states [19,21,22]. Appropriate combinations of the latter isolate the desired quantum numbers: momentum projection, parity, etc. For each strong-coupling eigenstate, we train a network on the analytic result and progressively fine-tune it at subsequent couplings.

Summarizing, our method consists in a set of individual and separate trainings, one for each eigenstate of the Hamiltonian. For each of them, we consider the analytic eigenfunction and eigenvalue at $1/g \rightarrow 0$, and train the neural network on a set of sampled configurations. At this point we save the result, restart by loading the model that we have just trained, and retrain it with a slightly different new coupling. At this point we do not have an analytic result anymore, and we are able to learn the solution by imposing only physical constraints. During the training we learn the new eigenfunction of that eigenstate and its energy (now treated as a training parameter). Once the training is completed, we move to a larger value of $1/g$, and repeat the procedure iteratively. In this way we learn how the eigenfunctions and their energies move along the renormalization flow of the theory, as the cutoff $1/a$ is pushed to infinity with increasing $1/g$. A schematic representation of the protocol is given by the Algorithm 1.

The idea of using PINNs comes from the fact that it is a form of unsupervised learning for a model (and potentially external parameters) without prior knowledge on the values of the target function. One of their advantages is that neural networks offer an easy way of implementing autodifferentiation, so that the derivatives of the model with respect to the inputs can be computed exactly. In this way one can

Algorithm 1. Pseudoadiabatic protocol for PINN training at coupling g^{-1} .

```

1: Input: Coupling  $g^{-1}$ , small step size  $\Delta g^{-1}$ 
2: if  $g^{-1} = 0$  then
3:   Initialize new model. Energy known exactly.
4:   Train with MSE loss on sampling points
5: else
6:   Load model from previous coupling.  $g_{\text{old}}^{-1} = (g^{-1} - \Delta g^{-1})$ 
7:   Energy not known, treated as training parameter.
8:   Train with composite PINN loss function.
9: end if
10: Output: Trained eigenfunction  $\psi$  and energy  $E(g^{-1})$ .

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impose differential and boundary conditions that completely identify the solution of a PDE. The element of innovation here is that we exploit the analytic results in a given coupling regime ($1/g \rightarrow 0$), and use them as a seed to flow adiabatically to other values of the coupling.

We remark that the above adiabatic argument is theoretical: our initial model will hardly be perfect, we do not know *a priori* how slowly we should change the coupling, and numerically we cannot enforce the normalization condition exactly. The latter limitation stems not simply from machine precision, but also from the fact that since at each iteration we do not know the eigenfunction at the new coupling, we inevitably commit sampling errors when estimating the normalization integral. However, up to these numerical approximation problems, we stress that the adiabatic theorem guarantees the validity of the protocol. Moreover, we can always check *a posteriori* the consistency of our results by, e.g., changing the coupling at lower rates, activating smoothly different contributions to the Hamiltonian, or even running the algorithm backward (from weaker toward stronger couplings), and verify that we get the same result at intermediate values.

B. Choice of the loss function

In this section we describe our choice for the loss function. We limit ourselves to pure-gauge theories, deferring the study of theories with fermions to a future work. The latter generalization does not add further differential operators, but requires to simply encode the dependency on the fermions configurations as well as the action of the Hamiltonian on the wave function.

In Sec. III A we have described how in principle one can take an eigenstate $|\phi_n\rangle$ in the strong-coupling limit and predict the coupling flow of its wave function and energy. We realize this by taking the analytic values of ϕ_n and training the model on them. For this we use the mean-square-error (MSE) loss function

$$\mathcal{L}^{(1/g \rightarrow 0)} = \frac{1}{N_{\text{pt}}} \sum_{i=1}^{N_{\text{pt}}} |\psi(\mathcal{U}_i) - \phi_n(\mathcal{U}_i)|^2, \quad (3.1)$$

where N_{pt} is the number of points sampled in configuration space, and the energy is fixed to its exact value during the training. This number can be changed at will for different couplings, while the strong-coupling provides a rough estimate for the necessary network size.

At progressively weaker couplings, we first load the model at the previous coupling, and enforce the time-independent Schrödinger equation both on the wave function ψ and energy E (which is now a trainable parameter). We use the following loss function:

$$\mathcal{L}^{(1/g \neq 0)} = \omega_{\text{PDE}} \mathcal{L}_{\text{PDE}} + \omega_{\text{norm}} \mathcal{L}_{\text{norm}} + \omega_{\text{symm}} \mathcal{L}_{\text{symm}}, \quad (3.2)$$

where ω_{PDE} , ω_{norm} , ω_{symm} are meta-parameters of the training that act as weights for the gradients of the loss function contributions. The individual terms are:

$$\mathcal{L}_{\text{PDE}} = \frac{1}{N_{\text{pt}}} \sum_{i=1}^{N_{\text{pt}}} |(H - E)\psi(\mathcal{U}_i)|^2, \quad (3.3)$$

$$\mathcal{L}_{\text{norm}} = \left(1 - \sqrt{\int d\mathcal{U} |\psi(\mathcal{U})|^2} \right)^2, \quad (3.4)$$

where $\mathcal{U}_i$ is the i th sampled configuration of links, $\mathcal{L}_{\text{symm}}$ is a term that enforces the specific symmetries of the eigenstate in question and gauge invariance through Gauss's law. The latter is imposed through a term $\mathcal{L}_{\text{Gauss}}$ in the loss function

$$\mathcal{L}_{\text{Gauss}} = \frac{1}{N_{\text{pt}}} \sum_{i=1}^{N_{\text{pt}}} \sum_{\vec{x}} \sum_a |G_a(\vec{x})\psi(\mathcal{U}_i)|^2 \quad (3.5)$$

In practice, for the eigenfunctions studied in this work, we found that it was sufficient to impose $\omega_{\text{PDE}} = \omega_{\text{norm}} = \omega_{\text{symm}} = 1$.

