Accurate Ground States of SU(2) Lattice Gauge Theory in 2 + 1D and 3 + 1D

Thomas Spriggs[1,*] Eliska Greplova[1] Juan Carrasquilla[2] and Jannes Nys[2,†]
[1]QuTech and Kavli Institute of Nanoscience, Delft University of Technology, 2628 CJ, Delft, The Netherlands
[2]Institute for Theoretical Physics, ETH Zürich, 8093, Switzerland

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We present a neural network wave function framework for solving non-Abelian lattice gauge theories in a continuous group representation. Using a combination of SU(2) equivariant neural networks alongside an SU(2) invariant, physics-inspired ansatz, we learn a parametrization of the ground state wave function of SU(2) lattice gauge theory in $2+1$ and $3+1$ dimensions. Our method, performed in the Hamiltonian formulation, has a straightforward generalization to $\mathrm{SU}(N)$. We benchmark our approach against a solely invariant ansatz by computing the ground state energy, demonstrating the need for bespoke gauge equivariant transformations. We evaluate the Creutz ratio and average Wilson loop, and obtain results in strong agreement with perturbative expansions. Our method opens up an avenue for studying lattice gauge theories beyond one dimension, with efficient scaling to larger systems, and in a way that avoids both the sign problem and any discretization of the gauge group.

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Introduction—The standard model is currently our best candidate for the fundamental theory of the physical forces of our Universe. Constituent elements of the standard model include matter and gauge fields that are described by quantum field theory. One of these fundamental forces, the strong nuclear force, has been the subject of immense study. To arrive at a regularized, well-defined theory, Wilson reformulated the theory of strong interactions from a continuous space-time to one on a discrete, Euclidean lattice where time is imaginary and periodic [1]. Soon after, Kogut and Susskind introduced the Hamiltonian formulation that allowed time to remain real and continuous but proved numerically more challenging to solve [2]. These lattice gauge theories (LGTs) offer rich avenues for simulating and studying quantum field theories in nonperturbative regimes.

A plethora of numerical techniques emerged to study the Euclidean formulation of LGTs; quantum Monte Carlo (QMC) [3], one of the most successful approaches to simulating LGTs, has led to a range of new insights into the properties of nonperturbative systems from neutron starts [4] to high-energy physics and nuclear physics [5], for example by giving insight into the hadronic spectrum using lattice QCD [6–8]. See Ref. [9] for a pedagogical introduction to LGTs. Within this field, many advancements have been made to improve the efficiency of generating configurations of gauge fields—often the most computationally intensive part of any LGT measurement. These range from the introduction of hybrid Monte Carlo algorithms [10–12], to machine learning approaches like normalizing flows [13–16]. Despite their remarkable success, QMC-based methods face limitations in certain parameter regimes of LGTs, particularly when dealing with finite baryon chemical potentials, topological θ terms, or out-of-equilibrium phenomena. In such scenarios, the well-known sign problem renders the QMC numerical approach ineffective and unreliable [17–22].

In part guided by the limitation imposed by the sign problem, several methods have thus been applied to the Hamiltonian formulation of LGTs.

Tensor networks (TNs) and the density matrix renormalization group algorithm, given their immense progress in the field of condensed matter, have become useful tools to simulate LGTs and extract information about their entanglement structure [23–27]. These methods have demonstrated significant success in simulating LGTs in $1+1$ dimensions for both Abelian and non-Abelian gauge groups [23,24,27–47]. More recently, they have been applied to Abelian LGTs in up to $3+1$ dimensions [48–51], and non-Abelian theories with truncated gauge fields in Refs. [52] and [53] for $2+1$D SU(2) and $3+1$D SU(3), respectively.

Another pair of approaches to the simulation of Hamiltonian LGTs are digital quantum devices [54–61] and analog quantum simulators [62–67] (see Ref. [68] for a recent review). These have been used as novel platforms to gain insight into emergent properties of gauge theories

*Contact author: t.e.spriggs@tudelft.nl
†Contact author: jannys@ethz.ch

[18,53,63,69–71]. Recent breakthroughs include the realization of discrete gauge symmetries and the observation of gauge-invariant phenomena like confinement and string-breaking dynamics in Abelian and non-Abelian theories [62,66,67,72]. Particularly significant is the demonstration of real-time dynamics in $\mathbb{Z}_2$ and U(1) lattice gauge theories, allowing controlled studies of thermalization, confinement dynamics, and the formation of topological defects [64,65]. Quantum simulations of non-Abelian lattice gauge theories, such as SU(2) and SU(3) in $1+1$D, have been explored on small lattices [73–75]. Limited simulations exist for $2+1$D [76], and $3+1$D is only recently being explored [53].

