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Four fermion interactions in non-Abelian gauge theory

Simon Catterall and Aarti Veernala

Department of Physics, Syracuse University, Syracuse, New York 13244, USA

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We continue our earlier study of the phase structure of a $SU(2)$ gauge theory whose action contains additional chirally invariant four fermion interactions. Our lattice theory uses a reduced staggered fermion formalism to generate two Dirac flavors in the continuum limit. In the current study we have tried to reduce lattice spacing and taste breaking effects by using an improved fermion action incorporating stout smeared links. As in our earlier study we observe two regimes; for weak gauge coupling the chiral condensate behaves as an order parameter differentiating a phase at small four Fermi coupling where the condensate vanishes from a phase at strong four Fermi coupling in which chiral symmetry is spontaneously broken. This picture changes qualitatively when the gauge coupling is strong enough to cause confinement; in this case we observe a phase transition for some critical value of the four Fermi coupling associated with a strong enhancement of the chiral condensate. We present evidence that this transition is likely first order. Furthermore, we observe that the critical four Fermi coupling varies monotonically with bare gauge coupling—decreasing, as expected, as the gauge coupling is increased. We have checked that these results remain stable under differing levels of smearing. These results argue against the appearance of new fixed points associated with chirally invariant four fermion interactions in confining non-Abelian gauge theories.

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I. INTRODUCTION

The primary purpose of the Large Hadron Collider (LHC) is to probe the nature of electroweak symmetry breaking in the Standard Model (SM). In the SM this is accomplished using a single scalar field—the Higgs. Unfortunately scalar field theories are known to suffer from fine-tuning and triviality problems and in consequence other extensions of the SM based on supersymmetry or new strong dynamics have been put forth to provide more natural explanations of electroweak symmetry breaking. One of the simplest realizations of dynamical electroweak symmetry breaking are technicolor models in which the SM is augmented with new fermions (techniquarks) which interact via a new strong technicolor gauge force. Strong interaction effects can then drive the formation of a techniquark chiral condensate which will in turn precipitate electroweak symmetry breaking if the electroweak gauge group appears as a subgroup of the chiral group of the techniquarks [1,2]. While theories with QCD-like dynamics are experimentally excluded they are far less stringent constraints on these models if the dynamics deviates dramatically from QCD. This is particularly true in light of the recent discovery of a light, Standard Model-like Higgs at the LHC. One way to produce such a light state in a strongly coupled beyond standard model (BSM) theory is to consider models lying close to the lower boundary of the conformal window. In this case it is conjectured that one might be able to identify the experimentally observed Higgs with a pseudo-Goldstone boson—the dilaton—arising from spontaneous breaking of approximate conformal symmetry. Such theories are often termed walking gauge theories since the gauge coupling should evolve slowly with energy scale [1,3] and possess other potentially useful features such as reduced contributions to the S parameter and flavor changing neutral currents.

The search for such walking gauge theories has led to numerous recent lattice studies—see the conference reviews [4–7]. However, the simplest technicolor models, while giving rise to masses for the gauge bosons, are incapable of generating masses for SM fermions. To achieve this more elaborate schemes such as extended technicolor [8–11] and top-condensation [12–15] have been invoked. At low energies these latter theories share a common framework; the actions contain additional four fermion interactions coupling both SM fermions and techniquarks. Indeed most theories of BSM physics can be expected to yield effective actions at low energy which contain additional four fermion terms.

In light of this it is important to study the structure of non-Abelian theories in the presence of additional chirally invariant four fermion interactions. This was the motivation behind our earlier work [16], where we explored the phase structure of a Nambu-Jona-Lasinio (NJL) model gauged under the $SU(2)$ group. This model has also been examined using truncated Schwinger-Dyson calculations in [17] where strong four Fermi interactions were claimed to lead to new universality classes of model with potentially interesting consequences for model building. Our work can also be seen as a nonperturbative check on these truncated Schwinger-Dyson results.

In our previous work we observed that the chiral condensate of the strongly coupled gauge theory underwent a strong enhancement for large values of the four Fermi coupling. The transition appeared very abrupt and therefore likely first order but we were unable to find definitive evidence of this in the earlier work. In addition we observed that the critical four Fermi coupling did not vary monotonically with the gauge coupling which led us to suspect that the results of those simulations might be plagued with large lattice spacing effects. To counter this we have revisited the model using an improved fermion action in which the usual gauge links are replaced by so-called *stout smeared* gauge links. The smeared gauge fields are obtained by a gauge invariant averaging procedure carried out over a local region in space. The essential idea is that this averaging procedure will tend to remove large UV fluctuations from the lattice gauge field while preserving the IR physics. Smeared actions have been shown to be very effective in lattice QCD [18–20]. The specific scheme we employ was developed in [21] for the case of $SU(3)$.