The norm entering in the loss of Eq. (3.4) is obtained at each training step as a Monte Carlo approximation over N_{pt} configurations

$$\int d\mathcal{U} |\psi(\mathcal{U})|^2 \approx \Omega \frac{1}{N_{\text{pt}}} \sum_{i=1}^{N_{\text{pt}}} |\psi(\mathcal{U}_i)|^2, \quad (3.6)$$

where Ω is the total Haar measure of all the links [1]. We remark that this introduces a sampling error, as we do not know yet the analytic form of the wave function and we necessarily have to sample from the one at the previous coupling. Moreover, even if we knew ψ exactly, the sampling could still remain a challenging task due to multimodalities of the $|\psi(\mathcal{U})|^2$ distribution. In the numerical calculations of this work it was sufficient to always finely sample the phase space uniformly. For future investigations, it would be interesting to consider Nested Sampling [23], which is well-suited for exploring multimodal distributions.

Work on applying this method to gauge theories is presently underway [24].

C. Network architecture and learning process

In this work we use fully connected neural networks (FCNNs) with $\tanh$ activation function, as model templates for the eigenfunctions. This choice is led by the universal approximation theorems of neural networks [25] and the fact that for the physical systems and regimes studied in this work, these networks proved to be complex enough to capture the physical features of the eigenstates. While the same choice was successful in other applications of PINNs [26–30], we recognize that it would be interesting to understand in a future work how different network architectures affect the efficiency.

Our networks take as inputs the angles parametrizing the links of the lattice, pass them to 2 hidden layers made of 512 neurons each throughout, and return the wave function value (see Fig. 2).

In order to avoid overfitting, we have included weight decay [31] using the AdamW algorithm [32] for minimization. The above choices were sufficient for our proof-of-principle application to demonstrate the method. We used the strong-coupling limit of the theory ($1/g \rightarrow 0$) to get an estimate of the above network size needed to capture the complexity of the wave functions. We used $N_{\text{pt}} = 10^4$ points throughout, obtained from a uniform sampling in configuration space. At intermediate couplings, we have checked that increasing the network size and number of points was keeping the results stable.

We conclude this section by reporting our strategy for the choice of the learning rate ϵ_r , responsible for the convergence speed toward the minimum of the loss function through gradient descent. If ϵ_r is too large, we make too coarse steps and we may never converge, while if it is too small we may spend too much time to find the solution and risk of falling in a local minimum. The tradeoff we adopted for our trainings in this work was to fix an initial learning rate, and use a “reduce on plateau” scheduler for its update [33].² In practice, we find empirically the initial value of ϵ_r and of the patience, so that during the training ϵ_r is automatically reduced when the optimizer is not reducing the loss function within a patience window.

During the network training we used the following stopping criterion. Since the energy E of the state is a trained parameter, we also construct during the training the following estimator:

$$E_{\text{est.}} = \frac{\int d\mathcal{U} \psi^*(\mathcal{U}) [H\psi(\mathcal{U})]}{\int d\mathcal{U} |\psi(\mathcal{U})|^2}, \quad (3.7)$$

²While this was sufficient for our study, for the future we plan to consider other unsupervised learning rate schedulers such as Twin [34].

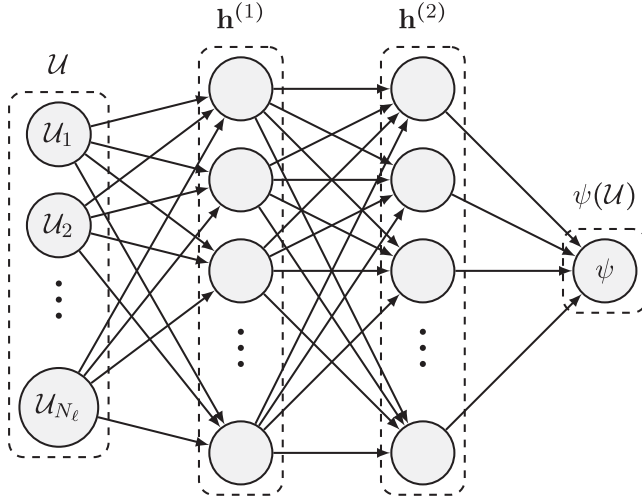


FIG. 2. Illustrative representation of the fully connected-neural network used in this work to train the eigenfunctions. The inputs are the gauge links of the lattice (in the form of the angles needed to parametrize them), which are passed to the hidden layers $h^{(1)}$, $h^{(2)}$ to output the wave function ψ . Each layer uses a $\tanh$ activation function.

which is the definition of the energy as expectation value. The ratio $r = \frac{(E - E_{\text{est}})}{E}$ gives a measure of the stability of the training. For the specific applications of this work it was sufficient to end the training either when ϵ_r went below 10^{-8} , or when reaching 10^5 epochs. In this way, we always obtain $r < 10^{-3}$ at the end of the training.

IV. RESULTS FOR THE SINGLE-PLAQUETTE SYSTEM

In this section we compare our findings with known analytical results for pure-gauge U(1) and SU(2) theories, in the limit of a single-plaquette system. The latter are obtained in a gauge-fixed Hamiltonian. We defer to Sec. B for a recap on gauge fixing and the corresponding construction of the Hamiltonian. For a single plaquette, fixing the gauge simplifies the training of the PINNs, as the time-independent Schrödinger equation reduces to an ordinary differential equation. A Python implementation is publicly available at Ref. [35].

Before presenting the specific case of U(1) and SU(2) we recall the following properties. The wave function has the form $\psi(\mathcal{U}_1, \dots, \mathcal{U}_{N_\ell})$, where $\mathcal{U}_k$ are the gauge links of the lattice. In the strong-coupling limit, $1/g \rightarrow 0$, the (electric) ground state ψ_0 is the identity function, and the Hilbert space of gauge invariant wave functions is spanned by traces of Wilson loops $\mathcal{L}$ applied to it [19,21,22]: $\text{Tr}[\mathcal{L}] \cdot \psi_0$. For a single-plaquette system, in this limit the eigenfunctions are the result of the repeated application of the only available Wilson loop (the plaquette operator) n times to the electric vacuum.

