The Coupled Cluster Method in Hamiltonian Lattice Field Theory

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Abstract

The coupled cluster or exp S form of the eigenvalue problem for lattice Hamiltonian QCD (without quarks) is investigated.

A new construction prescription is given for the calculation of the relevant coupled cluster matrix elements with respect to an orthogonal and independent loop space basis. The method avoids the explicit introduction of gauge group coupling coefficients by mapping the eigenvalue problem onto a suitable set of character functions, which allows a simplified procedure.

Using appropriate group theoretical methods, we show that it is possible to set up the eigenvalue problem for eigenstates having arbitrary lattice momentum and lattice angular momentum.
1 Introduction and Overview

The investigation of the eigenvalue problem for the lattice QCD Hamiltonian is considered to be an alternative to standard Lagrangian lattice Monte Carlo QCD, possibly giving new insight into the structure of such non-abelian gauge theories.

For pure SU(3) Yang-Mills theory without fermions in particular, many attempts have been made to attack the corresponding Kogut-Susskind Hamiltonian problem: for instance, there exist the strong coupling expansion, the exp(-tH) method or variational techniques. Up to now, none of these approaches could obtain results for excited states (e.g. glueball masses) comparable in control and accuracy to those within the Euclidean Monte Carlo method (there has been, however, some progress for ground states using the Greens function Monte Carlo method).

This also holds for the coupled cluster (exp S) method which attracted special attention in recent years. (Some encouraging results within this framework were obtained recently.) Here the basic idea is to incorporate manifestly the correct volume dependencies of observables by writing the ground state in the form $\psi_0 = e^S$ and putting $\psi = F\psi_0$ for excited states. The "Schroedinger" equation for the functions $S$ and $F$ can be formulated rigorously and it is tempting to define approximations by a suitable truncation of a loop space expansion of these quantities. (Some encouraging results within this framework were obtained recently.)

It is the purpose of this paper to further elucidate the structure of this coupled cluster method with the hope that the resulting insights may lead to improved calculations of the QCD spectrum.

We will concentrate our considerations on the treatment of the Kogut-Susskind Hamiltonian as the lattice regularization of an $SU(n)$ Yang Mills theory. A discussion of the full QCD and its treatment within a quenched approximation is possible, but this will be deferred to a future publication.

We now give an outline of our paper which summarizes at the same time our methods and our results.

Our basic tools will be group theoretical methods which will be introduced in section 2. The group of the link variables, the local lattice gauge group and the lattice Euclidean group will play a role.

As discussed in section 3, projection operators on representations of the lattice Euclidean group with given lattice momentum and lattice angular momentum allow one to introduce the notion of an intrinsic wavefunction related to the ground state function $S$ and to the "excitation operator" $F$.

This structure has been used in Refs. for the trivial representation; here we provide a systematic framework for general representations of the lattice Euclidean group.

The solution of the eigenvalue problem for the Kogut-Susskind Hamiltonian is then reduced to the determination of the intrinsic eigenfunctions.

For this purpose, a basis of suitable wavefunctions is needed which may be used for an expansion and which allows a computation of the relevant coupled cluster matrix elements. Within the Kogut-Susskind theory these have to be functions of the link variables which are invariant under the action of the local lattice gauge group.

The problem of setting up such a basis in an effective way is addressed in section. 4. There exist two strategies for the construction of such basis systems:

1) Choose first a basis for the functions of the individual link variables given by the standard D-functions. General polynomials of these functions with different link variables, combined with suitable $SU(n)$ coupling coefficients, form then the desired basis for the intrinsic hadron (or vacuum) wave functions. We call this set of functions the D-loop basis.
Details of this construction have been worked out in Ref.[1]. An application is the "exact linked cluster expansion" discussed in Ref.[2].

This method is limited by the necessity to handle an increasing number of $SU(n)$ coupling coefficients.

A clear merit of the procedure is that it provides an independent, orthogonal and (in the limit of increasing polynomial degree) complete basis of physical states.

2) An alternative system of physical states is provided by the set of character functions corresponding to an expansion in terms of suitable group characters. This approach was used in the recent calculations within the coupled cluster method[6, 7]. The obvious advantage here is that each term is manifestly locally gauge invariant, and no coupling with $SU(n)$ Clebsch Gordon coefficients is needed. The problem, however, is that the emerging system of wavefunctions is in general non-orthogonal and overcomplete.

In Refs.[6, 7, 8] the disease of having linear dependencies was cured with the help of a special form of the Cayley-Hamilton relation for $SU(n)$ matrices. This method, however, does not appear to be very systematic, and only calculations with wavefunctions generated from up to fourth order plaquette polynomials have been possible up to now.

In section 5 we will introduce a new procedure for working with the orthogonal and independent D-loop basis which combines the above two alternatives by constructing a suitable mapping of the character functions on the D-loop basis avoiding, however, the explicit handling of $SU(n)$ coupling coefficients. In this framework, the Cayley-Hamilton relationship in its general form is mainly used for systematically computing certain norm relations.

Our procedure relies essentially on the following observations:

1) The characteristic coupled cluster matrix elements emerge as a byproduct when the (non-orthogonal and overcomplete) character functions are set up systematically by an iteration procedure.

2) The D-loop functions can - up to a normalization factor - be uniquely characterized by the eigenvalue pattern of a certain set of commuting Casimir operators.

3) The matrix elements of these Casimir operators are computable within the character functions by the same methods which were used to set up these functions.

Diagonalizing all necessary Casimir operators in the space of character functions yields then the mapping on the D-loop states.

This solves the problem of linear dependencies among these functions by using the eigenvalue patterns of the Casimir operators and by computing the relative norms of the dependent eigenstates with the Cayley Hamilton relation.

The final calculations are in this way reduced to a calculation of the Kogut-Susskind eigenvalue problem within the D-loop basis expansion.