In the following section, we briefly describe our lattice theory and its connection to the gauged NJL model. Next we describe the method of stout smearing in the context of dynamical fermion simulations of an $SU(2)$ lattice gauge theory. Finally, we move on to our numerical results, where we discuss the phase structure resulting from varying both gauge and four Fermi couplings. We show that suppressing lattice spacing effects via smearing removes some of the technical issues associated with our earlier work but does not change the final conclusion: we see no evidence in confining gauge theories for new fixed points associated with strong four Fermi interactions. Instead, we present evidence that the lattice theory undergoes a first order phase transition for large four Fermi coupling. This transition is associated with a rapid enhancement of the chiral condensate and the generation of large fermion masses.

II. FOUR FERMION INTERACTIONS—ON AND OFF THE LATTICE

We will consider a model which consists of two flavors of massless Dirac fermions transforming in the fundamental representation of an $SU(2)$ gauge group and coupled through an $SU(2)_L \times SU(2)_R$ chirally invariant four Fermi interaction of NJL type. To avoid potential sign problems we have utilized two copies of this basic two flavor doublet yielding a four flavor theory. The action for a single doublet takes the form

$$S = \int d^4x \bar{\psi}(i\partial\!\!\!/ - A\!\!\!/)\psi - \frac{G^2}{2N_f}[(\bar{\psi}\psi)^2 + (\bar{\psi}i\gamma_5\tau^a\psi)^2] - \frac{1}{2g^2}\,\mathrm{Tr}[F_{\mu\nu}F^{\mu\nu}], \tag{1}$$

where G is the four Fermi coupling, g the usual gauge coupling and τ^a, $a = 1\ldots3$ are the generators of the $SU(2)$ flavor group.

To implement the theory in Eq. (1) on the lattice, it is convenient to reparametrize the four Fermi term in the continuum action via the use of scalar auxiliary fields. Specifically the fermion interaction term is replaced by the Yukawa terms

$$S_{\mathrm{aux}} = \int d^4x \frac{G}{\sqrt{N_f}}(\bar{\psi}\psi\phi_4 + \bar{\psi}i\gamma_5\tau^a\psi\phi_a) + \frac{1}{2}(\phi_4^2 + \phi_a^2). \tag{2}$$

We discretize the above action using a (reduced) staggered fermion formalism. This approach allows us to build a lattice theory which admits just two continuum flavors of fermion in the continuum limit without encountering rooting issues. Furthermore it allows us to write down lattice four Fermi terms which are invariant under a discrete subgroup of the continuum chiral symmetries [22,23]. Our work builds on earlier work on four fermion interactions [24–31] which employed either Wilson fermions or regular staggered fermions. In both of these cases, explicit chiral symmetry breaking mass terms were allowed. However, the presence of four Fermi interactions in our reduced staggered framework has an additional attractive feature—it allows us to study the lattice theory with exactly zero fermion mass where these discrete symmetries are exact [24].

In order to do this, we first rewrite the fermionic sector of the continuum theory in terms of a new set of matrix valued fields, Ψ and $\bar{\Psi}$ which naturally arise after twisting the original Lorentz symmetry with the flavor symmetry. We then expand these matrices on a basis corresponding to products of gamma matrices and associate these products with staggered fields χ, $\bar{\chi}$:

$$\Psi(x) = \frac{1}{8}\sum_b \gamma^{x+b}\chi(x+b), \tag{3}$$

$$\bar{\Psi}(x) = \frac{1}{8}\sum_b (\gamma^{x+b})^\dagger\bar{\chi}(x+b), \tag{4}$$

where $\gamma^{x+b} = \prod_{i=1}^4 \gamma_i^{x_i+b_i}$ and the sums correspond to the vertices in an elementary hypercube associated with lattice site x as the components vary $b_i = 0, 1$. The lattice theory thus far describes four flavors of continuum fermion. To reduce the flavor content further it is possible for massless fermions to restrict the single component fields χ and $\bar{\chi}$ to even and odd sites, respectively. In this way we arrive at the *reduced* staggered fermion action:

$$S = \sum_{x,\mu}\chi^T(x)\mathcal{U}_\mu(x)\chi(x+a_\mu) \times [\eta_\mu(x) + G\bar{\phi}_\mu(x)\epsilon(x)\xi_\mu(x)], \tag{5}$$

where

$$\mathcal{U}_\mu(x) = \frac{1}{2}[1+\epsilon(x)]U_\mu(x) + \frac{1}{2}[1-\epsilon(x)]U^*_\mu(x), \tag{6}$$

