

Lattice field theory analysis of the chiral Heisenberg model

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Motivated by ongoing interest in the universal behavior of the Hubbard model of spinning electrons on honeycomb and π -flux lattices at the semimetal–Mott insulator phase transition, we formulate the three-dimensional (3D) chiral Heisenberg model, a theory of relativistic fermions in three spacetime dimensions, as a lattice field theory using domain wall fermions. The contact interaction term preserves an $SU(2)$ global symmetry. We perform numerical simulations using the rational hybrid Monte Carlo algorithm on system sizes $L^3 \times L_s$, with $L \in \{8, \dots, 24\}$ and domain wall separation $L_s \in \{8, 16, 24\}$. We locate the phase transition corresponding to spontaneous $SU(2) \rightarrow U(1)$ breaking, yielding critical exponent estimates $\nu^{-1} = 0.63(3)$ and $\eta_\Phi = 1.42(8)$. These values are considerably removed from estimates obtained from simulations performed in $(2+1)D$, i.e., with the time and spatial directions treated differently, but align more closely with analytic estimates obtained using 3D covariant field theory. We also present results for the fermion correlator, ultimately needed for the determination of the exponent η_ψ , highlighting the need to rotate the fermion source to a common reference direction in isospace to obtain a signal.

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I. INTRODUCTION

The Hubbard model is a key tool in the modeling of strongly correlated electronic structure in materials. At half-filling, the Hamiltonian is of the form

$$H = - \sum_{\langle i,j \rangle; \sigma=\uparrow, \downarrow} t_{ij} [c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}] + U \sum_i \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right), \quad (1)$$

where $c^\dagger, c$ create and annihilate electrons of spin σ at the sites i of some lattice, the tunneling t_{ij} is nonzero only on nearest-neighbor sites $\langle i, j \rangle$, and the number of electrons at site i is $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \in \{0, 1\}$. The form of the on-site two-body interaction proportional to U is constrained by the Pauli exclusion principle. In two-dimensional systems, there is particular interest in the cases where either i, j denote the sites of a honeycomb lattice with constant $t_{ij} = t$ or i, j live on a square lattice and the product of the four t_{ij} around any elementary plaquette is constrained to equal -1 , yielding a π -flux. In either case the resulting low-energy electron dispersion vanishes at two Dirac points in the first Brillouin zone, around which the dispersion is linear, and propagation of single-particle excitations is described by the Dirac equation in the long-wavelength limit. At half-filling, the Fermi

energy equals zero, and particle or hole excitations can be interpreted as particles/antiparticles in a relativistic quantum field theory. For weak interactions, the resulting system is a semimetal. As U is increased, there may be a transition to a Mott insulator phase triggered by the opening of a gap at the Dirac points.

The field theory underlying the universality class of the phase transition is determined by the number of low-energy electronic degrees of freedom. For each of the lattices mentioned above, there are two sites per unit cell and two Dirac points per Brillouin zone; finally, there are two spin components, yielding $2 \times 2 \times 2 = 8$ components. In $d = 2 + 1$ dimensions, this naturally leads to a description in terms of $N = 2$ flavors of four-component Dirac spinors, to be set out in Sec. II. However, it is the symmetry of the interaction and its pattern of gap-driven breaking which characterize the universality class in this case. Defining the spin at site i ,

$$\vec{S}_i = \frac{1}{2} c_{i\alpha}^\dagger \vec{\tau}_{\alpha\beta} c_{i\beta}, \quad (2)$$

where $\vec{\tau}$ are Pauli matrices, we find, using $\sum_a \tau_{\alpha\beta}^a \tau_{\gamma\delta}^a \equiv 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta}$, that up to an irrelevant constant, the interaction in Eq. (1) can be recast as $-\frac{2U}{3} \sum_i \vec{S}_i \cdot \vec{S}_i$. Classically, this resembles the Hamiltonian of the Heisenberg model; the corresponding effective field theory of interacting relativistic fermions is known as the *chiral Heisenberg model*.

There have been many attempts to characterize the chiral Heisenberg universality class by estimating critical exponents. It is conventional to focus on the correlation length exponent ν and the exponent η_Φ defined by critical correlations of the order parameter field Φ ,

$$\langle \Phi(0)\Phi(r) \rangle_{U=U_c} \propto r^{-(d-2+\eta_\Phi)} \sim r^{-(1+\eta_\Phi)}. \quad (3)$$

Another exponent η_ψ characterizing critical correlations of the fermion field is needed for complete specification; since

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our results for the fermion correlator reviewed in Sec. IV are exploratory, we will not discuss η_ψ much in this work.

One group of estimates, motivated by closeness to the microscopic physics, emerges from numerical simulation of the Hubbard model in Eq. (1) using either quantum Monte Carlo (QMC), e.g., Refs. [1–7], or hybrid Monte Carlo (HMC) simulations [8–11] employing imaginary time. A distinct group of QMC simulations [12,13] employs the so-called SLAC formulation of the fermion hopping term, which better captures the symmetries of relativistic fermions at the price of introducing nonlocal tunneling. The Mott insulator phase is manifested in studies of solid-state materials like layered WSe₂ [14,15] and has recently even been observed experimentally [16], though critical exponents could not be extracted to date. A common feature of all these (2+1)D simulations is that, since ultimately a time continuum limit is needed, distinct approaches are taken to discretising time and space directions. As reviewed in Sec. III B, these simulation-based estimates tend to yield exponent estimates $\nu^{-1} \gtrsim 0.8$, $\eta_\phi \lesssim 1$, with a large spread, which has been attributed to the prevalence of severe finite volume effects [7].

Another group of estimates emerges from analytic or semianalytic calculations rooted in Euclidean quantum field theory: These include loop expansions about renormalizable models in the Gross-Neveu (GN) class in $d = 2$ [17] or Gross-Neveu-Yukawa (GNY) class [18] in $d = 4$ [17,19], large- N expansions in fixed dimensionality d [20], or functional renormalization group (FRG) approaches [21,22]. A unifying feature of such three-dimensional (3D) approaches is that Euclidean time is treated on the same footing as the spatial dimensions, up to boundary conditions. Since we are mainly interested in critical properties, the continuum limit may be taken uniformly across both temporal and spatial directions. Figure 5 shows that field theory-based estimates tend to have $\nu^{-1} \lesssim 0.9$, $\eta_\phi \gtrsim 1$, again with a large spread.

In this paper we will furnish a further estimate, based on a 3D lattice field theory simulation of the appropriate Euclidean theory. This aligns us very much with the latter group but, this time, based on a method with a completely different set of systematic but theoretically controllable errors, dictated by available computational resource. Our approach treats fermions ψ , $\bar{\psi}$ as independent Grassmann fields, formulated using domain wall fermions (DWFs), a lattice-based discretization specifically devised to reproduce the symmetries of continuum Dirac fermions as closely as possible. The DWF are defined on a $L^3 \times L_s$ hypercubic lattice, where open boundary conditions along an artificial third direction result in two domain walls separated by L_s . The dynamics of the target theory are then carried by near-zero modes of the DWF operator localized on either wall. It has been demonstrated both numerically [23] and analytically [24] that, in the limit $L_s \rightarrow \infty$, the desired $U(2N)$ symmetry of weakly interacting relativistic Dirac fermions is restored, in the sense that the resulting effective 3D Dirac operator D respects a 3D generalization of the Ginsparg-Wilson relations [25]. DWFs have previously been applied to the study of critical behavior in the 3D GN model [26,27] and the 3D Thirring model [28–30].

