Simulating Quantum Field Theories on the Lattice

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We discuss the lattice method of computing correlation functions of quantum field theories. The lattice allows *ab initio* calculations in *non-perturbative* regimes. Calculations on the lattice give rise to continuum results as the limit of the lattice spacing $a \to 0$ is taken by approaching criticality. Discretizing a continuum action on the lattice requires care, and we discuss the so-called "fermion doubling problem" that gives rise to extra physical fermion flavors for a single fundamental field. We explain lattice methods through the example of simulating a scalar ϕ^4 theory coupled to one or more fermion fields ψ via a Yukawa term $g\phi\bar{\psi}\psi$. Finally, we reproduce the expected phase diagram in the weak coupling regime via simulation, find the expected $1/n_f$ linear scaling in the phase transition points along a fixed g line, and demonstrate that indeed addition of the $\mathcal{O}(a)$ irrelevant term in the lattice action removes the fermion doublers as the continuum limit is taken.

I. INTRODUCTION

The Standard Model (SM) of physics is one of a class of *quantum field theories* (QFTs) that describe the quantum mechanical behavior of a set of fields defined over 4D spacetime. The features of the Standard Model have been compared to experimental results via a variety of techniques [1], and shown to provide a very accurate description of our world at a large range of scales. Yet, there are physical phenomena that do not fit within the description provided by the Standard Model: dark matter and neutrino masses, for example [2]. There are a number of proposed extensions to the Standard Model, collectively termed Beyond the Standard Model (BSM) physics, that seek to explain these phenomena. A major task for theorists is then to make concrete, verifiable predictions from both the SM and BSM models, allowing experiments to distinguish between them.

Physically observable quantites in QFTs are derived from the correlation functions of the theory, that are formally given by a path integral over field configurations weighted by the action [3]:

$$\langle \mathcal{O}_0[\Psi]\mathcal{O}_1[\Psi]...\rangle = \frac{1}{Z}\int \mathcal{D}\Psi(\mathcal{O}_0\mathcal{O}_1...)\exp\left(-iS[\Psi]\right)$$

where

$$Z = \int \mathcal{D}\Psi \exp\left(-iS[\Psi]\right)$$

the operators $\mathcal{O}_i[\Psi]$ are some complex-weighted combination of products of the fields, and the action $S[\Psi]$ is the time-integral of the kinetic energy minus the potential energy of the configuration. For most theories, this path integral cannot be explicitly evaluated (just like the partition function of statistical mechanics often cannot be explicitly solved), and we must use appropriate physical assumptions to make a bounded approximation of the result. To approximate the path integral calculation of correlation functions, a variety of tools are available to theorists.

Perturbation theory is commonly used to approximately calculate correlation functions in regimes where the coupling between fields of the physical theory are weak, allowing an order-by-order expansion in the degree of interactions. In regimes where coupling is strong, this expansion does not provide a good approximation to the physics at any finite order.

Effective field theories (EFTs) provide a systematic method of "integrating out" high-energy degrees of freedom to describe physics at lower energy scales [4]. If the lower-energy effective interactions are weakly coupled, one may approximately calculate correlation functions in terms of these effective degrees of freedom and interactions using perturbation theory. For infrared confined theories, the non-perturbative regime occurs at low energy scales, and EFTs allow computing correlation functions between composite objects that are weakly coupled. The strong nuclear force sector of the Standard Model describing quarks and gluons is one such theory, and specifically, Chiral Perturbation Theory is a low-energy EFT that describes nucleon and pion interactions [5]. Importantly, however, EFTs based on interactions between non-perturbatively described objects must draw their coefficients from elsewhere: either by fitting to experiment or another ab initio non-perturbative approach.

Lattice simulations provide such a non-perturbative ab initio approach. This paper focuses on lattice simulations in particular. In the remaining sections:

1. We justify why lattice simulations allow evaluation of continuum correlation functions (Section II).

2. We describe a simple scalar ϕ^4 theory formulated on a lattice (Section III) and subsequently extend the theory by adding a spin-$\frac{1}{2}$fermion field ψ coupled to the scalar via a Yukawa coupling $g\phi\bar{\psi}\psi$ (Section IV). We identify two issues with describing spin-$\frac{1}{2}$fermions on the lattice – the anticommuting nature of the field values and additional physical fermion flavors arising from lattice artifacts of the discrete Dirac equation – and identify solutions.

3. We explain the methods (Section V) and demonstrate the results (Section VI) of simulating the full Yukawa theory on a 2D lattice. In particular, we

reproduce the expected phase diagram of the theory and show the dependence of the critical point on the number of physical fermion flavors n_f, validating the existing of the extra fermion flavors and their removal.

II. LATTICE METHODOLOGY

In the lattice approach to calculating correlation functions, one *samples* the path integral to make numerical approximations to physical observables. This is typically performed by (1) rephrasing the quantum theory as a classical statistical theory, described by a real-weighted partition function, (2) discretizing the theory on a finite set of lattice points, and (3) sampling the resulting set of integrals via Monte Carlo methods generally applicable to statistical theories on discrete sets of points. While we discuss these steps in detail in the context of a specific theory in the next section, we take a moment to justify the physicality of step (2). Specifically, we argue that extrapolating lattice calculations of a given correlation function approaching a critical point of the theory gives the desired continuum result.

The path integral of QFT has parallels with a partition function of Mean Field Theory (MFT). In MFT, the continuum field theory is treated as an approximation to an underlying discrete theory. This is useful in weak-coupling regimes, as one can make use of continuum perturbation theory results to describe discrete physics. We are interested in strong-coupling regimes, however. Lattice discretization can be interpreted as following the MFT method in reverse: approximating a continuum theory by a discrete collection of degrees of freedom.

Just like in MFT, making physical predictions then requires us to evaluate in a regime where fluctuations are long-range, such that our replacement of fields by a lattice (or vice versa as in MFT) is well-justified [6, Chap 2]. As long as we consider calculations near a critical point where $\xi \to \infty$, this criterion is satisfied.