$$\bar{\phi}_\mu(x) = \frac{1}{16}\sum_b \phi_\mu(x-b) \quad (7)$$

and $\eta_\mu(x)$ is the usual staggered quark phase given by

$$\eta_\mu(x) = (-1)^{\sum_{i=1}^{\mu-1} x_i}. \quad (8)$$

Notice that the action involves a single staggered field χ defined over all lattice sites but coupled through a modified gauge field $\mathcal{U}_\mu(x)$. The two staggered tastes become the two physical quark flavors in the continuum limit. This action is invariant under the discrete shift transformations:

$$\chi(x) \to \xi_\rho(x)\chi(x+\rho), \quad (9)$$

$$U_\mu(x) \to U^*_\mu(x+\rho), \quad (10)$$

$$\phi_\mu(x) \to (-1)^{\delta_{\mu\rho}}\phi_\mu(x+\rho), \quad (11)$$

where $\xi_\mu = (-1)^{\sum_{i=\mu+1}^{4} x_i}$ These shift symmetries correspond to a *discrete* subgroup of the continuum axial flavor transformations which act on the matrix field Ψ according to

$$\Psi \to \Psi\gamma_\rho. \quad (12)$$

III. STOUT SMEARING

To reduce the magnitude of lattice spacing effects we replace the links $U_\mu(x)$ used in constructing the staggered fermion action by stout smeared links $U'_\mu(x)$ which are defined as

$$U'_\mu(x) = \{e^{Q_\mu(x)}\}U_\mu(x). \quad (13)$$

where the traceless, anti-Hermitian matrix Q_μ is given by

$$Q_\mu(x) = \frac{1}{2}[\Omega^\dagger_\mu(x) - \Omega_\mu(x)] - \frac{1}{2N}\,\mathrm{Tr}[\Omega^\dagger_\mu(x) - \Omega_\mu(x)], \quad (14)$$

with

$$\Omega_\mu(x) = C_\mu(x)U^\dagger_\mu(x), \quad (15)$$

and

$$C_\mu = \sum_{\mu\neq\nu}\rho[U_\nu(x)U_\mu(x+\nu)U^\dagger_\nu(x+\mu) + U^\dagger_\nu(x-\nu)U_\mu(x-\nu)U_\nu(x-\nu+\mu)]. \quad (16)$$

The parameter ρ can be tuned to optimize the smearing—in this work we have set $\rho = 0.1$. To leading order in ρ it is easily seen that this procedure generates a smeared link which is a weighted sum over the original link and its surrounding staples. In practice this procedure is iterated with the level n smeared fields $U^{(n)}_\mu$ being constructed from the fields $U^{(n-1)}_\mu$ at level $n-1$ via the obvious relation

$$U^{(n)}_\mu(x) = \{e^{Q^{(n-1)}_\mu(x)}\}U^{(n-1)}_\mu(x). \quad (17)$$

We have run our simulations using $n = 1$ and $n = 2$ levels of smearing. For details on how this smearing is implemented and the calculation of the smeared force term required by the rational hybrid Monte Carlo (RHMC) simulation we refer the reader to the Appendix.

IV. NUMERICAL RESULTS

Upon integration over the basic fermion doublet we obtain a Pfaffian $\mathrm{Pf}(M(U))$ depending in a complicated way on the original gauge field $U_\mu(x)$.[1] The required pseudofermion weight for two such doublets ($N_f = 4$ flavors) is then $\mathrm{Pf}(M)^2$. The pseudoreal character of $SU(2)$ allows us to show that this Pfaffian is purely real and so the four flavor simulations suffer from no sign problem. In practice we implement this weight in the path integral using a pseudofermion operator of the form $(M^\dagger M)^{-\frac{1}{2}}$ and a RHMC algorithm. A standard Wilson gauge action is employed for the gauge fields.

We have focused our study on a lattice of size 6^4 and a bare fermion mass $m = 0$. We have simulated a range of gauge couplings $\beta \equiv 4/g^2 = 1.8$–2.2 with additional runs at $\beta = 10.0$ to test the pure NJL model in which the gauge interactions are switched off. For each gauge coupling we have performed an extensive scan over a dozen or so values of the four Fermi coupling G. The range of β that was employed in the simulations was determined by examining the average plaquette and Polyakov line as β was varied holding the four Fermi coupling fixed at $G = 0.1$. In Fig. 1, we see a strong finite volume phase transition for $\beta > 2.2$ on a lattice with $L = 6$ and no smearing. Furthermore, this transition occurs at smaller bare gauge coupling, $\beta > 1.9$, when two levels of stout smearing are employed.