A. U(1) gauge theory

For U(1) we have only one generator in the Lie algebra, and each of the N_ℓ links is parametrized by a single angle. Therefore, a link and its canonical momentum admit the following representation:

$$\mathcal{U} = e^{i\phi}, \quad \phi \in [0, 2\pi], \quad (4.1)$$

$$L = -R = i \frac{\partial}{\partial \phi}. \quad (4.2)$$

The Hamiltonian reads

$$H = -\frac{g^2}{2} \sum_{k=1}^{N_\ell} \frac{\partial^2}{\partial \phi_k^2} - \frac{2}{g^2} \sum_{\square} \cos \phi_{\square}, \quad (4.3)$$

where $\phi_{\square}$ is the total phase accumulated by multiplying the links around a plaquette $\square$. When we restrict to a single plaquette and fix the gauge of the maximal tree, we get the following Hamiltonian [cf., Eq. (B4)]:

$$H = -2g^2 \frac{d^2}{d\omega^2} - \frac{2}{g^2} \cos \omega, \quad (4.4)$$

where ω is the angle that parametrizes the only active link. In this way, the eigenvalue equation $H\psi = E\psi$ in the variable $z = \omega/2$ becomes the Mathieu equation [14,15]

$$\left[\frac{d^2}{dz^2} + \alpha - 2q \cos(2z) \right] \psi(e^{i2z}) = 0, \quad (4.5)$$

where $\alpha = 2E/g^2$ and $q = -2/g^4$. From a purely mathematical viewpoint, the solutions are the Mathieu functions $\text{ce}_n(z, q)$ and $\text{se}_n(z, q)$, together with their pseudoperiodic partners from Floquet theorem (see, e.g., Refs. [36–39]). Of these solutions however, physically we can consider

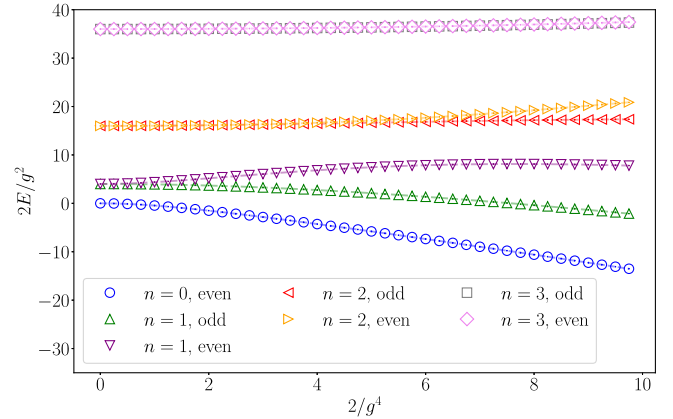


FIG. 3. First energy levels for the even and odd eigenfunctions of a U(1) single-plaquette system. The discrete points represent our prediction obtained with a PINN, while the dashed lines correspond to the exact analytic values.

only the π -periodic ones in z , as ψ has this period by construction.

In the strong-coupling limit $q \rightarrow 0$, and the eigenfunctions are the complex exponentials $\psi_n = e^{in\omega}$ with eigenvalues $E_n = 2g^2 n^2$. As anticipated before, we observe that these are indeed the result of the (untraced) plaquette operator applied to the electric vacuum.

As described in Sec. III, for each eigenstate we first train a model on its strong coupling limit ($q = 0$). From that model, we move to the weak-coupling regime (larger q) by imposing the normalization condition, the fulfillment of Eq. (4.5), and the correct periodicity and parity of the eigenfunction. In Fig. 3 we show the energies of the first few eigenstates determined with our PINN method, compared to the analytic results. In Fig. 4 we show the learned wave function's coupling flow, and in Fig. 5 we plot the

matching of the exact and trained eigenfunction. Finally, in Fig. 6 we show the typical behavior of the loss function and of the energy during the training.

B. SU(2) gauge theory

For SU(2) we have 3 generators in the Lie algebra, so that each of the N_ℓ links is parametrized by 3 angles. A possible choice of the basis for the k th link is [40]

$$\begin{aligned} \mathcal{U}_k &= \mathcal{U}(\omega_k, \theta_k, \phi_k) \\ &= \begin{pmatrix} \cos \frac{\omega_k}{2} - i \sin \frac{\omega_k}{2} \cos \theta_k & -i \sin \frac{\omega_k}{2} \sin \theta_k e^{-i\phi_k} \\ -i \sin \frac{\omega_k}{2} \sin \theta_k e^{i\phi_k} & \cos \frac{\omega_k}{2} + i \sin \frac{\omega_k}{2} \cos \theta_k \end{pmatrix}. \end{aligned} \quad (4.6)$$

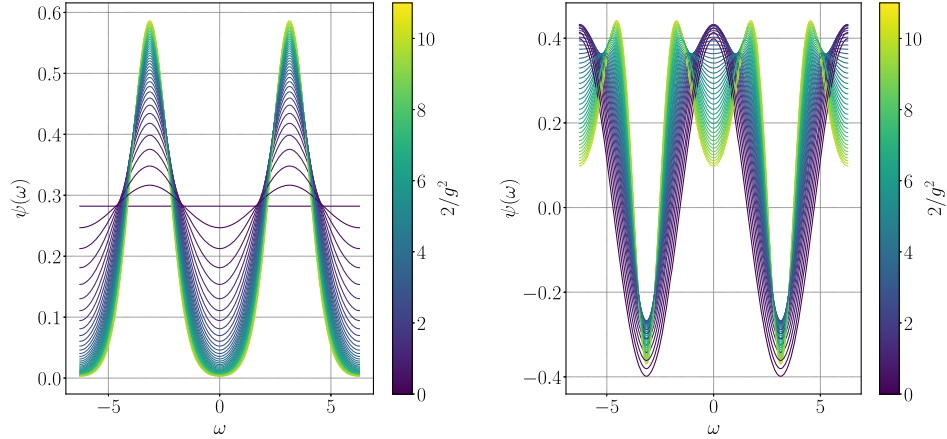


FIG. 4. Learned eigenfunction ψ for the ground state (left panel) and second excited state (right panel) of a single-plaquette U(1) system. On the horizontal axis, ω is such that $\cos \omega$ is the real part of the trace of the plaquette. Different curves correspond to different couplings, according to the color map on the side. Each curve is obtained by fine-tuning the model from the previous coupling. At $1/g \rightarrow 0$ the network is trained on the analytic expression.