One can also argue that physical results become valid near a critical point by demanding that we take the physical lattice spacing $a \to 0$ to make statements about the field theory [7]. Taking such a limit is not necessarily obvious, as we do not have direct control of the unitful a. As we tune closer to a lattice critical point, however, we can consider the length of the renormalization flow required to take us to a given temperature T with a fixed physical correlation length ξ. Approaching closer to the critical point implies a longer flow to reach a fixed T and ξ. In terms of the lattice spacing a, $\xi \sim ae^l$ with $l \to \infty$. Thus we must correspondingly have $a \to 0$ as we tune to the critical point. Creutz [8], provides a detailed RG analysis along these lines for the case of non-abelian gauge theories like QCD.

Having justified the lattice methodology, we proceed by describing a scalar field theory and an extension including fermions on the lattice.

III. SCALAR FIELD THEORY

We begin by considering a simple ϕ^4 scalar QFT, defined by the continuum action:

$$S_\phi^{\text{mink}}[\phi] = \int d^4x \left(-J \left(\partial_\mu \phi_x \partial^\mu \phi_x\right) - \frac{m^2}{2}\phi_x^2 - \lambda \phi_x^4 \right)$$

We use the repeated index summation convention $X_\mu X^\mu = X_\mu X_\nu \eta^{\mu\nu} = -X_t X_t + \sum_{i\in x,y,z} X_i X_i$ with a mostly-positive Minkowski metric $\eta = \text{diag}\,(-1,1,1,1)$. The two point correlator is given by:

$$\langle \phi_x \phi_0 \rangle = \frac{1}{Z} \int \mathcal{D}\phi \left(\phi_x \phi_0\right) \exp\left(-iS_\phi^{\text{mink}}[\phi]\right)$$

with

$$Z = \int \mathcal{D}\phi \exp\left(-iS_\phi^{\text{mink}}[\phi]\right)$$

This continuum field theory can be interpreted physically as a non-interacting Higgs field, without electroweak doublet structure (i.e. only a single scalar, instead of a two-component complex vector) [9, Sec 5.6]. When $m^2 < 0$, the saddle point solution picks out a constant configuration with non-zero expected value: $\phi_x^{sp} = \bar{\phi}$ with $\bar{\phi}^2 = \frac{-m^2}{4\lambda}$. In the full electroweak theory, this acquisition of a vacuum expectation value by the Higgs is responsible for W, Z boson and fermion masses [10]. Analysis of the critical points of this theory and its extensions is thus relevant for making predictions about the Higgs.

In the following, we discuss the lattice formulation of this theory (III A) and the sampling methods used to compute its correlation functions (III B).

A. Lattice formulation

To convert the continuum Minkowski theory described above into something tractable by simulation, we must massage the form. Specifically, we perform two transformations:

1. Convert the action into a Euclidean real-weighed integral via Wick rotation (III A 1).
2. Discretize the action and path integral for a finite number and spacing of spacetime points (III A 2).

1. *Wick rotation*

As we are ultimately interested in sampling this integral, we make the choice to *Wick rotate* [11] to a Euclidean metric via $t \to i\tau$. Performing this transformation replaces the Minkowski action with a Euclidean action (we drop the "mink" superscript for this new action), and removes the complex factor in the path integral:

$$\langle \phi_x \phi_0 \rangle = \frac{1}{Z} \int \mathcal{D}\phi \left(\phi_x \phi_0\right) \exp\left(-S_\phi\right) \tag{1}$$

$$S_\phi \equiv \int d\tau d^3x\, J(\partial_\tau \phi_x)^2 + J\left(\partial_i \phi_x \partial^i \phi_x\right) + \frac{m^2}{2}\phi_x^2 + \lambda \phi_x^4 \tag{2}$$

The effect of this rotation of our spacetime index is to phrase the path integral in terms of a positive, bounded weight e^{-S_ϕ}. Our correlators are now exactly the statistical mechanics variety of two-point functions: a pair of fields integrated against some probability distribution.

Our fields, and in particular our correlators, are now parameterized by Euclidean locations. We may ask: what does separation in the τ coordinate mean? If we treat our correlation function in the operator formalism, the value of the correlation function corresponds to the amplitude between a state created at $\tau = 0$ and $\tau = \tau'$. We may insert a complete set of energy eigenstates to compute the amplitude between a state created at $\tau = 0$ and annihilated at $\tau = \tau'$:

$$\langle \phi_{\vec{x},\tau'} \phi^\dagger_{\vec{x},0} \rangle = \sum_n \langle 0|\phi_{\vec{x},\tau'}|n\rangle \langle n|\phi^\dagger_{\vec{x},0}|0\rangle \tag{3}$$

$$= \sum_n \langle 0|\phi_{\vec{x},0} e^{iHt}|n\rangle \langle n|\phi^\dagger_{\vec{x},0}|0\rangle \tag{4}$$

$$= \sum_n |\langle 0|\phi_{\vec{x},0}|n\rangle|^2 e^{-E_n \tau'} \tag{5}$$

Thus, evolution in τ corresponds to non-unitary exponential decay of the amplitude of each energy eigenstate. Crucially, one can exploit this to extract the spectrum of a theory by making exponential fits.

By making a Wick rotation we have thus rephrased the path integral as integration over a Boltzmann-style probability distribution, $p[\phi] \propto e^{-S_\phi[\phi]}$, and have demonstrated the utility of the Euclidean correlation functions.

2. Lattice discretization

Having Wick rotated the theory, evaluation of the correlation functions reduces to a continuous path integral against a probability distribution. To make this computationally tractable, we discretize the Euclidean spacetime to a finite set of lattice points. This requires a discretized version of the fields, the path integral, and the action.

We choose to simply discretize the fundamental field by placing one value at every site of a 4D lattice, where the values are chosen from the same set as the general field. For the scalar field, this means a single real value per site. In principle, we could imagine different underlying lattice theories giving rise to the same "mean field" ϕ, but we choose the simplest possibility to make reasoning about the lattice theory easier. The measure of the path integral (1) is then naturally replaced by one integral per site.

