Monte Carlo evaluation of a fermion number violating observable in 2D.

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Abstract

We describe in some detail a computer evaluation of a ’t Hooft vertex in a two dimensional model using the overlap. The computer result agrees with the known exact continuum value, and in this sense our work is a first successful fully dynamical simulation of a chiral gauge theory on the lattice. We add some new data to numbers obtained earlier and provide a selfcontained description which should make it easy for others to reproduce and follow up on our work.

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1. Introduction

Unlike for QCD, a communal base of numerical experience about simulating chiral gauge theories on the computer is lacking. Even on what should be done in principle there is no consensus; in practice, handling the generically complex action is likely to present a formidable problem by itself. One approach for regularizing chiral gauge theories, the overlap [1], has been recently subjected to a full dynamical test for a simple model [2]. The result was positive and therefore a more detailed description of what was done in practice has become relevant. Previous publications emphasized theory and were brief on numerics. Here our objective is to collect all the technical details needed to carry out our test, so that the reader could reproduce and follow up on our numerical work without having to sift through several papers. The reader would be helped by QCD experience only to a limited extent; because of the presumed lack of familiarity with the overlap in practice our presentation will be quite explicit.

2. Continuum features.

Our particular model is a chiral abelian gauge theory in two Euclidean dimensions. The theory is defined on a torus of sides $l_1 = t$, $l_2 = l$. Matter consists of four left-handed Weyl fermions, $\chi_f$, of charge one and one right-handed Weyl fermion of charge two, $\psi$. The action is:

$$S = \frac{1}{4e_0^2} \int d^2 x F_{\mu\nu}^2 - \sum_{f=1}^4 \int d^2 x \bar{\chi}_f \sigma_\mu (\partial_\mu + iA_\mu) \chi_f - \int d^2 x \bar{\psi} \sigma_\mu (\partial_\mu + 2iA_\mu) \psi,$$

(2.1)

where $\sigma_1 = 1$, $\sigma_2 = i$ and $\mu = 1, 2$. The $U(1)$ gauge symmetry is anomaly free by $2^2 = 1^2 + 1^2 + 1^2 + 1^2$. The boundary conditions are:

$$\chi_f(x + l_\mu \hat{\mu}) = e^{2\pi ib^f_\mu} \chi_f(x)$$
$$\psi(x + l_\mu \hat{\mu}) = \psi(x)$$
$$F_{\gamma\nu}(x + l_\mu \hat{\mu}) = F_{\gamma\nu}(x)$$

(2.2)

for $\mu = 1, 2$. $\hat{\mu}$ is a unit vector in the $\mu$ direction. The $\bar{\chi}_f$ and $\bar{\psi}$ fields obey complex conjugate boundary conditions. The $b^f_\mu$ are given by:

$$b^1_1 = 0; \quad b^2_1 = 0; \quad b^3_1 = \frac{1}{2}; \quad b^4_1 = \frac{1}{2}; \quad b^1_2 = 0; \quad b^2_2 = \frac{1}{2}; \quad b^3_2 = 0; \quad b^4_2 = \frac{1}{2}.$$  

(2.3)

In the $t = l = \infty$ limit the following properties are relevant to the present work:
The physical Hilbert space can be written as a tensor product of two spaces which are not connected by the evolution operator. One of the spaces carries a representation of a massless conformal theory and the other describes a massive field theory. If we replaced $\psi$-matter by four right moving Weyl fermions of charge one the theory would be vectorial. Again, a similar factorization would hold and the massive factor would be isomorphic to the massive factor in our original chiral model.

The massless sector consists of six left moving Majorana Weyl fermions forming a sextet under the global $SU(4)$ acting on the $f$-index of the $\chi_f$’s. These particles are noninteracting. One can choose interpolating fields for these particles which are neutral objects local in the original fields:

$$\rho_{f_1 f_2} = -\rho_{f_2 f_1} = \frac{\pi^2 e^{-\gamma}}{e_0} [\chi_{f_1} \chi_{f_2} \bar{\psi} - \frac{1}{2} e^{f_1 f_2 f_3 f_4} \bar{\chi}_{f_3} \bar{\chi}_{f_4} \psi].$$

(2.4)

The prefactor is chosen so that $\rho$ becomes a canonical field at large distances. $\gamma$ is Euler’s constant. The mixing on the RHS is possible because fermion number is violated in quanta of two by instanton effects. The exact low energy effective Lagrangian of the model, written in terms of the $\rho$-fields, is

$$\mathcal{L} = \frac{1}{2} \sum_{f_1 > f_2} \rho_{f_1 f_2} \sigma \cdot \partial \rho_{f_1 f_2}. \quad (2.5)$$

Among the terms on the RHS we have a term proportional to a ’t Hooft vertex, $V(x)$, which we choose to define as:

$$V(x) = \frac{\pi^2}{e_0} \chi_1(x) \chi_2(x) \chi_3(x) \chi_4(x) \bar{\psi}(x) (\sigma \cdot \partial) \bar{\psi}(x). \quad (2.6)$$

This operator has a nonzero expectation value:

$$\langle V \rangle_{\infty} = \frac{e^{4\gamma}}{4 \pi^3} \approx 0.081.$$  

(2.7)

On the finite $t \times l$ lattice one has instead:

$$\langle V \rangle_{t \times l} = \frac{64\pi}{(tm_\gamma)^4} \exp \left[ -\frac{4\pi}{tm_\gamma} \coth \left( \frac{1}{2} tm_\gamma \right) \right] e^{4F(tm_\gamma)-8H(tm_\gamma,\xi)}, \quad (2.8)$$

where $m_\gamma^2 = \frac{4e^2}{\pi}$ and the functions $F(\xi)$ and $H(\xi,\tau)$ are defined below:

$$F(\xi) = \sum_{n>0} \left[ \frac{1}{n} - \frac{1}{\sqrt{n^2 + (\xi/2\pi)^2}} \right],$$

$$H(\xi,\tau) = \sum_{n>0} \frac{1}{\sqrt{n^2 + (\xi/2\pi)^2}} \frac{1}{e^{\tau \sqrt{(2\pi n)^2 + \xi^2}} - 1}. \quad (2.9)$$
We shall need $\langle V \rangle_{t \times l}$ at $t = l = \frac{3}{m_\gamma}$ and there its value is 0.0389, substantially smaller than the value at infinite volume.

