Improved projector Monte Carlo study of string tension and roughening in lattice QED in three dimensions

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We report on a faster version of the projector Monte Carlo, a method for stochastically simulating quantum Hamiltonian field theories. We also present a more accurate evaluation of the string tension for lattice U(1) gauge theory in 2+1 dimensions.

I. INTRODUCTION

This paper is the continuation of a study of string properties of Abelian lattice gauge theory in 2+1 dimensions. In our first paper¹ (hereafter referred to as I), we measured the ground state, string energies, and string width of that system in its Hamiltonian formulation using the projector Monte Carlo of Blankenbecler and Sugar.² In this report we wish to describe an improvement of the Monte Carlo method (the ensemble projector Monte Carlo, or EPMC) which allows the accumulation of data about an order of magnitude faster than the method of Blankenbecler and Sugar.

We have recalculated all the quantities of I with smaller error bars. In particular, the coupling dependence of the string tension is less erratic than in I, and compares well with strong- and weak-coupling predictions. Moreover, the computed ground-state energies follow closely Hofsass and Horsley's upper bound,³ now *from below* and deep into weak coupling.

About 100 CPU hours on a VAX 11/780 were needed to evaluate, within 5% error or less, string energies and string widths for 6 values of the coupling and 4 values of the string length, on a 6^2 lattice.

In Sec. II, we describe the EPMC method, and in Sec. III we show some results for string physics. Section IV contains our conclusions and some speculations for future work.

II. METHODOLOGY

Hamiltonian Monte Carlo algorithms have been used for some time now, especially in solid state and particle physics.⁴ The Monte Carlo technique used in this work is a variation of the projector Monte Carlo of Blankenbecler and Sugar.² It is identical to the one used by Campbell, DeGrand, and Mazumdar and by Hirsch and Schrieffer.⁵ It is based on the observation that the operator

$$u = e^{-\Delta \tau H} \tag{1}$$

is a projection operator for the ground state $|0\rangle$ (with energy E_0) of a Hamiltonian *H*. Indeed, for any states $|\chi\rangle$ and $|\psi\rangle$, not orthogonal to $|0\rangle$, the quantity

$$S_{M} \equiv \frac{\langle \chi \mid u^{M} \mid \psi \rangle}{\langle \chi \mid u^{M-1} \mid \psi \rangle}$$
(2)

has the limiting behavior

$$\lim_{M \to \infty} S_M = e^{-\Delta \tau E_0} \,. \tag{3}$$

Other Hamiltonian Monte Carlo studies use 1/H as the projector: in particular, Heys and Stump in their study of U(1) gauge theory in 2+1 and 3+1 dimensions, and Lee, Motakabbir, and Schmidt in a study of two-dimensional fermions.⁴ Otherwise the calculations we now describe are quite similar in spirit to theirs.

The goal of our calculation is to compute (2) and (3), for stringless and string states in compact threedimensional QED, whose Hamiltonian reads^{1,6}

$$H = \sum_{n,i} \frac{g^2}{2} (E_n^i)^2 + \sum_n \frac{1}{g^2} (1 - \cos B_n) .$$
 (4)

Here, E_n^i is the electric field operator on site $n = (n_1, n_2)$ and B_n is the magnetic field operator about a plaquette at site n,

$$B_n = A_n^1 + A_{n+1}^2 - A_{n+2}^1 - A_n^2.$$

Observe that Eq. (2) is based on the representation of states of the type $u | \psi \rangle$. Let us describe how they can be generated stochastically.

A prerequisite for such a task is the knowledge of the matrix element of the operator u in some basis. For our problem, a good basis is diagonal in the electric field. On a single link, $E_n^i | l_n^i \rangle = l_n^i | l_n^i \rangle$, while a complete lattice state $| \{ l_n^i \} \rangle$ is the direct product of single-link vectors.