We must then consider how to discretize the action S_ϕ given in (2). The spacetime integral must be broken down to a sum over lattice sites $\int d\tau d^3x \to a^4 \sum_x$, where a is the lattice spacing. The mass and ϕ^4 terms can be kept as they are. The continuum derivative may emerge from a number of possible lattice terms. For now, we choose a simple discretized derivative $(\partial_\tau \phi_x)^2 + (\partial_i \phi_x)^2 \to \frac{1}{a^2}\sum_\mu (\phi_{x+\hat{\mu}} - \phi_x)^2$. We will see that this ambiguity of underlying lattice terms as $a \to 0$ allows us to make judicious choices when fermion discrete derivatives present issues.

Finally, we can put together the discretized path integral and discretized action to write down our two-point correlator on the lattice:

$$\langle \phi_x \phi_0 \rangle = \frac{1}{Z} \int \prod_i d\phi_i \, (\phi_x \phi_0) \exp\left(-S^{\text{latt}}_\phi\right) \tag{6}$$

$$S^{\text{latt}}_\phi \equiv a^4 \sum_x \frac{J}{a^2} (\phi_{x+\hat{\mu}} - \phi_x)^2 + \frac{m^2}{2}\phi_x^2 + \lambda \phi_x^4 \tag{7}$$

B. Monte Carlo Sampling of the Path Integral

Having defined our lattice theory and discussed its physical relevance near a critical point, the natural next question is: how can we numerically simulate such a lattice theory? Specifically, we hope to numerically approximate the set of integrals on the lattice (6) that give us the two-point correlator. There is a host of literature on the subject [12–14]. For brevity, we provide only a general overview the Markov Chain Monte Carlo (MCMC) class of methods commonly applied in this situation. Appendix A 1 provides further details on the particular MCMC method used in our simulations.

First introduced by Metropolis et al. [15], Markov Chain Monte Carlo methods involve stochastically producing a sequence of lattice states that sample the path integral by using a Markovian update at every step. By choosing the update algorithm such that the equilibrium distribution has probabilities proportional to the Boltzmann weight per state $e^{-S^{\text{latt}}_\phi}$, one can approximate the path integral by averaging the value of the two-point correlator evaluated on some set of states in the sequence:

$$\langle \phi_x \phi_0 \rangle \approx \frac{1}{N} \sum_{i=1}^{N} \phi_x^{(i)} \phi_0^{(i)}$$

Metropolis et al. initially proposed one such update algorithm. At each step in the sequence, their method consists of randomly updating the previous state, $\phi^{(i)} \to \phi^{\text{new}}$, followed by either accepting the new state ($\phi^{(i+1)} = \phi^{\text{new}}$) or rejecting it and keeping the old ($\phi^{(i+1)} = \phi^{(i)}$). If the random state update is symmetric (equally likely to update $\phi^A \to \phi^B$ as $\phi^B \to \phi^A$), then setting the acceptance probability to

$$p_{\text{accept}} = \min\left(1, \exp\left(-S[\phi^{\text{new}}] + S[\phi^{(i)}]\right)\right) \tag{8}$$

ensures the equilibrium distribution is exactly the Boltzmann distribution [13, Sec 4.1].

IV. YUKAWA THEORY

While the scalar ϕ^4 theory provides a simplified model of the behavior of an isolated Higgs field, it does not give us a handle on the remainder of the Standard Model. Generally, we would additionally like to be able to discuss gauge bosons and fermions on the lattice. The former is outside the scope of this paper, but we focus on the latter by extending the scalar ϕ^4 theory with the inclusion of a fermion field ψ. By the Spin-Statistics theorem [16] all fermion fields must have half-integer spin. We focus our attention on spin-$\frac{1}{2}$fermions that are described by the Dirac equation, as all fermions in the Standard Model take this form. In the Standard Model, these fields are described by N_s-component complex-Grassmann-valued column vectors, where N_s is the number of spin components required by the Dirac equation and the Grassmann nature means the field values *anticommute*.

To enable probing our fermion field via lattice simulation, and to match the form of the SM Higgs-fermion coupling, we include an interaction between the ϕ and ψ via a *Yukawa coupling* term $g\phi\bar{\psi}\psi$ in the action, where $\bar{\psi}$ is the conjugate of ψ.

Both the anticommuting nature of the field values and the linear form of the Dirac equation present difficulties in simulations. Grassmann-valued integrals are tricky to evaluate numerically, but can instead be handled analytically. We discuss performing this evaluation and then rewriting the result in terms of integration over fictional *pseudofermion* fields that are N_s-component vectors over normal complex numbers (IV B). We then address additional physical fermion "doubler" flavors generated by a naive handling of the discretization of the Dirac equation (IV C). These additional flavors do not correspond to additional fermion fields in the Standard Model, and so simulating the Standard Model requires removing them. We summarze one technique to address this (IV D).

A. Continuum and lattice formulations

The complete action for the continuum theory (after Wick rotation to Euclidean metric) takes the form:

$$S_y = S_\phi + \int_x \left(g\phi_x\bar{\psi}_x\psi_x + \bar{\psi}_x\gamma^\mu\partial_\mu\psi_x + m_\psi\bar{\psi}_x\psi_x\right) \quad (9)$$

Here $\psi(\bar{\psi})$ is an N_s-component column(row) vector of complex-Grassmann values, and γ_μ are the d-dimensional $N_s \times N_s$ matrices that satisfy the Euclidean Clifford algebra $\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\nu = 2\delta_{\mu\nu}$. In the Standard Model, $d = 4$ and $N_s = 4$ as well. For a single spatial and single time dimension, $d = 2$ and $N_s = 2$. In our simulations we restrict to $d = 2$ due to limited computational resources.

To write down a lattice theory, we must discretize the new pieces of the action. We can represent the fermion fields $\bar{\psi}, \psi$ on the lattice by four-component complex-Grassmann vectors placed on every site. The interaction g and mass m_ψ terms can be represented identically on the lattice. The derivative term may be most simply discretized as:

$$\bar{\psi}_x\gamma^\mu\partial_\mu\psi \to \bar{\psi}_x\sum_\mu \frac{\gamma^\mu}{2a}\left(\psi_{x+\hat{\mu}} - \psi_{x-\hat{\mu}}\right) \quad (10)$$

We will see in IV C that this choice of derivative term results in additional physical fermion flavors arising in the lattice theory, but for now we press onward.