The objective of our numerical work is to reproduce this last continuum number on the lattice. Namely, we wish to evaluate the ratio of formal path integrals:

$$\frac{\int \prod_{f=1}^{4} [d\bar{\chi}^f d\chi^f] [d\bar{\psi} d\psi] \prod_{\mu=1}^{2} [dA_\mu] e^S V}{\int \prod_{f=1}^{4} [d\bar{\chi}^f d\chi^f] [d\bar{\psi} d\psi] \prod_{\mu=1}^{2} [dA_\mu] e^S} \equiv \langle V \rangle. \quad (2.10)$$

The path integrals are rendered finite by replacing the torus by a toroidal square lattice with spacing $a$. To preserve invariance under rotations by ninety degrees the two sides of the lattice are made equal. One wishes to show that the correct continuum number emerges in the limit $a \to 0$.

The following decomposition of $A_\mu$ simplifies the path integrals in the continuum:

$$A_1 = \partial_2 \phi + \frac{2\pi}{l} h_1 + ig^{-1} \partial_1 g, \quad A_2 = -\frac{2\pi q}{l^2} x_1 - \partial_1 \phi + \frac{2\pi}{l} h_2 + ig^{-1} \partial_2 g. \quad (2.11)$$

Above, $g$ is a periodic complex valued function on the torus with $|g(x)| \equiv 1$, representing the gauge degree of freedom. $\phi$ is a real periodic function on the torus and has no zero mode: $\int d^2 x \phi \equiv 0$. $h_\mu$ are two real constants restricted to the intervals $(-1/2, 1/2]$ which can be thought of as parameterizing two Polyakov loops on the torus. $q$ is an integer identifying the topological class. The pure gauge part of $S$ depends only on $\phi$ and $q$:

$$\frac{1}{4e_0^2} \int d^2 x F_{\mu \nu}^2 = \frac{1}{2e_0^2} \int d^2 x (\partial^2 \phi)^2 + \frac{2\pi^2 q^2}{(e_0 l)^2} \equiv S_0 + s_q. \quad (2.12)$$

The gauge measure $[dA_\mu]$ is replaced by $\sum_q [dg] [d^2 h][d\phi]$. Because the number of fermionic zero modes is determined by $q$, only the $q = 1$ term contributes in the sum over $q$ in the numerator of (2.10) and only the $q = 0$ term contributes to the denominator there. Thus, the sum over $q$ collapses to a single term. Gauge invariance implies that the integral over $g$ can be ignored. Only the fermionic part of the integrand depends on $h_\mu$.

3. Lattice formulation

On the lattice the “measurement” of $\langle V \rangle$ proceeds by two separate Monte Carlo simulations: one for the numerator and the other for the denominator in (2.10). To the numerator only gauge fields which induce exactly one fermionic zero mode for each charge one fermion and exactly two zero modes for the doubly charged fermion contribute. The denominator is entirely determined by configurations with strictly no fermion zero modes.
In principle, given a gauge configuration, one needs to perform some calculations to count the zero modes. However, by electing to work with a noncompact pure gauge action it becomes possible also on the lattice to predict the number of zero modes without a calculation simply by setting $q$. It is still up to the fermionic part of the system to “agree” with our prescribed $q$. We monitor for “disagreements” where the number of fermionic zero modes on the lattice is not what it should be for the given $q$. With our choice of parameters such disagreements are so rare that we never encounter them during our simulations. The main gain from this is that we can set $q$ by hand and our result does not suffer from the statistical noise inherent in simulating the prefactor $e^{-sq}$ from (2.12).

Our objective is to obtain the expectation value of the 't Hooft vertex in a fixed, rather small, physical volume. This is implemented by setting the bare coupling, $e_0$, to $1.5\sqrt{\pi}$ when we work on a finite $L \times L$ lattice. The continuum limit is taken by increasing $L$. Note that the parameter $m_\gamma$ was introduced as a bare parameter below equation (2.8). A priori, there is no guarantee that the lack of renormalization of the bare coupling in the continuum should hold also on the lattice. We assume that it does, and if our final result agrees with the continuum value we can say that the numerics are consistent with this assumption.

3A. Bosonic variables.