One of the challenges facing these first two methods is the infinite nature of either the continuous gauge group or electric field spectrum; these methods often require discretizing the group into a subgroup or truncating the gauge fields. These digitization methods can struggle at increasing spatial dimensions and certain regimes of LGTs [26,77].

One further approach is variational Monte Carlo (VMC). Early applications of VMC to LGTs relied on hand-crafted wave function parametrizations, often stemming from perturbative expansions of the theory [78–82]. The limited wave function parametrization has historically posed a limitation to VMC accuracies. Modern applications of VMC have overcome these limitations through the use of physics-agnostic, neural network parametrizations of the wave function, which has achieved impressive, and often state-of-the-art, results in the field of condensed matter [83–94], quantum chemistry [95–103], and nuclear and high-energy physics [104–106]. The application of these "neural wave functions" to LGT is limited to Abelian gauge theories: $\mathbb{Z}_2$ [107,108] and U(1) [109].

We present a scalable neural network wave function framework for simulating non-Abelian lattice gauge theories free of any discretizations of the gauge fields as well as the sign problem. Whilst the approach is general for any SU(N) theory, we focus on SU(2) in $2+1$ and $3+1$ dimensions. In order to respect gauge invariance while allowing for an expressive ansatz to represent the wave function, we introduce the lattice gauge neural wave function (LGNWF) ansatz, parametrized by expressive neural networks, containing equivariant and invariant blocks, well suited for VMC. To demonstrate the power of this ansatz we show that it finds ground states with lower energy than a prototypical physics-inspired ansatz and then present observables in $2+1$ and $3+1$ dimensions that agree with QMC calculations on similar sized lattices. Our framework allows for simple extensions to larger systems, higher dimensions, and different gauge groups; there is also a path to explore the inclusion of fermions, real-time evolution, and nonequilibrium dynamics.

Hamiltonian and representation—We focus on SU(2) pure gauge theory, where the gauge fields are defined on the links between spatial lattice sites. For a given lattice site x the directed link connecting x with its neighbor in the direction μ is denoted $U_\mu(x)$. These are related to the gauge fields from the continuum theory, $A_\mu^a(x)$, through $U_\mu(x) = \exp[-i\frac{1}{2}\sum_a \sigma^a A_\mu^a(x)]$, with $a = 1, 2, 3$ and $\boldsymbol{\sigma}^a$ being the Pauli matrices. An entire lattice of links will be denoted $\boldsymbol{U}$.

The Kogut-Susskind formulation of the SU(2) LGT Hamiltonian in D spatial dimensions is given by [68,78,110]

$$H = \frac{g^2}{2a_s^{D-2}} \sum_{l,a} E_l^a E_l^a + g^2 \lambda \frac{a_s^D}{a_s^4} \sum_{x,\nu>\mu} \left[1 - \frac{1}{2}\mathrm{Tr}P_{\mu,\nu}(x)\right]. \quad (1)$$

Here, l indexes each link in the lattice, and the sum over μ, ν, x encompasses each plaquette on the lattice. Moreover, g is the coupling constant, $\lambda = 4/g^4$, and a_s is the lattice spacing that we set to 1. Throughout this Letter, we will use a rescaled Hamiltonian instead, $(1/g^2)H$; see Supplemental Material [111] for more details. The (untraced) plaquette $P_{\mu,\nu}(x)$ is the product of four link operators forming a closed counterclockwise loop whose bottom left node is x. The electric field operators E^a are either the left, or right, generators of SU(2). They are defined through the commutators $[E^a, U] = \frac{1}{2}\sigma^a U$ or $[E^a, U] = U\frac{1}{2}\sigma^a$ for the left or right generators, respectively. The gauge links transform as $\mathcal{T}_\Omega U_\mu(x) = \Omega(x) U_\mu(x) \Omega(x+\mu)^\dagger$, where $\Omega \in \mathrm{SU}(2)$. As in the original Kogut-Susskind work [110], we deem states physical if they are annihilated by the generators of the gauge symmetry, which means that they are unchanged under that symmetry. Therefore, we will restrict ourselves to finding states that satisfy $\Psi(\mathcal{T}_\Omega \boldsymbol{U}) = \Psi(\boldsymbol{U})$.