Using these electric field eigenstates, we can express the vector $u \mid \psi \rangle$ as

$$|\psi\rangle = \sum_{\{l_k^j\}} a_{\{l_k^j\}}^{\psi} \left[\sum_{\{\overline{l}_k^j\}} \langle \{\overline{l}_k^j\} | u | \{l_k^j\} \rangle | \{\overline{l}_k^j\} \rangle \right].$$
 (5)

The expectation value $\langle \{\overline{l}_k^i\} | u | \{l_k^j\} \rangle$ is difficult to evaluate in general. This is why we break up the Hamiltonian in two parts, $H = H_1 + H_2$, and use the approximation

$$e^{-\Delta\tau H} = e^{-\Delta\tau H_{1}/2} e^{-\Delta\tau H_{2}} e^{-\Delta\tau H_{1}/2} + O(\Delta\tau^{3}) , \qquad (6)$$

where

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$$H_{1} = \sum_{n} \frac{g^{2}}{2} [(E_{n}^{1})^{2} + (E_{n+\hat{1}}^{2})^{2} + (E_{n+\hat{2}}^{1})^{2} + (E_{n}^{2})^{2}] + \frac{1}{g^{2}} (1 - \cos B_{n})$$
$$\equiv \sum_{\vec{n}} h_{1}(\mathbf{n})$$
(7)

with $\mathbf{n} \equiv (n_1, n_2)$, n_1 and n_2 being both even or odd. H_2

has the same form as
$$H_1$$
, except that n_1 is even (odd) and n_2 is odd (even). In other words, H_1 (H_2) contains the black (white) squares of a checkerboard.

The advantage of doing so is that $\langle \{ \} | e^{-\Delta \tau H_i} | \{ \} \rangle$ can be evaluated in a *local* way, i.e.,

$$\langle \{\overline{l}_{k}^{j}\} | e^{-\Delta \tau H_{1}} | \{l_{k}^{j}\} \rangle = \prod_{n}^{\text{black}} \langle \{\overline{l}_{n}^{\text{plaq}}\} | e^{-\Delta \tau h_{1}^{(n)}} | \{l_{n}^{\text{plaq}}\} \rangle.$$

In the right-hand side, each product depends only on one plaquette. The matrix elements of u are then expressed as

$$\langle \{\overline{I}_{k}^{j}\} | e^{-\Delta\tau H} | \{l_{k}^{j}\} \rangle = \sum_{\{\overline{l}_{k}^{j}\}\{\overline{l}_{k}^{j}\}} \left[\prod_{n}^{\text{black}} \langle \{\overline{I}_{n}^{\text{plaq}}\} | e^{-\Delta\tau h_{i}^{(n)}/2} | \{\widehat{I}_{n}^{\text{plaq}}\} \rangle \right] \left[\prod_{n}^{\text{white}} \langle \{\widehat{I}_{n}^{\text{plaq}}\} | e^{-\Delta\tau h_{2}^{(n)}} | \{\overline{I}_{n}^{\text{plaq}}\} \rangle \right] \left[\prod_{n}^{\text{black}} \langle \{\overline{I}_{n}^{\text{plaq}}\} | e^{-\Delta\tau h_{1}^{(n)}/2} | \{I_{n}^{\text{plaq}}\} \rangle \right].$$

$$(8)$$

Let us now describe the stochastic evaluation of $u | \psi \rangle$. The checkerboard breakup described earlier converts $\langle u \rangle$ into a product of single-plaquette matrix elements

$$\langle \{\overline{l}^{\text{plaq}}\} | e^{-\Delta \tau (1/2)^{2-i}h_i} | \{l^{\text{plaq}}\} \rangle.$$

We rewrite these matrix elements in terms of probabilities and scores, i.e.,

$$\langle \{\overline{l}^{\text{plaq}}\} | e^{-\Delta \tau (1/2)^{2-l} h_{i}} | \{l^{\text{plaq}}\} \rangle \equiv P^{(i)}_{\{\overline{l}^{\text{plaq}}\}, \{l^{\text{plaq}}\}} S^{(i)}_{\{\overline{l}^{\text{plaq}}\}, \{l^{\text{plaq}}\}} , \qquad (9)$$

where
$$0 \le P^{(i)} \le 1$$
 and $\sum_{\{j\}} P^{(i)}_{\{j\},\{\}} = 1$.