We use the same notation as in the continuum for $\phi, g, h, q$. The pure gauge action is

$$S_0 + s_q \equiv \frac{1}{2e_0^2} \sum_x (\Delta \phi)^2 + \frac{2\pi^2 q^2}{(e_0 L)^2}, \quad (3.1)$$

where

$$\Delta \phi(x) = \sum_\mu (\phi(x + \hat{\mu}) + \phi(x - \hat{\mu})) - 4\phi(x), \quad \phi(x + L\hat{\mu}) \equiv \phi(x). \quad (3.2)$$

All site index components $x_\mu$ are between 0 and $L - 1$ and if they appear outside this range in any of our equations one has to use the appropriate boundary conditions to bring them back within range. The field $\phi$ is constrained by $\sum_x \phi(x) = 0$. In Fourier space this constraint is trivially implemented. The pure gauge integration measure is taken as:

$$\sum_{q \in \mathbb{Z}} e^{-sq} \int d\mu \cdots \equiv \sum_{q \in \mathbb{Z}} e^{-sq} \int \prod_x dg(x) \int_{-1/2}^{1/2} d^2 h \int \sum_{x, \phi(x)=0} \prod_x d\phi(x)e^{-S_0(\phi)} \cdots \quad (3.3)$$

and the pure gauge partition function is

$$Z = \sum_{q \in \mathbb{Z}} e^{-sq} N; \quad N = \int d\mu. \quad (3.4)$$
Both Monte Carlo simulations carried out to get \( \langle V \rangle \) will calculate the expectation value of appropriate “fermion observables” in an ensemble governed by \( d\mu \). In other words, both the numerator and the denominator of (2.10) are divided by \( \mathcal{N} \). The “fermion observables” are functions of \( g, h, \phi \) that represent lattice versions of what in continuum is viewed as the result of carrying out the Grassmann integral in a fixed gauge background. With \( q \) fixed the pure gauge action depends only on \( \phi \), just like in the continuum. The “fermion observable” depends also on \( g \), in addition to \( h_\mu \). Hence, the \( g \) integral cannot be dropped.

We generate gauge fields using the pure gauge action and treat the fermion integrals in a fixed gauge field background as observables in the pure gauge theory. In our Monte Carlo implementation there is a difference between the numerator and the denominator. The measure for generating the variables \( h \) is flat in (3.3). We shall keep it this way for the numerator. In the denominator however, we replace the flat measure for \( h \) by a measure including the known \( h \)-dependent factor from the continuum fermionic contribution. This factor is extracted back from the fermionic observable (the equivalent of the chiral determinant), so the answer is unchanged. We are thus exploiting the fact that the dependence on \( h \) factorizes from the fermionic determinant in the continuum and from the pure gauge action both in the continuum and on the lattice. This trick significantly reduces the statistical error of the Monte Carlo simulation “measuring” the denominator.

For the numerator the \( h_\mu \) are generated randomly in the interval \([-1/2, 1/2]\). For the denominator the \( h_\mu \) are generated by a weight proportional to:

\[
|\theta(2h_1, 2h_2)|^2 = \left| \sum_{n=\infty}^{\infty} e^{-\pi(n+2h_2)^2+2i\pi n 2h_1} \right|^2. \tag{3.5}
\]

The other gauge variables are simulated in a standard way: \( S_0 \) defined in (3.1) and (3.2) can be written in momentum space as

\[
S_0 = \frac{1}{2\pi} \sum_{k_0, k_1=0}^{L-1} \tilde{\phi}(k)\tilde{\phi}(-k) \left[ 4 \sin^2\left(\frac{\pi k_0}{L}\right) + 4 \sin^2\left(\frac{\pi k_1}{L}\right) \right]^2, \tag{3.6}
\]

where

\[
\phi(x) = \frac{e_0}{L\sqrt{\pi}} \sum_{k_0, k_1=0}^{L-1} \tilde{\phi}(k) e^{2\pi ik_0 x}, \quad \tilde{\phi}(k) = \tilde{\phi}^*(k); \quad \tilde{\phi}(0) = 0 \tag{3.7}
\]

and \(-k_\mu \equiv \text{mod}(L-k_\mu, L)\). If \( k \neq -k \), we generate two random numbers, \( u_1, u_2 \), normally distributed according to

\[
\int du \exp \left[ -\frac{u^2}{\pi} \left[ 4 \sin^2\left(\frac{\pi k_0}{L}\right) + 4 \sin^2\left(\frac{\pi k_1}{L}\right) \right] \right]
\]

and set \( \tilde{\phi}(k) = u_1 + iu_2 \). If \( k = -k \), we generate one random number, \( u \), normally distributed according to
\[ f \, du \exp \left[ -\frac{u^2}{2\pi} \left( 4 \sin^2 \left( \frac{\pi k}{L} \right) + 4 \sin^2 \left( \frac{\pi k}{L} \right) \right) \right] \] and set \( \tilde{\phi}(k) = u \). We then use (3.7) to obtain several independent \( \phi(x) \) configurations.

For the denominator we can therefore replace \( d\mu \) in (3.3) by

\[
\int \prod_{x} dg(x) \int_{-1/2}^{1/2} d^{2} h \int_{-1/2}^{1/2} d^{2} r \prod_{\mu} \left[ \delta_{h_{\mu}, \frac{r_{\mu}}{L}} + \delta_{h_{\mu}, \frac{r_{\mu} - r_{\mu+1}}{L}} \right] \frac{|\theta(r_{1}, r_{2})|^{2}}{z_{t}}
\]

(3.8)

where \( z_{t} = 4 \int_{-1/2}^{1/2} d^{2} r |\theta(r_{1}, r_{2})|^{2} \) and the last factor is thought of as part of the observable. In this manner we obtain \( h_{\mu} \) in the range \([-1/2), (1/2)]\) distributed according to (3.7). Note that \( q \) is presumed fixed already. For the numerator, there are no \( r, z_{t} \) variables and the factors containing them are absent. Finally, the gauge variables \( g(x) \) are U(1) gauge transformations randomly generated at each site \( x \). Each gauge configuration we generate is statistically independent of the previous ones if we assume a high quality random number generator. We used RANLUX at luxury level 4. *

