GREEN’S FUNCTION MONTE CARLO APPROACH TO SU(3) YANG-MILLS THEORY IN (3+1)D

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A ‘forward walking’ Green’s Function Monte Carlo algorithm is used to obtain expectation values for SU(3) lattice Yang-Mills theory in (3+1) dimensions. The ground state energy and Wilson loops are calculated, and the finite-size scaling behaviour is explored. Crude estimates of the string tension are derived, which agree with previous results at intermediate couplings; but more accurate results for larger loops will be required to establish scaling behaviour at weak coupling.

1 Introduction

Classical Monte Carlo simulations provide a very powerful and accurate method for the study of Euclidean lattice gauge theories. In the Hamiltonian formulation, on the other hand, the corresponding quantum Monte Carlo methods have been somewhat neglected. Here we present a study of SU(3) Yang-Mills theory in (3+1) dimensions, using the Green’s Function Monte Carlo approach.

Heys and Stump\cite{ref1} and Chin et al.\cite{ref2} pioneered the use of “Green’s Function Monte Carlo” (GFMC) or “Diffusion Monte Carlo” techniques in Hamiltonian LGT, in conjunction with a weak-coupling representation involving continuous gauge field link variables. This was successfully adapted to non-Abelian Yang-Mills theories\cite{ref3,ref4} with no minus sign problem arising. In this representation, however, one is simulating the wave function in gauge field configuration space by a discrete ensemble or density of random walkers: it is not possible to determine the derivatives of the gauge fields for each configuration, or to enforce Gauss’s law explicitly. the ensemble always relaxes back to the ground state sector. In order to compute the string tension or mass gap, one must measure an appropriate correlation function, and estimate the mass gap as the inverse of the correlation length. We have introduced the ‘forward-walking’ technique, well-known in many-body theory\cite{ref5} to measure the expectation values and correlation functions. The technique has been demonstrated for the cases of the transverse Ising model in (1+1)D\cite{ref6} and the U(1) LGT in (2+1)D\cite{ref7}.

Here we apply the technique for the first time to a non-Abelian model, namely SU(3) Yang-Mills theory in (3+1)D. The ground state energy and Wilson loop values are calculated, and approximate values are extracted for the string tension in the weak-coupling regime. Comparisons are made with
earlier calculations, where they are available.

2 Method

2.1 Lattice Hamiltonian

The Green’s Function Monte Carlo formalism has been adapted to SU(2) Yang-Mills theory by Chin, van Roosmalen, Umland and Koonin, and sketched for the SU(3) case by Chin, Long and Robson.

The SU(3) lattice Hamiltonian is given by

\[ H = \frac{g^2}{2a} \left\{ \sum_l E_l^a E_l^a - \frac{\lambda}{3} \sum_p Tr(U_p + U_p^\dagger) \right\} \] (1)

where \( E_l^a \) is a component of the electric field at link \( l \), \( \lambda = 6/g^4 \), the index \( a \) runs over the 8 generators of SU(3), and \( U_p \) denotes the product of four link operators around an elementary plaquette. We will work with the dimensionless operator

\[ H = \frac{1}{2} \sum_l E_l^a E_l^a - \frac{\lambda}{6} \sum_p Tr(U_p + U_p^\dagger) \] (2)

The link variables are elements of the group SU(3) in the fundamental representation

\[ U = \exp(-i \frac{1}{2} \lambda^a A^a) \] (3)

2.2 Green’s Function Monte Carlo method

The Green’s Function Monte Carlo method employs the operator \( \exp(-\tau(H - E)) \), i.e. the time evolution operator in imaginary time, as a projector onto the ground state \( |\psi_0\rangle \):

\[ |\psi_0\rangle \propto \lim_{\Delta \tau \to 0, N \Delta \tau \to \infty} \exp(-N\Delta\tau(H - E))|\Phi\rangle \] (4)

where \( |\Phi\rangle \) is any suitable trial state. To procure some variational guidance, one performs a “similarity transformation” with the trial wave function \( \Phi \), and evolves the product \( \Phi|\psi_0\rangle \) in imaginary time. The heart of the procedure is the calculation of the matrix element corresponding to a single small time step \( \Delta \tau \). Chin et al.\[4\] show that