Combining these results, the lattice version of the path integral can be written:

$$\langle\phi_x\phi_0\rangle = \frac{1}{Z}\int\prod_i d\bar{\psi}_i d\psi_i d\phi_i \left(\phi_x\phi_0\right)\exp\left(-S_y^{\text{latt}}\right) \quad (11)$$

$$S_y^{\text{latt}} \equiv S_\phi^{\text{latt}} + \sum_{x,y}\bar{\psi}_x D_{xy}\psi_y \equiv S_\phi^{\text{latt}} + S_\psi^{\text{latt}} \quad (12)$$

$$\begin{aligned} D_{xy}[\phi] \equiv{}& \delta_{xy}\mathbb{1}^{N_s\times N_s}\left(g\phi_x + m_\psi\right) \\ &+ \sum_\mu \frac{\gamma^\mu}{2a}\left(\delta_{x+\hat{\mu},y} - \delta_{x-\hat{\mu},y}\right) \end{aligned} \quad (13)$$

B. Replacing fermions with pseudofermions

The integrals over $\bar{\psi}, \psi$ are Grassmann-valued and thus difficult to handle numerically. However, we can actually handle these analytically. Grassmann Gaussian integration gives:

$$\langle\phi_x\phi_0\rangle = \frac{1}{Z}\int\prod_i d\phi_i \det\left(D[\phi]\right)\left(\phi_x\phi_0\right)e^{-S_\phi^{\text{latt}}} \quad (14)$$

This form could be sampled, but requires many evaluations of $\det D$, a costly procedure as D is $NN_s \times NN_s$ (with N the number of lattice sites). Instead, this path integral is typically rephrased in terms of the pseudofermion field η that has the same vector structure as $\bar{\psi}, \psi$ but takes normal complex values rather than complex Grassmann values. Using γ_5-hermiticity of D [13, Sec 5.4.3], we have:

$$\det D = \det\left(\gamma_5 D\right) = \det\left(\gamma_5 D\gamma_5 D\right)^{1/2} = \det\left(D^\dagger D\right)^{1/2}$$

Introducing Gaussian integrals over this fictional field, we can then absorb the square-root determinant:

$$\langle\phi_x\phi_0\rangle = \frac{1}{Z}\int\prod_i d\eta_i d\phi_i \left(\phi_x\phi_0\right)e^{-S_\phi^{\text{latt}} - S_\eta^{\text{latt}}} \quad (15)$$

$$S_\eta^{\text{latt}} \equiv a^4\sum_x \eta_x^\dagger\left(D^\dagger D\right)^{-1}\eta_x \quad (16)$$

This finally gives us a form of the path integral that is accessible to numerical approximation.

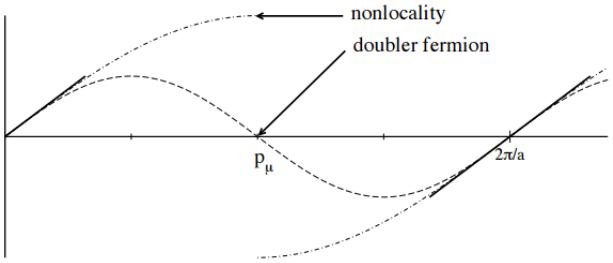

FIG. 1: Using the naive discretized derivative for ψ, we get an additional zero of the lattice fermion coupling, occurring at $q = \pi/a$. Generally, if we demand continuity and linear behavior about zero, an additional zero is forced. Figure courtesy of [18].

C. Fermion doubling

The linear nature of the Dirac equation presents another issue to simulating fermions on the lattice. Let us briefly revisit the naive derivative term (10) we chose in discretizing the derivative. Fourier transforming this component of S_ψ^{latt} gives:

$$S_\psi^{\text{latt}} \supset \frac{\text{const.}}{a} \int_q \bar{\psi}_q \sum_\mu \gamma_\mu (e^{iq_\mu a} - e^{-iq_\mu a}) \psi_q \tag{17}$$

$$\propto \frac{i}{a} \int_q \bar{\psi}_q \left(\sum_\mu \gamma_\mu \sin(q_\mu a) \right) \psi_q \tag{18}$$

In QFTs, the poles of the Fourier-space correlator $\langle \bar{\psi}_q \psi_q \rangle$ define the physical particles of the theory [17, Sec 3.4]. Intuitively, a pole of the correlator corresponds to a momentum mode of the field that will "ring forever" if kicked. Based on the fermion piece of the lattice action described above, a pole occurs wherever $\sin(q_\mu a) = 0$, which occurs when all $q_\mu = n\pi/a$. As q is a lattice wavevector, the inequivalent values can be located in the first Brillouin zone with bounds $[0, 2\pi/a]$ in every dimension. Thus for our simple discretization we have an inequivalent pole for every point in the Brillouin zone of the form $q = (0, 0, ...)$, $(\pi/a, 0, ...)$, $(0, \pi/a, ...)$, $(\pi/a, \pi/a, ...)$, etc. This is diagrammed for one dimension in Figure 1. In d dimensions, we thus have included 2^d physical fermions in the theory!

As discussed in III A 2, we have freedom in choosing the lattice discretization of the derivative since the continuum extrapolation takes $a \to 0$. Can we choose a better form of the derivative by introducing $\mathcal{O}(a)$ terms that reduces these extra fermions, while still matching the continuum form? A famous theorem by Nielson and Ninomaya [19] has the implication for our fermions [20] that as long as we maintain (1) translational symmetry, (2) locality, (3) the proper continuum derivative about $p = 0$, and (4) D anticommuting with γ_5, we cannot have an odd number of fermion flavors. Intuitively, we can see this topologically: the conditions demand a smooth function that is positive at the beginning of the Brillouin zone and negative at the end (Figure 1), mandating a zero-crossing in the continuum limit. This argument can be generalized to multiple dimensions.