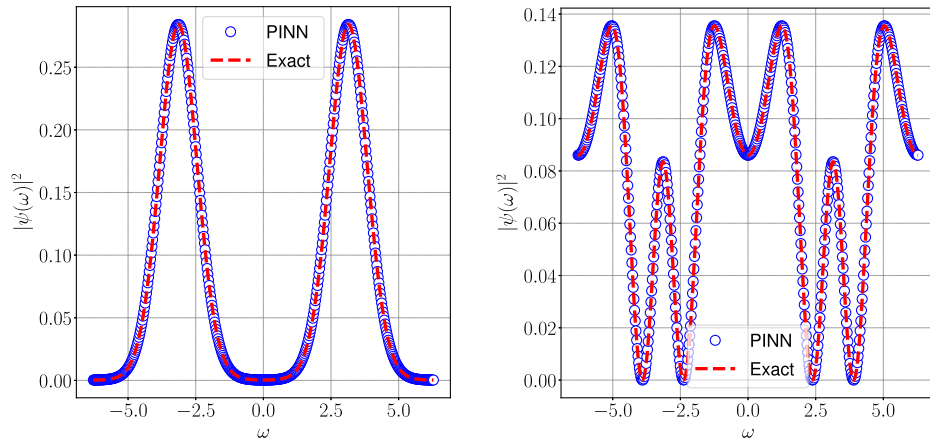


FIG. 5. Comparison of learned eigenfunction (open points) and exact result (dashed line) at the intermediate coupling $2/g^2 = 5.0$. The left and right panel correspond respectively to the ground state and 2nd excited state eigenfunctions, for a U(1) single-plaquette system.

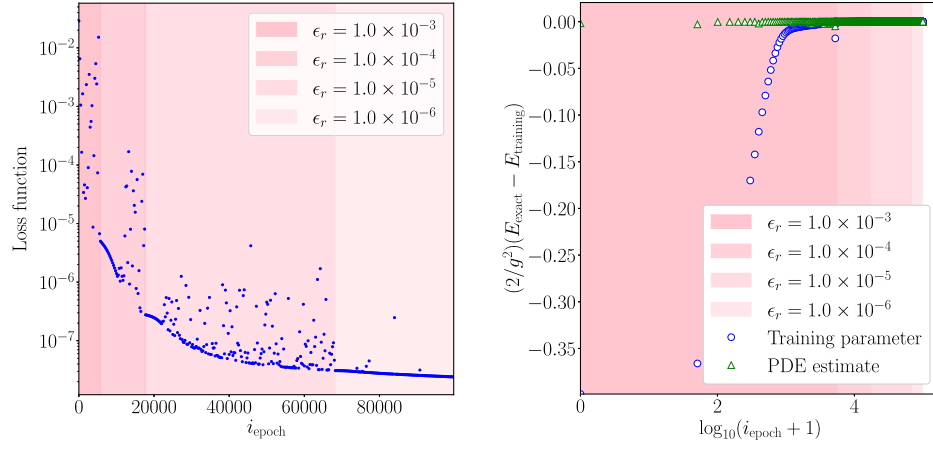


FIG. 6. Loss function (left) and energy (right) during the training, for the ground state of a single-plaquette U(1) system, at $2/g^2 = 5.0$. The different color bands correspond to different learning rates ϵ_r , scheduled according to a reduction-on-plateau criterion. The right panel shows the convergence of the energy parameter and the estimator of Eq. (3.7) to the exact value.

In this basis the Hamiltonian reads (see Sec. A)

$$H = \frac{g^2}{2} \sum_{k=1}^{N_\ell} \left[\frac{\mathbb{L}^2(\theta_k, \phi_k)}{4 \sin^2 \frac{\omega_k}{2}} - \frac{\partial^2}{\partial \omega_k^2} - \cot \frac{\omega_k}{2} \frac{\partial}{\partial \omega_k} \right] - \frac{2}{g^2} \sum_{\square} \cos \varphi_{\square}, \quad (4.7)$$

where:

$$\mathbb{L}^2(\theta_k, \phi_k) = -\frac{\partial^2}{\partial \theta_k^2} - \cot \theta_k \frac{\partial}{\partial \theta_k} - \frac{1}{\sin^2 \theta_k} \frac{\partial^2}{\partial \phi_k^2}, \quad (4.8)$$

and $\cos \varphi_{\square}$ is the real part of the trace of the product of links around a plaquette $\square$.

When considering a single plaquette in SU(2), we have only one active link (see Sec. B). If we call ω , θ , ϕ the angles parametrizing it, the Hamiltonian becomes [cf., Eq. (B4)]

$$H = 2g^2 \left[\frac{\mathbb{L}^2(\theta, \phi)}{4 \sin^2 \frac{\omega}{2}} - \frac{\partial^2}{\partial \omega^2} - \cot \frac{\omega}{2} \frac{\partial}{\partial \omega} \right] - \frac{4}{g^2} \cos \frac{\omega}{2}. \quad (4.9)$$

We realize that $\mathbb{L}^2$ is the square of the usual angular momentum operators [9], whose eigenfunctions are the spherical harmonics $Y_\ell^m(\theta, \phi)$. Moreover, for this system, the Gauss's law generators are the angular momentum operators in the angles θ and ϕ [40]. Thus, Gauss' law restricts the physical subspace to the states with $\ell = m = 0$, and all gauge-invariant wave functions have the form

$$\psi(\omega, \theta, \phi) = Y_0^0(\theta, \phi) \frac{u(\omega)}{\sin \omega/2} \quad (4.10)$$

In this way the time-independent Schrödinger equation becomes separable in ω , with a trivial dependence on

θ, ϕ fixed by gauge invariance. The latter is a special feature of SU(2) and this choice of angular basis.