In what follows, in Sec. II, we first specify the Euclidean action of the continuum 3D field theory in the chiral Heisenberg universality class, sharing the same symmetries and

particle content at low energies as the original Hubbard model in Eq. (1), followed by its DWF discretization. The action is phrased in terms of a real scalar auxiliary boson triplet $\vec{\phi}$ which, using particle physics parlance, we will refer to as an *isotriplet*. The numerical simulation is performed using the rational HMC (RHMC) algorithm [31]; some simplifying features, applicable since $\vec{\phi}$ is only defined on the domain walls, are noted. Appendix A shows that the continuum model has a real positive fermion determinant and that the sign problem introduced by DWFs is likely to be mild and safe to ignore. As already noted, the approach differs from most simulations in condensed matter physics in treating spatial and temporal directions alike; it also differs from particle physics applications in having no symmetry-breaking parameter, such as an explicit fermion mass, to guide the direction of symmetry breaking. In Sec. III A, it is shown how, in the resulting simulation, the auxiliary $\vec{\phi}$ explores the manifold of allowed ground states in a fairly uniform manner, so that a pragmatic choice of pseudo-order parameter $|\Phi|$ is needed, defined in Eq. (13) below. A series of simulations of varying system size L^3 , with $L \in \{8, \dots, 24\}$, and domain wall separation $L_s \in \{8, 16, 24\}$ are performed with $|\Phi|$ as the principle observable, and a critical coupling is identified, first using the Binder cumulant and next with more precision using a finite volume scaling (FVS) analysis, leading to estimates for critical exponents. Particular attention is paid to the stability of the results as L_s is increased toward the limit where the symmetries of the continuum model are expected to be restored. Next, in Sec. III B, we set things in context by comparing our predictions for ν^{-1} and η_ϕ with a compendium of other results found in the recent literature.

In Sec. IV, we switch attention to the fermion sector where ultimately a controlled analysis will be needed to extract the exponent η_ψ ; a possible route is sketched in Ref. [32]. Our lattice sizes are too small to reach the Euclidean time separations needed to establish critical scaling; rather, we present exploratory work, first in Sec. IV A defining the correlation function to be studied in terms of the component remaining after tracing over Dirac indices, yielding a timeslice correlator $S_m(x_0)$ which is antisymmetric about the lattice midpoint $x_0 = L/2$. To have a nonvanishing signal following the drift of $\vec{\phi}$ around the vacuum manifold, we must introduce a rotation $S_m \mapsto \tilde{S}_m$ to align the source along the third isodirection. Further details are presented in Appendix B. Finally, Sec. IV B presents an analysis of $\tilde{S}_m$ for various couplings and lattice volumes using the Truncated Hankel correlator (THC) method [33] and masses of the lowest excited state and overlap amplitudes for the lowest excited state extracted. Section V gives a brief summary of our conclusions.

II. FORMULATION AND SYMMETRY

Our starting point is the continuum Lagrangian density for the chiral Heisenberg model

$$\begin{aligned} \mathcal{L} = & \bar{\psi}(\partial_\mu \gamma_\mu \otimes \mathbb{1}_{2 \times 2} + g\vec{\phi} \cdot \mathbb{1}_{4 \times 4} \otimes \vec{\tau})\psi \\ & + \frac{1}{2}\vec{\phi} \cdot \vec{\phi} \equiv \bar{\psi}\mathcal{M}\psi + \frac{1}{2}\vec{\phi} \cdot \vec{\phi}. \end{aligned} \quad (4)$$

Here, ψ , $\bar{\psi}$ represent two flavors of a four-component spinor. In our notation γ_A are 4×4 traceless Hermitian matrices

acting on spinor indices satisfying $\{\gamma_A, \gamma_B\} = \delta_{AB}$, with $A \in \{0, 1, 2, 3, 5\}$, and the $\bar{\tau}$ act on flavor. Spacetime indices are denoted by $\mu \in \{0, 1, 2\}$. The following invariances of the kinetic term [i.e., with $g = 0$ in Eq. (4)] generate a global U(2) invariance of the free fermion Lagrangian:

$$\begin{aligned} \psi &\mapsto e^{i\alpha} \psi, & \bar{\psi} &\mapsto \bar{\psi} e^{-i\alpha}, & \psi &\mapsto e^{\alpha\gamma_3\gamma_5} \psi, & \bar{\psi} &\mapsto \bar{\psi} e^{-\alpha\gamma_3\gamma_5}, \\ \psi &\mapsto e^{i\alpha\gamma_3} \psi, & \bar{\psi} &\mapsto \bar{\psi} e^{i\alpha\gamma_3}, & \psi &\mapsto e^{i\alpha\gamma_5} \psi, & \bar{\psi} &\mapsto \bar{\psi} e^{i\alpha\gamma_5}. \end{aligned}$$

In the interaction, $\vec{\phi}$ is a real three-component scalar auxiliary field. It is readily integrated out to recover a four-Fermi contact interaction resembling that of the Hubbard model in Eq. (1), but the form in Eq. (4) is more convenient to handle, with a manifest invariance under a global SU(2) rotation

$$\psi \mapsto U\psi, \quad \bar{\psi} \mapsto \bar{\psi}U^\dagger, \quad \phi \mapsto O\phi, \quad (5)$$

with $U \in \text{SU}(2)$, $O_{ij} = \frac{1}{2}\text{tr}[\tau_i U^\dagger \tau_j U] \in \text{SO}(3)$. This model corresponds to the case $\tilde{N}_D = 1$, $M = 3$ in the classification of GNY models presented in Ref. [18]. Because ϕ is real, the interaction term breaks the U(2) invariance of free Dirac fermions in 3D to $\text{U}(1) \otimes \text{U}(1)$.

Our simulations are performed using DWFs on a $L^3 \times L_s$ lattice, where open boundary conditions along an artificial third direction result in two domain walls separated by L_s . In the limit $L_s \rightarrow \infty$, the desired U(2) symmetry of weakly interacting relativistic Dirac fermions is restored, in the sense that the resulting effective 3D Dirac operator D respects the 3D generalization of the Ginsparg-Wilson relations [24]

$$\{\gamma_3, D\} = 2aD\gamma_3D, \quad \{\gamma_5, D\} = 2aD\gamma_5D, \quad [\gamma_3\gamma_5, D] = 0. \quad (6)$$

In the long-wavelength limit $aD \rightarrow 0$ (where a is the physical lattice spacing, implicitly set to unity almost everywhere), this guarantees U(2) restoration.

Here, we present the discretized action $S = S_{\text{kin}} + S_{\text{int}} + S_\phi = \bar{\Psi}\mathcal{M}\Psi + S_\phi$ in detail, following the discussion in Ref. [27]. The fermion kinetic term uses the 3D domain wall operator defined in Refs. [23,24]

$$S_{\text{kin}} = \sum_{x,y} \sum_{s,s'} \bar{\Psi}(x,s) [\delta_{s,s'} D_W(x|y) + \delta_{x,y} D_3(s|s')] \Psi(y,s'), \quad (7)$$

where $\Psi, \bar{\Psi}$ are four-component isodoublet spinors defined in $2+1+1$ dimensions. The relation with the fields $\psi, \bar{\psi}$ living in the $(2+1)\text{D}$ target space is

$$\begin{aligned} \psi(x) &= \mathcal{P}_- \Psi(x, 1) + \mathcal{P}_+ \Psi(x, L_s), \\ \bar{\psi}(x) &= \bar{\Psi}(x, L_s) \mathcal{P}_- + \bar{\Psi}(x, 1) \mathcal{P}_+, \end{aligned} \quad (8)$$

with projectors $\mathcal{P}_\pm = \frac{1}{2}(1 \pm \gamma_3)$. Here, D_W is the 3D Wilson operator defined on spacetime volume V ,

$$\begin{aligned} D_W(M)_{x,y} &= -\frac{1}{2} \sum_{\mu} [(1 - \gamma_\mu) \delta_{x+\hat{\mu},y} + (1 + \gamma_\mu) \delta_{x-\hat{\mu},y}] \\ &\quad + (3 - M) \delta_{x,y}, \end{aligned} \quad (9)$$

with the domain wall height parameter M set to unity throughout, and D_3 controls hopping along the third dimension between the walls at $s = 1$ and $s = L_s$,

$$D_{3,s,s'} = -[\mathcal{P}_- \delta_{s+1,s'} (1 - \delta_{s',L_s}) + \mathcal{P}_+ \delta_{s-1,s'} (1 - \delta_{s',1})] + \delta_{s,s'}. \quad (10)$$