If we enforce all of the above conditions, we cannot remove the doubler fermions entirely. To remove the doublers, then, we must choose a condition and carefully break it.

D. Solutions to fermion doubling

There are many methods to address the fermion doubling problem on the lattice. Common techniques are: Staggered fermions [21], Domain Wall fermions [22], and Wilson fermions [23]. We focus on the latter because of its simplicity in implementing on the lattice, however the various options each have their merits.

Wilson fermions eliminate the unwanted extra poles by explicitly breaking condition (4) described above: that D anticommute with γ_5. Specifically, Wilson suggests modifying the Fourier transform of the derivative piece of S_ψ^{latt} (18) to read [13]:

$$S_\psi^{\text{deriv}} \propto \frac{i}{a} \sum_\mu \gamma_\mu \sin(q_\mu a) + \mathbb{1} \frac{1}{a} \sum_\mu (1 - \cos(q_\mu a)) \tag{19}$$

At points of the Brillouin zone where n components of q_μ are π/a, this term takes value $\sim \frac{n}{a} \to \infty$ in the continuum limit, while at $q = (0, 0, ..., 0)$ this term still goes to zero linearly with $\mathcal{O}(a)$ corrections. Thus by introducing this extra term, all correlator poles except $q = (0, 0, ..., 0)$ are given infinite masses and correspondingly should have no effect on the continuum theory.

Implementing this term involves inverse Fourier transforming the cosine term which gives additional couplings between further separated ψ_x. Further details can be found in [13, Sec 5.2.3].

V. METHODS

To demonstrate the effects of fermions on the scalar theory, and specifically to identify the existence of fermion doublers, we performed simulations of the Yukawa model in 2D on an 8×8 lattice. A Hybrid Monte Carlo method was used to generate the Markov chain of lattice states, with N_0 tuned to achieve acceptance rates generally in the range $0.6 - 1.0$ (see Appendix A 1).

Following [24], we rewrite our lattice action $S_\phi^{\text{latt}} + S_\eta^{\text{latt}}$ as given in (15) and (16) to combine J and m^2 into a single β-like parameter. Specifically, we define $\hat{J} \equiv a^2 J$, $\hat{\lambda} \equiv a^4 \lambda$, $\hat{g} \equiv a^4 g$, and $\hat{m}_\psi \equiv a^4 m_\psi$, and fix $a^4 \frac{m^2}{2} \stackrel{!}{=}$

$\left(1-2d\hat{J}-2\hat{\lambda}\right)$, Rewriting S_ϕ^{latt} and S_η^{latt} then gives:

$$\begin{aligned} S_\phi^{\text{latt}} &= \sum_x \hat{J} \sum_\mu (\phi_{x+\hat{\mu}} - \phi_x)^2 \\ &\quad + \left(1-2d\hat{J}-2\hat{\lambda}\right)\phi_x^2 + \hat{\lambda}\phi_x^4 \end{aligned} \tag{20}$$

$$\begin{aligned} &= \sum_x -2\hat{J}\sum_\mu \phi_x\phi_{x+\hat{\mu}} + \hat{\lambda}\left(\phi_x^2-1\right)^2 \\ &\quad + \phi_x^2 + \text{const.} \end{aligned} \tag{21}$$

$$S_\eta^{\text{latt}} = \eta^\dagger \left(\hat{D}^\dagger \hat{D}\right)^{-1} \eta,\ \hat{D} \equiv D[\phi, \hat{g}, \hat{m}_\psi] \tag{22}$$

We expect temperature $T \sim 1/\hat{J}$. Throughout, we fix $\hat{m}_\psi$ to 1.0, and tune the coupling strength through $\hat{g}$.

VI. RESULTS

Throughout, we compare results against a Higgs-Fermion model implemented by Bulava et al. [24], using their phase terminology [25].

A. Uncoupled scalar ϕ^4 theory

We first demonstrate that the uncoupled ($\hat{g}=0$) scalar field theory, as described in Section III reproduces the relevant features of the field theory. Specifically, we find that there are three phases: a ferromagnetic (FM) phase, an antiferromagnetic (AFM) phase, and a symmetric (SYM) phase. These are characterized by two order parameters: magnetization $\langle m \rangle$ and staggered magnetization $\langle s \rangle$, defined by:

$$\langle m \rangle \equiv \frac{1}{N} \langle | \sum_x \phi_x | \rangle \tag{23}$$

$$\langle s \rangle \equiv \frac{1}{N} \langle | \sum_x (-1)^{x_0+x_1} \phi_x | \rangle \tag{24}$$

Intuitively, the magnetization is a measure of an overall uniform expectation value acquired by the field, while the staggered magnetization is a measure of an overall alternating-sign expectation value acquired by the field. These order parameters characterize the phases by:

$$\langle m \rangle \neq 0, \langle s \rangle = 0 \rightarrow \text{FM}$$

$$\langle m \rangle = 0, \langle s \rangle \neq 0 \rightarrow \text{AFM}$$

$$\langle m \rangle = 0, \langle s \rangle = 0 \rightarrow \text{SYM}$$

The results are shown in Figure 2. Based on the behavior of $\langle m \rangle$ and $\langle s \rangle$ we have identified the phases and transition values of $\hat{J}$ by hand. The critical $\hat{J}$ values for

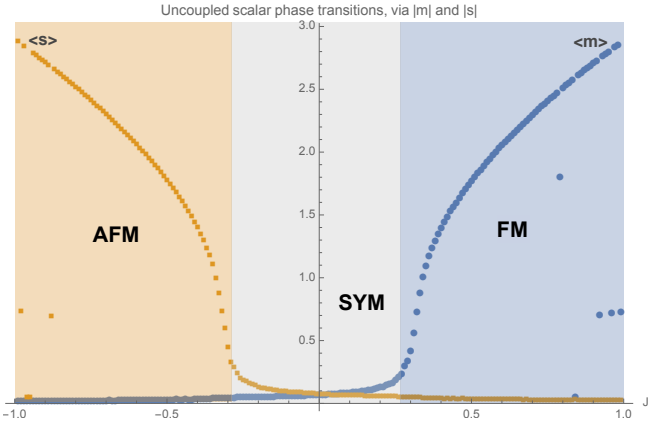

FIG. 2: Plot of $\langle m \rangle$ and $\langle s \rangle$ in the uncoupled model ($\hat{g}=0$) against $\hat{J} \sim T^{-1}$. We see three distinct phases characterized by the behavior of the two order parameters. As expected for the uncoupled theory, the phases are symmetric under $\hat{J} \leftrightarrow -\hat{J}$.