The ω -dependent part of the Hamiltonian on the physical space reads

$$H = 2g^2 \left(-\frac{d^2}{d\omega^2} - \cot \frac{\omega}{2} \frac{d}{d\omega} \right) - \frac{4}{g^2} \cos \frac{\omega}{2}. \quad (4.11)$$

When acting on $\frac{u(\omega)}{\sin \omega/2}$ the time-independent Schrödinger equation $H\psi = E\psi$ simplifies to

$$\left[-\frac{d^2}{d\omega^2} - \frac{1}{4} - \frac{2}{g^4} \cos \frac{\omega}{2} \right] u(\omega) = \frac{E}{2g^2} u(\omega). \quad (4.12)$$

In the variable $z = \omega/4$, Eq. (4.12) becomes the Mathieu equation [14,15] (similarly to the U(1) case of Sec. IV A)

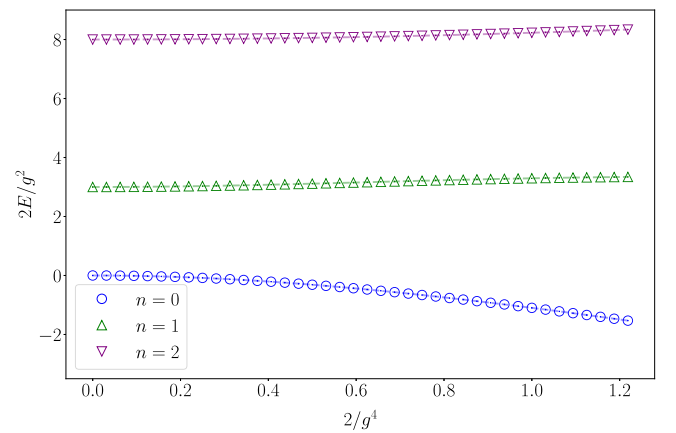


FIG. 7. Energy levels for a SU(2) single-plaquette system. The discrete points represent our prediction obtained with a PINN, while the dashed lines correspond to the exact values.

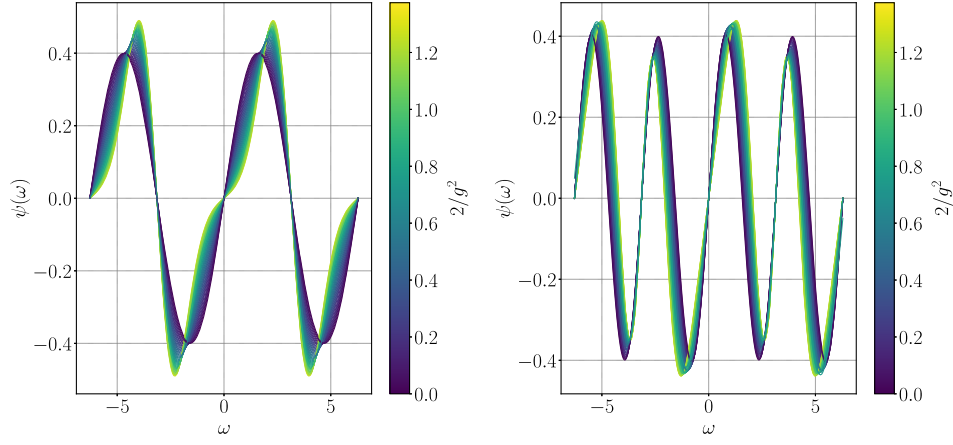


FIG. 8. Learned eigenfunction ψ for the ground state (left panel) and first excited state (right panel) of a single-plaquette SU(2) system. On the horizontal axis, ω is such that $2 \cos(\omega/2)$ is the real part of the trace of the plaquette. Different curves correspond to different couplings, according to the color map on the side. Each curve is obtained by fine-tuning the model from the previous coupling. In the limit $1/g \rightarrow 0$ the network is trained on the analytic expression.

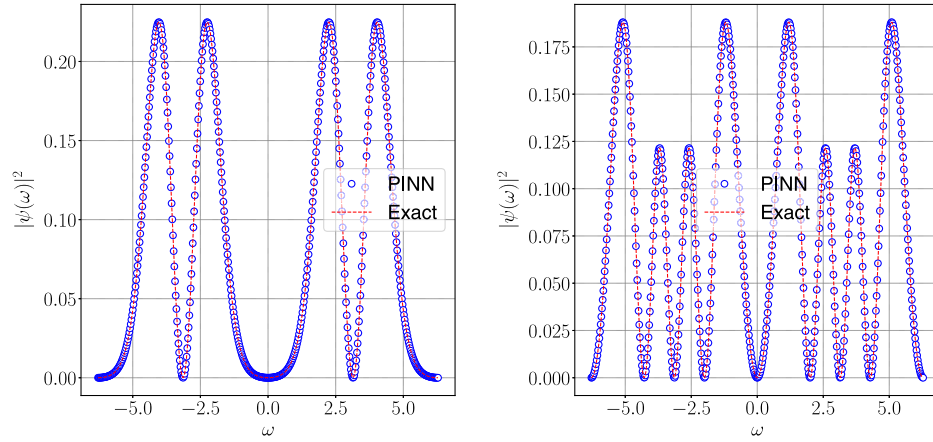


FIG. 9. Comparison of learned eigenfunction (open points) and exact result (dashed line) at the intermediate coupling $2/g^2 = 1.0$. The left panel is the ground state and the right one the 2nd excited state eigenfunction.