The DWF formulation of the interaction term is defined solely in terms of fields on the domain walls

$$\begin{aligned} S_{\text{int}} &= \sum_x \vec{\phi}(x) \cdot [\bar{\Psi}(x, L_s) \mathcal{P}_- \bar{\tau} \Psi(x, 1) \\ &\quad + \bar{\Psi}(x, 1) \mathcal{P}_+ \bar{\tau} \Psi(x, L_s)]. \end{aligned} \quad (11)$$

As originally noted in Ref. [26], restriction of the scalar degrees of freedom to the domain walls implies that the Pauli-Villars kernel normally needed to cancel unphysical contributions from bulk modes has no ϕ dependence and therefore can be omitted from the simulation dynamics. Finally, the auxiliary action

$$S_\phi = \beta \sum_x \vec{\phi}(x) \cdot \vec{\phi}(x), \quad (12)$$

with the dimensionless parameter $\beta = ag^{-2}$. All terms in S are invariant under the SU(2) global symmetry in Eq. (5).

It is shown in Appendix A that the continuum theory in Eq. (4) is free of a sign problem, while the DWF-regularized version has a mild sign problem expected to vanish as $L_s \rightarrow \infty$. Accordingly, we simulate $N = 1$ flavor (i.e., a single isodoublet of fermion four-spinors) using the RHMC [31] algorithm, which updates using the positive functional measure $(\det \mathcal{M}^\dagger \mathcal{M})^{\frac{1}{2}}$. Further details of the algorithm are presented in Ref. [28].

III. NUMERICAL RESULTS

A. Finite volume scaling

Our goal is to study the spontaneous breaking $\text{SU}(2) \rightarrow \text{U}(1)$ expected at some critical coupling β_c . In the infinite volume limit, the symmetry-broken phase is signaled by long-range order, namely, a nonzero scalar field expectation $\langle \vec{\phi} \rangle \neq \vec{0}$. In a finite system, however, in the absence of explicit symmetry breaking such as a fermion mass, the mean direction $\vec{\phi}/|\phi|$ drifts around the $\text{SO}(3)$ manifold, so on long enough simulation timescales, $\langle \vec{\phi} \rangle \approx 0$, as illustrated in Fig. 1. This demonstrates that our simulations are ergodic and cover the entire phase space efficiently. To study symmetry breaking, a pragmatic alternative is therefore the *pseudo-order parameter*

$$|\Phi| = \frac{1}{L^3} \sqrt{\sum_{a=1}^3 \left(\sum_x \phi_a(x) \right)^2}. \quad (13)$$

Pilot studies of the 3D GN model using DWFs [27] have found the large- L_s limit needed for the GW symmetries in Eq. (6) is for practical purposes recovered by $L_s \sim \mathcal{O}(20)$, which is relatively modest compared with recent studies of the 3D Thirring model [30,34]. To corroborate this, we make separate simulations using $L_s = 8, 16$, and 24 .

We have simulated on $L^3 \times L_s$, using $L = 8, 12, 16, 20, 24$, with $|\Phi|$ the principal observable. For each of $L_s = 8, 16, 24$, a total of 55 datasets were generated, each of between 300 (for $L = L_s = 24$) and 50 000 (for $L = L_s = 8$) measurements. The $L_s = 16$ dataset is shown in Fig. 2.

First consider the Binder cumulant

$$B = 1 - \frac{(|\Phi|^4)}{3(|\Phi|^2)^2}, \quad (14)$$

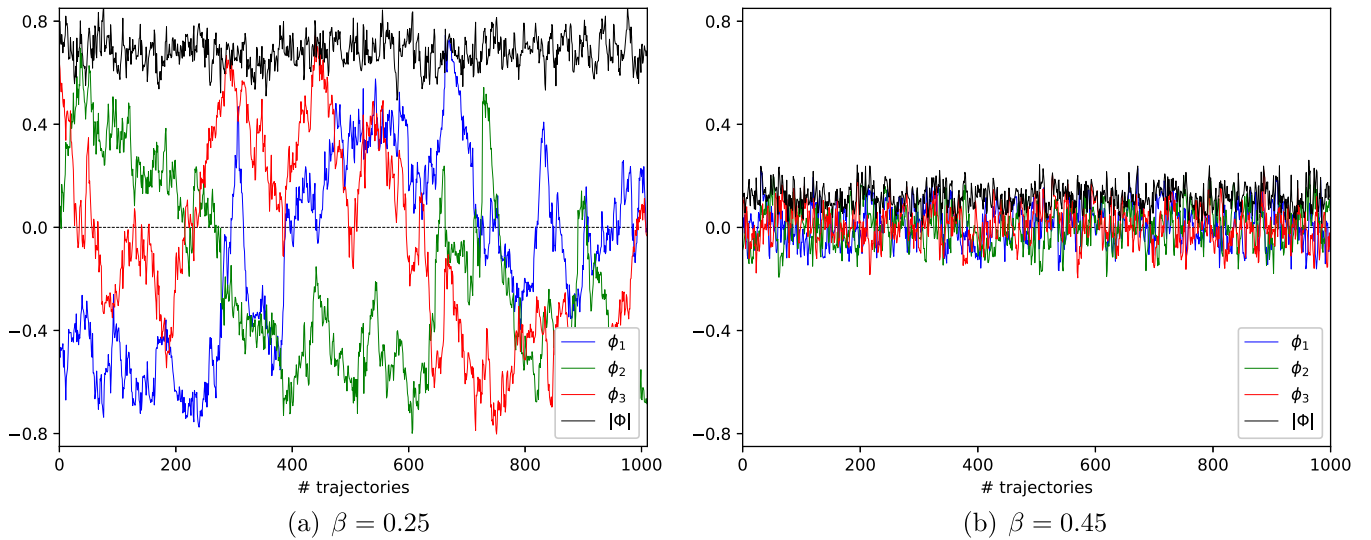


FIG. 1. Scalar field histories over 1000 RHMC trajectories on $12^3 \times 8$. Colored lines show the component $\phi_{i=1,\dots,3}$; the black line is $|\Phi|$ [see Eq. (13)].

proportional to the excess kurtosis (the fourth moment of the distribution) of the order parameter. At a phase transition, B becomes volume independent, and in consequence, lines corresponding to different L values should cross at the critical coupling β_c . The Binder cumulant has been plotted for $L_s = 16$ in Fig. 3, which suggests a critical coupling $\beta_c \approx 0.45$. The noise level of B is rather high so that the resulting estimation of β_c has a low precision. It can, however, serve as an independent sanity check for the critical coupling extracted in the following via the far more accurate finite-volume scaling (FVS).

To extract critical exponents β_Φ and ν , for each L_s , we fit to a FVS form

$$|\Phi| L^{\frac{\beta_\Phi}{\nu}} = f(t L^{\frac{1}{\nu}}), \quad (15)$$

with the dimensionless reduced coupling $t \equiv (\beta - \beta_c)/\beta_c$. We performed fits using both quadratic $f(x) = A + Bx + Cx^2$

and cubic $f(x) = A + Bx + Cx^2 + Dx^3$ Ansätze, in all cases including the 36 datapoints from within a window $|x| \leq 1.5$. To increase the fit stability, we used initial guesses for the critical exponents obtained with the method from Ref. [8], which approximates the data by cubic splines for every L and minimizes the integrals between the different resulting curves. These results were also compatible with our subsequent fits, which makes us confident that the polynomial approximations did not introduce a significant bias. The fitted values for the critical parameters are given in Tables I and II and data collapse for the cubic fits plotted in Fig. 4. The χ^2 values quoted for the cubic fits were obtained first by fitting for all seven parameters and then fixing the critical parameters and refitting A, B, C, D , yielding values $O(10\%)$ smaller.