\[ \langle x'|\Phi e^{-\Delta\tau(H-E)}\Phi^{-1}|x\rangle = \prod_l \langle U_l' | N \left\{ \exp(-\frac{1}{2}\Delta\tau E_l^a E_l^a) \exp[\Delta\tau E_l^a (E_l^a \ln \Phi)] \right\} |U_l \rangle \]

\[ \exp\{\Delta\tau[E - \Phi^{-1}H\Phi(x)]\} + O(\Delta\tau^2) \]

\[ \equiv p(x', x)w(x) + O(\Delta\tau^2) \] (5)
where $\mathbf{x} = \{U_l\}$ denotes an entire lattice configuration of link fields.

The product $\Phi|\psi\rangle$ is simulated by the density of an ensemble of random walkers. At the kth step, the ‘weight’ of each walker at $x_k$ is multiplied by $w(x_k)$. The effect of $p(x_{k+1}, x_k)$ is to alter each link variable $U_l$ in $\{X_k\}$ to $U'_l$ by a Gaussian random walk plus a “drift step” guided by the trial wave function:

$$U' = \Delta U U_d U \tag{6}$$

where $U_d = \exp[i \frac{1}{2} \lambda^a (i \Delta \tau E^a \ln \Phi)]$ is the drift step, and $\Delta U$ is an SU(3) group element randomly chosen from a Gaussian distribution around the identity, with variance $\langle \Delta s^2 \rangle = 8 \Delta \tau$ (i.e. $\Delta \tau$ for each index $a$), where

$$\langle \Delta s^2 \rangle \approx \sum_a A^a A^a = 8 \Delta \tau, \tag{7}$$

for small $A^a$.

The simulation is carried out for a large number of iterations $\Delta \tau$, until an equilibrium distribution $\Phi|\psi_0\rangle$ is reached. The energy $E$ in (5) is adjusted after each iteration so as to maintain the total ensemble weight constant. The average value of $E$ can then be taken as an estimate of $E_0$, the ground-state energy.

As time evolves, the weights of some walkers grow larger, while others grow smaller, which would produce an increased statistical error. To avoid this, a “branching” process is employed, whereby a walker with weight larger than some threshold is split into two independent walkers, while others with weights lower than another threshold are amalgamated.

### 2.3 Trial Wave Function

The trial wave function is chosen to be the one-parameter form

$$\Phi = \exp[\alpha \sum_p Tr(U_p + U_p^\dagger)] \tag{8}$$

Then the drift step for each link is

$$U_d = \exp[-i \frac{\lambda^a}{2} A^a_l], \tag{9}$$

$$A^a_l = -i \Delta \tau \frac{\alpha}{2} \sum_{p \in l} Tr[\lambda^a U_p U_p^\dagger - h.c.] \tag{10}$$

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Finally, the trial energy factor is

\[ \Phi^{-1} H \Phi = \sum_{l} \left\{ \frac{\alpha^2}{8} \left( \sum_{p \in l} \text{Tr}[\lambda^a U_l U_l^\dagger - h.c.] \right)^2 + \left( \frac{2\alpha}{3} - \frac{\lambda}{24} \right) \sum_{p \in l} \text{Tr}(U_p + U_p^\dagger) \right\} \].

(11)

(12)

2.4 Forward Walking estimates

The “forward walking” technique is used to estimate expectation values. Its application to the U(1) lattice gauge theory in (2+1)D was discussed by Hamer et al. It is implemented for an operator Q (assumed diagonal, for simplicity) by recording the value \( Q(x_i) \) for each “ancestor” walker at the beginning of a measurement; propagating the ensemble as normal for \( J \) iterations, keeping a record of the “ancestor” of each walker in the current population; and taking the weighted average of the \( Q(x_i) \) with respect to the weights of the descendants of \( x_i \) after the \( J \) iterations, using sufficient iterations \( J \) that the estimate reaches a ‘plateau’.