(

The P's and S's are otherwise arbitrary (we assume here that u is positive definite). For our simulation of QED, we have used the same probabilities and scores as in Ref. 1 [see Eq. (11) there] and imposed periodic boundary conditions. In terms of these quantities, the vector $u | \psi \rangle$ reads [Eqs. (8) and (9) in (5)]:

or, in a more compact notation

$$u \mid \psi \rangle = \sum_{i,j} a_i^{\psi} \mathscr{P}_{ij} \mathscr{S}_{ij} \mid j \rangle .$$
 (10b)

In the original method of Ref. (1) the state $u | \psi \rangle$ would consist of N states, each selected with probability P and weighted by a factor S. We modify that procedure by performing a further sampling which allows the number of states in the ensemble to fluctuate.

We take $|\psi\rangle$ to be some collection of N (electric field) states which diagonalize H in strong coupling (and do not exclude the possibility that some of the states are identical). We apply u to $|\psi\rangle$ as follows. From each state $|\{l_k^I\}\rangle$ of this ensemble, first generate one new state $|\{l_k^I\}\rangle$ with probability \mathscr{P} (i.e., a successive application of $P_{\hat{I}\hat{I}}^{(1)}P_{\hat{I}\hat{I}}^{(2)}P_{\hat{I}\hat{I}}^{(1)}$). Then, retain a number of copies of the new state, the number of which being determined as follows.

Let us rewrite (10) as

$$u \mid \psi \rangle = \widetilde{\mathscr{S}} \sum_{i,j} a_i^{\psi} \mathscr{P}_{ij} \mathscr{R}_{ij} \mid j \rangle$$

with

$$\mathcal{R}_{ij} = \mathcal{S}_{ij} / \tilde{\mathcal{S}}$$
 .

So far \mathscr{F} is chosen arbitrarily. If $0 \le \mathscr{R} \le 1$, we generate a random number r with a uniform distribution between 0 and 1. If $\mathscr{R} \le r$ keep $|\{\overline{l}_k^i\}\rangle$. If $\mathscr{R} = J + \delta$, J > 1 (J is an integer), keep J copies, plus one more with probability δ . The collection of all these copies is called $|\psi^{(1)}\rangle$.

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(11)

This is how we generate the vector $u | \psi \rangle$ stochastically. If interested in $uu | \psi \rangle$, repeat the above procedure with the states of $| \psi^{(1)} \rangle$, in order to get $| \psi^{(2)} \rangle$.

Let us stress that

$$\widetilde{\mathscr{S}} | \psi^{(1)} \rangle \neq u | \psi \rangle ,$$

but instead

$$\widetilde{\mathscr{S}} \mid \langle \{l_k^j\} \mid \psi^{(1)} \rangle \mid \simeq \mid \langle \{l_k^j\} \mid u \mid \psi \rangle \mid$$

Taking $|\chi\rangle$ to be a broad state $(\langle \chi | \psi \rangle = N^{(0)})$ and $\langle \{l_k^j\} | u | \psi\rangle$ real and greater than zero, we have

$$\begin{split} \langle \mathcal{X} \mid u \mid \psi \rangle &= \sum_{\{l_k^j\}} \langle \mathcal{X} \mid \{l_k^j\} \rangle \langle \{l_k^j\} \mid u \mid \psi \rangle \\ &= \sum_{\{l_k^j\}} \langle \{l_k^j\} \mid u \mid \psi \rangle \\ &\simeq \sum_{\{l_k^j\}} \widetilde{\mathscr{S}} \langle \{l_k^j\} \mid \psi^{(1)} \rangle = \widetilde{\mathscr{S}} N^{(1)} \end{split}$$

and

$$\frac{\langle \chi \mid u \mid \psi \rangle}{\langle \chi \mid \psi \rangle} = \frac{\tilde{\mathscr{P}} N^{(1)}}{N^{(0)}} .$$
(12)

The strength of this method is as follows. u is a projection operator, so repeated application of u to $|\psi\rangle$, generating $|\psi^{(1)}\rangle$, $|\psi^{(2)}\rangle$, ..., etc., builds states which are better and better approximations to the ground state. So,

$$\frac{\langle \chi \mid u \mid \psi^{(n)} \rangle}{\langle \chi \mid \psi^{(n)} \rangle} \simeq e^{-\Delta \tau E_0} .$$
(13)