The cubic fits are of significantly better quality than the quadratic, but the fitted critical parameters are compatible. Data have been taken in both broken and symmetric phases.

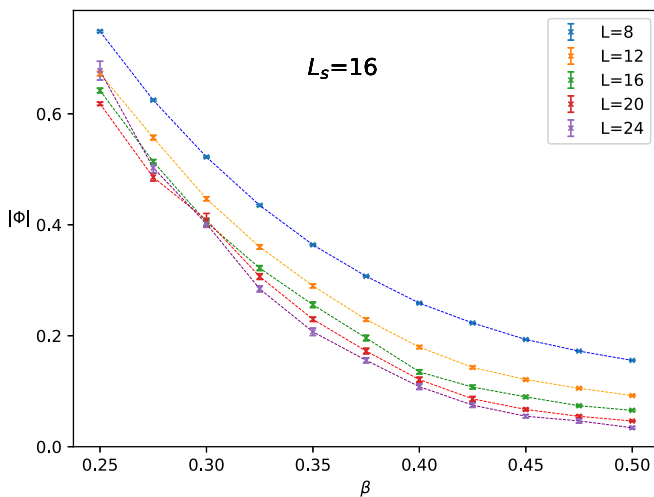


FIG. 2. Pseudo-order parameter $|\Phi|$ [see Eq. (13)] vs coupling β for five spacetime volumes L^3 , with $L_s = 16$. Data from $L_s = 8, 24$ are virtually indistinguishable.

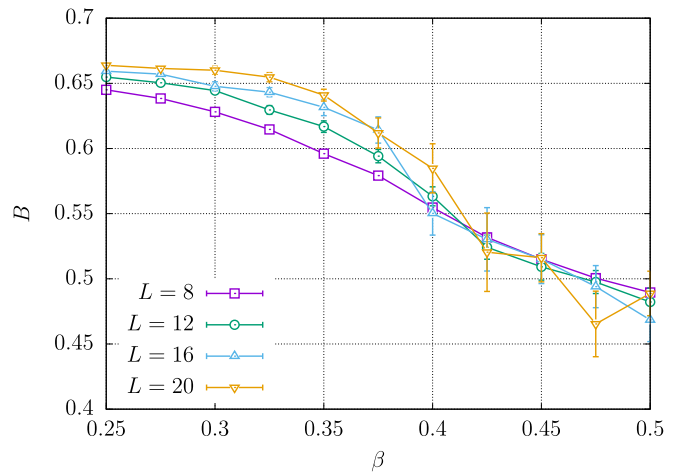


FIG. 3. Binder cumulant B as a function of the coupling β for $L_s = 16$. The plots look very similar for $L_s = 8, 24$. Error bars for $L \leq 12$ are too small to be visible on this scale; results for $L = 24$ are very noisy and have been omitted.

TABLE I. Critical coupling β_c and exponents ν^{-1} , η_Φ obtained via FVS in Eq. (15) fits using a quadratic scaling function.

L_s	β_c	β_Φ/ν	$1/\nu$	χ^2/dof
8	0.470(6)	1.22(2)	0.631(26)	3.3
16	0.468(5)	1.20(2)	0.627(22)	5.6
24	0.469(6)	1.21(2)	0.630(28)	4.6

Importantly and encouragingly, there is no sign of any systematic drift of the fitted critical parameters as L_s is increased from 8 to 24, which suggests the results are obtained in a regime where the global symmetries are those of continuum Dirac fermions. This has proved to be a much more troublesome issue in DWF simulations of the 3D Thirring model [30], where data from L_s as large as 120 were required for the analysis. We quote the $L_s = 24$ results

$$\beta_c = 0.465(11), \quad \frac{\beta_\Phi}{\nu} = 1.21(4), \quad \frac{1}{\nu} = 0.633(26), \quad (16)$$

TABLE II. Critical coupling β_c and exponents ν^{-1} , η_Φ obtained via FVS in Eq. (15) fits using a cubic scaling function. Fits are visualized in Fig. 4.

L_s	β_c	β_Φ/ν	$1/\nu$	χ^2/dof
8	0.453(9)	1.17(4)	0.634(28)	1.2
16	0.461(5)	1.18(4)	0.629(22)	0.8
24	0.465(11)	1.21(4)	0.633(26)	1.4

using the errors output from the least squares routine.

B. Comparison with previous work

Taken at face value our results suggest $\frac{1}{\nu} = 0.63(3)$, $\eta_\Phi = 2\frac{\beta_\Phi}{\nu} - 1 = 1.42(8)$, where we assume hyperscaling. Table III (based on table V in Ref. [17]) presents a nonexhaustive list of estimates for these exponents obtained using both

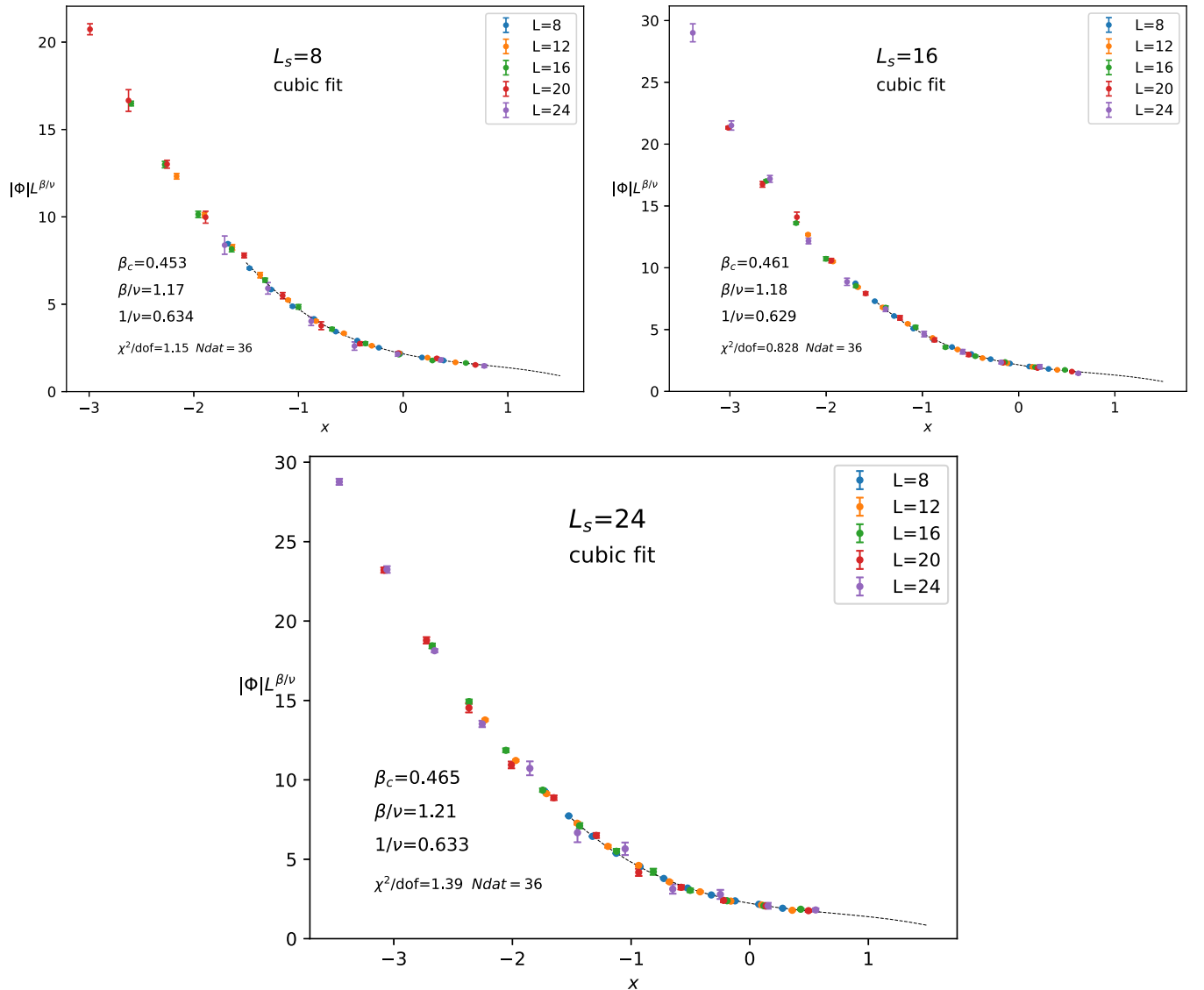


FIG. 4. Data collapse for the FVS in Eq. (15) using cubic fits. Results are provided in Table II. The panels differ in domain wall separation L_s .