The primary observable used in this study is the chiral condensate which is computed from the gauge invariant one link operator

$$\sum_x \langle\chi(x)(\mathcal{U}_\mu(x)\chi(x+e_\mu) + \mathcal{U}^\dagger_\mu(x-e_\mu)\chi(x-e_\mu))\rangle\epsilon(x)\xi_\mu(x). \quad (18)$$

Because of the absence of spontaneous symmetry breaking in finite volume we measure the absolute value of this operator. In a chirally broken phase we expect this to approach a constant as the lattice volume is sent to infinity. Conversely if chiral symmetry is restored this observable will approach zero in the same limit. We have also used the auxiliary scalar field to monitor this observable.

Having used these simple gauge observables to determine an appropriate range for the gauge coupling β we now turn to the behavior of the system as the four Fermi coupling is varied. As a benchmark we have examined the system for a small value of the gauge

[1]Note that the fermion operator appearing in Eq. (5) is antisymmetric and hence a Pfaffian rather than a determinant results after integrating over the single fermion field χ.

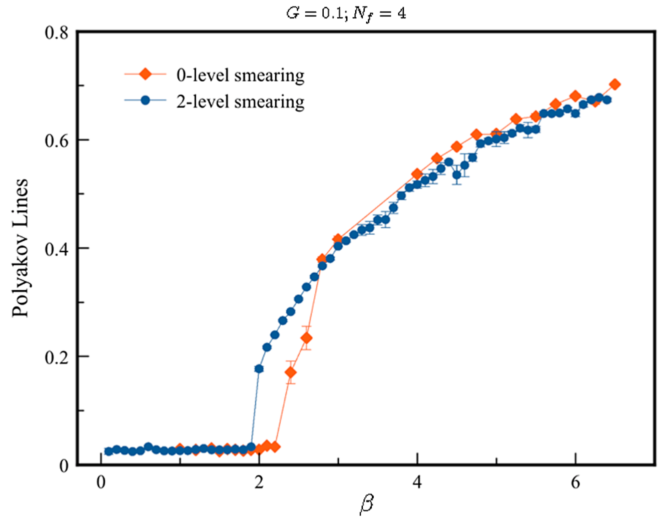

FIG. 1 (color online). Polyakov line vs β at $G = 0.1$ for four flavors.

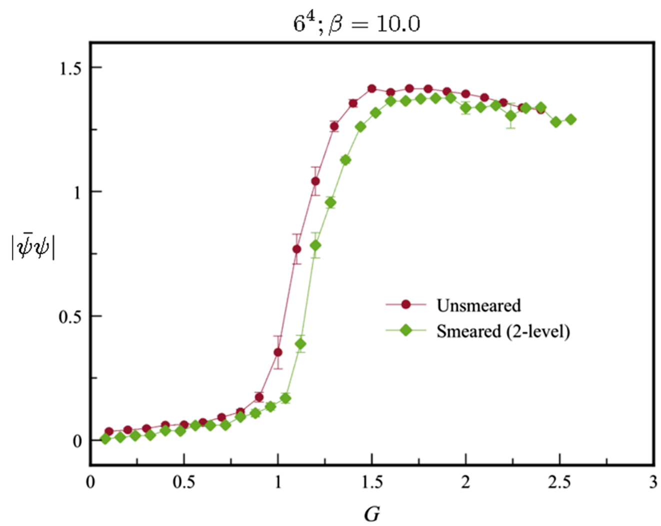

FIG. 2 (color online). $|\langle\bar{\chi}\chi\rangle|$ vs G for $\beta = 10.0$, 6^4 lattice.

coupling at $\beta = 10.0$.[2] The condensate is shown in Fig. 2 as the four Fermi coupling varies. The plot reveals evidence for a phase transition separating a chirally symmetric phase at small G from a broken phase for $G > G_c$. The relatively smooth behavior is consistent with earlier work using sixteen flavors of naive fermion reported in [30] which identified a line of second order phase transitions in this region of parameter space. It also agrees with the behavior seen in previous simulations of staggered quarks [31].

We now turn to our results at nonzero gauge coupling, corresponding to smaller values of β (stronger gauge coupling). Figure 3 shows results for the condensate in the confining theory at $\beta = 1.8$ for several levels of smearing.

[2]Note that gauge coupling g^2 varies as $\frac{1}{\beta}$. This region corresponds to the high temperature phase.