If at the same time one adjusts $\widetilde{\mathscr{S}}$ so that on the average, $N^{(n+1)} \simeq N^{(n)}$ (which can be done by setting $\widetilde{\mathscr{S}}_{n+1} = \widetilde{\mathscr{S}}_n N^{(n+1)} | N^{(n)}$), $\widetilde{\mathscr{S}}$ will also converge to an equilibrium value. After that point, the ground-state energy can be read off from $\widetilde{\mathscr{S}}$ [see (12)]:

$$e^{-\Delta\tau E_0} = \langle \tilde{\mathscr{S}}_n \rangle , \qquad (14)$$

where the average is over some values of n (as the wave functions $|\psi^{(n)}\rangle$ are correlated from step to step, it is necessary to average $\tilde{\mathscr{S}}_n$ on only every few steps).

Similarly, for operators diagonal in the electric field basis, we have

$$\langle 0 | 0 \rangle \simeq \left\langle \frac{\langle \psi^{(n)} | 0 | \psi^{(n)} \rangle}{\langle \psi^{(n)} | \psi^{(n)} \rangle} \right\rangle_{n} .$$
(15)

For our problem, we have worked with $\Delta \tau = 0.1$ and 0.05, $N^{(i)} \simeq 500 - 3000$ (see below); about 10 steps were required to equilibrate $\tilde{\mathscr{S}}$, and data were taken every 4 steps thereafter, to a maximum of 50 to 100 steps. Moreover, expressions (14) and (15) have been evaluated many times (run with different random number generator seed and $\tilde{\mathscr{S}}_0$); the results reported in the next section are averages over these runs.

The ensemble projector Monte Carlo gives much more accurate energies for an equivalent amount of computer time than the projector Monte Carlo of Blankenbecler and Sugar where one measures \mathscr{S}_N directly as a ratio of product of scores:

$$\langle u^{N} \rangle = \sum_{\{i\},\{j\},\{k\}} \cdots S_{\{i\},\{j\}} S_{\{i\}\{k\}} \cdots S_{\{y\}\{z\}} \times \langle \chi \mid \{i\} \rangle \langle \{z\} \mid \phi \rangle .$$
(16)

The difficulty with this method is that fluctuations in u^M grow with M. If the average score is S and its typical fluctuation Δs , then

$$\langle u^M \rangle \sim \langle (s + \Delta s)^M \rangle \sim \langle s \rangle \left[1 + M \frac{\Delta s}{s} \right].$$
 (17)

One needs large M to project onto the ground state; however, large M leads to large fluctuations in the average score and in the energy measurements. The method described here "effectively" takes M=1 since at each time step, we begin with a new state (i.e., the $|\psi^{(m)}\rangle$'s). It can show systematic effects with the number of states in the ensemble since only a finite number of states are retained simultaneously; in the projector Monte Carlo, the "ensemble" is built one state at each time and can be arbitrarily large. For the lattice gauge model we discuss here, energies do not appear to be sensitive to "number of states" systematics if we keep more than about 2000 states, on a 6² lattice, in a strong or intermediate coupling.

No significant improvements in terms of CPU time have been reached regarding the evaluation of matrix elements. In the projector Monte Carlo, this expectation value is given by the $\langle \chi | u^{NO} | \psi \rangle$ computed by applying U^{N} to one state in $|\psi\rangle$ at a time. [See Eq. (5) in I.] On the other hand, this quantity is obtained in the EPMC by summing the $\langle \{l_{b}^{i}\} | 0 | \{l_{b}^{i}\} \rangle$, weighted by the square of the number of copies of $|\{l_{b}^{i}\}\rangle$ in the ensemble $|\psi^{(i)}\rangle$ under consideration. This number cannot be obtained from a straight energy calculation: extra time is needed as one has to scan through the ensemble [this process involves the comparison of $N^{(i)}(N^{(i)}-1)/2$ lattice configurations].