3 Results

Simulations were carried out for \( L \times L \times L \) lattices up to \( L=8 \) sites, using runs of typically 4000 iterations and an ensemble size of 250 to 1000 depending (inversely) on lattice size. Time steps \( \Delta \tau \) of 0.01 and 0.05 “seconds” were used, with each iteration consisting of 5 sweeps and 1 sweep through the lattice, respectively, followed by a branching process. The first 400 iterations were discarded to allow for equilibration. The data were block averaged over blocks of up to 256 iterations, to minimize the effect of correlations on the error estimates.

The results taken at \( \Delta \tau = 0.01 \) and \( \Delta \tau = 0.05 \) were extrapolated linearly to \( \Delta \tau = 0 \). The variational parameter \( c \) was given values as used by Chin et al., obtained from a variational Monte Carlo calculation. We checked that these were approximately the optimum values for small lattices.

Forward-walking measurements were taken over \( J \) iterations, where \( J \) ranged from 20 to 100, depending on the coupling \( \lambda \). Ten separate measurements were taken over this time interval, in order to check whether the value measured by forward-walking had reached equilibrium. A new measurement was started soon after the previous one had finished.
3.1 Ground-state Energy

The dependence of the ground-state energy per site on lattice size is illustrated in Figure 1, at two fixed couplings $\lambda = 3.0$ and $\lambda = 5.0$. In the “strong-coupling” case, $\lambda = 3.0$, it can be seen that the results converge exponentially fast in $L$, whereas in the “weak-coupling” regime, $\lambda = 5.0$, the convergence is more like $1/L^4$ at these lattice sizes. This behaviour merits some further explanation.

A similar phenomenon occurs in the case of the U(1) theory in (2+1)D. In the strong-coupling regime, where the mass gap is large, the usual exponential convergence occurs. In the weak-coupling regime, however, where the mass gap $M$ is very small, the finite-size scaling behaviour for small lattice sizes is that of a massless theory, and it is only at much larger lattice sizes $L \approx 1/M$ that a crossover to exponential convergence occurs. An “effective Lagrangian” corresponding to free, massless gluons (non-interacting QCD) should describe the finite-size behaviour in the present case, in line with the idea of asymptotic freedom. By analogy with the (2+1)D case, we expect a $1/L^4$ dependence for the corrections to the ground-state energy per site. We hope to pursue this analysis further at a later date.

An anomalous feature in Figure 3b) is that the $L = 8$ point lies well out of line with the others. This occurs at other couplings also. We suspect that the results for $L = 8$ are not reliable, and that the trial wave function will have to be further improved to give reliable results for such large lattices.

We have made estimates of the bulk limit, extrapolating mainly from the smaller $L$ values where possible. The estimates for the bulk ground-state energy per site are graphed as a function of coupling in Figure 2, where they are compared with previous estimates obtained by an ‘Exact Linked Cluster Expansion’ (ELCE) procedure, and with the asymptotic weak-coupling series. The Monte Carlo results agree very well with the ELCE estimates, and appear to match nicely onto the expected weak-coupling behaviour for $\lambda \geq 6$.

3.2 Wilson Loops

The forward-walking method was used to estimate values for the $m \times n$ Wilson loops, $W(m, n)$. A graph of the ‘mean plaquette’ $W(1, 1)$ versus the variational parameter $c$ is shown in Figure 3. A problem is immediately apparent. The estimate for $W(1, 1)$ is not independent of $c$, in fact it depends linearly on $c$ over this range, and the size of the variation is such that the probable systematic error due to the choice of $c$ is an order of magnitude larger than the random statistical error in the results. Thus it would be advantageous in future studies to put more effort into improving the trial wave function, rather than merely
improving the statistics.

The finite-size behaviour for the Wilson loops is similar to that of the ground-state energy. The estimates for the mean plaquette in the bulk limit are graphed as a function of coupling $\lambda$ in Figure 4, and compared with series estimates at strong and weak coupling. The agreement is quite good.