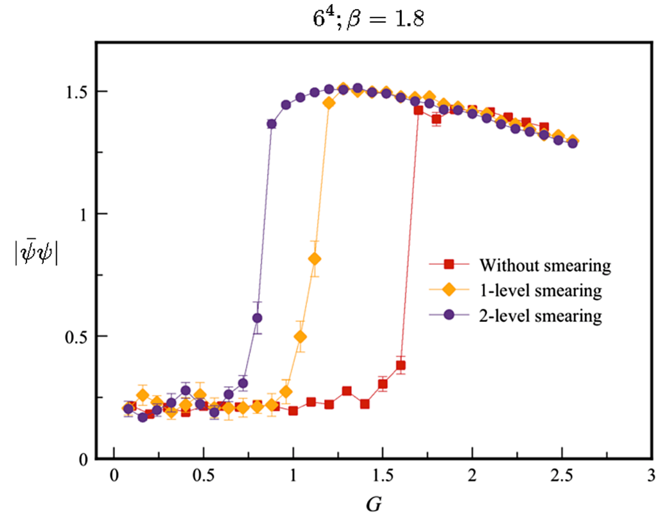

FIG. 3 (color online). $\langle\bar{\chi}\chi\rangle$ vs G at $\beta = 1.8$ for 6^4 lattice.

Notice that the chiral condensate is now nonzero even for vanishing four Fermi coupling consistent with spontaneous chiral symmetry breaking in the pure gauge theory. However, it jumps abruptly to much larger values when the four Fermi coupling exceeds some critical value. Notice that while the limiting values of the condensate in both small G and large G phases do not depend on how much smearing is done, the position of the transition itself depends on the smearing level. This should not be particularly surprising; the magnitude of critical couplings associated with lattice phase transitions generically depends on details at the scale of the lattice spacing. However, notice that the chiral condensate, being an IR quantity, does not show this sensitivity.

Figure 3 appears to show that the jump in the chiral condensate is markedly discontinuous in character—reminiscent of a first order phase transition. Further evidence for this first order behavior is seen in Figs. 4–7 which

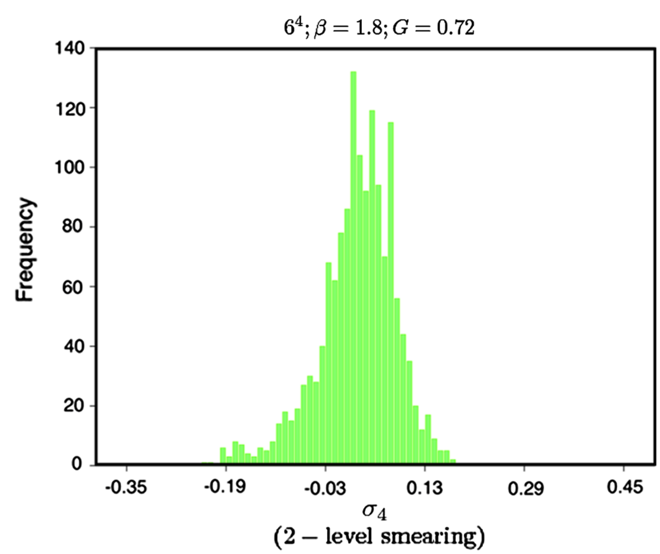

FIG. 4 (color online). Histogram of σ_4 for $G = 0.72$.

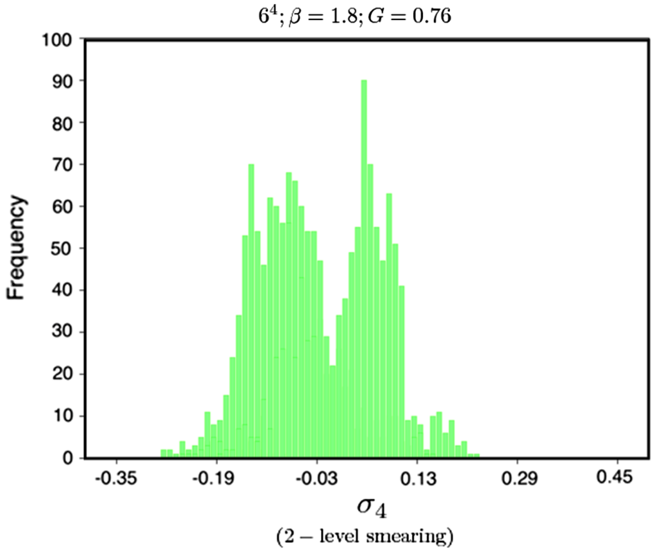

FIG. 5 (color online). Histogram of σ_4 for $G = 0.76$.