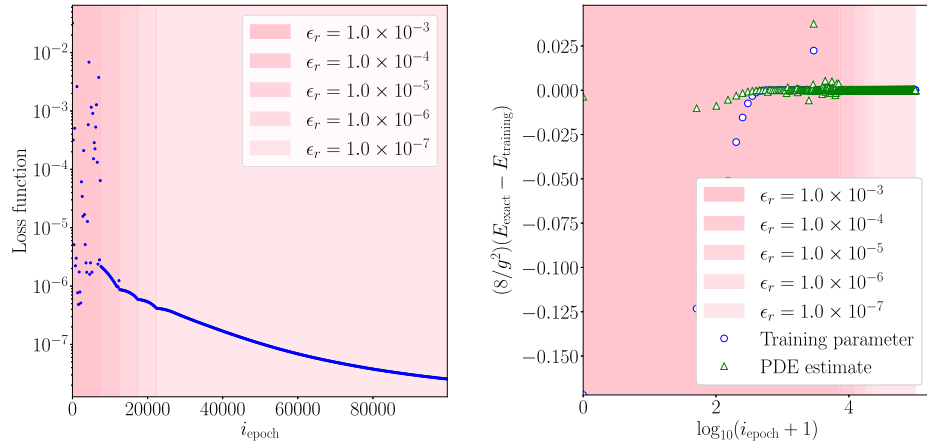


FIG. 10. Loss function (left) and energy (right) during the training, for the ground state of a single-plaquette SU(2) system, at $2/g^2 = 1.0$. Right panel: convergence of the energy parameter and the estimator of Eq. (3.7) with respect to the exact value. The different color bands correspond to different learning rates ϵ_r , scheduled according to a reduction-on-plateau criterion.

$$\left[\frac{d^2}{dz^2} + \alpha - 2q \cos(2z) \right] u(4z) = 0, \quad (4.13)$$

where $\alpha = (4 + 8E/g^2)$ and $q = -16/g^4$. In this case, the physical solutions $u(\omega)$ are the subset of Mathieu functions that are odd and π -periodic in z . In fact, the gauge invariant states are generated by traces of loops (and their powers). In SU(2), the latter depend on ω only through $\cos \omega/2$, which is even. Thus, $\psi(\omega) \sim \frac{u(\omega)}{\sin(\omega/2)}$ is even too, and 4π -periodic in ω by construction.

As described in Sec. III [and as we did for U(1) in Sec. IV A], we move to larger q by imposing a unit normalization, the fulfillment of Eq. (4.13), the correct periodicity, and the correct symmetry of the eigenfunction under a parity transformation. In Fig. 7 we show the learned energies of the first few eigenstates, as a function of the gauge coupling. In Fig. 8 we show the wave functions of the first few eigenstates at different couplings, and in Fig. 9 we compare to the exact results. Finally, in Fig. 10 we show the typical behavior of the loss function and of the energy during the training.

V. CONCLUSIONS AND OUTLOOK

In this work, we have introduced a neural network framework for solving SU(N_c) lattice gauge theories, verifying its applicability in the case of the single-plaquette spectrum of U(1) and SU(2) pure-gauge theories.

By incorporating the relevant physical constraints directly into PINNs, we have shown that one can reproduce the gauge coupling dependence of eigenfunctions and eigenvalues starting from the strong-coupling limit. This is achieved with a novel method based on an adiabatic flow of the Yang-Mills gauge coupling: from a known analytic eigenstate and its energy at $1/g \rightarrow 0$, it is possible to determine its dependence at larger values of $1/g$. The training process works by tuning the network to reproduce the correct wave function and learns its corresponding eigenvalue. At $1/g \neq 0$, this is achieved by enforcing physical constraints on the wave function, without the need of a validation set from the exact solution.

The input to the network is a set of sampled gauge configurations. This feature makes our PINN method a candidate for a scalable, multigrid-style path to approximate eigenstates of lattice gauge theories: one can train “coarse” representations (in configuration space), and progressively refine the sampling to fine-tune the eigenfunctions models. Finally, the proposed adiabatic PINNs method provides a transparent avenue to the calculation of matrix elements from the definition.

Future developments will focus on extending this framework to theories with fermionic degrees of freedom, to larger lattice volumes, and to gauge groups with higher color number N_c .

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DATA AVAILABILITY

The data that support the findings of this article can be reproduced with the open-source library available at Ref. [35].

APPENDIX A: HAMILTONIAN OF SU(N_c) GAUGE THEORIES ON THE LATTICE

The lattice action of an SU(N_c) gauge theory reads [1]

$$S = S_{\text{YM}}[\mathcal{U}] + S_{\text{F}}[\psi, \bar{\psi}, \mathcal{U}], \quad (\text{A1})$$

where the gauge links $\mathcal{U}_\mu(x) \in \text{SU}(N_c)$ and the fermionic fields $\psi(x), \bar{\psi}(x)$ are the degrees of freedom of the theory. The Yang-Mills action S_{YM} describes the dynamics of the bosonic fields and their self-interactions, while the fermionic action S_{F} describes fermions and their interactions with the bosons. There exist multiple regularizations for the lattice actions that differ only at nonvanishing lattice spacing. In this work we limit our attention to pure-gauge Yang-Mills (YM) theories, in the standard Wilson regularization [44,45]

$$S_{\text{YM}}^{\text{Wilson}} = -\frac{2}{g^2} \sum_x \sum_{\mu=0, \nu < \mu}^{d-1} \text{Re Tr}[\mathcal{U}_{\mu\nu}(x)]. \quad (\text{A2})$$

The above sum runs over all spacetime points x , d is the total number of dimensions and

$$\mathcal{U}_{\mu\nu}(x) = \mathcal{U}_\mu(x) \mathcal{U}_\nu(x + \mu) \mathcal{U}_\mu^\dagger(x + \nu) \mathcal{U}_\nu^\dagger(x). \quad (\text{A3})$$

The invariance under SU(N_c) transformations allows to fix a gauge. In the Weyl gauge ($\mathcal{U}_0(x) = \mathbb{1}$), using the transfer matrix formalism on the quantum theory and in the limit of vanishing temporal lattice spacing, we find the Kogut-Susskind Hamiltonian [44–47]³:

³This expression is consistent with, e.g., Refs. [44–47]. In the literature one can also find an additional factor (1/2) in front of H_B (see, e.g., Refs. [14,15,40]). The reason is that the choice of the constant K in front of H_B is just a convention in the definition of g and of the lattice spacing a [48]. Two different choices of K are related by matching the eigenvalues of the Hamiltonian in physical units: $(K_2/K_1) = (a_2/a_1)^2 = (g_2/g_1)^4$.