The fermions do not depend on the noncompact fields directly. They only depend on ordinary, compact, link variables. Thus, if one wished to replace the noncompact pure fermionic action by a compact one the fermionic part of our code would remain unchanged. The connection between the variables \( g, h, \phi, q \) we generate as described above and the link fields transmitted to the fermions is given by:

\[
U_{1}(x) = \begin{cases} 
    g(x) e^{\frac{2\pi i h_{1}}{2} e^{\phi(x) - \phi(x-\hat{1}) e^{\frac{2\pi i q}{L} x_{2}} g^{*}(x + \hat{1})} & \text{if } x_{1} = L - 1 \\
    g(x) e^{\frac{2\pi i h_{1}}{2} e^{\phi(x) - \phi(x-\hat{1})} g^{*}(x + \hat{1})} & \text{otherwise} 
\end{cases}
\]

(3.9)

\[
U_{2}(x) = g(x) e^{\frac{2\pi i h_{2}}{2} e^{\phi(x-\hat{2}) - \phi(x) e^{-\frac{2\pi i q}{L} x_{1}} g^{*}(x + \hat{2})}.
\]

Note that for \( q \neq 0 \) we take care of the needed twist at the boundary in the first line of (3.9). The noncompact character of the pure gauge action is reflected in that the mapping \( \{ g, h, \phi, q \} \to \{ U_{\mu} \} \) is many to one.

* Subtract-and-borrow random number generator proposed by Marsaglia and Zaman, implemented by F. James with the name RCARRY in 1991, and later improved by Martin Lüscher in 1993 to produce “Luxury Pseudorandom Numbers”. Fortran 77 coded by F. James, 1993 [3].
The right handed fermions live on the lattice the gauge fields are defined on. The parallel transporters between neighboring sites for these doubly charged fermions are \( U_\mu(x)^2 \). Up to gauge transformations the \( U_\mu(x) \) are quite close to the identity. The \( U^2 \) fields will be a little farther from the identity. The deviations of \( i(1-U^2) \) from \( 2A \) are cutoff effects of some typical magnitude. Similar cutoff effects also exist for the singly charged fermions and there is no numerical reason to try to make them smaller than the ones for the doubly charged fermions. We can thus put the charge one fermions on a twice as coarse lattice, thereby saving some computer time without increasing the ultraviolet cutoff effects.

3B. Fermionic variables.

The definition of the fermionic observables is in terms of fermionic creation and annihilation operators associated with the continuum Grassmann variables. Unlike their continuum counterparts, these operators are Dirac spinors (not Weyl spinors) thus ending up with twice as many components. The charge 2 \( \psi(x) \) field is represented by \( b(x;\alpha) \) where \( \alpha = 1,2 \) is the extra spinor index. The charge 1 \( \chi_f(x) \) fields are represented by \( a_f(y;\alpha) \).

The sites \( y \) are on the coarse lattice and their integer components range sequentially from 0 to \( \frac{L}{2} - 1 \). \( L \) is always even. Whenever a site index is outside its fundamental range one has to use the following boundary conditions to bring it back within range:

\[
\begin{align*}
  b(x + L\hat{\mu}_x;\alpha) &= b(x_\mu;\alpha), \\
  a_f(y + \frac{L}{2}\hat{\mu}_y;\alpha) &= e^{2\pi ib^f_\mu}a_f(y;\alpha),
\end{align*}
\]

where \( b^f_\mu \) are given by (2.3). The operators \( a, b \) obey canonical anti-commutation relation and act on the usual Fock space. \( \mu_x \) and \( \mu_y \) are elementary links on the fine and coarse lattices respectively.

For the numerator we need to discretize (2.6). To this end we introduce the operators \( \eta_{f_1,f_2}(y) \) below:

\[
\eta_{f_1,f_2}(y) = a_{f_1}(y;2)a_{f_2}(y;2)b^\dagger(2y;2).
\]

The site argument of \( b \) is relative to the fine lattice. All operators in (3.11) reside at the same physical site. The spinorial indices are chosen to match the continuum Lorentz transformation properties of the original fields. Thus, the \( \eta \)’s are lefthanded and \( U(1) \) neutral. With the help of the \( \eta \)’s we can produce a gauge invariant point split discretization of \( V \). The \( \eta \) fields also appear in the definition of the \( \rho \) field in (2.4).

The central object of the overlap is a Hamiltonian that acts on the Fock space irreducibly representing the complete algebra of anti-commutators. The Hamiltonian is bilinear and separable by flavor. These two properties represent the bilinearity and separability of the continuum action. The Hamiltonian (with implicit summations over spin...
and site indices) is given by:

\[ H = b^\dagger H^b(U^b)b - \sum_{f=1}^{4} a_f^\dagger H^a(U^a)a_f. \]  

(3.12)

The single particle Hamiltonians appearing in (3.12) are given below:

\[ H^{a,b}(U^{a,b}) = \begin{pmatrix} B(U^{a,b}) - m & C(U^{a,b}) \\ C^\dagger(U^{a,b}) & -B(U^{a,b}) + m \end{pmatrix}, \]  

(3.13)

\[ C(z, z'; U) = \frac{1}{2} \sum_{\mu=1}^{2} \sigma_{\mu} \left[ \delta_{z', z + \mu_x} (U^\mu(z)) - \delta_{z, z' + \mu_x} (U^\mu(z')) \right], \]  

(3.14)

\[ B(z, z'; U) = \frac{1}{2} \sum_{\mu=1}^{4} \left[ 2\delta_{z, z'} - \delta_{z', z + \mu_x} (U^\mu(z)) - \delta_{z, z' + \mu_x} (U^\mu(z')) \right]. \]  

(3.15)