TABLE III. Compendium of results for the critical exponents ν^{-1} , η_ϕ obtained using various methods.

Method	Year	ν^{-1}	η_ϕ
RHMC (DWF) (this work)	2026	0.63(3)	1.42(8)
$(2 + \varepsilon)$, $(4 - \varepsilon)$ interpolate [17]	2022	0.83(12)	1.01(6)
$(4 - \varepsilon)$ (4 loops) [19]	2017	0.64	0.98
Large- N [$O(N^{-2})$ + Padé] [20]	2018	0.85	1.18
FRG (NLO derivative expansion) [22]	2017	0.80	1.03
FRG (local potential approx) [21]	2014	0.77	1.01
QMC (SLAC) [13]	2025	0.98(2)	0.73(1)
QMC (hcmb) [7]	2026	0.90(10)	0.79(2)
QMC (π -flux) [4]	2020	0.95(4)	0.75(4)
QMC (hcmb+ π -flux) [2]	2015	0.98(1)	0.47(7)
QMC (hcmb) [6]	2021	1.11(4)	0.80(9)
QMC (hcmb) [3]	2018	1.14(9)	0.79(5)
QMC (hcmb+ π -flux) [1]	2014	1.19(6)	0.70(15)
QMC (π -flux) [5]	2020	1.10(8)	0.55(2)
HMC (hcmb) [9]	2021	0.84(4)	0.52(1)
HMC (hcmb) [8]	2020	0.84(4)	0.85(13)
HMC (hcmb) [11]	2018	1.08	0.62
HMC (hcmb) [10]	2018	0.86	0.87(4)

continuum-based approaches such as $(4 - \varepsilon)$, $(2 + \varepsilon)$, and large- N expansions and FRG as well as lattice-based simulations such as determinantal QMC [35] and HMC [36,37]. The discretizations admitting eight relativistic fermionic components in the low-energy limit include both honeycomb and square lattices, the latter with both π -flux lattice (equivalent to staggered fermions) and SLAC discretizations. We have distinguished between approaches rooted in 3D covariant field theory (upper part), and those (2+1)D simulations in which the time direction is essentially distinct (lower).

Significantly, our extracted results for both ν^{-1} and η_ϕ are outliers, as becomes very apparent in Fig. 5, where the values from Table III are visualized. Noncovariant (2+1)D simulation-based estimates for ν^{-1} tend to cluster around 1.0 and for η_ϕ to be significantly less than 1.0. Covariant 3D approaches such as this one find smaller ν^{-1} and larger η_ϕ ; even so, our values lie at the extremes of the range.

Figure 5 demonstrates that not only is there a very clear separation between the 3D and (2+1)D estimators, but there is also a very clear overall anticorrelation between ν^{-1} and η_ϕ . Our result is an outlier in both critical exponents, but it is reproducing this anticorrelation very well. Generally, it appears to be relatively easy to estimate the sum $\nu^{-1} + \eta_\phi$ (or something similar), but the distinction between the two exponents is very hard. Put differently, probably their (anti-)correlation is greatly underestimated in the uncertainties of most calculations (including ours).

IV. FERMION CORRELATOR

A. Specification of observable

Here, we introduce observables based on the fermion correlator

$$\mathcal{S}(x, s; y, s') = \langle \Psi(x, s) \bar{\Psi}(y, s') \rangle. \quad (17)$$

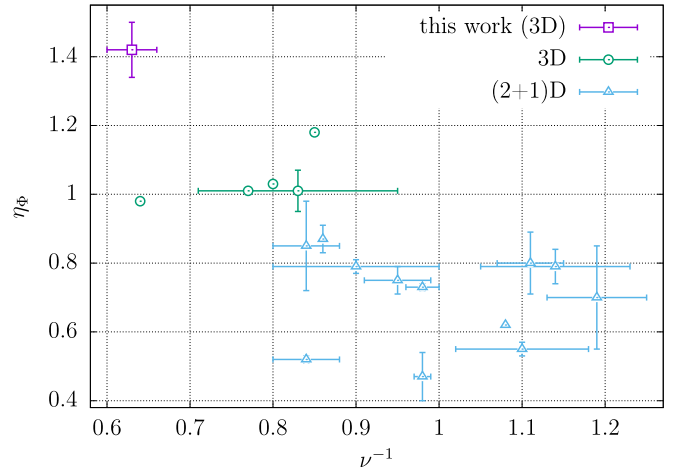


FIG. 5. Critical exponents ν^{-1} , η_ϕ from Refs. [1–13,17,19–22], as listed in Table III. Points labeled 3D (including this work) correspond to covariant methods with fully preserved Lorentz symmetry in three dimensions and are listed in the upper part of the table. Points labeled (2+1)D correspond to noncovariant methods that distinguish two spatial dimensions from one separate temporal dimension and are listed in the lower part of the table. The absence of error bars indicates that no uncertainties were provided in the references, respectively.

Following Eq. (8), the 3D propagator depends only on fields on the domain walls at $s = 1, L_s$. Define timeslice correlators [32]

$$\begin{aligned}
 S_\gamma(x_0) &\equiv \frac{1}{4} \text{tr} \gamma_0 \mathcal{S}(x_0) = \frac{1}{4} \sum_{\vec{x}} \\
 &\times \text{tr} \gamma_0 [\mathcal{P}_- \mathcal{S}(0, 1; x, 1) + \mathcal{P}_+ \mathcal{S}(0, L_s; x, L_s)], \\
 S_m(x_0) &\equiv \frac{1}{4} \text{tr} \mathcal{S}(x_0) = \frac{1}{4} \sum_{\vec{x}} \\
 &\times \text{tr} [\mathcal{P}_- \mathcal{S}(0, 1; x, L_s) + \mathcal{P}_+ \mathcal{S}(0, L_s; x, 1)], \quad (18)
 \end{aligned}$$

where the traces are taken over Dirac indices. Empirically, the following relations are recovered on a generic ϕ background in the $L_s \rightarrow \infty$ limit:

$$\begin{aligned}
 (S_\gamma)_{11} &= (S_\gamma)_{22}^*, & (S_\gamma)_{12} &= -(S_\gamma)_{21}^*, \\
 (S_m)_{11} &= -(S_m)_{22}^*, & (S_m)_{12} &= (S_m)_{21}^*,
 \end{aligned} \quad (19)$$

where the subscripts are flavor indices, consistent with the global SU(2) symmetry in Eq. (5). For practical purposes, it is thus sufficient to invert on just a single source flavor. For efficient sampling, we implement five evenly spaced but randomly shifted wall sources [32] for each ϕ configuration, performing five RHMC trajectories between measurements. Our simulation then reveals the only nonvanishing observables (up to noise) to be $\langle \text{Re}(S_\gamma)_{11} \rangle$, $\langle \text{Re}(S_m)_{11} \rangle$, $\langle \text{Re}(S_m)_{12} \rangle$, and $\langle \text{Im}(S_m)_{12} \rangle$ as well as those related by Eq. (19); below, we will label the three S_m components by an isoindex $a = 3, 1, 2$, respectively.