We hope that this will allow future numerical Hamiltonian lattice QCD calculations which may go to higher order than the previous attempts[6, 7, 8, 9].

Also, our procedure yields a natural truncation prescription for the corresponding coupled cluster equations because the D-loop basis is orthogonal and unique.

Some details of a computational strategy are described in section 6.

2 Group Theoretical Structures

We shall first give the definitions and notations for the $SU(n)$ lattice Yang-Mills theory, especially its group theoretical content.

The general framework was given by Kogut and Susskind[1]. Accordingly, one has to define
a Hilbert space $\mathcal{H}$ given by the set of “top” wave functions depending on $N$ link variables

$$\mathcal{H} = \{\Psi(U_1, .. U_N)\}$$

(1)

where the quantities $U_l$ ($l = 1, .. , N$) are elements of the gauge group $SU(n)$ and $N$ is the number of oriented links in a D-dimensional lattice (D is the number of space dimensions).

As in thermodynamics we shall work with a finite volume, i.e. with a finite lattice, for definiteness. However, our computational framework allows one to take an infinite volume limit ($N \to \infty$) at any later stage.

The scalar product is given by an $N$-fold Haar measure integral.

The group theoretical nature of the link variables $U_l$ gives us a natural orthogonal and complete basis of $\mathcal{H}$ all $N$-fold products of $SU(n)$ D-functions, e.g. for $SU(2)$ we have the functions

$$D_{j_1 m_1}^{j_2 m_2} (U_1) D_{j_3 m_3}^{j_4 m_4} (U_2) .. D_{j_N m_N}^{j_N' m_N'} (U_N)$$

(2)

The group of (time independent) local lattice gauge transformations is abstractly given by

$$G_{loc} = [SU(n)]^M$$

(3)

where $M$ is the number of sites of the lattice.

Elements of $G_{loc}$ are written as $g = g(x)$ where $x$ denotes any lattice site. A unitary representation of $G_{loc}$ on $\mathcal{H}$ is then given by

$$(\rho(g) \Psi)(U_1, .. U_N) = \Psi(U_1^g, .. U_N^g)$$

(4)

where the link variables are transformed like parallel transporters:

$$U_i^g = g(x) U_l g^{-1} (x + \epsilon e_j)$$

(5)

if the link $l = (x, e_j)$ connects the sites $x$ and $x + \epsilon e_j$ ($\epsilon$ is the lattice spacing, $e_j$ is a positive unit vector in $j$-direction).

The physical Hilbert space is defined by the subspace of $\mathcal{H}$ corresponding to the trivial part of the decomposition of the representation $\rho$, i.e. by the gauge invariant states

$$\mathcal{H}_{phys} = \{\Psi \in \mathcal{H} | \rho(g) \Psi = \Psi \text{ for all } g \in G_{loc}\}$$

(6)

A systematic construction of a basis of $\mathcal{H}_{phys}$ generalizing Refs.[11, 7] will be the main topic of this paper and is described in section 4.

We want to impose on this basis the classification of being characterized by the irreducible representations of the lattice Euclidean group, which is a strict symmetry group of the lattice Kogut-Susskind Hamiltonian. The lattice Euclidean group is a discrete remnant of the standard continuum Euclidean group and is defined as follows:

Let

$$R_{latt}^D = \{x = \epsilon \sum_{j=1}^D n_j e_j | \ n_j = \text{integer}\}$$

(7)

be the set of lattice sites of an infinite lattice. The lattice translation group $G_{lt}$ is then isomorphic to $R_{latt}^D$ and given by the mapping of $R_{latt}^D$

$$x \to x + a$$

(8)

for any $a \in R_{latt}^D$. The lattice rotation group $G_{lr}$ is the restriction of the group $O(D)$ leaving $R_{latt}^D$ invariant. We call $G_{lr}$ the cubic group[13], it is discrete and has 8 elements for $D = 2$.
and 48 elements for \( D = 3 \). The structure of this cubic group and its representations are well known [13]. The Euclidean group \( G_E \) is then the semidirect product \( G_E = G_{lr} \otimes_s G_{lt} \) defined for \( u = (R, a) \in G_E \) by the mapping of \( R^D_{latt} \)

\[
x \rightarrow ux = Rx + a
\]  

(9)

Since the mappings \( u \) may change the orientation (i.e. it may be that \( det(R) = -1 \)), the group \( G_E \) acts on the set of links with both orientations. We use the notation \( \lambda = (l, \sigma), \sigma = \pm 1 \) for these generalized links:

- \((l, 1)\) stands for the links with the originally chosen orientation, i.e. they have the structure \((l, 1) = (x, e_j)\), connecting \( x \) to \( x + \epsilon e_j \) \((x \in R^D_{latt})\) where \( e_j \) is positive.
- \((l, -1) = (x + \epsilon e_j, -e_j)\) connects then \( x + \epsilon e_j \) to \( x \).

Writing \( \lambda = (x, c_j) \) for a general link, \( c_j \) being a positive or negative lattice unit vector, the action of \( u = (R, a) \in G_E \) is simply given by

\[
\lambda \rightarrow u\lambda = (ux, Rc_j)
\]  

(10)

This allows us to define a unitary representation \( T \) of the lattice Euclidean group \( G_E \) on the Kogut-Susskind wave functions as a combination of the corresponding permutation of the link variables and the mapping \( U \rightarrow U^{-1} \) if the link in question is reoriented: If \( \Psi \) depends on the variables \( U_{l_1}, \ldots, U_{l_r} \) and if we put \( u(l_\alpha, 1) = (n_\alpha, \sigma_\alpha) \) \((\alpha = 1, \ldots, r, \sigma_\alpha = \pm 1)\), then \( T(u)\Psi \) depends on the variables \( U_{n_1}, \ldots, U_{n_r} \) and we have

\[
(T(u)\Psi)(U_{n_1}, \ldots, U_{n_r}) = \Psi(U_{\sigma_1 1}, \ldots, U_{\sigma_r r}).
\]  

(11)

As in the formal continuum limit, the operators \( T(u) \) commute with the Kogut-Susskind Hamiltonian for all \( u \in G_E \).