(3.13) displays the dependence on spin indices in matrix format while (3.14-15) define the site dependence explicitly. When using (3.13-15) in (3.12), equation (3.10) must be employed to obtain the correct form of \( H \), with site index coordinates restricted to \([0, L - 1]\) for \( b \) and to \([0, L/2 - 1]\) for \( a_f \). \( U^{a,b} \) are the link variables as seen by the appropriate fermions. In our case the \( a \) fermions reside on the coarse lattice and the \( U^a \) link variable live on the links of that coarse lattice. The \( U^b \) link variables are on the original lattice and are chosen as identical to the link variables \( U \) introduced in (3.9). The \( U^a \) link variables are locally defined in terms of the \( U^\mu \)’s as follows: The parallel transporter between \( y \) and \( y + \hat{\mu}_y \) on the coarse lattice, \( U^a_\mu(y) \), is given by:

\[ U^a_\mu(y) = \frac{W}{|W|}, \]

\[ W = U^\mu(2y)U^\mu(2y + \hat{\mu}_x) + U^\nu(2y)U^\mu(2y + \hat{\nu}_x)U^\mu(2y + \hat{\mu}_x + \hat{\nu}_x)U^\nu(2y + 2\hat{\mu}_x) + U^\nu(2y - \hat{\nu}_x)U^\mu(2y - \hat{\nu}_x + \hat{\mu}_x)U^\nu(2y + 2\hat{\mu}_x - \hat{\nu}_x), \quad \nu \neq \mu. \]  

(3.16)

To obtain a proper description for chiral fermions one needs to pick \( 0 < m < 1 \). In practice, we used \( m = .5 \). This is a value empirically tuned to minimize potentially UV divergent effects due to a dynamically generated Thirring coupling.

The fermionic observables are matrix elements of fermionic operators made out of \( a, b \) in a way corresponding to the continuum expression in terms of Grassmann variables. The matrix elements are taken between two different states: The “ket” is the ground state of \( H \), \( |0\rangle^\text{WB} \), with the phase fixed in a manner which is dependent on the topology:

\[ ^\text{WB}_1^\text{WB} |((\tilde{a}_1^\dagger(2)\tilde{a}_1(1)\tilde{b}(1)\tilde{b}^\dagger(2))|0\rangle^\text{WB} \]  

(3.17)

9
is real and positive if $q = 0$ and

$$
\sum_{f_1, f_2, f_3, f_4 = 1}^4 \sum_{\mu = 1}^2 \sum_y \epsilon_{f_1 f_2 f_3 f_4} \sigma_\mu \left| \langle \eta_{f_1 f_2 (y)} \eta_{f_3 f_4 (y + \hat{\mu}_y)} |0\rangle^\text{WB}_U \right|
$$

is real and positive if $q = 1$. The phase of the state $\left| \langle 0 \rangle \right|_U^\text{WB}$ is immaterial since it does not depend on $U$. The sum over $y$ is over all sites on the coarse lattice. $\tilde{a}_1(\alpha) = \sum_y a_1(y; \alpha)$ is the operator associated with a single particle zero momentum state for the $q = 1$ fermion that has periodic boundary conditions in both directions and the sum on $y$ is over all points on the coarse lattice. Similarly, $\tilde{b}(\alpha) = \sum_x b(x; \alpha)$ is the operator associated with a single particle zero momentum state for the $q = 2$ fermion while the sum on $x$ is over all points on the fine lattice. These operators create states that carry no momentum. The combinations are also charge neutral. All insertions are best thought of as acting to the left and defining a $U$-independent reference state used to fix the phase of the ground state of the $U$-dependent system. The reference state is a Lorentz scalar and carries no $U(1)$ charge.

The “bra” state in the matrix element representing the result of the Grassmann integration, $\langle 0 \rangle$, is $U$-independent and given by the ground state of an ultralocal Hamiltonian, similar to (3.12) only that the single particle Hamiltonians (3.13) are diagonal having only mass terms with the parameter $m$ there replaced by a negative number. The phase choice for the “bra” is immaterial as long as it keeps the state $U$-independent.

With these definitions in place we finally can write down the lattice formula for (2.10) in the overlap formalism on an $L \times L$ lattice as:

$$
\langle V \rangle = \frac{2\pi^2}{(\epsilon_0 L)^4} e^{-\frac{2\pi^2}{(\epsilon_0 L)^2}} \frac{N}{D} = 0.024204\frac{N}{D},
$$

$$
N = \frac{L^2}{24} \sum_{f_1, f_2, f_3, f_4 = 1}^4 \sum_{\mu = 1}^2 \sum_y \epsilon_{f_1 f_2 f_3 f_4} \int \frac{d\mu}{N} \langle 0| \eta_{f_1 f_2 (y)} \eta_{f_3 f_4 (y + \hat{\mu}_y)} |0\rangle^\text{WB}_U, \quad (3.20)
$$

$$
D = \int \frac{d\mu}{N} \langle 0|0\rangle^\text{WB}_U. \quad (3.21)
$$

The sum over $y$ in (3.20) is over all points on the coarse lattice.

Expressions (3.20) and (3.21) are still not in an explicit enough form to transcribe directly into a program. First we need to rewrite (3.20) and (3.21) in first quantized forms. To this end, we diagonalize the single particle Hamiltonians (3.13):

$$
H_O = O \Lambda. \quad (3.22)
$$
The $\Lambda$ are diagonal matrices and the real elements along the diagonal are in decreasing order top to bottom. We work with five Hamiltonians: four are $L^2/2 \times L^2/2$ matrices and differ by the boundary conditions on the unit charged fermions. The fifth is an $2L^2 \times 2L^2$ matrix representing the doubly charged fermion.