We find the flavor-singlet component S_γ is insensitive to the coupling β . Just as for the GN model [27], S_γ is symmetric under Euclidean time reversal. By contrast, S_m is odd under Euclidean time reversal, again echoing the GN model

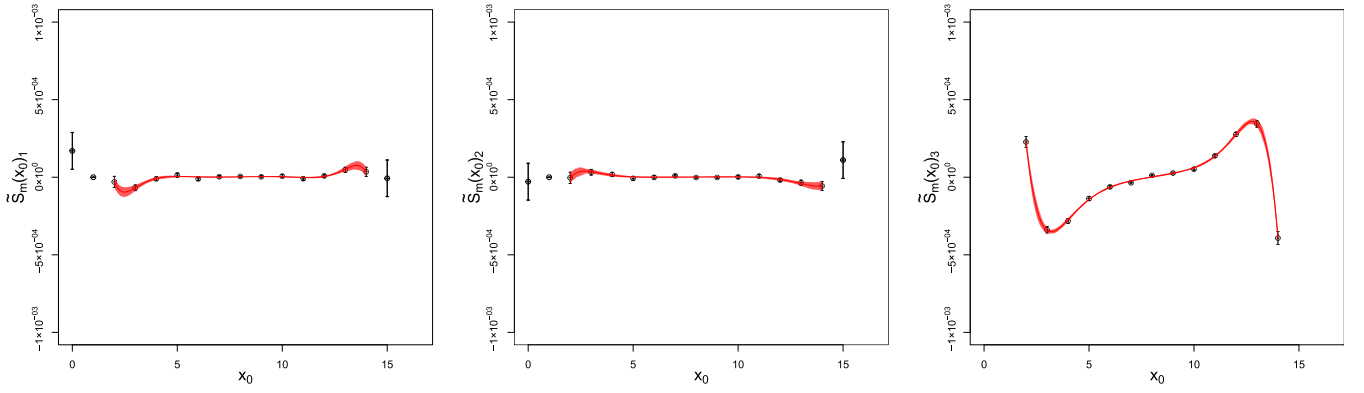


FIG. 6. Expectation values $\tilde{S}_m(x_0)$ of the $a = 1, 2, 3$ components (left to right) of the fermion correlator after rotation of the time slice $t = 1$ into positive 3-direction for $L = 16$, $L_s = 24$, coupling $\beta = 0.375$. The red curves show a simultaneous 8-state fit to the 2×2 matrix $\tilde{S}_m$ including error bands obtained with the THC method.

[27]. This time, we find a clear β dependence, so we focus subsequent analysis on the S_m component.

Since there is no symmetry-breaking term in the simulation, $\vec{\phi}$ drifts uniformly around its $SO(3)$ manifold during the course of the simulation, as shown in Fig. 1, so none of the three nonvanishing components of S_m should be privileged over sufficiently long run times. Noting that the $L_s \rightarrow \infty$ limit in Eq. (19) implies $S_m(x_0) = \vec{\tau} \cdot \vec{Q}$, our analysis first applies a global rotation $S_m \rightarrow \tilde{S}_m$ such that $\vec{Q}(x_0 = 1) = (0, 0, Q_3)$, in effect rotating the source along the third isodirection. Further details are given in Appendix B.

B. THC fit results

After rotation, we fit the full 2×2 matrix-valued fermion correlator $\tilde{S}_m(x_0)$. This simultaneous fit is made feasible in an automated way by the THC method [33]. The THC is a fully algebraic method providing a near-optimal set of energies E_l and matrix elements c_l for any given truncation k approximating

$$(\tilde{S}_m(x_0))_{\alpha\beta} = \sum_{l=1}^k c_{\alpha\beta,l} e^{-E_l x_0}, \quad (20)$$

with a tower of exponentials. Antisymmetry in this setting is realized by pairs of energies $E_l = -E_{l'}$ and coefficients $c_{\alpha\beta,l} = -e^{E_l L} c_{\alpha\beta,l'}$. (Anti-)symmetries of this type can be captured exactly by the THC method without the necessity to constrain the parameters *a priori*. We use the implementation in the HADRON package [38].

An example of such a matrix-valued THC fit is visualized in Fig. 6. In this case, we required $k = 8$ states to adequately describe the behavior for $2 \leq x_0 \leq L - 2$. The correlator is antisymmetric to a very good approximation, which means that the data are effectively described by four hyperbolic sine functions

$$(\tilde{S}_m(x_0))_{\alpha\beta} = \sum_{l=1}^{k/2} \tilde{c}_{\alpha\beta,l} \sinh[E_l(x_0 - L/2)]. \quad (21)$$

The most important result of all our simultaneous fits is that the $\{\alpha, \beta\} = \{1, 2\}$ components are always compatible with zero. In other words, once the gauge-fixing rotation aligns the

correlators at $x_0 = 1$ into the 3-direction, the entire fermion correlator remains within this one-dimensional subspace up to statistical fluctuations. Physically, this confirms that the residual $U(1)$ acting in the 12-plane following $SU(2)$ symmetry breaking remains unbroken as expected.

Once the 3-component has been isolated and numerically verified to be the only significant signal, we can simplify the analysis and fit this component exclusively. Fit results for two very different values of the coupling β are depicted in Fig. 7. Both cases are described well by four exponential or two sinh states. Their major difference is the greatly decreased amplitude for larger β .

Surprisingly, the quantification of this difference is rather elusive. The ground-state energy E_0 remains approximately constant over the entire region of β , as can be seen in Fig. 8. That is, the fermion remains massive across the phase transition, and only its interaction with the field changes.

An alternative observable related to the amplitude of the correlator is the ground-state contribution to the slope of the correlator at half time $\tilde{c}_0 E_0$. We see the amplitude decrease in Fig. 7, reflected in a decrease of this slope in Fig. 9. Since the slope decreases equally quickly for all lattice sizes, it does not feature a phase transition signature either. The leading factor appears to be inversely proportional to the squared volume $V = L^3$ and has been included in Fig. 9 to achieve an approximate data collapse. This needs to have little to do with the underlying fermion propagation and is conceivably due to the decreased sampling efficiency of the global rotation $S_m \rightarrow \tilde{S}_m$ as the spatial extent of correlated patches of ϕ field decreases with increasing β . However, given the considerable finite volume artifacts for free DWFs discussed in Ref. [32], we should be wary of drawing firm conclusions from relatively small systems.

V. SUMMARY

We have investigated the $SU(2)$ chiral Heisenberg model as a 3D covariant lattice field theory of GN type. It lends its name to a well-populated universality class of phase transitions. However, to date, lattice simulations of other models within the chiral Heisenberg universality class were limited to (2+1)D; that is, they have a distinct (noncovariant) time