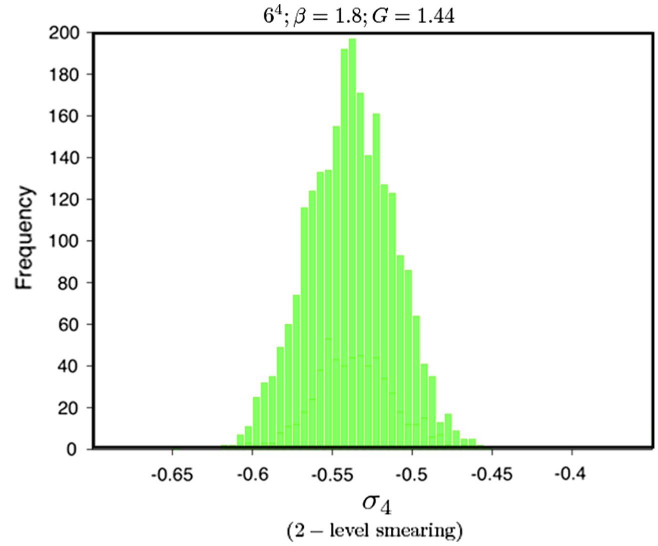

FIG. 7 (color online). Histogram of σ_4 for $G = 1.44$.

show histograms of the condensate (as measured by the scalar field average σ_4) for several four Fermi couplings G around the phase transition. The histograms tell a clear story; for G both below and above the transition a single peak is seen. In contrast for values of G close to the jump in the condensate the double peak structure indicates that the condensate has tunneled back and forth between two different states over the course of the run. Such tunneling behavior is generally taken as a smoking gun sign of the presence of a first order transition. We have also examined the dependence of these features on the magnitude of the gauge coupling β. Figure 8 shows a plot of the condensate vs G for $N_f = 4$ for a fixed lattice size $L = 6$ and using two levels of smearing. Two regimes are clearly visible; for $\beta < 1.9$ or so the chiral condensate is nonzero for small G corresponding to a strongly coupled, confining and chirally broken gauge theory even in the absence of four Fermi terms. Conversely for $\beta > 2.0$ the chiral condensate goes to zero for vanishing four Fermi coupling and the system is deconfined in the absence of the four Fermi coupling. This is not a surprise; it corresponds to the usual deconfinement one sees when the lattice size becomes smaller than the confinement scale.

Notice that the onset of the crossover occurs for smaller values of the critical four Fermi coupling, G_{cr}, as we increase the strength of the gauge coupling (corresponding to decreasing β). This monotonic dependence of the critical four Fermi coupling contrasts with the situation seen earlier in our study with an unsmeared action [16]. In the strong coupling regime, since the chiral symmetry is already broken, the crossover occurs quickly at a small (weak) four Fermi coupling. As one approaches the weak

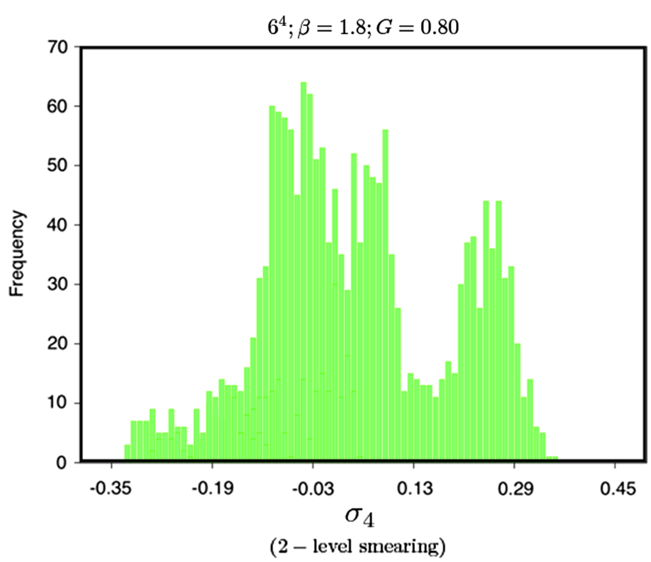

FIG. 6 (color online). Histogram of σ_4 for $G = 0.80$.