$$H = H_E + H_B = \frac{g^2}{2} \sum_{\vec{x}} \sum_{\mu=1}^{d-1} \sum_{a=1}^{N_g} (L_a)_\mu^2(\vec{x}) - \frac{1}{g^2} \sum_{\vec{x}} \sum_{\mu=1, \nu < \mu}^{d-1} \text{Tr}[U_{\mu\nu}(\vec{x}) + U_{\mu\nu}^\dagger(\vec{x})]. \quad (\text{A4})$$

H_E and H_B are the *electric* and *magnetic* contributions to the Hamiltonian. The sum in Eq. (A4) extends over the spatial lattice points and dimensions, and $U_\mu(\vec{x})$ and $(L_a)_\mu(\vec{x})$ are now operators in the Hilbert space $\mathcal{H}$. N_g is the number of generators of the gauge group's Lie algebra: $N_g = 1$ for $U(1)$ and $N_g = N_c^2 - 1$ for $SU(N_c)$. The *magnetic* basis for $\mathcal{H}$ is given by the configurations of links

$$|\mathcal{U}\rangle = \bigotimes_{\vec{x}} \bigotimes_{\mu=1}^{d-1} |\mathcal{U}_\mu(\vec{x})\rangle, \quad U_\mu(\vec{x})|\mathcal{U}\rangle = \mathcal{U}_\mu(\vec{x})|\mathcal{U}\rangle. \quad (\text{A5})$$

The canonical momenta, for each $\vec{x}$ and μ , are the left and right generators L_a, R_a . They satisfy the following properties and canonical commutation relations with their conjugated link U [45]

$$[L_a, R_b] = 0, \quad L_a^2 = R_a^2, \quad (\text{A6})$$

$$[L_a, L_b] = if_{abc} L_c, \quad [R_a, R_b] = if_{abc} R_c, \quad (\text{A7})$$

$$[L_a, U] = -\tau_a U, \quad [R_a, U] = U \tau_a, \quad (\text{A8})$$

where f_{abc} are the structure constants of $\mathfrak{su}(N_c)$ and τ_a its generators in color space. The residual gauge symmetry is generated by the Gauss's law operator, so that the physical states are only the subset of $\mathcal{H}$ satisfying

$$G_a(\vec{x})|\psi\rangle_{\text{phys}} = \left[\sum_{\mu=1}^d (L_a)_\mu(\vec{x}) + (R_a)_\mu(\vec{x} - \mu) \right] |\psi\rangle_{\text{phys}} = 0. \quad (\text{A9})$$

In the wave function formalism, in the links basis, the state of a system is described by a functional $\psi(\mathcal{U}) \in \mathbb{C}$. The

operators $U_\mu(\vec{x})$ are represented as $SU(N_c)$ matrices, and the L_a, R_a by Lie derivatives [45,49]

$$(L_a)_\mu(\vec{x})\psi(\dots, \mathcal{U}_\mu(\vec{x}), \dots) = -i \frac{d}{d\omega} \psi(\dots, e^{-i\omega\tau_a} \mathcal{U}_\mu(\vec{x}), \dots) \Big|_{\omega=0}, \quad (\text{A10})$$

$$(R_a)_\mu(\vec{x})\psi(\dots, \mathcal{U}_\mu(\vec{x}), \dots) = -i \frac{d}{d\omega} \psi(\dots, \mathcal{U}_\mu(\vec{x}) e^{i\omega\tau_a}, \dots) \Big|_{\omega=0}. \quad (\text{A11})$$

The latter equation implies that these are 1st-order differential operators. They can be also expressed in terms of the variables $(\theta^a)_\mu(\vec{x})$ parametrizing the $\mathcal{U}_\mu(\vec{x})$ as $\mathcal{U}_\mu(\vec{x}) = \exp(i(\theta^a)_\mu(\vec{x})\tau_a)$. At given N_c , the coefficients in front of each partial derivative ∂_{θ^a} can be found using the Maurer-Cartan 1-form (see Ref. [45] for a derivation).

APPENDIX B: GAUGE FIXING

In this section we provide a concise recap on gauge fixing, focusing on the peculiarities of the one-plaquette system discussed in Sec. IV.