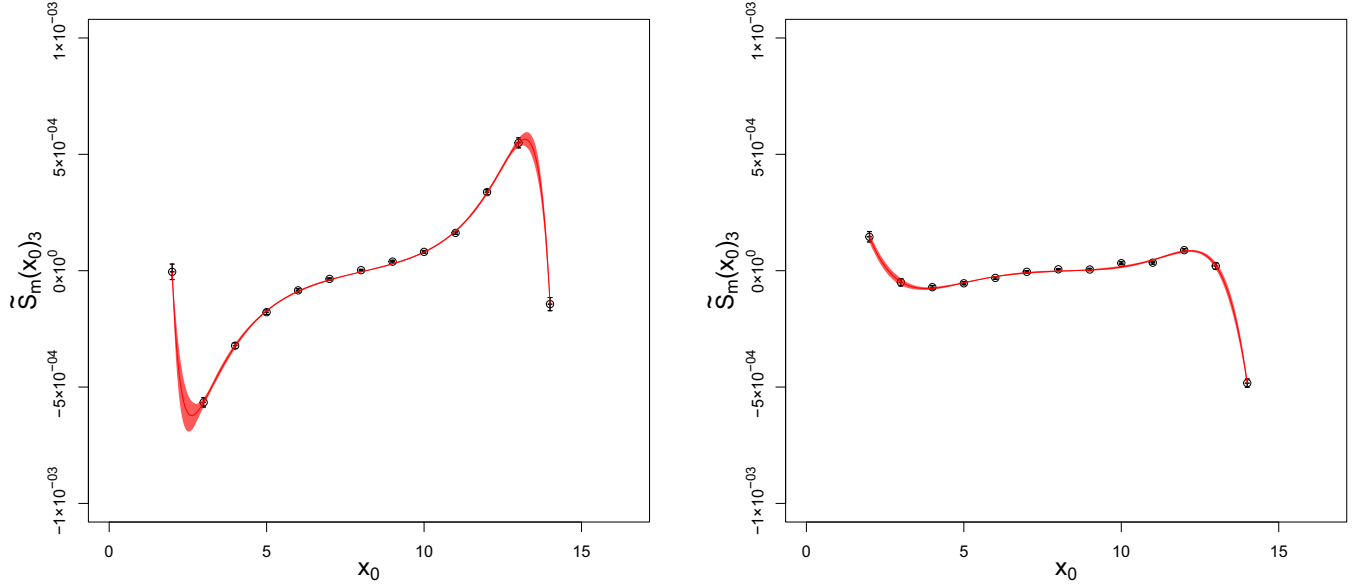


FIG. 7. Expectation value $\tilde{S}_m(x_0)$ of the 3-component of the fermion correlator after rotation of the time slice $x_0 = 1$ into positive 3-direction. Both panels used $L = L_s = 16$. Left: Coupling $\beta = 0.35$, right: $\beta = 0.475$. The red curves show 4-state fits including error bands obtained with the THC method.

dimension. This includes but is not limited to the Hubbard model on honeycomb and π -flux lattices. GN models, on the other hand, have primarily been investigated perturbatively so far. In contrast, in this work, we have performed a nonperturbative DWF simulation using the RHMC algorithm.

We have treated the absolute value $|\Phi|$ of the volume-averaged three-vector $\vec{\phi}$ that encodes the bosonic fields as an order parameter. At a critical coupling β_c the SU(2) symmetry is broken spontaneously to a residual U(1), and $|\Phi|$ develops a nonzero expectation value for all smaller couplings $\beta < \beta_c$. First, we have determined the Binder cumulant B (see Fig. 3) and observed simultaneously a crossing of B for different volumes. While this is a clear signature of a phase transition, we found the Binder cumulant too noisy for a quantitative analysis. Instead, we performed a data collapse fit

assuming universal FVS, see Fig. 4. The FVS *Ansatz* allowed us to extract the critical coupling $\beta_c = 0.465(11)$ as well as the critical exponents $\frac{\beta_\Phi}{\nu} = 1.21(4)$ and $\frac{1}{\nu} = 0.633(26)$. The numerical fits underpinning these results are stable and particularly show no sensitivity to the domain wall separation L_s , suggesting that the $L_s \rightarrow \infty$ limit needed to recover the symmetries of fully relativistic fermions is readily reached in this model, corroborating earlier findings in the 3DGN model [27].

Our result for β_c is uncontroversial, but our critical exponents are clear outliers compared with practically all findings in earlier work. We have visualized 18 distinct tuples $(\frac{1}{\nu}, \frac{\beta_\Phi}{\nu})$ from various literature sources in Fig. 5 together with our values. It would also be very interesting to compare with

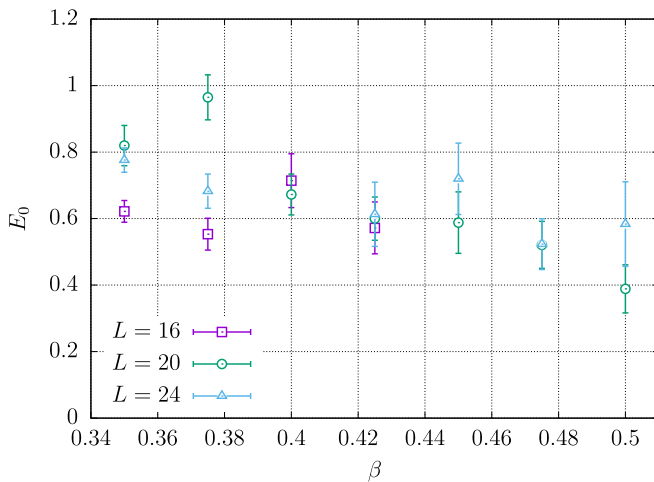


FIG. 8. Ground-state energies E_0 of the fermion correlators as a function of the coupling β for $L_s = 16$. The plots look very similar for $L_s = 8, 24$.

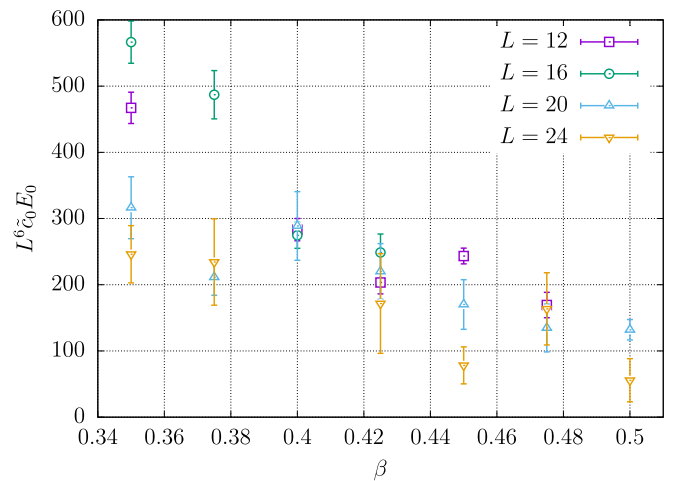


FIG. 9. Ground-state contribution to the slope $\tilde{c}_0 E_0$ of the correlator at the zero crossing at $x_0 = L/2$ rescaled by the squared volume $V = L^3$ as a function of the coupling β for $L_s = 16$. The plots look very similar for $L_s = 8, 24$.

anticipated results from the conformal bootstrap. Most literature values are not mutually compatible; however, there are two trends apparent. First, the results are completely split into two almost disjoint clusters, one stemming from methods using 3D models (including ours) and another based on (2+1)D models. The second trend is a strong anticorrelation between $\frac{1}{\nu}$ and $\frac{\beta_\Phi}{\nu}$ over all the results. Our understanding of this anticorrelation is that the two critical exponents are very hard to distinguish methodologically and that systematic uncertainties that result from this difficulty are vastly underestimated in (almost) all determinations including our own. We encourage the community to contemplate this behavior in the hope to pin down the characteristics of the chiral Heisenberg universality class conclusively.

Subsequently, in Sec. IV, we have investigated the fermion correlator. Since we did not introduce any explicit symmetry breaking or bare fermion mass to our simulations, the correlator is a Hermitian 2×2 matrix with the full SU(2) symmetry preserved and antisymmetric in time. This made the analysis nonamenable to standard techniques like plateau fits. To obtain a nonvanishing signal, we needed to rotate each ensemble into a fixed reference frame prior to averaging. A fit to the full matrix-valued correlator with the THC method [33] then allowed us to describe the correlator with a tower of sinh functions. It showed the expected unbroken U(1) subsymmetry on both sides of the phase transition. We further found that the ground-state energy hardly depends on the coupling β , which demonstrates that the fermion remains massive across the phase transition. Its interaction with the bosonic fields, on the other hand, changes with β , reflected in a decreasing amplitude of the correlator (see Figs. 7 and 9). The fermionic correlator data do not feature a phase transition signature, which certainly warrants further investigation in future work on larger lattices.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [40]. We used FORTRAN for the DWF simulations [42]. Our data analysis relied heavily on the standalone package COMP-AVG [41] as well as the HADRON [38] package implemented in R [43].