We also define some gauge field independent reference matrices $O_0$: These will be used in implementing the Wigner-Brillouin phase definition. We shall need a realization of the bra state in (3.17) and (3.18) after being acted on by the $\tilde{a}_1$ and $\tilde{b}$ operators.

$$H_0O_0 = O_0\Lambda_0.$$  

(3.23)

$H_0$ is one of the five free Hamiltonian obtained by setting the gauge links to unity. The boundary conditions are maintained. For a trivial gauge configuration one can diagonalize the matrices by Fourier transform. Except for fermions which are periodic in both directions the ordering of $\Lambda_0$ is the same as above. For periodic fermions there are zero momentum eigenstates and the action of the $\tilde{a}_1$ and $\tilde{b}$ operators is implemented by switching the position of the positive eigenvalue corresponding to zero total momentum with the position of the negative eigenvalue corresponding to zero momentum. This induces a switch of two columns in $O_0$

It is convenient to partition the $O$ matrices into the following pattern:

$$O_a^f = \begin{pmatrix} O_{LL}^f(U^a) & O_{LR}^f(U^a) \\ O_{RL}^f(U^a) & O_{RR}^f(U^a) \end{pmatrix}, \quad f = 1, 2, 3, 4; \quad O_b = \begin{pmatrix} O_{LL}(U^b) & O_{LR}(U^b) \\ O_{RL}(U^b) & O_{RR}(U^b) \end{pmatrix}.$$  

(3.24)

The submatrices have half as many rows as the original $O$ matrices. These rows are indexed by a site index, running over $L^2$ values for $O_b$ (defined on the fine lattice) and over $L^2/4$ values for $O_a^f$ (defined on the coarse lattice). The first columns of $O$ contain the eigenvectors corresponding to positive eigenvalues of $H$. This set of columns defines the horizontal partition of the $O$ matrices. (Exactly zero eigenvalues of $H$ are possible but are non-generic.) The $O_0$ reference matrices are partitioned into square submatrices $O_{0LL}, O_{0LR}, O_{0RL}, O_{0RR}$ similarly to (3.24).

We define a configuration to have zero lattice topology (in practice, these are configurations with $q = 0$) when all submatrices are square. The lattice topological number will be unity (in practice, these are configurations with $q = 1$) when all $O_a^f$ are rectangular with $L^2/4 + 1$ columns and $O_{LL}$ is rectangular with $L^2 + 2$ columns. When the lattice topological number is unity we associate with the rectangular matrices the following site dependent square matrices:
\[ O_{LL}^f(U^a; y) = \left( \begin{array}{c} O_{LL}^f(U^a) \\ v_{RL}^f(U^a; y) \end{array} \right), \]
\[ O_{RR}^f(U^b; x_y, \mu) = \left( O_{RR}^f(U^b), v(x_y) \right), \]
\[ O_{LR}^f(U^b; 0, 0) = \left( O_{LR}^f(U^b), 0, 0 \right). \]

The site \( y \) is on the coarse lattice. \( x_y \equiv 2y \) identifies a site on the fine lattice that also resides on the coarse lattice. \( \hat{\mu}_y \) connects two sites of the coarse lattice. \( v_{RL}^f(U^a; y) \) is the \( y \)th row of \( O_{RL}^f(U^a) \). \( v(x_y) \) is a column vector of length \( L^2 \) that is zero everywhere except at the site \( x_y \) and “0” denotes a zero column vector. The \( O_{LL}^f(U^a; y) \) are \( (L^2/4+1) \times (L^2/4+1) \) matrices. \( O_{RR}^f(U^b; y, \mu) \) and \( O_{LR}^f(U^b; 0, 0) \) are \( L^2 \times L^2 \) matrices. The site dependence of the square matrices defined in (3.24) corresponds to the sites of the \( \eta \) operators in (3.20).

We need some extra rectangular reference matrices for the case of unit lattice topology:
\[ O_{0LL}^f(0) = \left( O_{0LL}^f, 0 \right), \quad O_{0RL}^f(y) = \left( O_{0RL}^f, v(y) \right). \]

Now we can write down the single particle representations of the matrix elements in (3.20) and (3.21). The overlap appearing in (3.21) has the following explicit form:

\[ \langle 0 | 0 \rangle_{U}^\text{WB} = \prod_f \det O_{LL}^f(U^a) \det O_{RR}^f(U^b) e^{i\phi(U)} \]

with

\[ e^{i\phi(U)} = \left[ \frac{\det WB_{RR}(U^b)}{\det WB_{RR}(U^b)} \right] \prod_f \left[ \frac{\det WB_{LL}^f(U^a)}{\det WB_{LL}^f(U^a)} \right]. \]

In (3.28),
\[ WB_{RR}(U^b) = [O_{RR}^f(U^b)]^\dagger O_{0RR} + [O_{LR}^f(U^b)]^\dagger O_{0LR}, \]
\[ WB_{LL}^f(U^a) = [O_{LL}^f(U^a)]^\dagger O_{0LL} + [O_{RL}^f(U^a)]^\dagger O_{0RL}. \]

The overlap appearing in (3.20) becomes (no sum over \( f_i \)),
\[ \langle 0 | \eta_{f_1 f_2}(y) \eta_{f_3 f_4}(y + \hat{\mu}) | 0 \rangle_{U}^\text{WB} = \epsilon_{f_1 f_2 f_3 f_4} \det O_{LL}^f(U^a; y) \det O_{LL}^f(U^a; y) \]
\[ \det O_{LL}^f(U^a; y + \hat{\mu}_y) \det O_{RR}^f(U^b; x_y, \mu) e^{i\phi(U)} \]

with
\[ e^{i\phi(U)} = \frac{wb(U)}{|wb(U)|}. \]