There are two features to this theory that prove difficult for contemporary quantum simulation methods (such as quantum simulations and TNs): representing the continuous nature of the gauge group and respecting the gauge symmetry.

The continuous nature has several workarounds that involve some level of digitization of the gauge fields. The search for efficient bases of LGTs is an active area of research in itself [77,116]. One approach is to employ the quantum link model formulation [18,54,117–122] where the representation is discrete but the link variables are no longer unitary—a relic that must be removed before this model can be compared with the original theory. Alternatively, remaining with the Kogut-Susskind form, one can construct explicit basis representations known as the electric or magnetic bases [see Ref. [123] for an overview of bases in $1+1$D SU(2)]. The former basis involves constructing a basis of a finite number of irreducible representations of the electric field operator, relying on an explicit truncation on the number of irreducible representations to keep the basis finite; however, this truncation is known to be increasingly less reliable at smaller values of g, when the dimensionality of the system increases, or when trying to approach the continuum limit of the theory [26,77]. The latter, the magnetic basis, involves direct parametrizations of the group elements of the theory: this is the approach taken in this Letter. For implementations on quantum simulators or TNs the magnetic basis is truncated either by sampling the continuous group or using a discrete subgroup [36,124]. In our Letter no such restrictions are added and we work with the full, continuous gauge group.

As for respecting the gauge symmetry, several works are formulated in a basis that is gauge-invariant by construction. These go by the name of dressed site formulations in TNs for which we refer the reader to Ref. [26]. In the context of VMC, Ref. [125] showed that the states of $\mathrm{SU}(N)$ can be represented using a discrete spin-j angular momentum representation, which has dimension $2j+1$. Using the straightforward representation of the symmetry in this basis, the model can be made global $\mathrm{SU}(N)$ symmetric by construction. This was then extended to *local* $\mathrm{SU}(N)$ symmetry [126]. Nevertheless, as pointed out in Ref. [127], working only with these gauge-invariant bases severely limits the tractability in higher dimensions and the expressive power of the neural networks.

Our approach to representation works with the continuous gauge group without any discretization on truncation at any point. We achieve this by writing Eq. (1) not in terms of operators acting on *elements* of SU(2) but in terms of the *algebra* of the group instead, as was originally done in Ref. [78]. This leads to a continuous theory in S^3 that can be tackled using VMC. Furthermore, we will present a gauge-invariant trial wave function that exactly respects the symmetry without resorting to a restricted basis.

To be explicit, we use a spherical representation for the link variables (ρ, θ, ϕ),

$$U_\mu(x) = \cos\left(\frac{\rho}{2}\right)\mathbb{I} - i\boldsymbol{n}\cdot\boldsymbol{\sigma}\sin\left(\frac{\rho}{2}\right), \tag{2}$$

where $\boldsymbol{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ given $0 \le \rho \le 2\pi$, $0 \le \theta \le \pi$, and $0 \le \phi \le 2\pi$. In this representation, only the electric field term of the Hamiltonian changes: it becomes the Laplace-Beltrami operator on S^3,

$$E^2 = -\frac{1}{4}\nabla^2_{S^3}. \tag{3}$$

Further details relating to the spherical representation are given in Supplemental Material [111].

Variational model—As previously stated, our variational wave function needs to be gauge-invariant, and while neural networks can approximate a rich class of functions, and thus one could possibly learn the gauge symmetry through training, we take the approach of explicitly baking gauge symmetry into our variational model. We will now present two ways that this can be achieved.

The simplest approach is to work with only gauge-invariant constructions, the smallest of which is the traced plaquette

$$W_{\mu,\nu}(x) = \frac{1}{2}\mathrm{Tr}P_{\mu,\nu}(x). \tag{4}$$

The first ansatz we consider does not contain a neural network. Instead, traced plaquettes are combined to form a physics-informed, two-body Jastrow ansatz [128], the output of which remains invariant under any gauge transformation of the input,

$$\Psi(\boldsymbol{U}) = \prod_{\mu<\nu,x} e^{\alpha_\mu W_{\mu,\nu}(x)} \prod_{\mu'<\nu',x'} e^{\beta^{\mu,\nu,\mu',\nu'}_{d(x,x')} W_{\mu,\nu}(x) W_{\mu',\nu'}(x')}. \tag{5}$$

Here, α and β are complex variational parameters, where the latter depends on the relative distance $d(x,x')$ between sites x and x', yielding a translationally invariant, yet nonlocal model. Setting $\beta = 0$ yields the single-plaquette model from Refs. [78,79,81,82].