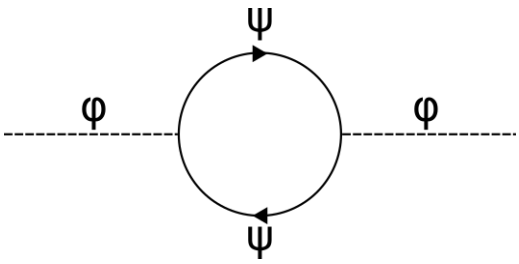

FIG. 3: The first-order correction to ϕ-ϕ coupling is given by a fermion loop when $\hat{g}$ is small.

the ferromagnetic and antiferromagnetic transitions are related by a sign exchange. This property is protected by the symmetry of the theory that maps every other $\phi_x \rightarrow -\phi_x$ and simultaneously changes $\hat{J} \rightarrow -\hat{J}$ (one can check that the Hamiltonian is preserved and the phase space is mapped back to itself). On the other hand, once we introduce a non-zero Yukawa coupling $\hat{g}\phi\bar{\psi}\psi$, this symmetry is explicitly broken, and we should not expect the critical $\hat{J}$ to be related by a sign flip.

B. Yukawa theory

Introducing the Yukawa coupling involves including the fermion determinant in the simulation via the pseudofermion action as shown in (15) and (16). Dialing the coupling $\hat{g}$ allows us to investigate the behavior of the two phase transitions of the ϕ^4 theory. Intuitively, introducing a weakly coupled fermion field modifies to first order only the $\hat{m}^2$ term of the ϕ via the loop diagram shown in Figure 3. We tried to pin $\hat{m}^2$ to $1-2d\hat{J}-2\hat{\lambda}$ in (20), but this suggests that under a renormalization group analysis we will necessarily reintroduce a generic $\hat{m}^2$ term. As we dial $\hat{J} \sim 1/T$, then, we should expect some kind

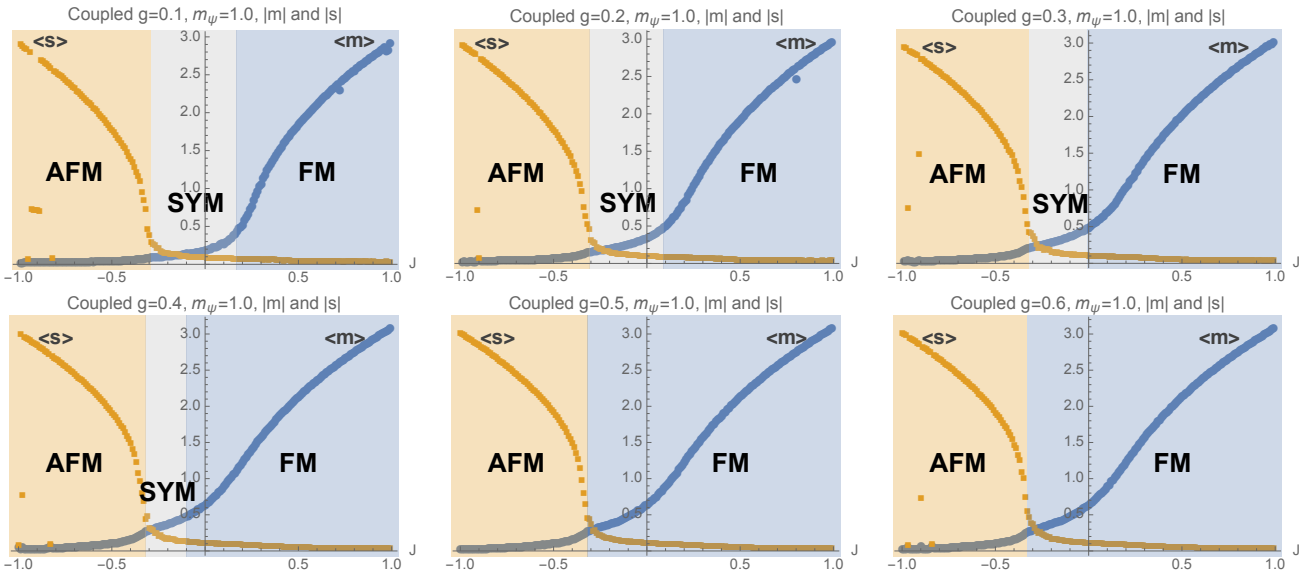

FIG. 4: The six plots above show the $\langle m \rangle$ and $\langle s \rangle$ order parameters as a function of $\hat{J}$ for $\hat{g} = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6$ repectively. The shading corresponds to manually identified phases. As $\hat{g}$ is increased, the FM-SFM transition shifts towards more negative $\hat{J}$, until at $\hat{g} = 0.5$ we begin to see a direct FM-AFM transition.

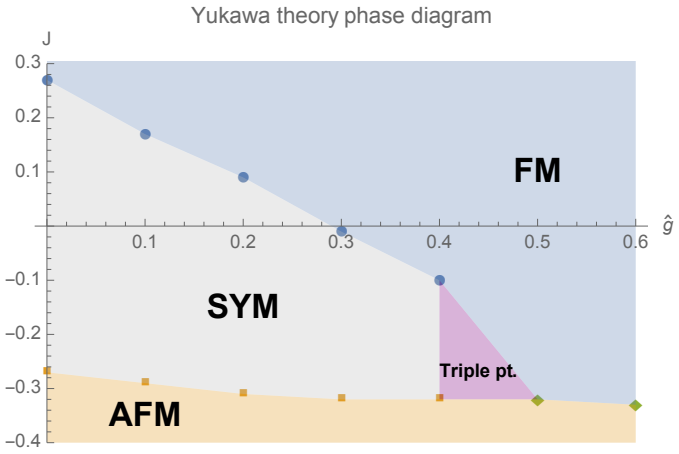

FIG. 5: Plotting the manually identified transitions, we roughly map out the shape of the SYM phase in the weak-coupling, small-$\hat{J}$ region. The purple region indicates a rough bound on the triple-point location where the FM-SYM and AFM-SYM transitions merge into a single FM-AFM transition line. This phase diagram closely matches the results of [24].

of skew due to this effective $\hat{m}^2$. While it would require a detailed RG analysis to determine exactly how we expect the critical points to move, we confirm the skew via lattice simulation.