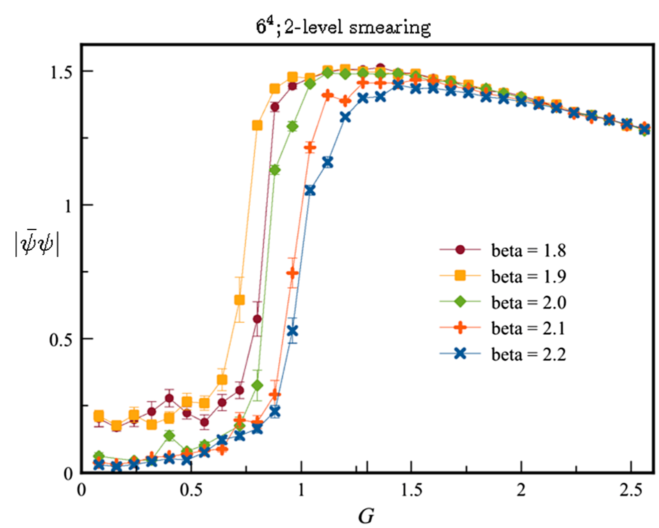

FIG. 8 (color online). $\langle \bar{\chi}\chi \rangle$ vs G for varying β. Two-level smearing has been implemented here.

coupling limit, the model is less influenced by the gauge interactions and the chiral symmetry remains intact until the four Fermi coupling becomes strong enough to break the symmetry.

V. SUMMARY

In this paper we have conducted numerical simulations of a four flavor non-Abelian gauge theory in the presence of additional chirally invariant strong four fermion interactions. The latter are expected to be present in generic effective theories of BSM physics including (walking) technicolor, top quark condensation and little Higgs theories. We employ a reduced staggered fermion lattice action which preserves a discrete subgroup of the continuum chiral symmetry. In addition we have improved this action using stout smearing techniques.

We have examined the exactly massless theory for a modest lattice size of 6^4 over a range of gauge couplings β, and four Fermi interaction strength G. In the NJL limit $\beta \rightarrow \infty$ we find evidence for a continuous phase transition corresponding to the expected spontaneous breaking of chiral symmetry due to strong four Fermi interactions. The location and character of this transition is, not surprisingly, insensitive to the smearing. However, for gauge couplings β that generate confinement and a nonzero chiral condensate even at $G = 0$, this crossover appears much sharper and indeed we show that it is consistent with first order phase transition. Such a phase transition would preclude the existence of any new continuum limits in the model. The location of this transition occurs at a critical four Fermi coupling which depends on the level of smearing and decreases monotonically with increasing gauge coupling.

Thus our results are consistent with the idea that the second order phase transition which exists in the pure NJL theory ($G = \infty$) survives in the presence of weak gauge interactions. However our results suggest that this line of transitions becomes first order at a point at which the gauge coupling becomes strong enough to cause confinement. In a finite volume this occurs at a finite β but presumably this first order region extends all the way to $\beta = \frac{1}{g^2} = \infty$ in infinite volumes. Ideally, one would like to investigate this model for larger volumes to be sure that such first order behavior persists in the infinite volume limit.

The gauged NJL model we study in this paper was examined using a truncated Schwinger-Dyson analysis in [17] in which it was claimed that the phase diagram of the gauged NJL model should include a new critical line along which critical exponents such as the mass anomalous dimension vary continuously. Our results are *inconsistent* with this scenario but are consistent with the approximate analysis performed in [32] which argues for a strong enhancement of the chiral condensate for large four Fermi coupling. While our results seem to exclude new universality classes due to strong four Fermi couplings in confining gauge theories it is still logically possible that this conclusion might be very different in a gauge theory which is conformal at $G = 0$.

ACKNOWLEDGMENTS

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APPENDIX: CALCULATION OF THE STOUT SMEARED FORCE IN $SU(2)$

Stout smearing is implemented in our code in two parts. The first involves replacing the gauge links in the fermionic action by the smeared links, $U_\mu^{(n)}(x)$ as given in Eq. (17). The second, and the nontrivial, part of implementing smearing lies in the calculation of the smeared force $F_\mu(x)$ needed in the auxiliary molecular dynamics evolution which forms the kernel of the dynamical fermion algorithm. The force $F_\mu(x)$ is defined as

$$F_\mu(x) = U_\mu(x)\frac{\partial S(U^{(n)})}{\partial U_\mu(x)}. \quad \text{(A1)}$$

The complication that arises at this point is that we have no explicit representation of the smeared action in terms of the original gauge links—indeed such an expression would be very complicated given that the smeared links are determined iteratively. Instead we follow the approach of [21] and derive an iterative expression for the smeared force by considering the rate of change of the action over a fictitious (simulation) time t:

$$\frac{\partial}{\partial t}S(U^{(k)}) = 2\,\mathrm{Re}\sum_{\mu,x}\mathrm{Tr}\left[f_\mu^{(k)}(x)\frac{\partial}{\partial t}U_\mu^{(k)}(x)\right]. \quad \text{(A2)}$$