Extending beyond this, recent work focusing on using neural networks for sampling gauge configurations has demonstrated that it is feasible to construct gauge-equivariant neural networks for lattice gauge theories using continuous group representations [13,14,129,130]. This offers a powerful approach to capturing correlations in lattice gauge theories, and offers a promising extension to tackle continuous-group theories beyond one dimension. We now introduce the LGNWF ansatz, composed of two such gauge-equivariant neural networks.

In our first type of neural transformation, we update a link $U_\mu(x)$ through updating the eigenvalues of an untraced plaquette operator $P_{\mu,\nu}(x)$ [which contains $U_\mu(x)$]. This is done using a neural network that takes all traced plaquette loops W as an input, i.e.,

$$P_{\mu,\nu}(x) = Ve^{i\lambda}V^\dagger \to P'_{\mu,\nu}(x) = Vf(\lambda, \boldsymbol{W})V^\dagger, \tag{6}$$

$$U_\mu(x) \to U'_\mu(x) = P'_{\mu,\nu}(x)P_{\mu,\nu}(x)^\dagger U_\mu(x), \tag{7}$$

where $\lambda = [\lambda_1, \lambda_2]$ is a vector of the sorted eigenvalues of P, V are the corresponding eigenvectors, and f is a convolutional neural network architecture taking all invariant traced plaquettes as input. The transformation in Eqs. (6), (7) was introduced in [13] and is referred to here as a "plaquette equivariant layer." The second neural transformation combines all untraced plaquettes that start and end at x, i.e., $C^i_{\mu,\nu}(x) = \{P_{\mu,\nu}(x), P_{\mu,-\nu}(x), P_{-\mu,\nu}(x), P_{-\mu,-\nu}(x)\}^i$. We then parametrize a transformation of $U_\mu(x)$ as

$$\epsilon_\mu(x) = e^{i\sum_i \xi_{\mu,i}[C^i_{\mu,\nu}(x)]_{aH}} \tag{8}$$

$$U_\mu(x) \to U'_\mu(x) = \epsilon_\mu(x)U_\mu(x), \tag{9}$$

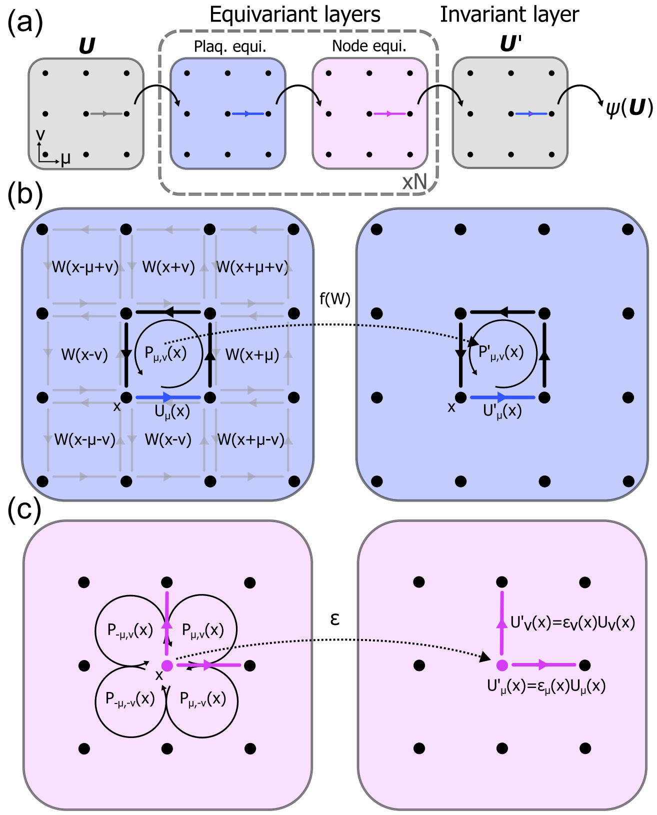

FIG. 1. Example configuration of the LGNWF ansatz. (a) Schematic of updating a lattice of links, $\boldsymbol{U}$, through N blocks of equivariant layer-to-layer transforms (b) and (c). (b) Plaquette equivariant network updating the link $U_\mu(x)$ through Eqs. (6) and (7) conditioned on nonlocal information W. (c) Node equivariant layer acting on $U_\mu(x)$ and $U_\nu(x)$ through Eqs. (8) and (9), acting only on plaquettes originating at x.

where $\xi_{\mu,i}$ are variational parameters for the transformation along direction μ, and aH is shorthand for the anti-Hermitian component; this transformation was introduced in Ref. [129]. We refer to this transformation as a "node equivariant layer".

