Analytic Variational Investigation of Euclidean SU(3) Gauge Theory

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Analytic variational techniques for lattice gauge theories based on the Rayleigh-Ritz (RR) method were previously developed for euclidean SU(2) gauge theories in 3 and 4 dimensions. Their extensions to SU(3) gauge theory including applications to correlation functions and mass gaps are presented here.

1. Introduction

Despite impressive strides made in the Monte Carlo (MC) studies of lattice gauge theories, a satisfactory understanding of the wavefunctionals of these theories is still lacking. Motivated by the success of variational methods of quantum mechanics in addressing such issues, a program of developing these methods for lattice systems was undertaken. At first these methods were applied to spin systems, both discrete and continuous, in two dimensions, with success. Subsequently, the much harder problem of applying these methods to 4-dimensional gauge theories was undertaken and successfully solved for the case of U(1) and SU(2) gauge theories. Details of these and other related works along with the relevant references can be obtained from [1].

The basic idea is to apply the RR technique to the spectrum of the transfer matrix, denoted symbolically by $T$. One makes an ansatz for the largest eigenvalue state guided by the usual intuitions of nodelessness, symmetry etc.

The simplest such ansatz for a lattice gauge theory is

$$\psi = \exp(\alpha \sum Retr P_i)$$

where $P_i$ are the relevant plaquette variables lying on a “time” slice with tr being taken over some irr. of the group, and $\alpha$ a variational parameter. Recall that $T$ connects configurations on neighbouring time slices. The estimate for the largest eigenvalue is then given by

$$\Lambda_0 = \max_\alpha (\psi, T\psi)/(\psi, \psi)$$

(2)

The denominator in (2) is the partition function of a 3-dimensional theory with coupling $2\alpha$, while the numerator can be interpreted as the partition function of a generalised 3-dimensional theory where the links per site are doubled and with anisotropic couplings $\alpha + \beta/2$, $\beta$.

Our idea was to construct the appropriate transfer matrices for these lower dimensional problems and then apply the RR method to their spectra, and so on. Under the simplifying assumption justified a posteriori, that the same variational parameters are used for all the subsequent ansätze, one arrives at the variational estimate for the free energy per site of the form

$$-F_4 = \max_\alpha [F^H(\beta_H) + G(\alpha)]$$

(3)

where $F^H$ is the free energy for a 4-dimensional unit hypercube with coupling $\beta_H = 3/2\alpha + \beta/4$, while $G(\alpha)$ is expressible in terms of the norms of the various ansätze (details are given in [1]). The unit hypercube partition function as well as $G(\alpha)$ are evaluated by making use of group character expansions

$$\exp(x Retr_f(g)) = \sum d_r tr_r(g) b_r(x)$$

(4)

where $tr_i(g)$ is the character in the i-th irrep. whose dimension is $d_i$. For SU(2) $b_r(x) = I_{2r+1}(2x)/x$ where the $I_r(x)$ is a modified Bessel function. For SU(3) their analytic form is not known. $f$ corresponds to the fundamental rep.

The main result which made the analytic investigation of the SU(2) case possible is the explicit

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expression for the partition function of a unit hypercube in terms of a product of 16 SU(2) 6-j symbols. This result was obtained by generalising the graphical rules of Yutsis, Vanagas and Levinson. Symbolically expressed, this result reads
\[ e^{-F^H} = \sum d_{r_1} b_{r_1} \cdots d_{r_{24}} b_{r_{24}} \prod 6j's \]  
(5)

For SU(3), however, there are additional complications due to i) the complex nature of irreps, ii) multiplicity problems associated with weights and tensor decompositions. These are being investigated at present. However, substantial contribution to (5) comes from surfaces that only depend on \( d_i \) and the number of singlets \( N_{rst} \) contained in the tensor product of 3 irreps. Even though the latter is affected by multiplicity problems too, a programme was developed based on the elegant prescription given in [1].