Here, $f_\mu^{(k)}(x) = \frac{\partial S(U^{(k)})}{\partial U_\mu^{(k)}(x)}$. In order to simplify notation, we denote the k level fields with a prime and the $(k-1)$ level fields without a prime. Using Eq. (13), we have

$$\frac{\partial}{\partial t}U'_\mu(x) = \left(\frac{\partial}{\partial t}e^{Q_\mu(x)}\right)U_\mu(x) + e^{Q_\mu(x)}\left(\frac{\partial U_\mu(x)}{\partial t}\right). \quad \text{(A3)}$$

The matrix exponentials can be handled using the $SU(2)$ identities:

$$e^{Q} = (\cos q)I_{2X2} + \frac{\sin q}{q}Q, \quad \text{(A4)}$$

where q, the eigenvalues of the traceless anti-Hermitian matrix Q, are given by

$$q^2 = -\frac{1}{2}\mathrm{Tr}(Q^2). \quad \text{(A5)}$$

Using this the derivatives of e^Q can be expressed as

$$\frac{\partial}{\partial t}e^{Q_\mu(x)} = \mathrm{Tr}\left[Q_\mu(x)\frac{\partial Q_\mu(x)}{\partial t}\right]B + \frac{\sin q}{q}\left(\frac{\partial Q_\mu(x)}{\partial t}\right), \tag{A6}$$

with

$$B_\mu = \frac{\sin q}{2q} - \frac{(\cos q - \sin q/q)}{2q^2}Q_\mu. \tag{A7}$$

Using these results Eq. (A2) can be expressed as

$$\sum_{\mu,x}\mathrm{Tr}\left[f'_\mu(x)\frac{\partial}{\partial t}U'_\mu(x)\right] = \sum_{\mu,x}\left[\mathrm{Tr}\left(f'_\mu(x)e^{Q_\mu(x)}\frac{\partial}{\partial t}U_\mu(x)\right) - \mathrm{Tr}\left(\Lambda_\mu(x)\frac{\Omega_\mu(x)}{\partial t}\right)\right], \tag{A8}$$

where

$$\Lambda_\mu(x) = -[\Gamma^\dagger_\mu(x) - \Gamma_\mu(x)] + \frac{1}{N}\mathrm{Tr}[\Gamma^\dagger_\mu(x) - \Gamma_\mu(x)], \tag{A9}$$

and

$$\Gamma_\mu(x) = \mathrm{Tr}[f'_\mu(x)B_\mu(x)U_\mu(x)]Q_\mu(x) + \frac{\sin q}{q}U_\mu(x)f'_\mu(x) \tag{A10}$$

and $\Omega_\mu(x)$ is given by Eq. (15). Using the cyclic properties of the trace we ultimately obtain

$$f_\mu(x) = f'_\mu(x)\left(\cos q I_{2X2} + \frac{\sin q}{q}Q\right) - C^\dagger_\mu(x)\Gamma_\mu(x) + \rho\sum_{\mu,x}\Theta_{\mu\nu}(x), \tag{A11}$$

where

$$\begin{aligned}\Theta_{\mu\nu}(x) = {} & U_\nu(x+\mu)U^\dagger_\mu(x+\nu)U^\dagger_\nu(x)\Lambda_\nu(x) + U^\dagger_\nu(x+\mu-\nu)U^\dagger_\mu(x-\nu)\Lambda_\nu(x-\nu)U_\mu(x-\nu)\\ & - U^\dagger_\nu(x-\mu+\nu)U^\dagger_\mu(x-\nu)\Lambda_\nu(x-\nu)U_\nu(x-\nu) - \Lambda_\nu(x+\mu)U_\nu(x+\mu)U^\dagger_\mu(x+\nu)U^\dagger_\nu(x)\\ & + U_\nu(x+\mu)U^\dagger_\mu(x+\nu)\Lambda_\mu(x+\nu)U^\dagger_\nu(x) + U^\dagger_\nu(x+\mu-\nu)\Lambda_\nu(x+\mu-\nu)U^\dagger_\mu(x-\nu)U_\nu(x-\nu).\end{aligned} \tag{A12}$$

Equation (A11) gives $f_\mu(x) \equiv f^{(k-1)}_\mu(x)$ in terms of $f'_\mu(x) = f^{(k)}_\mu(x)$ at level k. Given an initial "naive" force at level n $f^{(n)}_\mu = \frac{\partial S(U^{(n)})}{\partial U^{(n)}_\mu}$ it may be iterated to yield $f^{(0)}_\mu(x)$ and hence the final smeared force needed by the molecular dynamics equations

$$F_\mu(x) = U_\mu(x)f^{(0)}_\mu(x). \tag{A13}$$

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