Current Status of the Numerical Simulations of d=3 SU(2) Lattice Gauge Theory in the Dual Formulation.

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We have continued our systematic investigations of the numerical simulations of lattice gauge theories in the dual formulation. These include: i) a more practical implementation of the quasi-local updating technique, ii) a thorough investigation of the sign problem, iii) issues related to the ergodicity of the various update algorithms, iv) a novel way of measuring conventional observables like plaquette in the dual formalism and v) investigations of thermalisation. While the dual formulation holds out a lot of promises in principle, there are still some ways to go before it can be made into an attractive alternative lattice formulation.

1. INTRODUCTION

We are reporting on our continuing investigations of SU(2) lattice gauge theory in the dual formulation. A brief introduction to the formalism as well as to the techniques that have been developed for numerical simulations was presented at LATTICE’99 [1]. As was stated there, the partition function of the conventional LGT can be converted, upon using the techniques of character expansion and group integrations, into the dual form [2] (for another perspective on this issue see [3]):

\[ Z_d = \sum_{\{j\}} \prod (2j + 1) C_{ja} (\beta) \prod_{i=1}^{5} \left\{ a_i \ b_i \ c_i \ d_i \ e_i \ f_i \right\} \] (1)

This partition sum is defined over the dual lattice where \(\{ja\}\) live over the links and \(\{jb\}\) over the diagonals to the plaquettes. The convention for the diagonals is that they connect the vertices of the odd sublattice. We have collectively designated \(\{ja\}\), \(\{jb\}\) by \(\{j\}\). Each cube of the dual lattice is seen to be spanned by 5 tetrahedra of which one is spanned entirely by \(\{jb\}\) while four are spanned by three \(\{ja\}\) and three \(\{jb\}\). These features are illustrated in fig.1 which exhibits a two-cube cell on the dual lattice. The b-links are shown by dashed lines while the a-links are shown by solid lines. Each tetrahedron carries a weight factor which is the SU(2) 6-j symbol \(\left\{ a \ b \ c \ d \ e \ f \right\}\).

Periodic b.c for the original lattice is crucial for this construction.

One immediate advantage of the dual approach is that variables are now discrete and for all practical purposes can be represented by short integers. Other advantages of this method have already been commented upon in [1].

1.1. Conventional Observables

Usually when one goes to the dual description, observables in the original formulation become very complicated in the dual picture and vice versa (for a discussion of the Wilson loop in the dual picture see [3]). It is therefore curious to see that, in the present context, a whole class of conventional observables are just as easily measured in both the formulations. In the conventional formulation, the expectation value of the normalized plaquette is given by

\[ \langle P \rangle = \frac{1}{N_p} \frac{\partial \log Z(\beta)}{\partial \beta} \] (2)

where \(N_p\) is the number of plaquettes in the lattice. In the dual picture it can be easily verified...
that this expectation value is given by
\[ < P > = \langle \frac{d \log C_j(\beta)}{d\beta} \rangle \] (3)
where the average on the r.h.s is over the distribution of \( j \)-values on the a-links of the dual lattice. This formula can be generalized to the case of any function of the plaquette variable and more importantly to the two-point correlation functions of plaquettes or of functions of plaquette variables. This allows for a direct comparison between the dual and the conventional pictures.

2. UPDATES

In [1] we introduced two types of updating algorithms: local and quasi-local. It was already pointed out there that the local updates are not ergodic as they are unable to change integer spins to non-integer spins and vice versa. We illustrate the local update algorithm with the help of fig.1.

Figure 1. Illustrating the local updates.

The b-link shown as a dotted line is contained in 6 tetrahedra (two of them containing only b-links); it is also contained in 6 triangles again two of which contain only b-links. For each triangle containing this link, one forms \( j_{max}^i = j_1^i + j_2^i \) and \( j_{min}^i = |j_1^i - j_2^i| \) where \( j_{1,2}^i \) are the remaining two spins in the \( i \)-th triangle containing the link to be updated. One then forms \( j_{max} = \min_i \{j_{max}^i\} \) and \( j_{min} = \max_i \{j_{min}^i\} \) and updates the link to a value in the range \((j_{min}, j_{max})\). Clearly this does not change half-integers to integers and vice versa and the move is not ergodic by itself.

In addition to the problem of ergodicity, there are two additional problems with this method. Every now and then one may face a situation where \( j_{min} = j_{max} \) in which case the move can not change the value of the link. Our code keeps track of this possibility through a counter \texttt{irange} and whenever this happens one skips the particular site and moves on to the next one. The other problem has to do with the fact that \( 6j \)'s occasionally vanish even when all the triangle relations hold. Very rarely it so happens that every new value of the link is such that the product of \( 6j \)'s over the tetrahedra (four in the case of local updates of a-links and six in the case of b-links) vanishes and the new configuration is to be eliminated because it does not contribute to either the partition sum or to any of the expectation values. This is kept track of by the counter \texttt{ispecial}.