In order to keep our total CPU time within reasonable limits, while striving for accurate energies, we have made two different sets of runs. The first set involved $N^{(i)} \simeq 3000$ and was dedicated to energy and string-tension calculations. In the second set, the vacuum expectation values of string-width operators were computed, with $N^{(i)} \simeq 500-1500$.

III. ON-AXIS STRING CALCULATIONS

A. String energy

The string tension in computational three-dimensional QED has been studied by several authors, with varying degrees of success.⁷⁻¹¹ Here, we are interested not as much in comparing our results with theirs as in the improvements brought by the EPMC over the projector Monte Carlo.

We have recalculated the string energies studied in I. The EPMC needs one tenth the CPU time and one half the number of field configurations to achieve twice the accuracy of the method in Ref. 1.

The ground state and the string state differ in their initial configuration $|\psi\rangle$. The initial lattice configuration for the ground state has zero electric flux on all links, or in the case of a string, a lattice which is fluxless except on the links supporting the string, which carry one unit of flux. Let us mention that static sources can be also handled explicitly in the Euclidean formulation of lattice three-dimensional QED, by including them in the action.⁷

Figure 1 shows the ground-state energy for $0.57 \le g \le 2.0$. The smooth curve represents the upper bound



FIG. 1. Ground-state energy (per plaquette) versus the coupling constant. The smooth curve is the upper bound found by Hofsass and Horsley (Ref. 3).

computed by Hofsass and Horsley.³ Not shown is the comparison of the data with strong-coupling prediction in the range $2.0 \le g \le 10.0$: our calculation agrees well with $E_0 = 1/g^2$ within 1%, as expected.

Contrary to the data in I (Ref. 1, Fig. 2), all of the numbers obtained here are below, and follow quite closely Hofsass and Horsley's curve. Both data are within one standard deviation of each other. This makes us confident about the validity of the computations.

As mentioned earlier, it appears that E_0 (and E_L) is not very sensitive to number of states systematics as we used about 3000 states.

The string state energies have been computed in the same coupling range. As in I, because E_L was roughly linear with respect to the length (L) (it is in fact even



FIG. 2. The string tension versus the coupling constant. The solid and dashed curves correspond to strong and weak coupling, respectively.

more linear here), the string tension T was deduced by fitting the straight line

$$E_L = E_0^{\text{fit}} + T^{\text{fit}}L$$
 /area.

As in I again, the value for E_0^{fit} gives a consistency check on the values displayed in Fig. 1 (it is indeed consistent).

The coupling dependence of the tension T is shown in Fig. 2. The continuous curve represents the first-order strong-coupling prediction $(g^2/2)$; the dashed line corresponds to Suranyi's variational estimate in Hamiltonian formulation^{8,9}

$$\frac{4\sqrt{8}}{g^2}\exp(-4.4/g^2)$$
.

This expression is consistent, up to a factor in g, with other Hamiltonian variational studies;^{6,9} it is also similar to the weak-coupling lower bound of the string tension in Euclidean Villain theory.¹⁰

The data leaves the strong-coupling curve in the range $g \simeq 1.5$, to follow the weak-coupling prediction from above. It is impossible to evaluate T at g < 0.5, because of its smallness, $T < 10^{-10}$ at g < 0.3.

B. String width

The expectation values $\langle \sum E_{\parallel}^2 \rangle$ and $\langle \sum X_{\perp}^2 E_{\parallel}^2 \rangle$ were calculated using Eq. (15). For reasons explained in Sec. II, the collections $|\psi^{(m)}\rangle$ contained only 500 to 1500 states, and it was used for both operators; the strings had length L = 0, 3, 4, 5, and the coupling set to g = 2.00, 1.50, 1.16, and 0.75.



FIG. 3. The string width $W_L(g)$ versus the string length L.



FIG. 4. The string width at length L = 4, versus the inverse of the number of states $N^{(i)}$ (averaged over number of time steps).

We have computed the ratio

$$W_{L} \equiv \frac{\langle \sum X_{\perp}^{2} E_{\parallel}^{2} \rangle_{L,g}}{\langle \sum E_{\parallel}^{2} \rangle_{L,g}}$$

which serves as a good signal for roughening. As shown in Ref. 1, although its magnitude is volume dependent, it appears that its L dependence *is not:* in the two lattices investigated (6^2 and 8^2), the length dependence changes abruptly at the roughening point (see Figs. 5–8 there).