In practice, the sum (5) is evaluated by finding the contribution of all possible closed surfaces that can be embedded in the unit hypercube. A complete classification of such surfaces is given in [2]. For example, each surface of area \( A \) and topology of a sphere contributes \( \sum d_i^2 b_i^A \) to (5), while each surface with area \( A \) and torus topology contributes \( \sum b_i^A \). There are, for example, 8 spheres with \( A=6 \) and 3 torii with \( A=16 \) in the unit hypercube. Likewise, surfaces obtained by gluing 3 disks of area \( A_r \), \( A_t \) and \( A_s \) in irreps \( r \), \( t \) and \( s \), contribute \( \sum N_{rst} d_i d_t d_s b_i^r b_t^t b_s^s \). More complicated surfaces require a knowledge of the 6-j symbols. The sum in the above formulae (except (5)) is only over nontrivial irreps.

The \( b_i(x) \) for SU(3) were calculated by generating their series expansions up to \( x^{100} \) using an algorithm to find the number of times the irrep \( r \) occurred in \( (f \oplus \bar{f})^n \) by a recursion relation. The resulting \( b_i \)'s were checked against a numerical evaluation of their integral representation for \( x \) as large as 10, and agreement was seen to double precision accuracy. A weak coupling expansion was also developed using the symbolic manipulation package FORM and again good agreement was seen with the series expansion.

At the moment we have restricted the sum(5) to only those surfaces for which one at most needs the \( N_{rst} \). It is encouraging (also from the point of more accurate extensions of this method) that in the range \( 0 < \beta < 2.25 \) (this corresponds to the range \( (0, 6.75) \) for the coupling used in literature) this truncation works quite well as will be shown by the results.

2. Correlation Functions And Mass Gaps

There are three classes of plaquette-plaquette correlations within the unit hypercube that are relevant for the study of mass-gaps; these are a) when the plaquettes on both the time-slice are in the same spatial plane and b) when they are in planes orthogonal to one another (this class will be called dh3). Case a) further splits into a1) when the two plaquettes can be embedded in a cube (dh2) and a2) otherwise (dh1). It is useful to factor out \( b_0(x)^{24} \) in (5) (here 0 refers to the trivial irrep) and write

\[ e^{-F^H} = 24lnb_0(x) + ln(1 + A) \]  
(6)

where \( A \) is the sum of contributions from various surfaces, examples of some having been given before, except that \( b_i \)'s in those expressions should be replaced by \( B_r = b_r/b_0 \). The average plaquette (normalised) is then given by

\[ \langle P \rangle = B_f(\beta_H) + 1/72A'(1 + A)^{-1} \]  
(7)

The connected correlation function between two given plaquettes \( P_1 \) and \( P_2 \) can be obtained as follows: let the coupling for these two be \( \beta_1 \) and \( \beta_2 \) with all other couplings being \( \beta_H \). The free energy in that case is given by

\[ e^{-F^H} = b_0(\beta_H)^{22} b_0(\beta_1) b_0(\beta_2)(1 + A(\beta_1, \beta_2)) \]  
(8)

Here \( A \) contains contributions only from surfaces in which both the plaquettes \( P_1 \) and \( P_2 \) are embedded. The connected correlation function (normalised) is given by

\[ 0 \langle P_1 P_2 \rangle = 1/9(\partial \beta_1 \partial \beta_2)(e^{-F^H})|_{\beta_1=\beta_2=\beta_H} \]  
(9)

It is clear from the above that a lot fewer surfaces contribute to the connected correlation lengths than to \( \langle P \rangle \). At low \( \beta_H \), the dominant contribution to the average plaquette is \( B_f(\beta_H) \), and
all connected correlation functions nearly vanish. Only dh2 receives contribution from one out of the 8 spheres of area 6. With increasing $\beta_H$ other surfaces start contributing and all the three classes become appreciable.