2.1. Quasi-local Updates

As already discussed in [1], if we were to change a link from half-integer (henceforth referred to as fermionic) to integer (bosonic) or vice versa, in general the change proliferates throughout the lattice as at least two links have to be \( Z_2 \)-flipped in every triangle. What one needs are flippings involving the smallest cluster of links. Two categories of such quasi-local updates were identified in [1]. At an even site of the lattice, the update algorithm called \texttt{globeven} involves the interior links of a cluster of 8 tetrahedra as shown in fig.2. Likewise, at odd sites the corresponding update is

Figure 2. Quasi-local updates at even sites.
called *globodd* and it involves the 6 a-links and 12 b-links in the interior of the 8-cube cluster involving 32 tetrahedra as shown in fig.3. In both these schemes of quasi-local updates, one keeps all the links on the outer surface fixed and $Z_2$-flips all the interior links. The changes should be so made as to satisfy all the triangle inequalities. In [1], the basic idea of achieving this goal was briefly mentioned. This is done using variables originally introduced by Bargman [3] and developed by [4]. This will be discussed in detail in [7]. While this method based on the K(agency)-variables is the systematic approach to the quasi-local updates, it is pretty involved and time consuming. A simplified algorithm was proposed in [1] which consisted of simply shifting all spin values on the interior links by $\frac{1}{2}$ which can be seen to preserve all the triangle inequalities. But this can result in substantial changes in the Boltzman weight resulting in abrupt changes. In the current investigations we modified this by following the fixed $Z_2$-flip by randomly selecting a set of configurations satisfying the triangle inequalities and then performing heatbath or metropolis in the subspace of these configurations.

3. THE SIGN PROBLEM

It was already emphasised in [1] that one of the main drawbacks of the dual formulation is the lack of positivity of the Boltzman weight which arises out of the 6j’s not being of a particular sign. There we had proposed to use the trick of generating important samples with probabilities that are the modulus of the weights occurring in eqn (1) but by absorbing the sign of the configuration into the observables. It was soon pointed out to us by Wosiek [6] that no matter how small the local probability of a wrong sign, in the thermodynamic limit there will be an almost equal fraction of configurations with the two signs. This meant that the average value of the sign is very close to zero making the procedure questionable. One way out is to regroup the terms in eqn(1) so that for each group the weight is positive. But it is not clear how to do this. To make some progress we decided to adopt another strategy based on the fact that sign changes in the configurations come about through completely local sources. To see this, let us look at the expression for the average of a generic observable $O$:

$$\langle O \rangle_p = \frac{\langle O \epsilon \rangle_{\tilde{p}}}{\langle \epsilon \rangle_{\tilde{p}}}$$

where $\{\tilde{p}_i = |p_i|\}$ with $P = \sum_i |p_i|$ and $p_i$ are the weights occurring in eqn(1) and are not necessarily positive. Further, $\epsilon_i$ is the sign of $p_i$. Now if it so happens that when thermal equilibrium is reached the average value of $O$ (in the usual sense) is insensitive to the sign of the configuration in the sense that the average over positive sign configurations is very close to the average over negative sign configurations, the numerator in eqn(4) is also proportional to $\langle \epsilon \rangle_{\tilde{p}}$ and we can simply ignore the sign problem.

We wish to argue that this is very likely to happen for relatively local observables and also for the correlation functions of relatively local observables. The reason for this is the fact that the source for the change of sign of the configuration is ultralocal. Combining this with the expectation that both signs become equally likely as the system size increases, one is led to surmise that the configurational average of reasonably local observables as well as the correlation functions of reasonably local observables are insensitive to the sign of the configuration. So far most of our runs have borne out this expectation. We found that whenever there was a reasonable fraction of configurations with each sign, the averages of in-
ner and outer tetrahedra were indeed insensitive to the sign in the limit of thermalisation (to be more precise, in the limit of nearly stationary expectation values). We are investigating this with other classes of observables. We also propose to make a systematic study of the sign problem by studying the way the signs fluctuate locally as well by studying their correlations over the lattice.

4. METROPOLIS AND HEATBATH

For the local updates both the metropolis and heatbath methods work in fairly standard ways because the allowed range of values for the new link are very small. But for the quasi-local moves the situation is quite different. Even in the case of the quasi-local updates at even sites, we are dealing with the space of allowed spin values on six links. Truncating the maximum value of spins at $\frac{9}{2}$ as we did, we have $10^6$ values to check for triangle inequalities and subsequently picking a new element from among the list. This is a hopeless task. Even using the K-variable method\[7\] is time consuming. So what we did was to apply the fixed $Z_2$-flip and select the first a-link randomly from its allowed possibilities, the second a-link randomly from its allowed values (which depends on the random choice made for the first a-link) and so on. For metropolis algorithm, after selecting a sextuplet of values, the new set was accepted or rejected according to the usual metropolis rule. For the heatbath method we likewise selected a certain number of sextuplets before the $Z_2$-flip and an equal number after the flip. The heatbath algorithm was then applied to this manageable subset. At present we do not have a more rigorous argument to justify our heatbath method. For the globodd update the problems are even more severe and we have again adopted the same pragmatic approach.