### 3.3 String Tension

Having obtained estimates for the Wilson loop values on the bulk lattice, one can extract estimates for the ‘spacelike’ string tension using the Creutz ratios:

$$K a^2 \simeq R_n = -\ln \left( \frac{W(n, n)W(n - 1, n - 1)}{W(n, n - 1)^2} \right)$$

The results are shown in Figure 5. Also shown in Figure 5 are some previous estimates derived from the ‘axial’ string tension, obtained using an ‘Exact Linked Cluster Expansion’ (ELCE) method. The axial string tension $aT$ is calculated as an energy per link, and must be converted to a dimensionless, ‘spacelike’ tension by dividing by the ‘speed of light’ $c$. We have also used the weak-coupling relationship between the scales of Euclidean and Hamiltonian lattice Yang-Mills theory calculated by Hasenfratz et al to plot the results against the Euclidean coupling $\beta = 6/g_E^2$.

It can be seen that the present GFMC results are in rough agreement with the axial string tension results in the region $4 \leq \beta \leq 5$, which is also the region where the ‘roughening’ transition occurs in the string tension. For $\beta > 5$, however, the Creutz ratio $R_2$ runs above the ELCE estimate, and shows no sign of the expected crossover to an exponentially decreasing scaling behaviour at $\beta \simeq 6$. We presume that this is a finite-size effect, and that the Creutz ratios $R_n$ for larger $n$ will show a substantial decrease in the ‘weak-coupling’ regime $\beta \geq 6$. That is certainly the pattern seen in the Euclidean calculations, or in the $U(1)_{2+1}$ model. Unfortunately, however, our present results for the larger Wilson loops are not of sufficient accuracy to allow worthwhile estimates of $R_n$ for $n \geq 2$.

### 4 Conclusions

Some significant problems with the GFMC method have emerged from this study. The ‘forward-walking’ technique was introduced specifically to avoid any variational bias from the trial wave function. As it turns out, however, the results for the Wilson loops show a substantial dependence on the trial wave function parameter $c$. The systematic error due to this dependence is
an order of magnitude larger than the statistical error, so it would pay to put
more effort in future studies into improving the trial wave function, rather
than simply increasing the statistics. Furthermore, the effective ensemble size
decreases during each measurement as the descendants of each ‘ancestor’ state
die out, and this produces a substantial loss in statistical accuracy at weak
coupling, as well.

It would be preferable if one were able to do away entirely with all the
paraphernalia of trial wave function, weights, branching algorithms, etc, and
just rely on some sort of Metropolis-style accept/reject algorithm to produce
a correct distribution of walkers. Within a quantum Hamiltonian framework,
a way is known to do this, namely the Path Integral Monte Carlo (PIMC)
approach. We conclude that the PIMC approach may be better suited than
GFMC to the study of large and complicated lattice Hamiltonian systems.

Acknowledgments

This work is supported by the Australian Research Council. Calculations
were performed on the SGI Power Challenge Facility at the New South Wales
Centre for Parallel Computing and the Fujitsu VPP300 vector machine at the
Australian National University Supercomputing Facility: we are grateful for
the use of these facilities.

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Figure 1: Ground-state energy per site graphed against $1/L^4$, where $L$ is the lattice size: a) at coupling $\lambda = 3.0$, b) at coupling $\lambda = 5.0$. The lines are merely to guide the eye.

Figure 2: The bulk ground-state energy per site graphed against coupling $\lambda$. The points are our Monte Carlo estimates; the solid line represents earlier ELCE estimates[19]; and the dashed line represents the asymptotic weak-coupling behaviour.

Figure 3: Estimated value for the mean plaquette $W(1,1)$ as a function of the variational parameter $c$, for $L = 6, \lambda = 5.0$. 
Figure 4: The mean plaquette $W(1,1)$ for the bulk system graphed against coupling $\lambda$. The solid line represents the strong-coupling series expansion [19], and the dashed line the asymptotic weak-coupling behaviour.

Figure 5: The string tension $K\alpha^2$ graphed against coupling $\beta$. The circles are obtained from ELCE estimates of the axial string tension [19]; the triangles are Monte Carlo estimates of $R_2$. 