We now construct projection operators on subspaces of \( \mathcal{H} \) or \( \mathcal{H}_{phys} \) corresponding to specific irreducible representations of \( G_E \):

For translations we have a “lattice momentum projection”

\[
\Pi_{lt}(p) = \sum_{a \in R^D_{latt}} e^{-i\alpha p_j}T(R = 1, a)
\]  

(12)

where \( p \in R^D \) is restricted to the first Brillouin zone \((-\pi \leq \epsilon p_j \leq \pi)\).

If \( d^F_{\nu, \nu'} \) denote the D-functions for the irreducible representations (including inversions) of the cubic group \( G_{lr} \)[13], a projection on ”lattice angular momentum” \( \Gamma \) is given by

\[
\Pi_{lr}(\Gamma; \nu, \nu') = \sum_{R \in G_{lr}} d^F_{\nu, \nu'}(R)T(R, a = 0)
\]  

(13)

By construction these definitions guarantee for any \( \Psi \in \mathcal{H} \) the characteristic relations

\[
T(1, a)\Pi_{lt}(p)\Psi = e^{ip_j\alpha_j}\Pi_{lt}(p)\Psi
\]

\[
T(R, 0)\Pi_{lr}(\Gamma; \nu, \nu')\Psi = \sum_{\nu''} d^F_{\nu, \nu''}(R)\Pi_{lr}(\Gamma; \nu'', \nu')\Psi
\]  

(14)

A combination of both projections yields states with “good” momentum and angular momentum in the sense that we have for

\[
\Psi_{\nu, \nu'}^{\Gamma p} = \Pi_{lt}(p)\Pi_{lr}(\Gamma, \nu, \nu')\Psi
\]  

(15)
the relations

\[
T(1,a)\Psi_{\nu\nu'}^{p} = e^{i\rho_{\nu} a_{\lambda}} \Psi_{\nu\nu'}^{\Gamma p}
\]

\[
T(R,0)\Psi_{\nu\nu'}^{p} = \sum_{\nu''} d_{R\nu''}^{\Gamma p} \Psi_{\nu''\nu'}^{\Gamma p}
\]

(16)

The basic problem of a “lattice Yang Mills theory” is then to find in \( \mathcal{H}_{\text{phys}} \) (approximate) eigenfunctions of the type \( \Psi_{\nu\nu'}^{p} \) of the Kogut-Susskind Hamiltonian \[ H_{KS} = \frac{g^2}{2\pi} H \] with

\[
H = E_{la} E_{la} - xV
\]

\[
V = \sum_{\Box} \chi_{\Box}
\]

\[
x = \frac{2}{g^4}
\]

(17)

where \( g \) is the coupling constant and \( a \) is a colour index \((a = 1, \ldots, n^2 - 1)\). Summation over repeated indices is always assumed; \( \Box \) labels the plaquettes, and \( \chi_{\Box} \) is given by

\[
\chi_{\Box} := \text{tr} \, U_{l_1}^{\sigma_1} U_{l_2}^{\sigma_2} U_{l_3}^{\sigma_3} U_{l_4}^{\sigma_4}
\]

(18)

when \( \Box = (l_1, \sigma_1, \ldots, l_4, \sigma_4) \). The “colour-electric field operators” \( E_{la} \) generate - in analogy to the standard momentum operator - a left multiplication of group elements in the arguments of the wave functions. They are quantum operators conjugate to the link operators \( U_{l} \) obeying the commutation relations

\[
[E_{la}, U_{l'}] = \delta_{ll'} \lambda^{a} U_{l}
\]

(19)

where the SU(n) generators \( \lambda^{a} \) are normalized according to \( \text{tr} \, \lambda^{a} \lambda^{b} = \delta^{ab}/2 \).
3 The exp S method and intrinsic wave functions

A motivation for the introduction of the coupled cluster or exp S method is given by the following considerations:

Given a Hamiltonian $H$, a standard and often successful method to get the approximate spectrum of the low lying energy states is provided by the Lanczos approach: Choose some trial state $\phi$ and diagonalize $H$ restricted to the finite-dimensional space spanned by $(\phi, H\phi, H^2\phi, ..., H^n\phi)$. There are many cases where this gives reliable results if $n$ is large enough.

However, for our lattice Yang Mills case, this procedure is doomed to fail\[14\] because we have here a situation analogous to nuclear matter, for instance. In the infinite volume limit ($N \to \infty$) - where we want to formulate our approach - the groundstate energy $E_0$ and excitation energies $E - E_0$ of $H_{KS}$ have the behaviour

$$
E_0 \propto N \\
E - E_0 \propto 1
$$

(20)

Also the groundstate wavefunction displays a characteristic “pathology” in sense that its norm (defined by the N-fold Haar measure integral) has an essential singularity for $N \to \infty$. Its precise structure will be given below, within perturbation theory it is related to the appearance of disconnected diagrams.

It has been known for a long time that this difficulty is cured by rewriting the eigenvalue problem within the exp S framework (see Ref.\[15\] for the standard many-body theory and Ref.\[16\] for the Kogut-Susskind theory).

For our case, the method consists of introducing the ansätze

$$
\Psi_0(U) = \exp S(U) \\
(21) \\
(U = (U_1, ..., U_N))
$$

for the ground state and

$$
\Psi(U) = F(U) \exp S(U) \\
(22)
$$

for excited states.

The mentioned “pathology” of the ground state consists then in the fact that we have the norm relation $|S|^2 \propto N$ for the function $S(U)$ appearing in the exponent with respect to $\Psi_0$!