In (3.31),
\[ wb(U) = \sum_{f_1, f_2, f_3, f_4 = 1}^4 \sum_{\mu=1}^2 \sum_y [\epsilon_{f_1 f_2 f_3 f_4}]^2 \sigma_{\mu} \det WB_{LL}^f(U^a; y) \det WB_{LL}^f(U^a; y) \]
\[ \det WB_{LL}^f(U^a; y + \hat{\mu}_y) \det WB_{LL}^f(U^a; y + \hat{\mu}_y) \det WB_{RR}(U^a; x_y, \mu). \]
The matrices appearing in (3.32) are given by

\[
\begin{align*}
WB_{LL}^f(U^a; y) &= [O_{LL}^f(U^a)]^\dagger O_{0LL}(0) + [O_{RL}^f(U^a)]^\dagger O_{0RL}(y), \\
WB_{RR}(U^b; x_y, \mu) &= [O_{RR}(U^b; x_y, \mu)]^\dagger O_{0RR} + [O_{LR}(U^b; 0, 0)]^\dagger O_{0LR}.
\end{align*}
\] (3.33)

3C. The Monte Carlo procedure.

We have seen that the bosonic variables are integrated over by Monte Carlo while the fermionic variables are “integrated” out “exactly”. The bosonic integration has two stages, consisting of two Monte Carlo processes, one running within the other. The outer process (for either \( q = 0 \) or \( q = 1 \)) averages over gauge orbits, generating the fields \( \phi(x) \) and \( h_\mu \).

The links on the coarse and fine lattice are then defined up to a gauge transformation. Setting \( g(x) \equiv 1 \) in (3.9) this gives us a representative of an orbit. Loosely, we can refer to this as the “Landau” gauge representative, since in the continuum, setting \( g \) to unity in (2.11) would imply \( \partial_\mu A_\mu = 0 \). We then compute the needed determinants (3.27-33), depending on the topological sector we are in.

The internal Monte Carlo procedure averages over gauge transformations after a “Landau” configuration (an orbit) has been selected and the fermionic observables have been calculated. For each \( x \) we randomly draw a unimodular complex number \( g(x) \). When the links are replaced by gauge transformed links (see (3.9)) the dependence of the the Hamiltonians \( H^{a,b} \) in (3.13) on the gauge transformation \( g \) can be absorbed into a unitary matrix \( G^{a,b} \) which conjugates the “Landau” gauge \( H^{a,b} \). \( G^a \) (\( G^b \)) is a diagonal \( L^2/2 \times L^2/2 \) \((2L^2 \times 2L^2)\) matrix whose rows and columns are indexed by sites and spin components. The entries on the diagonal are the appropriate \( g \) for the site. Thus the Hamiltonians after the gauge transformation are expressed in terms of the “Landau” gauge Hamiltonians as:

\[
H^{a,b}(\text{gauge transformed links}) = [G^{a,b}] H^{a,b}(\text{Landau gauge links}) [G^{a,b}]^\dagger. \quad (3.34)
\]

The effect of the conjugation in (3.34) is to multiply the “Landau” gauge \( O^f_a \) and \( O_b \) from the left by \( G^{a,b} \). The submatrices (3.24) and (3.25) also get multiplied from the left by appropriate diagonal submatrices of \( G^{a,b} \). The determinant factors in (3.27) and (3.30) change by gauge factors given by the product of the five determinants of these diagonal submatrices. Because of gauge invariance, the dependence on the site \( y \) in (3.30) cancels out from its gauge factor and both gauge factors turn out to be given by \( \prod_x g(x) [\prod_y g(y)]^4 \) (we remind the reader that the \( x \)'s are sites on the fine lattice and the \( y \)'s are sites on the embedded coarse lattice).

The diagonal matrices implementing the gauge transformations on the matrices \( O \) get caught in between the matrices multiplied in (3.29) and (3.33) and the related determinants.
in (3.28) and (3.32) have to be recomputed. Since no rediagonalization of the Hamiltonians is necessary, and since the changes in (3.27) and (3.30) are simple, the total amount of computation needed to account for link updates along gauge orbits is smaller than for link updates changing gauge orbit.

Every orbit we generate is completely independent statistically (assuming an ideal random number generator) from every other orbit. Similarly, all gauge transformations we generate are mutually independent. The absence of correlations implies that statistical error analysis is relatively simpler here than in standard Monte Carlo. Of course, since our observables are non-local, one needs to look at their distributions to ascertain that they are reasonable and that our numerical approach hasn’t been rendered hopeless by large fluctuations. For sizes $L = 8 - 24$ the fluctuations are manageable and we can make quite accurate statistical determinations. The ability to control the fluctuations is helped by the adjustment of the coupling constant with $L$ which keeps the physical volume finite.

For a given gauge configuration the number of floating point operations is quite high, $\sim 10^{11}$ for the highest $L$’s. The evaluations of the gauge averages of the imaginary parts involve some cancelations which are roundoff sensitive. Thus, it is necessary to use double precision floating point arithmetic throughout (except in the generation of the random numbers).

4. Numerical results.

We evaluated the quantities $N$ and $D$ ((3.20-21)) for all even $L$’s between 8 and 24. For a single gauge configuration, the evaluation of a $D$-contribution is faster than the evaluation of an $N$-contribution. This is countered somewhat by smaller fluctuations for $N$. We aimed at comparable accuracies in $N$ and $D$ and ended up spending ten times as much computer time on evaluating $N$ than on calculating $D$ for the larger $L$’s. For a fixed gauge configuration and asymptotic $L$, $N$ is an $L^8$ computation while $D$ is an $L^6$ computation.

It was determined that reasonable values could be obtained for $D$ with 100 orbits plus 100 gauge transforms per orbit. For $N$ 20 orbits with 40 gauge transforms sufficed. This yielded relative errors (single standard deviation) in $N$ and $D$ of a few percent.