2.1. Mass Gap estimates

Having obtained a variational “ground” state $|0\rangle^t$ for the transfer matrix, we can extend the technique to obtain estimates for the lower eigenvalues and hence the mass gaps. There are some important technical differences in implementing this strategy for lattice systems as compared to quantum mechanics. We summarise these points and present the details elsewhere: a) in the variational treatment of quantum mechanical systems, the ansatz for the excited states can be chosen quite independently of the ground state ansatz. But in the RR applied to lattice theories the trial excited state functionals have to be of the form $F[\psi] = \sum \theta_r \psi_r$ with $\theta_r$ a basis for such projectors, a necessary condition for the problem determining the eigenvalues of the transfer matrix to be well defined is

$$\frac{\langle 0| T \theta_r | 0 \rangle^t}{\langle 0 | T | 0 \rangle^t} = \frac{\langle 0 | \theta_r | 0 \rangle^t}{\langle 0 | 0 \rangle^t} \quad (10)$$

Otherwise, the problem of determining the eigenvalues of $ND^{-1}$ where the matrices $N$ and $D$ are given by $N_{rs} = \left[ \theta_0 | 0 \rangle | 0 \rangle^t \right]$ and $D_{rs} = \left[ \theta_0 | r \rangle | 0 \rangle^t \right]$, becomes ill-defined in the sense that while $D_{rs}$ grows as volume in the thermodynamic limit, $N_{rs}$ grows as $vol^2$.

Situations where (10) is satisfied automatically are i) due to symmetry reasons both $\langle 0 | T \theta_r | 0 \rangle^t$ and $\langle 0 | \theta_r | 0 \rangle^t$ vanish; this happens, for example, in the X-Y model when $\theta_r$ are rotationally non-invariant. ii) when $|0\rangle^t$ is an exact eigenstate of $T$. iii) when $|0\rangle^t$ of the form $exp(\sum \mu_r \theta_r)$ where $(\mu_r)$ are determined variationally, in which case (10) are the conditions for the stationarity of $\Lambda_0$ w.r.t $(\mu_r)$.

In view of the last remark we should build the excited state projectors only out of $P$'s. Nevertheless, in the case of $SU(2)$, Wilson loops of length 6 could also be considered as it was seen that in the range of $\beta$-values of interest, (10) was satisfied quite well. But $D_{rs}$ in that case required the knowledge of 6j symbols; hence for $SU(3)$ we have restricted our attention to only plaquettes in the fundamental rep. Following standard procedure, one then constructs linear combinations of these that transform irreducibly under the cubic group. With this choice, $N$ and $D$ are already diagonal. To the accuracy considered the various cubic irreps were nearly degenerate in mass (which is not the true situation) and hence only the lowest (scalar) mass estimates will be shown in the table.

3. Results

In the strong and weak coupling ends the analysis can be carried out to yield $\alpha$ in analytic form. In the intermediate regions the analysis has to be made numerically but without MC.

The first four terms of the exact free energy in both these ends are reproduced for all gauge groups and dimensions (space-time); actually for $d=4$ the coefft of the fourth term in the weak coupling is numerically very close, but not exactly equal to, the exact result. The variational parameter $\alpha = \beta/2 + c\beta^2$ for small $\beta$ and equals 7/9$\beta$ for large $\beta$.

In the case of $SU(2)$ the average plaquette for $d=3$ was indistinguishable from high statistics MC; in $d=4$ it agreed to within 1% everywhere except the crossover region where the maximum discrepancy was about 2%. The specific heat in $d=4$ also agreed very well. The string tension and mass gap average very well up to the crossover but beyond there was a noticeable deterioration. For further details see [1]. In the mass gap estimates inclusion of operators in higher irreps. made practically no difference while there was a dramatic decrease in the mass gap when the effective dimensionality of the transfer matrices was increased. Also inclusion of larger Wilson loops improved the estimates.