$SU(N_c)$ gauge-symmetric field theories are invariant under local group transformations [17]. On the lattice, the degrees of freedom transform as [1]

$$\psi(x) \rightarrow \Omega(x)\psi(x) \quad (\text{fermionic fields}), \quad (\text{B1})$$

$$\mathcal{U}_\mu(x) \rightarrow \Omega(x)\mathcal{U}_\mu(x)\Omega^\dagger(x + a\hat{\mu}) \quad (\text{gauge links}), \quad (\text{B2})$$

where $\Omega(x)$ is a group element in the fundamental representation, a is the lattice spacing and $\hat{\mu}$ is the unit vector in the μ th axis. As a consequence, the description of the system contains some redundancy: some of the gauge links can be mapped to the identity without changing the content of the theory. Using the symmetry to fix some of the links to $\mathbb{1}$ is called *gauge fixing*, and the set with the largest number of gauge-fixable links constitutes a *maximal tree* [14,44]. Geometrically, the latter corresponds to a maximal set of links on the lattice that do not form any

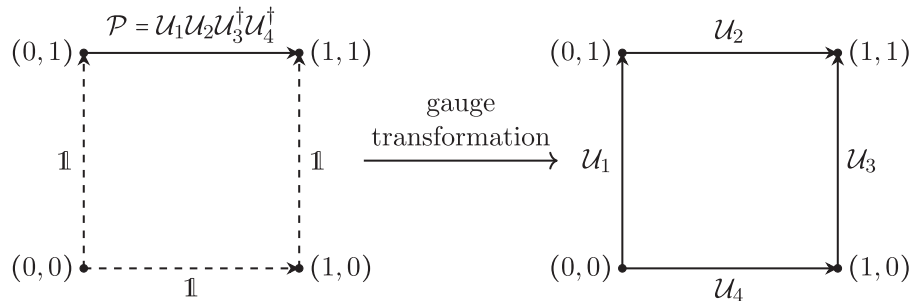


FIG. 11. Left: maximal tree (dashed lines) and active link (solid line) for a single plaquette system with open boundary conditions. Every value of the active link can be gauged to an arbitrary configuration of the four links (right), as in Eq. (B3).

closed loop. For a single plaquette with open boundary conditions for instance, the gauge-invariant combination $\mathcal{P} = \mathcal{U}_1 \mathcal{U}_2 \mathcal{U}_3^\dagger \mathcal{U}_4^\dagger$ is the only *active* link, from which any link configuration is obtained by a gauge transformation [40]

$$\begin{aligned} |\mathbb{1}, \mathcal{U}_1 \mathcal{U}_2 \mathcal{U}_3^\dagger \mathcal{U}_4^\dagger, \mathbb{1}, \mathbb{1}\rangle &\rightarrow |\mathbb{1}, \mathcal{U}_1 \mathcal{U}_2, \mathcal{U}_4 \mathcal{U}_3, \mathbb{1}\rangle \\ &\rightarrow |\mathbb{1}, \mathcal{U}_1 \mathcal{U}_2, \mathcal{U}_3, \mathcal{U}_4\rangle \\ &\rightarrow |\mathcal{U}_1, \mathcal{U}_2, \mathcal{U}_3, \mathcal{U}_4\rangle, \end{aligned} \quad (\text{B3})$$

where 1, 2, 3, 4 indicate the indices of the links in the plaquette as in Fig. 11.

In the Hamiltonian formalism, gauge symmetry is a result of the residual gauge freedom in the Weyl gauge, $U_0(x) = \mathbb{1}$, at each time slice [44]. In practice, when solving the theory we can either impose gauge-symmetry by hand through Gauss's law, work in a gauge-fixed Hilbert space directly or, equivalently, formulate the Hamiltonian and the Hilbert space in terms of gauge-invariant operators.

For the purpose of this work and in the context of pure-gauge $SU(N_c)$ gauge theories, we recall here the hybrid approach adopted in Ref. [40]. In fact, it turns out that we can write the Hamiltonian in terms of loop operators (and their canonical momenta) that are gauge invariant up to a gauge transformation at the origin of the lattice. Figure 12 provides a sketch of the loops construction in 2 spatial dimensions.

In particular, for the case of the one-plaquette problem analyzed in Sec. IV, the gauge-fixed Hamiltonian of Eq. (A4) reads

$$H = H_E + H_B = 2g^2 L_a^2(\kappa) - \frac{2}{g^2} \text{ReTr} P(\kappa), \quad (\text{B4})$$

where κ is the only active link of the one-plaquette system, $P(\kappa)$ the corresponding loop variable and $L_a(\kappa)$ are its

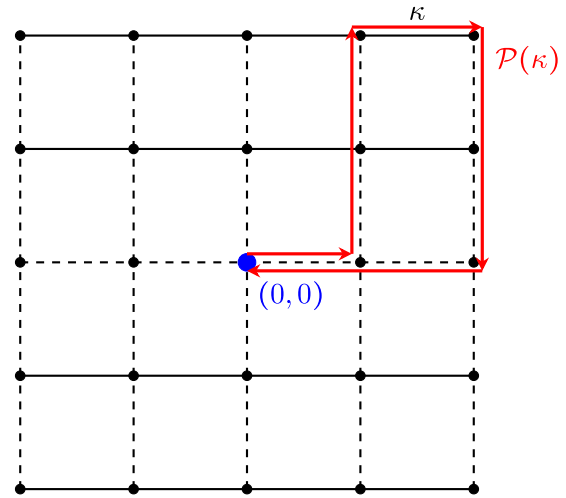


FIG. 12. Construction of loop operators on a lattice with 2 spatial dimensions, analogous to Ref. [40]. The dashed lines correspond to the links gauged to $\mathbb{1}$ in the maximal tree, while the solid lines are the active links. The loop is built walking from the origin and going through the respective active link. An explicit construction is shown for $P(\kappa)$, corresponding to an active link κ . The (untraced) loops are still gauge-variant under a gauge transformation at the origin.

associated canonical momenta. In the magnetic basis, $L_a(\kappa)$ is a differential operator in the angles defining $P(\kappa)$ [45]. If we use $\omega = \text{Arg}(\text{Tr} P(\kappa))$ as one of the angles, H_B will depend only on ω . In particular, for $U(1)$ and $SU(2)$ there is only one Casimir operator, thus H_E can depend only on ω because of gauge invariance. As a result, the time-independent Schrödinger equation for a one-plaquette system reduces to an ODE for the eigenvalues. For $N_c > 1$ the gauge is not fully fixed, and we also need to impose the fulfillment of the PDE corresponding to Gauss's law at the origin [14,40].

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