Figure 4 shows the results of the phase transition as $\hat{g}$ is dialed through 0.1, 0.2, 0.3, 0.4, 0.5, and 0.6. The AFM-SYM transition slowly shifts towards more negative $\hat{J}$, while the FM-SYM transition more quickly moves towards negative $\hat{J}$, ultimately squeezing out the SYM phase entirely, producing a first order transition between AFM and FM directly [26]. Plotting the manually identified phase transition locations in the $\hat{J}$-$\hat{g}$ plane, we map out the extent of the SYM phase and the nearby AFM and FM regions in Figure 5.

C. Counting fermion flavors

The Yukawa coupled model also allows us to investigate the number of physical fermion flavors produced by the theory. Per Bulava et al. [24], we expect a linear deviation of the phase transition boundaries at points away from the $1/n_f \to 0$ analytic limit when we fix the parameters $\tilde{\lambda} \equiv \hat{\lambda}/n_f$, $\tilde{g} \equiv \hat{g}\sqrt{n_f}$, and set $\hat{m}^2 = n_f - 2\tilde{\lambda} - 2dJ$.

We have two methods of modifying the n_f in the theory: (1) add additional naive flavors by including more copies of ψ (and thus η for simulation) and (2) include (exclude) the Wilson term that forbids (allows) the four fermion doublers. We explore both of these options.

Plotting the phase transitions determined in each of these cases against $1/n_f$ in Figure 6 we see the expected linear behavior when we take into account the removal of doublers effected by the Wilson term in the AFM-SYM transition. Curiously, the FM-SYM transition showed rather poor results. In the analysis of these results, the phase transitions became less clear as $1/n_f$ was increased. We hypothesize that at some boundary value of n_f the phase transition FM-SYM is actually destroyed. Clarifying this FM-SYM behavior would be interesting future work.

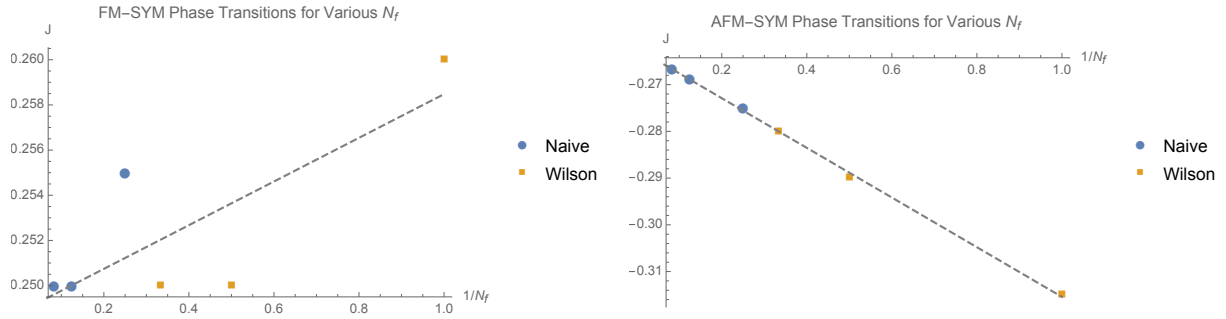

FIG. 6: We plot the critical J and a linear fit against $1/n_f$ for both the FM-SYM and AFM-SYM transitions. The critical values were identified manually based on the behavior of the order parameters $\langle m \rangle$ and $\langle s \rangle$ respectively. We see the expected linear behavior as $1/n_f$ in the AFM-SYM transition, but get poor results for the FM-SYM transition.

VII. DISCUSSION AND CONCLUSION

Lattice simulations provide a tool to theorists to make predictions for QFTs in non-perturbative regimes. In comparise to EFTs, lattice simulations produce ab initio results, allowing theorists to directly evaluate the fundamental model directly. Fundamentally the lattice calculations become physically relevant due to the shrinking of physical scales relative to the correlation length about the critical point. In much the same way that this enables MFT analyses, this allows us to formulate a quantum field theory in terms of a computation on the lattice.

Simulating scalar fields turns out to be relatively accessible on the lattice. Markov Chain Monte Carlo methods give accurate results with low computational cost. On the other hand, extending simulations to spin-$\frac{1}{2}$fermions or to gauge bosons with additional gauge structure is difficult. As one encounters both of these types of fields when describing the Standard Model, for example, we must address these challenges.

In this paper, we focused on addressing the difficulties of simulating spin-$\frac{1}{2}$fermions that obey the Dirac equation. The anticommuting nature of the fields requires analytically integrating and rewriting the interaction matrix determinant in terms of fictional pseudofermion fields coupled via the inverse interaction matrix. Handling the inverse matrix is costly, but tractable. We also find that introducing a single naive lattice fermion field generates 2^d physical fermions, with properties that do not match those found in the Standard Model. By choosing more complex discretizations of the derivative term, such as the Wilson fermion term (19), we can reduce the number of physical fermions to 1.

Our simulations of a specific model incorporating a scalar field Yukawa-coupled to a fermion field demonstrated the described lattice methods. Matching previous work [24], we found three distinct phases (antiferromagnetic, symmetric, and ferromagnetic) in the weak coupling regime, and a linear scaling in $1/n_f$ of the antiferromagnetic-symmetric phase transition. The behavior of the ferromagnetic-symmetric phase transition demonstrated poor results, possibly due to a breakdown of the phase transition for small n_f.