In $d=3$ our variational results for $SU(3)$ looked qualitatively very much like the results for $SU(2)$ in $d=3$; there was a noticeable peak in the specific
Table 1: SU(3): Local Quantities

| $\beta_H$ | $\beta$ | $\langle P \rangle$ | $\langle P \rangle_{4}$ | $\langle P \rangle_{an}$ |
|----------|--------|------------------|-----------------|------------------|
| 0.6      | 0.6000 | 0.1138           | 0.1168          | 0.1164           |
| 1.0      | 0.9950 | 0.2028           | 0.2078          | 0.2040           |
| 1.2      | 1.1880 | 0.2501           | 0.2566          | 0.2517           |
| 1.4      | 1.3720 | 0.3012           | 0.3017          | 0.3012           |
| 1.6      | 1.5410 | 0.3512           | 0.3592          | 0.3522           |
| 1.8      | 1.6960 | 0.4019           | 0.4330          | 0.4044           |
| 2.0      | 1.8500 | 0.4586           | 0.4821          | 0.4554           |

Table 2: SU(3): Correlations and Masses

| $\beta_H$ | $\Delta h^2$ | $\Delta h^2(an)$ | Mass |
|----------|--------------|-----------------|------|
| 0.8      | -.00002      | .00006          |      |
| 1.0      | .00005       | .00018          | 5.5  |
| 1.2      | .00046       | .00041          | 4.4  |
| 1.4      | .00076       | .00078          | 4.6  |
| 1.6      | .00132       | .00121          | 3.6  |
| 1.8      | .00198       | .00148          | 4.0  |
| 2.0      | .00237       | .00129          | 4.2  |

heat curve which however was not as sharp as the one in $d=4$. Here we did not compare the results with MC data. In the weak coupling region analytical results were obtained with the help of FORM and the first four terms of the free energy density agreed with exact results. The details of this case have not been given here but will be reported elsewhere. Efforts are under way to enlarge the scope of these calculations by considering more complicated ansätze. Inclusion of fermions is also being considered.

The results for $SU(3)$ in $d=4$ are summarised in two tables. A two-fold check with MC was performed. The first of these consisted in simulating the unit hypercube itself; the ‘infinite’ lattice was simulated on a $4^4$ lattice. One noticed that when $\beta_H$ was small there was no appreciable difference between $\langle P \rangle$ obtained by the two simulations. But as $\beta$ increased there was a considerable difference between them. But when the $\langle P \rangle$ of the hypercube simulation at $\beta_H$ was compared with that of the 4-site simulation at $\beta$, there was very good agreement. This can be viewed as a MC realisation of the method described here.

On the other hand, since in our $SU(3)$ studies we have not been able to include all the possible surfaces in (5), the MC of the hypercube served as a check on the accuracy of the analytical results represented by $\langle P \rangle_{an}$ in table 1 and by $\Delta h^2(an)$ in table 2. The hypercube MC was performed with 50,000 sweeps each. The tables show that as far as $\langle P \rangle$ is concerned, upto $\beta \sim 2.25$ the RR estimate is very good. Comparison of the connected correlations is trickier; at low $\beta$ these are very very small and MC is unable to measure them reliably. At larger $\beta$, however, the error in $\langle P \rangle_{an}$ becomes significant due to the neglect of many surfaces in (5). Thus reliable comparison can be made only in the window (1.2-2.2) which fortunately covers the interesting range. But even in this range only $\Delta h^2$ could be sensibly compared.

3.1. Future Prospects

From the behaviour of the mass gap in both $SU(2)$ and $SU(3)$ cases it is clear that the ansatz (1) works very well for local quantities like $\langle P \rangle$ but in the region close to the crossover it is not so efficient in describing long distance correlations. On the other hand this was the simplest ansatz one could have considered and it is surprising that it worked as well as it did. It is clear that larger operators have to be included; also the weakest link in the present implementation is at the stage where the same type of ansatz was used for the 2-dim transfer matrix. But in that case the ansatz predicts strictly vanishing $d=2$ correlations (connected). Any further improvement must circumvent this. An effective way of introducing larger operators is to choose $T^n|0\rangle$ as the trial ground state. This will then involve the enumeration of surfaces embedded in larger hypercubes. This is under study.

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