The data is displayed in Fig. 3 and confirms the general picture presented in I, namely, the existence of the roughening transition at $g_R \simeq 1.16$. The g=1.50, 1.16, and 0.75 data is consistent with I. For g=2.00 the EPMC gives results two standard deviations lower than in I; however, in either case, $W_L(g=2.00)$ is very small, around 0.04 to 0.05.

Because of the small ensembles involved here, the number of states systematics can be substantial for less than 500 states in the ensemble (see Fig. 4). As a general rule, for fixed g and L, W_L and the difference $\Delta(g,L,N) \equiv W_L(g,N) - W_L(g,N')$ decrease with increasing N, while $\Delta(g,L,N)$ decreases with decreasing g.

The data reported in Fig. 3 involves the following number of states (for all L):

$$g = 2.00 \rightarrow N^{(i)} \simeq 1000 ,$$

$$g = 1.50 \rightarrow N^{(i)} \simeq 1000 ,$$

$$g = 1.16 \rightarrow N^{(i)} \simeq 500 ,$$

$$g = 0.75 \rightarrow N^{(i)} \simeq 500 .$$

By comparing with the W_4 's in Fig. 4 for different $N^{(i)}$, one sees (at least for $g \le 1.50$) that the $N^{(i)}$ systematics have been brought pretty much under control.

It is unfortunately impossible to determine accurately the exact location of g_R . Our lattice was rather small (6²) and finite-size effects impose a cutoff on the magnitude of $\langle \sum x_{\perp}^2 E_{\parallel}^2 \rangle$.¹ Moreover, the transition is much smoother than in the case of an infinite lattice.

IV. SPECULATIONS FOR FUTURE WORK

The EPMC is a faster version of the projector Monte Carlo. The only drawback is the obligation to store all of the states of the collections $|\psi^{(M)}\rangle$ and $|\psi^{(M-1)}\rangle$ at the same time, which is hard on memory: consideration of larger lattices meant for us smaller $N^{(M)}$, and thus bad statistics. This, however, should not deter any potential users with access to larger machines.

Another aspect of lattice three-dimensional QED that could be studied with EPMC is off-axis string behavior. This calculation is more involved because of the high degeneracy related to off-axis string configurations.¹¹ The determination of the zeroth-order state (which is to be the starting collection $|\psi\rangle$) is a formidable problem in itself. We have investigated short off-axis strings in strong coupling, and found $W_L(g)$ to be of the order of 1, as expected [in contradistinction with the on-axis case where $W_L(g)\simeq 0$].

Finally, it should be interesting to apply the EPMC to SU(2) lattice thereby. Formally, one could still checkerboard the Hamiltonian, which has the same structure as Eq. (7):¹²

$$H_{\rm SU(2)} = \frac{g^2}{2a} \left[\sum_{\rm links} E^2 - \frac{2}{g^4} \sum_{\rm plaq} {\rm Tr} u u u u + {\rm H.c.} \right]$$

 E^2 is the Casimir operator for SU(2), and $u_{n,\nu} = \exp[igaT^{\alpha}A_{n,\nu}^{\alpha}]$. Unfortunately, satisfying the requirements of gauge invariance is much more difficult for SU(2) than for U(1). The eigenstates of the electric field operator are rotation matrices, and satisfying Gauss's law at a site for a *d*-dimensional theory involves coupling up to 2*d* angular momenta together, a forbidding prospect, to say the least.

We have been able to study the roughening transition in three-dimensional U(1) gauge theory; of immediate interest is the investigation of this phenomenon in non-Abelian gauge theories, where it has also been shown to exist (see Refs. in I). Recently, Fukugita and Niuya¹³

have numerically investigated the coupling behavior of the string width in Euclidean SU(2) theory. Although they have been able to study the width below the roughening point, the small size of their Wilson loops have prevented them from seeing the transition itself. More work needs to be done on this subject.

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