The validity of these volume dependencies is related to a characteristic linked cluster structure of $S(U)$ and $F(U)$, which follows from rewriting the Schrödinger equation in terms of these functions, resulting in the non-linear equation

$$
S_{\mu\mu} + S_\mu S_\mu - xV = E_0 \\
(23)
$$

for $S$ and in the linear equation

$$
F_{\mu\mu} + 2S_\mu F_\mu = (E - E_0)F \\
(24)
$$

for the excitation operator $F$.

Here, we use the abbreviation

$$
\mu = (l, a) \\
(25)
$$

and the notation

$$
f_\mu = [E_{l;a}, f] , \\
f_{\mu\mu} = [E_{l;a}, [E_{l;a}, f]]
$$

(26)

for any function $f(U)$.
Note that the “coupled cluster equations” (23) and (24) are still rigorous.

The linked cluster structure of the functions $S(U)$ and $F(U)$ follows from the fact that they may be expressed with the help of the projection operators (12) and (13) as in (15) in terms of “intrinsic” functions. These intrinsic functions are given by linked clusters and are defined as follows.

Suppose that $F\Psi_0$ describes a state with Euclidean quantum numbers $(p, \Gamma, \nu, \nu')$ (see eq. (15)). We then write $F$ and $S$ in the form ($S$ has to have trivial quantum numbers)

$$F(p, \Gamma, \nu, \nu') = \Pi_{lt}(p) \Pi_{lr}(\Gamma; \nu, \nu') F_{\text{int}}(p, \Gamma, \nu, \nu')$$

$$S = \Pi_0 S_{\text{int}}$$

$$\Pi_0 = \Pi_{lt}(0) \Pi_{lr}(0, 0, 0)$$

If $F\Psi_0$ corresponds in the continuum limit to a bound state, we expect that $F_{\text{int}}$ may be chosen to describe a localized state. This is analogous to non-relativistic many-body theory where bound states can be separated into square integrable functions of the relative coordinates and an overall center of mass motion, described here with projection operators.

In analogy to nuclear matter for instance, the same localization holds true for the vacuum function $S_{\text{int}}$ because correlations have a finite range.

The validity of these properties of the intrinsic functions is seen below through the structure of the expansion of these functions in terms of a localized basis, i.e. a basis of linked clusters.

We shall first characterize this basis through its general properties and then describe the concrete construction in section 4.

We call the basis

$$\chi^\alpha(U_{l1}, ..., U_{lm_\alpha}) \quad \alpha = 1, 2, 3, ..$$

and impose the following conditions:

1) $\chi^\alpha$ should be gauge invariant.

2) $\chi^\alpha$ should be “linked”, see section 4 for the precise definition. A main consequence is that $m_\alpha$ is finite for any $\alpha$, though not limited.

3) $\chi^\alpha$ should be “standardized”, i.e. the equation

$$T(u)\chi^\alpha = \lambda \chi^\beta \quad (u \in G_E)$$

should only have solutions for $\alpha = \beta$.

4) $\chi^\alpha$ should be a strong coupling eigenfunction, i.e.

$$\sum_a E_{t,a} E_{t,a} \chi^\alpha = \epsilon_{t} \chi^\alpha$$

It will be convenient to specify $\chi^1$ as the “plaquette function” by putting

$$\Pi_0 \chi^1 = 4(D - 1)V$$

and to distinguish the constant function via

$$\chi^0 = 1$$

$\chi^0$ fulfils the relation

$$\Pi_0 \chi^0 = s_0 N \chi^0$$

where the symmetry factor $s_0 = |G_{lr}|$ is equal to 8,48 for $D = 2, 3$, respectively.
Simplifying (27) by writing $F = \Pi F_{\text{int}}$ and introducing the functions $\tilde{S}(S)$ and $\tilde{F}(S,F)$ by

\[
(\Pi_0 S_{\text{int}})_{\mu}(\Pi_0 S_{\text{int}})_{\mu} = \Pi_0 \tilde{S}
\]
\[
(\Pi F_{\text{int}})_{\mu}(\Pi_0 S_{\text{int}})_{\mu} = \Pi \tilde{F}
\]

the coupled cluster equations (23) and (24) can be rewritten as

\[
(S_{\text{int}})_{\mu\mu} + \frac{x}{4(D-1)} \chi^1 = s_0 \frac{E_0}{s_0 N} \]
\[
(F_{\text{int}})_{\mu\mu} + 2 \tilde{F} = (E - E_0) F_{\text{int}}
\]

The “linked cluster theorem” for our lattice Yang-Mills theory consists then in the statement that if (for $N \to \infty$) we have the norm relation $|S_{\text{int}}|, |F_{\text{int}}| \propto 1$, we have also $|\tilde{S}|, |\tilde{F}| \propto 1$.

The norm relations for $S_{\text{int}}$ and $F_{\text{int}}$ are fulfilled because of their localized nature, those for $\tilde{S}, \tilde{F}$ follow then as a result of the fact that the “derivative” $S_\mu F_\mu$ selects only linked clusters. We shall prove this structure by suitable expansions in terms of the linked cluster basis (28).