We capture higher-order correlations through these gauge-equivariant neural transformations on the configurations $\boldsymbol{U}$, before entering them into the invariant form in Eq. (5), to arrive at a gauge-invariant ansatz whose input is not simply gauge-invariant constructs. A schematic of the LGNWF ansatz is shown in Fig. 1.

This approach can be easily generalized to larger lattices. Even after training, the LGNWF can be fine-tuned on larger lattices requiring only one extra parameter for each new unique distance, $d(x, x')$, introduced by the larger lattice. Furthermore, while these will be applied to the spherical representation of SU(2), the LGNWF ansatz can also be applied to any SU(N) LGT. For more details about these transformations, including various configurations and neural network architectures, and the scaling of this method, we refer the reader to Supplemental Material [111].

The parameters of the LGNWF ansatz are found through VMC: at every iteration of training we estimate the energy and the gradient of the energy (with respect to the variational parameters) using Markov chain Monte Carlo. The variational parameters are then adjusted according to these gradients for the next iteration of training. Automatic differentiation is used to compute the electric term in the Hamiltonian (details of which are elucidated in Supplemental Material [111]) as well as gradients of the ansatz (see Ref. [131] and references therein for a comprehensive explanation of VMC).

Observables—To capture the improved performance of the LGNWF ansatz, we define the relative energy change achieved by this ansatz, compared to the purely invariant Jastrow ansatz from Eq. (5), as

$$\delta E = \frac{E_{\text{LGNWF}} - E_{\text{Jastrow}}}{E_{\text{Jastrow}}}. \tag{10}$$

Beyond the energy of the ground state, there remains the question of whether these neural wave functions capture other physical properties of the ground state. To answer this question, we consider the scaling of traced plaquettes of size $l \times h$, $\langle W^{l\times h}\rangle$. One expects that in the limit of small λ (known often as the "strong" coupling limit) the expectation value of the plaquette should scale with the area of the plaquette, whereas at large λ it should scale with its perimeter. The Creutz ratio was introduced in [132] to isolate the amount of area law scaling. The Creutz ratio is defined as

$$\chi = \frac{1}{N_x}\sum_x -\ln\left(\frac{\langle W^{2\times 2}(x)\rangle\langle W^{1\times 1}(x)\rangle}{\langle W^{1\times 2}(x)\rangle\langle W^{2\times 1}(x)\rangle}\right) \tag{11}$$

for N_x lattice sites x.

Results—For the following results we performed VMC calculations for a fixed number of iterations: 14 000 (19 000) for the two (three) dimensional lattices. This includes training on smaller lattices and then using these to initialize larger systems. Training was performed using 1024 samples per iteration, this was increased for the observables reported in this Letter and will be mentioned alongside the result. For further details see Supplemental Material [111].

To establish that the nonlocal information sharing and increased expressivity facilitated by the LGNWF ansatz improves the variational estimate of the ground state, Fig. 2 (left) shows the energy improvements of the LGNWF ansatz over the Jastrow ansatz for a system of 12×12 links. It is clear that the LGNWF consistently finds a variational state with lower energy and is thus a better representation of the ground state. Furthermore, the improvement in energy increases with increased λ. Negligible improvement at small λ is to be expected; in Ref. [78] the authors show that in the limit of small λ the wave function should resemble a one-body Jastrow ansatz