Lattice simulations have thus far had a large impact in simulating Quantum Chromodynamics, the strong nuclear force sector of the Standard Model. Lattice calculations have produced ab initio predictions of hadron spectra, scattering amplitudes, and decay constants [1, Sec 18]. Yet, lattice calculations are limited by computational resources, and new techniques continue to be developed to more effeciently perform computations. This is an important tool for theorists attempting to map the bounds of the Standard Model and find evidence for a theory beyond the Standard Model.

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Appendix A: Methods and Detailed Calculations

1. Hybrid Monte Carlo

As discussed in Section III B, MCMC methods are often used to sample configurations to approximate path integral evaluation. While the accept/reject step of MCMC ensures the correct equilibrium distribution for any symmetric update step, different choices of update steps trade off computation and equilibration time.

The original Metropolis method applied to a collection of particles distributed in space. Their update step moved a single particle per accept/reject step. For a more complex theory, single-particle or single-site updates result in slow equilibration, and more advanced techniques generally perform full state updates. In our simulations, we use Hybrid Monte Carlo (HMC) [27], a method of performing fictional dynamical evolution of the fields based on a carefully constructed Hamiltonian.

In HMC, proposing a new lattice state consists of the following steps:

1. Generate a fictional set of momenta π_x conjugate to the primary fields ϕ_x.
2. Simulate Hamiltonian evolution based on the classical energy $H[\pi,\phi] \equiv \frac{1}{2}\sum_x \pi_x^2 - S_\phi^{\text{latt}}[\phi]$. Fields are evolved by discrete integration of Hamilton's equations of motion. In our simulation, we use the leapfrog integrator [13, Sec 8.2.1] with fixed dimensionless evolution time 1.0 but tunable number of steps N_0.
3. Accept or reject the final state ϕ with probability $p = \min\left(1, \exp\left(-\Delta H\right)\right)$. Increasing N_0 allows more faithful integration, thus reducing ΔH and increasing the acceptance rate at the cost of more computation.

Analytically determining Hamilton's equations of motion from the action requires some care. We explicitly derive the form used for our simulations in Appendix A 2.

2. Yukawa HMC Equations

As is standard for HMC incorporating pseudofermions [14, Sec 2.5.1], we extend the HMC method to include an initial step generating a random Gaussian-weighted η. Under the Hamiltonian, $\dot{\eta} = 0$, thus we leave the field fixed to this value throughout a single HMC evolution.

We now derive the equations of motion for the HMC dynamics of the remaining fields using the full action defined in (22). The dynamics of ϕ is easy to write down:

$$\dot{\phi_x} = \frac{\partial H}{\partial \pi_x} = \pi_x \tag{A1}$$

$$\phi_x(t+\epsilon) = \phi_x(t) + \epsilon \pi_x(t) \tag{A2}$$

The dynamics of π require functional differentiation of the action with respect to ϕ. We break the action into S_ϕ^{latt} and S_η^{latt} and evaluate:

$$\begin{aligned}\nabla_\phi S_\phi^{\text{latt}} =& 2\phi_x + 2\hat{\lambda}(\phi_x^2 - 1)2\phi_x \\ & - 2\hat{J}\sum_\mu \phi_{x+\hat{\mu}} + \phi_{x-\hat{\mu}}\end{aligned} \tag{A3}$$

$$\begin{aligned}=& \left(2 - 4\hat{\lambda}\right)\phi_x + 4\hat{\lambda}\phi_x^3 \\ & - 2\hat{J}\sum_\mu \phi_{x+\hat{\mu}} + \phi_{x-\hat{\mu}}\end{aligned} \tag{A4}$$

$$\begin{aligned}\nabla_\phi S_\eta^{\text{latt}} =& -\left(\left(D^\dagger D\right)^{-1}\eta\right)^\dagger \\ & \times \nabla_\phi\left(D^\dagger D\right)\left(\left(D^\dagger D\right)^{-1}\eta\right)\end{aligned} \tag{A5}$$

$$\nabla_{\phi_z}\left(D^\dagger D\right) = \hat{g}\delta^{(z)}D + \hat{g}D^\dagger\delta^{(z)} \tag{A6}$$

$$= \hat{g}\left(D^{(z)} + (D^\dagger)^{(z)}\right) \tag{A7}$$

$$\nabla_\phi S_\eta^{\text{latt}} = 2\hat{g}\left(\left(D^\dagger D\right)^{-1}\eta\right)^\dagger \odot D\left(D^\dagger D\right)^{-1}\eta \tag{A8}$$

Above, we use the matrix identity $\frac{\partial M^{-1}}{\partial \phi} = -M^{-1}\frac{\partial M}{\partial \phi}M^{-1}$. We also write the final functional derivative of S_η^{latt} in terms of the Hadamard product ($\odot$) which in this context is defined as a point-wise multiply in the site index, but a dot product in the spinor indices.

Finally, we have the complete equations of motion:

$$\phi_x(t+\epsilon) = \phi_x(t) + \epsilon\pi_x(t) \tag{A9}$$

$$\pi_x(t+\epsilon) = \pi_x(t) - \epsilon\nabla_\phi S_\eta^{\text{latt}}(t) - \epsilon\nabla_\phi S_\phi^{\text{latt}}(t) \tag{A10}$$

On a practical note, computing $\left(D^\dagger D\right)^{-1}\eta$ generally dominates the cost of a lattice simulation involving fermions [14, Sec 2.5.2]. While the matrix D can generally be represented in terms of a few local terms, the inverse is generally a dense $NN_s \times NN_s$ matrix. For moderately large N the cost of generating and storing the inverse explicitly becomes intractable. Since we have $D^\dagger D$ Hermitian, however, the eigenvalues are guaranteed to be positive definite, which allows application of more efficient numerical solving techniques, such as the Conjugate Gradient method [28, Sec 10.2]. Evaluating $\nabla_\phi S_\eta^{\text{latt}}$ requires a single solve of $\left(D^\dagger D\right)^{-1}\eta$ per step, and, using Conjguate Gradient, it is therefore computationally tractable.