Introducing the summation conventions

\[
\sum_{a} = \sum_{a=1,2,\ldots}
\]
\[
\sum'_{a} = \sum_{a=0,1,2,\ldots}
\]

the expansions of the intrinsic wavefunctions read (specifying again the Euclidean quantum numbers)

\[
S_{\text{int}}(U) = \sum_{a} S_a \chi^a(U)
\]
\[
F_{\text{int}}(p, \Gamma, \nu, \nu'; U) = \sum'_{a} F_a(p, \Gamma, \nu, \nu') \chi^a(U)
\]

The coupled cluster equations (23) and (24) may then equivalently be formulated as equations for the coefficients $S_a$ and $F_a(p, \Gamma, \nu, \nu')$

\[
\epsilon_a S_a + \sum_{\beta,\gamma} C_{\alpha}^{\beta\gamma} S_{\beta} S_{\gamma} = \frac{x}{4(D-1)} \delta_{a1} + \frac{E_0}{s_0 N} \delta_{a0}
\]
\[
\epsilon_a F_a(p, \Gamma, \nu, \nu') + 2 \sum_{\beta,\gamma,\nu_1} C_{\alpha}^{\beta\gamma}(p, \Gamma, \nu_1, \nu') S_{\beta} F_{\gamma}(p, \Gamma, \nu, \nu_1) = (E - E_0) F_a(p, \Gamma, \nu, \nu')
\]
\[
\epsilon_a = \sum_{I} \epsilon_{aI}
\]

The crucial quantities in these equations are the coupled cluster matrix elements $C_{\alpha}^{\beta\gamma}$ and $C_{\alpha}^{\beta\gamma}(p, \Gamma, \nu_1, \nu')$ defining the expansion of the functions $\tilde{S}$ and $\tilde{F}$, respectively, which are obtained as follows:

Determine first the set of numbers $c_{\alpha}^{\beta\gamma}(u \in G_E)$ defined by

\[
\sum_{\mu, u \in G_E} \chi_\mu^a(T(u) \chi^\gamma)_\mu = \sum_{\alpha, u} c_{\alpha}^{\beta\gamma} T(u) \chi^\alpha
\]
This yields then
\[ C_{\gamma}^{\alpha \beta}(p, \Gamma, \nu, \nu') = \sum_{u=(R,a)} C_{\gamma R,a}^{\alpha \beta} d_{\nu u'}^\Gamma(R^{-1}) e^{-ip_{j}a_{j}} \tag{40} \]
\[ C_{\gamma}^{\alpha \beta} = C_{\gamma}^{\alpha \beta}(0, 0, 0, 0) \]

A proof hereof is given in the appendix. The linked cluster theorem guaranteeing the correct volume dependencies of the relevant quantities discussed above is now given by the fact that, due to the localized nature of the functions \( \chi^\alpha \), the r.h.s. sums in eqs. (39) and (40) run only over a finite number of terms.

The coupled cluster equation (38) also have the property that approximate solutions generated by truncations (see e.g. Refs.[6, 7]) display correctly all relevant volume dependencies.

The important task is now to compute the matrix elements \( c_{\alpha u}^{\beta v} \) for which one needs an efficient and systematic way to set up and handle the basis elements \( \chi^\alpha \).

### 4 Construction of the loop space basis

In principle, an orthogonal basis of the type \( \chi^\alpha \) has been constructed in Ref.[11]: for simplicity, we will formulate the method for \( SU(2) \) and \( D = 2 \), but the generalization is obvious, though technically more difficult.

Suppose \( \chi^\alpha \) (\( \alpha \) fixed) depends on the link variables \((U_1, \ldots, U_r)\). This basis function is then - up to a normalization factor - uniquely characterized by the following set of angular momenta:

1) We have a set \((J_1, \ldots, J_r)\), i.e. one (half integer) angular momentum for each link.

2) We have an angular momentum \( J_{ab} = J_{cd} \) for each quadruplet of links \( l_a, \ldots, l_d \) forming a 4-point vertex in the link pattern \((l_1, \ldots, l_r)\). Here the convention is that the links \((l_a, l_b)\) are oriented such that they are going into, and \((l_c, l_d)\) are leaving, the common site.

These angular momentum quantum numbers are constrained by \( J_a = J_b \) if \((l_a, l_b)\) form a 2-point vertex and by the condition that the coupling \( J_a + J_b \rightarrow J_c \) should be possible if \((l_a, l_b, l_c)\) form a 3-point vertex.

For instance, putting \( r = 7 \) and choosing the link pattern of Fig. 1, one has just three angular momenta \((J_1 (= J_2 = J_3), J_4 (= J_5 = J_6), J_7)\) yielding the basis elements \((\alpha = (J_1, J_4, J_7))\)

\[ \chi^\alpha = \sum_{M_1, \ldots, M_{10}} D_{M_{11}, M_{12}}^{J_1}(U_1) D_{M_{21}, M_{22}}^{J_2}(U_2) D_{M_{31}, M_{32}}^{J_3}(U_3^{-1}) \]
\[ \left( \begin{array}{c} J_1, J_7, J_4 \\ M_8, M_{10}, M_4 \end{array} \right) D_{M_{71}, M_{10}}^{J_7}(U_7) \left( \begin{array}{c} J_1, J_7, J_4 \\ M_1, M_7, M_9 \end{array} \right) \]
\[ D_{M_{41}, M_{51}}^{J_4}(U_4^{-1}) D_{M_{51}, M_{61}}^{J_5}(U_5^{-1}) D_{M_{61}, M_9}(U_6) \tag{41} \]

We call this orthogonal set of functions the “D-loop basis”.

In Ref.[12] this framework was used for estimating observables within the ELCE method, but higher order calculations were limited by the necessity to handle an increasing number of \( SU(n) \) couplings. Also it should be mentioned that in Refs.[11, 12] the linked cluster form of the lattice Yang-Mills many-body problem was taken into account within a different computational framework.