4.1. INITIAL CONFIGURATIONS

As initial configurations we chose from among three classes: i) cold start - here we set all the a-links and b-links to $j = 1$. This configuration clearly satisfies all the triangle inequalities. ii) extreme cold start - here all a-links and b-links were set equal to $j = 0$. It is worth noting that the extreme cold start configuration is a fixed point of the local update algorithms. iii) hot start - here a-links and b-links are randomly chosen in a way that all triangle inequalities are satisfied. A practical way of reaching such configurations is to first start with a cold start configuration and go on choosing links randomly in their allowed ranges. After sweeping the lattice sufficiently many times one gets to a hot start configuration.

5. RESULTS

We carried out our simulations on a $8^3$ lattice at various $\beta$-values. We simulated with the absolute values of the weights given by eqn(1) and monitored the fluctuations in the sign of the configurations. In a few runs we noticed that the sign changed very few times. In those cases, the average values of the inner (outer) tetrahedra for the positive sign and negative sign configurations did not approach the same values even after many iterations. But for these cases $\langle \epsilon \rangle \tilde{p}$ is not close to zero and one can safely use eqn (4). On the other hand for a majority of runs, the sign fluctuated quite a bit and even when $\langle \epsilon \rangle \tilde{p} \simeq 0.5$, the average values for the two cases were very close to each other bearing out the surmise made earlier. This was so for all the classes of update algorithms, initial states and metropolis/heatbath. We plan to study this issue for a larger class of observables.

In our simulations using only the local updates, we found that while the results of metropolis and heatbath converged for given initial states, the results did not converge for trials with different initial states. We have interpreted this as due to the non-ergodic nature of the local updates. The results for the quasi-local updates were not so clear cut. We also ran the code with the updating algorithms being chosen randomly; at the first instance we have run the code such that all updating algorithms are equally likely. Here we find that while the runs for the cold-start and hot-start converged, the results for metropolis and heat bath are widely divergent. We have not really understood the reason for this.
6. CONCLUSION

Clearly a lot more work needs to be done before establishing the dual framework as a viable alternative for numerical simulations of Gauge and Spin systems. The most pressing problem is to gain a satisfactory understanding and control of the sign problem. While our surmise in this direction is well borne out by the initial runs, we are yet to show its correctness in a controlled manner. One interesting possibility is to study the model defined by the absolute value of weights in its own right and we plan to undertake that study shortly. But we still have to understand the lack of convergence between the different runs before we can take any of the conclusions seriously. To this end, we are going to investigate the efficacy of our metropolis and heat bath methods by studying them in contexts where we can get results by deterministic as opposed to stochastic methods.

Another line of attack we are contemplating is to look for simple models that are analytically tractable but which nevertheless have all the essential ingredients of the dual formulation studied here. Indeed, such models were encountered in the study of analytic variational methods for euclidean lattice gauge theories [8] and in the analytic evaluation of the partition function of the unit hypercube for $d = 4$ SU(2) lattice gauge theories [9]. We are hoping that the insights so gained will enable us to complete the investigations reported here.

There are a large class of very important problems that belong to the same calculational scheme as what we have attempted here. The most notable are: the $d = 4$ version of these results as obtained by Halliday and Suranyi [10], the class of models considered by Ooguri [11] and their non-topological descendants etc. Language and techniques very similar to the ones used in the dual picture are also becoming increasingly popular in treatments of quantum gravity [12]. Replacing the 6j’s by q-deformed 6j’s would immediately relate these developments to the well known Turaev-Viro models and their generalizations. Clearly it is of great importance to make further progress in the numerical simulations of theories in the dual formulation.

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REFERENCES

1. N.D. Hari Dass, Proceedings of the XVIIth International Symposium on Lattice Field Theory, Nucl. Phys. B (Proc.Suppl.) 83-84(2000) 950 - 952.
2. R. Anishetty, Srinath Cheluvaraja, H.S. Sharatchandra and Manu Mathur, Phys. Letts. B 314 (1993) 387.
3. V. Bargman, Reviews of Modern Physics, Vol 34, Number 4, October 1962.
4. R. Anishetty, G.H. Gadiyar, Manu Mathur and H.S. Sharatchandra, Phys. Letts. B 271(1991) 391.
5. Robert Oeckl and Hendryk Pfeiffer, The dual of the pure non-Abelian lattice gauge theory as a spin foam model, hep-th/0008097.
6. J. Wosiek, Private Communication.
7. N.D. Hari Dass, in these proceedings.
8. N.D. Hari Dass and P.G.Lauwers, Nucl. Phys. B235 (1984) 535.
9. N.D. Hari Dass, On the Analytic Evaluation of the Partition Function of an Unit Hypercube in 4 Dimensions, NIKHEF 12/1984.
10. I. Halliday and P. Suranyi, Phys. Letts. B 350(1995) 189.
11. H. Ooguri, Mod. Phys. Letts. A7(1992) 2799.
12. J.C. Baez, An introduction to Spin foam models, gr-qc/9905082.