Numerically, $N$ and $D$ are dominated by ultraviolet effects. When $L$ is large we expect the following asymptotics:

$$\log(N) = n_0 L^2 + n_1 \log L + n_2 + \frac{n_3 \log L}{L^2} + \frac{n_4}{L^2} + \cdots$$

$$\log(D) = d_0 L^2 + d_1 \log L + d_2 + \frac{d_3 \log L}{L^2} + \frac{d_4}{L^2} + \cdots$$

(4.1)
$n_0$ and $d_0$ are evaluated from the noninteracting theory:

$$n_0 = d_0 = 0.242586.$$ (4.2)

A regularized version cannot reproduce (2.1) exactly in the continuum limit because an exactly marginal (in the renormalization group sense) coupling exists and obeys all symmetries. This is the “Thirring” coupling:

$$g_{Th}(\sum_f \bar{\chi}_f \chi_f) \bar{\psi} \psi.$$ (4.3)

$g_{Th}$ can have either sign. Depending on it we can have $n_1 > d_1$ or $n_1 < d_1$.

Generically, by tuning a free parameter in the regularization one can adjust the approach to continuum to have $n_1 = d_1$. In our case this is approximatively achieved by choosing $m = .5$ (see paragraph after (3.16)). Of course, the tuning cannot be exact, so we will expect $N/D$ to either diverge or go to zero as $L$ becomes truly large. But, as long as $|n_1 - d_1| \log L$ is numerically negligible $\log(N/D)$ is dominated by $n_2 - d_2$. The first subleading correction is of order $1/L^2$ since there are no dimension three irrelevant operators to contribute to the action or the operator. The exact result quoted in section 2 is essentially $n_2 - d_2$ for the case $n_1 = d_1$.

Schematically, we would expect the following behavior of the ratio as a function of $1/L^2$:

![Expected Schematic Behavior](image)

**Figure 1** Effect of Thirring coupling.
The data would follow either ABC or ABD, depending on the sign of $g_{Th}$. The better we tuned $m$ the closer will B by to E, the exact result for $g_{Th} = 0$. This is only the simplest scenario for what happens around B. Since various terms make comparable contributions the curves may get more complicated there.

The $1/L^2$ corrections that come from the operator (rather than from the action) can be evaluated at $g_{Th} = 0$ in the continuum. This yields a correction factor (point-split factor) of:

$$ps = \exp\{-\int_0^\infty \frac{d\tau}{\tau} e^{-\frac{1}{3}(\tau+\frac{1}{\tau})} + 1.15443133 + 2 \log \frac{3}{L}\}.$$  \hspace{1cm} (4.4)

The factor $ps$ can be used to improve convergence. The number 1.15443133 above is two times Euler’s constant and $3/L$ comes from $2e_0/\sqrt{\pi}$. We use the complete formula for $ps$, including all subleading terms in $1/L^2$.

Figure 2  Data obtained with gauge averaging. Convergence improves by inclusion of the point-split factor $ps$.

Figure 2 contains our results for the logarithm of the vertex, $\log <V>$. The exact continuum limit is also shown ( $\log <V> (L = \infty) = -3.247$ ). Quite clearly, we see convergence towards the exact continuum number for $L$ between 8 and 18. $ps$ indeed “improves” the observable. The data for $L$ between 20 and 24 show a certain amount of instability. It is conceivable that this reflects region B in our schematic figure. We cannot say anything conclusive without better statistics and additional results for higher $L$’s.
Most of the computation time is spent on gauge averaging. By discarding gauge averaging we can increase statistics. A simple gauge invariant way to avoid gauge averaging is to replace the integrands in (3.20) and (3.21) by their absolute values. The corresponding quantities in the continuum are positive. In figure 3 we show data obtained using the absolute values exploiting the same runs as in figure 1. We also add four more data points in the range $L = 18$ to 24 with higher statistics: $N$ is evaluated from 100 orbits and $D$ from 200. We see that the higher statistics, while supportive of some structure around $L = 20$, still do not lead us to a definite confirmation of the qualitative scenario that would relate it to a Thirring term.

To be sure that using the absolute value rather than the gauge averaged results is not a source of contamination as far as the possibility of a structure around $L = 20$ is concerned we compare in figure 4 the two (absolute value and gauge averaged) vertices for the entire set of available orbits. We see that the difference is quite insignificant numerically and, therefore, how gauge invariance is recovered is unimportant.

In figure 5 we display $N$ and $D$ individually. We subtract the large numbers $n_0L^2 = d_0L^2$ from the logarithms of $N$ and $D$ and plot the results together with the logarithm of the ratio $(\log(N/D) = 0.474$ in the continuum limit). We see that the bulk of $D$ and $N$ is given by the free field terms we subtracted, and that the remainder consists of numbers of
Figure 4  A comparison of data obtained with gauge averaging to data obtained without for the same sample of orbits.

Figure 5  log $N$ and log $D$ after subtracting the quadratic divergence are small numbers. The logarithm of $N/D$ is also shown. The numbers were obtained with gauge averaging.
order unity.

5. Summary.

Although the tuning of the Thirring coupling is not fully understood numerically, overall, our simulation confirms the validity of the overlap regularization method of the model in (2.1). More work would be needed to understand the possible role of a dynamically generated $g_{Th}$. Other two dimensional models can be tested by similar methods. Going to higher dimensions would require some algorithmical improvements, as the simulations presented here took a considerable amount of time on machines of various types.

Based on our work, we express our hope that the problem of simulating chiral gauge theories has been turned from one of principle to one of practicality.

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