An alternative for the construction of a basis is related to an exp S generalization of the Lanczos idea and was pursued in Refs.[6-10] for trivial representations of the Euclidean group. We will define this method here in such a way that it allows the computation of arbitrary Euclidean representations and also a transition to the independent, orthogonal D-loop basis. This yields especially a systematic way of eliminating linear dependencies.
Starting with $\phi^{1,1} = \chi^1$ from (31) we define “character functions” $\phi^{\delta,1}, ..., \phi^{\delta,n_\delta}$ by the iterative condition that the following expansion should hold (we put $\phi^{0,1} = 1, n_0 = n_1 = 1$)

$$
\phi^{\delta_1,k_1}(T(u))\phi^{\delta_2,k_2}(T(v)) = \sum_{v \in G} \sum_{0 \leq \delta_1 + \delta_2,k_1 \leq n_\delta} \zeta^{\delta_1,k_1\delta_2,k_2} T(u) T(v) \phi^{\delta,k}
$$

(42)

$$k_1 \leq n_{\delta_1} \quad k_2 \leq n_{\delta_2}
$$

Because of the “derivative” $\mu$, the functions $\phi^{\delta,k}$ are by definition linked - both terms on the l.h.s. have to have a common link variable for a non-vanishing result - and they also can be chosen to be standardized - i.e to obey the condition (29) - because we included the Euclidean operator $T(v)$ on the r.h.s. of (42).

The definition of the functions $\phi^{\delta,k}$ is made complete and unique by the condition that it should be just a product of characters, i.e. for each $(\delta,k)$ there should exist a set of $L_1, ..., L_r$ defined by the generalized links

$L_j = (l_{j1}, \sigma_{j1}, ..., l_{jm_j}, \sigma_{jm_j})$

(43)

such that

$$
\phi^{\delta,k} = \Pi_{j=1}^r tr(U_{l_{j1}}^{\sigma_{j1}} ... U_{l_{jm_j}}^{\sigma_{jm_j}})
$$

(44)

Hereby, for $SU(3)$, the loops $L_1, ..., L_r$ should have all possible orientations compatible with the standardization of $\phi^{\delta,k}$. For $SU(2)$, however, all loops should have the same (fixed) orientation which is no loss of generality because of the relation $trg = trg^\dagger$ for $g \in SU(2)$.

The result of the l.h.s. of (42) may be expanded in such terms because of an inductive argument: $\phi^{1,1}$ has the form (44). Assuming the form (44) for the two terms of the l.h.s. of (42) which we call, specifying for simplicity only the dependence on a certain (common) link variable $U_l = V$, $tr(AV)$ for the first term and $tr(BV^\sigma)$ for the second term $(\sigma = \pm 1)$, the “differentiation” with respect to $\mu = (l,a)$ may be evaluated using eq. (19) and the standard property of the $SU(n)$ generators $\lambda^a$:

$$
\sum_a \lambda^a_{ij} \lambda^a_{ij'} = \frac{1}{2} (\delta_{ij} \delta_{jj'} - \frac{1}{n} \delta_{ij} \delta_{ij'})
$$

(45)

yielding

$$
\sum_a (tr(AV))_{l,a} (tr(BV^\sigma))_{l,a} = \sigma \left( \frac{1}{2} tr(V^\rho AV^\rho B) - \frac{1}{2n} tr(AV) tr(BV^\sigma) \right)
$$

(46)

where $\rho = (\sigma + 1)/2$. If the variable $V = U_l$ also occurs in functions $A(U)$ or $B(U)$, additional terms arise on the r.h.s. due to the product rule of differentiation, but these terms will again display a loop space structure of the same type. The same happens if the first term has the form $tr(AV^{-1})$. In this sense, (46) describes the “generic” case.

Each character function $\phi^{\delta,k}$, constructed in this way, is uniquely characterized by the set of “geometric” loops indicated in (44). For $SU(2)$ and $D = 2$, examples up to third order are given in Figs. 2 and 4. For this dimension and for $SU(2)$, the number of loop space functions is 4, 16 for the orders $\delta = 2, 3$, respectively.

5 The D-Mapping

Of course, the system of loop space functions $\phi^{\delta,k}$ is neither orthogonal nor linearly independent. For $SU(2)$, for instance, the number of independent functions is known to be respectively 1,3,10 up to third order.
However, the construction yields directly the expansion coefficients needed in (39) by taking in (42) the sum over \( u \in G_E \).

The main problem which remains is to select an independent subset in the space of the functions \( \phi^{\delta,k} \).

In Refs. [7, 10] independent functions were determined using besides \( trg = trg^\dagger \) the relation
\[
tr(gg') = tr(gtrg') - tr(g^\dagger g') \quad \text{for} \quad g, g' \in SU(2).
\]

The emerging functions were in general neither orthogonal nor unique.

Within this paper, we propose a different strategy, namely, to relate the functions \( \phi^{\delta,k} \) - divided into convenient subsets - directly to the orthogonal “D-loop basis” \( \chi^\alpha \) by a characteristic mapping, called D-mapping.

This allows us to do the final calculation, i.e. to solve (approximately) eq. (38), with respect to the D-loop basis. But, at the same time, the crucial matrix elements \( c_{\alpha,u}^{\beta\gamma} \) may be computed in terms of the character functions using the D-mapping, while avoiding any explicit \( SU(n) \)-coupling or recoupling. We hope that this simpler structure will finally allow calculations of the type of Ref. [7, 8, 10] to higher order and/or for \( D = 3 \).

The construction of the (non-invertible) D-mapping relies on the following structure of the D-loop basis already indicated in section 4. For any \( \chi^\alpha = \chi^\alpha(U_{l_1}, ..., U_{l_{r_\alpha}}) \) (\( \alpha \) fixed) there exists a maximal set of commuting operators \( (A_1, ..., A_{M_\alpha}) \) with the property that
\[
A_\alpha^\lambda \chi^\alpha = a_\lambda \chi^\alpha \quad (47)
\]
and such that the state \( \chi^\alpha \) is uniquely characterized by the eigenvalues \( (a_1, ..., a_{M_\alpha}) \).