APPENDIX A: SIGN OF THE DETERMINANT

In the continuum Lagrangian density in Eq. (4), the fermion matrix $\mathcal{M}$ is the sum of anti-Hermitian and Hermitian terms, so its eigenvalues are complex in general. If, following a unitary rotation on ψ [23], we replace the interaction term by the U(2)-equivalent form $g\vec{\phi} \cdot \vec{\psi} i\gamma_3 \otimes \vec{\tau} \psi$, then both terms are anti-Hermitian, and the spectrum of $\mathcal{M}$ is pure imaginary. Since $\mathcal{M}$ is even dimensional, this proves the determinant $\det \mathcal{M}$ is real. The more conventional route uses the identity $\mathcal{M}^\dagger = \gamma_5 \mathcal{M} \gamma_5$ to show $\det \mathcal{M} = (\det \mathcal{M})^*$. This is important because this proof extends to lattice regularizations such as DWFs. We will proceed on the assumption that $\det \mathcal{M}$ is real, for both target and regularized theories.

Theories with a real determinant can still have a sign problem, but its nature is significantly constrained. Eigenvalues of $\mathcal{M}$ either come as complex (λ, λ^*) pairs or lie on the real axis. If the real eigenvalues can move independently along the axis, then it is possible for an odd number to become negative, flipping the sign of $\det \mathcal{M}$. Theories with isolated real eigenvalues are interesting because, under smooth evolution (e.g., under HMC flow), the eigenvalue must remain on the real axis until it meets another isolated eigenvalue, whereupon both have the opportunity to move back into the plane as part of a conjugate pair.

To see which case applies here, write the eigenvalue equation

$$[\partial_\mu \gamma_\mu \otimes \mathbb{1} + i\vec{\phi} \cdot \gamma_3 \otimes \vec{\tau}] \Psi = \lambda \Psi. \quad (\text{A1})$$

Now consider a related mode $\tilde{\Psi} = \mathcal{C} \gamma_5 \otimes \tau_2 \Psi$, where the (Dirac-basis dependent) matrix $\mathcal{C}$ has the properties

$$\mathcal{C} \gamma_\mu \mathcal{C}^{-1} = -\gamma_\mu^*, \quad \mathcal{C}^{-1} = -\mathcal{C}, \quad \mathcal{C}^* = \mathcal{C}, \quad [\mathcal{C}, \gamma_5] = 0, \quad (\text{A2})$$

satisfying

$$[\partial_\mu \gamma_\mu^* \otimes \mathbb{1} - i\vec{\phi}^* \cdot \gamma_3^* \otimes \vec{\tau}^*] \tilde{\Psi} = \lambda \tilde{\Psi}, \quad (\text{A3})$$

where we have also used $\tau_2 \vec{\tau} \tau_2 = -\vec{\tau}^*$. We conclude $\tilde{\Psi}^*$ is another eigenmode of $\mathcal{M}$ with eigenvalue $\lambda^* = -\lambda$. Since every nonzero eigenvalue is a member of a conjugate pair, $\det \mathcal{M}$ is real and positive. We can develop an analogous argument using the Hermitian interaction term if instead we focus on the Hermitian matrix $\gamma_5 \mathcal{M}$ to show that all eigenvalues are real and that both λ and $-\lambda$ feature in the spectrum, with corresponding modes $(\Psi, \mathcal{C} \otimes \tau_2 \Psi^*)$. Since $\det \gamma_5 = 1$, and by construction $\dim(\mathcal{M})$ is a multiple of 4, this is enough to prove the same result.

Things get interesting when we go to the lattice regularization since DWFs contain a Hermitian term in $\mathcal{M}$ proportional to $\mathbb{1} \otimes \mathbb{1}$; therefore, $[\gamma_5 \otimes \mathbb{1}, \mathcal{C} \otimes \tau_2] = 0$ spoils the $\lambda \rightarrow -\lambda$ symmetry for $\gamma_5 \mathcal{M}$. The mode $\tilde{\Psi}^*$ satisfies a different equation to Ψ ; we cannot deduce spectral symmetry; and we conclude $\det \mathcal{M}$ is not positive in general. Since we expect to recover the target theory in the limit $L_s \rightarrow \infty$, it seems reasonable to hope that the resulting sign problem is mild and can be ignored.

APPENDIX B: GAUGE FIXING (ROTATIONS INTO z BASIS)

Let us consider an observable S , for instance, S_m from Eq. (19), of the form

$$S = \begin{pmatrix} x_3 & x_1 - ix_2 \\ x_1 + ix_2 & -x_3 \end{pmatrix} \quad (\text{B1})$$

$$\equiv x_k \sigma_k, \quad (\text{B2})$$

i.e., S is a traceless Hermitian matrix that can be represented by a three-vector x as coefficients to the Pauli spin matrices. Here, S has a global degree of freedom under the adjoint representation of $\mathfrak{su}(2)$ so that we can act on S with an arbitrary matrix $U \in \text{SU}(2)$,

$$S \mapsto \tilde{S} = U^\dagger S U, \quad (\text{B3})$$

maintaining the physically relevant information. We can choose U so that $\tilde{S}$ becomes diagonal

$$\tilde{S} = \tilde{x}_3 \sigma_3, \quad (\text{B4})$$

where $\tilde{x}_3 = ||x||$. The rotation matrix U leading to this result is not unique, but for our purpose, it is enough to find one particular realization. Since we measure the observable $S(\tau)$ at different values of the Euclidean time τ , we must find one realization U_0 that diagonalizes $S(\tau_0)$ and then apply the same transformation

$$S(\tau) \mapsto \tilde{S}(\tau) = U_0^\dagger S(\tau) U_0, \quad (\text{B5})$$

for all times.

It is essential to perform this rotation on every individual measurement before averaging over the MC history. Since there is no other gauge-fixing mechanism, otherwise, S would average to 0. In practice, the equal-time correlator for $\tau = 0$ is typically not representative for the other values of τ . Therefore, we used $\tau_0 = 1$, which has the maximally significant signal among $\tau > 0$.

From the relation between $\text{SU}(2)$ and $\text{SO}(3)$ or, more intuitively, the equivalence between S and x , it becomes clear that we can reduce the diagonalization problem to a rotation by $O \in \text{SO}(3)$ with

$$Ox = \tilde{x}. \quad (\text{B6})$$

The diagonality condition in Eq. (B4) together with $x'_3 > 0$ then translates to

$$\frac{x}{||x||} = O^\top e_3. \quad (\text{B7})$$

At this point, we make the *Ansatz* to write O as a product of planar rotations

$$O = R_\theta R_\varphi, \quad (\text{B8})$$

$$R_\varphi = \begin{pmatrix} \cos \varphi & -\sin \varphi & 0 \\ \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (\text{B9})$$

$$R_\theta = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta \\ 0 & \sin \theta & \cos \theta \end{pmatrix}. \quad (\text{B10})$$

The right-hand side in Eq. (B7) then becomes

$$O^\top e_3 = \begin{pmatrix} \sin \theta \sin \varphi \\ \sin \theta \cos \varphi \\ \cos \theta \end{pmatrix}. \quad (\text{B11})$$

Setting this equal to the left-hand side of Eq. (B7) allows us to solve for φ and θ , yielding

$$\begin{aligned} \varphi &= \text{atan2}(x_1, x_2), \\ \theta &= \text{atan2}\left(\sqrt{x_1^2 + x_2^2}, x_3\right), \end{aligned} \quad (\text{B12})$$

where atan2 denotes the two-argument arctangent. It is implemented in most programming languages. By definition, $\text{atan2}(y, x)$ returns the unique 2π -periodic angle between the coordinate (x, y) and the positive x axis.

Thus, the transformation in Eq. (B5) of S can be expressed by the rotation

$$x(\tau) \mapsto \tilde{x}(\tau) = R_\theta R_\varphi x(\tau), \quad (\text{B13})$$

where φ and θ are determined by Eq. (B12) using $x(\tau_0)$. Simple sanity checks for the correctness of the rotation are that $\tilde{x}(\tau_0) = (0, 0, ||x(\tau_0)||)^\top$ and $||\tilde{x}(\tau)|| = ||x(\tau)||$ for all τ .

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