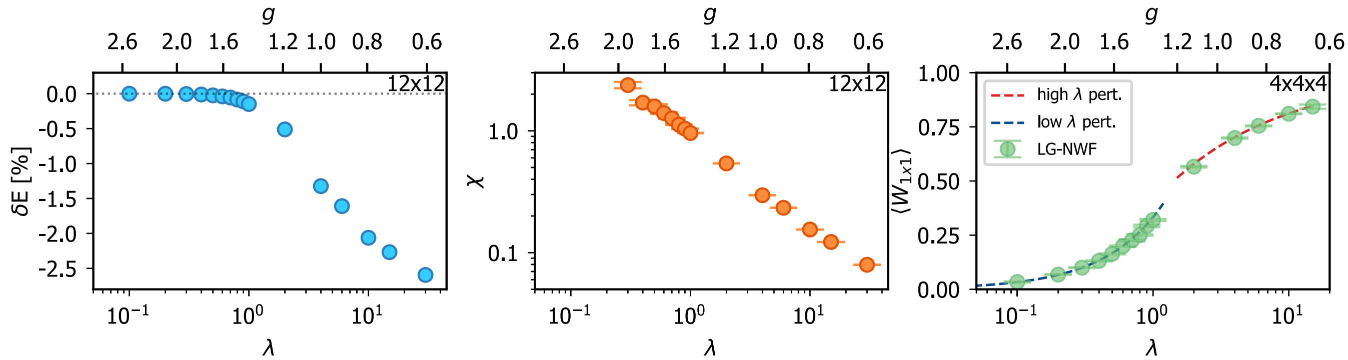

FIG. 2. The relative change in energy, defined in Eq. (10), achieved using the LGNWF ansatz compared to the two-body Jastrow ansatz (left). Data are shown against λ and g, where $\lambda = 4/g^4$. The Creutz ratio measured on the ground states found using the LGNWF ansatz (center). The average traced plaquette (divided by 2 for normalization) of the ground states compared to perturbative expansions from [78] (right). The Monte Carlo errors for the energy are too small to be distinguished from zero and are thus omitted, whereas for the Creutz ratio and plaquette they are the standard error on the mean across the 144 (64) different lattice sites for the two (three) dimensional lattice.

and therefore the one- and two-body Jastrow ansatz that we are comparing to already contains the optimal solution at small λ. These data were measured using 65 536 samples and the resulting MC error across this ensemble is too small to be discerned visually; however, this error does not account for any uncertainties related to the VMC procedure converging. See Supplemental Material [111] for further discussions on the related uncertainties and the equivalent data for the 3D lattice.

With ground state neural wave functions in hand, what remains is to show that these representations capture more than just a low energy. Figure 2 (middle) shows the Creutz ratio χ decreasing monotonically with increasing λ, consistent with the predictions that the scaling of the plaquette goes from area-dominated to perimeter-dominated. These data were measured using 524 288 samples. Figure 2 (right) shows the expectation value of the 1×1 traced plaquette averaged over all of the lattice sites for the $4 \times 4 \times 4$ system using 65 536 samples alongside the perturbative expansions from Ref. [78]. There is clearly very strong agreement between the data and theory in both small and large λ regimes (known as the strong and weak coupling expansions, respectively). This changeover from the weak coupling to strong coupling behaviors occurs in the range $1 \leq \lambda \leq 2$, in agreement with earlier estimations on similar sized lattices using VMC with a Jastrow ansatz [78], QMC [133,134], and the density of states [135].

Conclusion and outlook—In this Letter we present a flexible yet gauge-invariant ansatz for simulating SU(2) lattice gauge theory in the full continuous representation. We employed bespoke gauge-equivariant neural networks with a physics-informed gauge-invariant final layer to the task of finding the ground state of the SU(2) LGT Hamiltonian. In doing so we highlighted the improvements that can be made with the inclusion of these gauge-equivariant networks and showed that measurements taken on these ground states agree well with theoretical predictions. Our combination of various gauge-equivariant layers, alongside their inclusion in the framework of VMC, opens up a new avenue to study non-Abelian gauge theories; moreover, these techniques are scalable, applicable to any SU(N) LGT, and facilitate the advancements in condensed matter and quantum information be carried over into the study of high-energy physics.

Theories with gauge symmetries are also found beyond the realms of LGTs. There are, for example, interesting formulations of the Hubbard model with auxiliary fields where continuous gauge symmetries emerge [136,137]. A promising avenue would be to apply the gauge-equivariant VMC ansatz proposed in this Letter to systems with gauge symmetries outside of LGTs.

A natural next step for applications to LGTs is to incorporate dynamical fermionic fields, leveraging recent neural representations of fermionic Hamiltonians [87,90,95,138–141]. Another is to target low-energy eigenstates [95,141] and thermal states [142–144]. Beyond static properties, our framework is compatible with variational real-time evolution, providing access to nonequilibrium phenomena in gauge theories beyond one spatial dimension. In particular, variational Monte Carlo with expressive neural quantum states has recently emerged as a powerful approach for simulating dynamics in 2D and 3D [145–151], including continuous representations [146,150], fermionic degrees of freedom [146], and thermal state dynamics [144]. Extending our approach to include these features could shed light on open problems related to such issues as identifying the mechanisms determining the timescales of the thermalization and the sensitivity of the dynamics to the initial conditions in field theories [18].

The simulations performed in this Letter were carried out with a custom-developed code based on JAX [152] and NetKet [131].

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Data availability—The data that support the findings of this article are openly available [154,155].

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