In the case \( SU(2) \) and \( D = 2 \), these operators are apparently given by a combination of the two sets
\[
\sum_a E_{\lambda a} E_{\lambda a} \quad \lambda = l_1, ..., l_{r_\alpha} \quad (48)
\]
and all operators
\[
\sum_a (E_{ba} + E_{ca})(E_{ba} + E_{ca}) \quad (49)
\]
which fulfil the condition that \((b,c)\) are outgoing links of a four point vertex in the link set related to \( \chi^\alpha \).

The more general case may be extracted from Refs. [11, 12]. Important for our purpose is that each \( A_\lambda \) is a Casimir operator of the local lattice gauge group \( G_{loc} \), i.e. it is a certain polynomial in the operators \( E_{l,a} \) of the type given above. For \( SU(3) \), two generalizations have to be taken into account: The third order Casimir operators have to be added to the set (47). In addition, suitable permutation operators have to be included if the \( SU(3) \) Clebsch Gordan decompositions generalizing eq. (41) have the property that the same irreducible representations occurs several times. (For \( SU(2) \), an example for the definition of such a permutation operator is given in the appendix A3.)

The main point for the construction of the D-mapping is that the evaluation of the operators \( A_\lambda \) on the states \( \phi^{\delta,k} \) can be done in precise analogy to the computation in eq. (46). The important ingredient is again the relation (45) and a corresponding third order generalization for \( SU(3) \) (see, e.g. [17]). In other words, it is possible to compute the matrix elements of \( A_\lambda \) defined by
\[
A_\lambda \phi^{\delta,k} = \sum_{\delta' \leq \delta,k'} (A_\lambda)^{\delta,k}_{\delta',k'} \phi^{\delta',k'} \quad (50)
\]
These matrices related to \( A_\lambda \) are finite \((\delta' \leq \delta)\) and stay small, in general. This is because the terms on the r.h.s. have to be consistent with the loop pattern of the variables of the l.h.s. Since link variables may be removed by \( A_\lambda \) (see eq. (46) for \( \sigma = -1 \)), this consistency also
allows terms with removed variables on the r.h.s.. In the classification of the states as D-loop functions, this corresponds to the possibility that one of the link angular momenta may be zero. The loop pattern of $\phi^{\delta,k}$ also determines the choice of the possible operators $A_\lambda$ in (45). More details are given in section 6 where it is also shown that with the knowledge of the matrices of $A_\lambda$ it is sufficient to work out (42) without the derivatives.

Eq. (50) corresponds to an evaluation of the operators $A_\lambda$ with respect to a non-orthogonal and overcomplete basis. Because the $A_\lambda$ are hermitian and commute with each other, they must nevertheless be simultaneously diagonalizable. Therefore, there must exist combinations

$$\varphi^\gamma = \sum_{\delta,k} C^\gamma_{\delta,k} \phi^{\delta,k}$$

such that

$$A_\lambda \varphi^\gamma = a^{\gamma}_{\lambda} \varphi^\gamma \quad \lambda = \gamma_1, \ldots, \gamma_r$$

The choice of the operators $A_\lambda$ is determined by the loop pattern of the variables occurring in $\varphi^\gamma$.

Any state $\varphi^\gamma$ is by construction proportional to a D-loop basis function characterized by the eigenvalues $a^{\gamma}_{\lambda_1}, \ldots, a^{\gamma}_{\lambda_r}$.

Consequently, the states $\varphi^\gamma$ are - up to a normalization factor and a possible Euclidean mapping (11) - equal if and only if their eigenvalue patterns are equal.

Some subset of the functions $\varphi^\gamma$ are then independent and orthogonal. They fulfill all conditions of (28) and can be identified with a certain subset of the $\chi^\alpha$. The D-mapping is just the restriction of (51) to such independent solutions and to the computation of the relative normalization factors for the dependent states $\varphi^\gamma$. Having determined the D-mapping, eqs. (51) and (42) contain all ingredients for the computation of the crucial matrix elements (39).

6 Computational strategy and examples

We now describe the computational steps which - put into the language of a suitable computer program - would lead to the possibility to determine approximate glueball spectra. We shall elucidate these steps by some examples of low order for $D = 2$.

1) Set up the character functions.

In order to minimize the computational effort, we propose to divide the character functions into subsets of the following type.

Introduce first the set of “generic” functions

$$A^\delta_{\delta,k} \quad \delta = 1, 2, \ldots \quad k = 1, \ldots, n_\delta$$

of $\delta$-fold linked, standardized plaquette products.

For $SU(2)$, all plaquettes should have the same orientation.

For $D = 2$, we have for $SU(2)$ $n_\delta = 1, 2, 4$, for $SU(3)$ $n_\delta = 1, 4, 12$ up to $\delta = 3$. Fig. 2 gives the corresponding loop patterns for $SU(2)$.

The relevance of this set of functions is two-fold:

i) They determine the possible elements of the D-loop basis occurring up order $\delta$. They are given by the link patterns of the generic set and the coupling rules of as many fundamental representations (and its adjoint) as there exist common links. Hereby, a double counting with lower order states has to be avoided. Fig. 3 exemplifies the related elements of the D-loop basis for $SU(2)$ and $D=2$ up to $\delta = 3$. 

ii) The set (53) is “generic” because each element defines a characteristic subspace given by functions
\[ \Lambda^{\delta,k,\nu} ; \nu = 1, \ldots, M(\delta, k) \]  
which is left invariant under the action of any Casimir operator of the lattice gauge group. Hereby, of course, only a finite number Casimir operators is relevant for any given \((\delta, k)\). The set of character functions \(\phi^{\delta,\kappa}\) is contained in the set (54), (i.e. for a given \(\delta\) there exists for each \(\kappa\) a pair \((k(\kappa), \nu(\kappa))\) such that that \(\phi^{\delta,\kappa} = \Lambda^{\delta,k(\kappa),\nu(\kappa)}\)) an explicit construction is not necessary because it is more convenient to work with (54).

2) Compute the Casimir operator matrices.

The set (54) is generated by applying the relevant Casimir operators on (53) yielding the matrix elements (50) as a system of - in general small - submatrices
\[ A_{\lambda} \Lambda^{\delta,k,\nu} = \sum_{\nu'=1}^{M(\delta,k)} A^{\nu'}_{\nu}(\lambda, \delta, k) \Lambda^{\delta,k,\nu'} \]  
Applying the product rule and (46) for the evaluation of the Casimir operators yields for the loop structure of the subspaces (54) \((\delta, k)\) fixed) the simple geometrical condition that they are generated from the plaquette systems (54) by “cutting and gluing” doubly occurring links. Up to third order, the related \(SU(2)\) loop structures for \(D = 2\) are given in Fig. 4, some examples of the corresponding Casimir operator matrices are presented in the Appendix A2.

Note that the sets (54) may also contain elements of lower order if they occur during the cutting and gluing procedure. Also a standardization is not done. This is convenient since this makes the “Casimir matrices” (55) especially simple.

3) Fix the D-Mapping.

The next step is the diagonalization of the Casimir matrices (56) giving eigenfunctions
\[ \varphi^{\nu}(\delta, k) = \sum_{\nu'} C^{\nu'}_{\nu}(\delta, k) \Lambda^{\delta,k,\nu'} \]  
obeying
\[ A_{\lambda} \varphi^{\nu}(\delta, k) = a_{\lambda}(\nu, \delta, k) \varphi^{\nu}(\delta, k) \]  
For the construction of the D-mapping one first may put with a suitable enumeration \(\bar{\alpha}(\nu, \delta, k)\)
\[ \varphi^{\nu}(\delta, k) = N(\nu, \delta, k) T(\bar{u}(\nu, \delta, k)) \chi^{\bar{\alpha}(\nu, \delta, k)} . \]  
Hereby, linear dependencies are eliminated by the identification prescription
\[ \bar{\alpha}(\nu, \delta, k) = \bar{\alpha}(\nu', \delta', k') \Leftrightarrow a_{\lambda}(\nu, \delta, k) = a_{\lambda}(\nu', \delta', k') \ for \ all \ \lambda . \]  
Of course, equality of the eigenvalue patterns guarantees the equality of the corresponding eigenfunctions only up to a (non-zero) factor \(N(\nu, \delta, k)\) and up to a Euclidean transformation \(T(\bar{u}(\nu, \delta, k))\).

For the computation of the normalization factors \(N(\nu, \delta, k)\) we observe that within our exp S framework (including a possible truncation) it is not necessary to work with basis states which are normalized to one. Hence only the relative factors are needed, i.e. we may put \(N(\nu, \delta, k) = 1\) if the D-loop function \(\chi^{\bar{\alpha}(\nu, \delta, k)}\) occurs for the first time when increasing the order \(\delta\). Also we may set for this first case \(\bar{u}(\nu, \delta, k) = 1\). As a result we may find for each quantum number \(\alpha\)
an eigenfunction (56) characterized by \((\tilde{\delta}(\alpha), \tilde{\nu}(\alpha), \bar{k}(\alpha))\) defining an expansion of the elements of the D-loop basis in terms of the character functions

\[
\chi^\alpha = \sum_{\nu'} \xi^\alpha_{\nu'} (\tilde{\delta}(\alpha), \bar{k}(\alpha)) \Lambda^{\tilde{\delta}(\alpha), \bar{k}(\alpha), \nu'}.
\]  

(60)

For each \((\delta, k)\), the matrices \(C^\nu_{\nu'}(\delta, k)\) may be inverted, yielding with (58) the inverse mapping

\[
\Lambda^{\delta, k, \nu} = \sum_{\nu'} D^\nu_{\nu'}(\delta, k) N(\nu', \delta, k) T(\tilde{u}(\nu', \delta, k)) \chi^{\delta(\nu', \delta, k)}.
\]  

(61)

Equation (61) - together with the inversion (60) - constitutes the D-mapping in a form which is sufficient for the computation of the coupled cluster matrix elements (39).

We still have to give a recipe to compute the normalization factors \(N(\nu, \delta, k)\). In principle, they could be determined by evaluating Haar measure integrals. This can be avoided, however, by rewriting the states \(\varphi^\nu(\delta, k)\) in a (up to the normalization factors) unique form by using the usual procedure of eliminating linear dependences via the Cayley Hamilton relations

\[
tr g^\dagger = tr g
\]  

(62)

\[
g^2 = g tr g - 1 \quad (g \in SU(2))
\]  

(63)

and

\[
tr g^2 = (tr g)^2 - 2tr g^\dagger
\]  

(64)

\[
g^3 = g^2 tr g - g tr g^\dagger + 1 \quad (g \in SU(3))
\]  

(65)

This allows us to introduce a standardization of the functions \(\Lambda^{\delta, k, \nu}\) by eliminating for \(SU(2)\) \((SU(3))\) all structures of the type \(tr g^n g^\dagger\) with \(n \geq 2\) \((n \geq 3)\). For this purpose, eq. (61) respectively (63) have to be iterated yielding formulas of the type \(g^n = a g^2 + b g + c\) where \(a, b, c\) are polynomials in \(tr g\) and \(tr g^\dagger\). (For \(SU(2), a = 0\) and \(b, c\) become polynomials in \(tr g\) only.)

For \(SU(3)\) and \(n = 2\), also terms of the type \(tr g^2\) in (44) may be standardized with the help of (64).

For the examples where the Casimir matrices (55) are computed, we give in the Appendix A2 also a construction of the corresponding part of the D-mapping.

4) The incorporation of the Euclidean group.

For the computation of the matrix elements (39) it is sufficient to work out (42) disregarding the derivatives, i.e. to determine the coefficients \(\eta_{\gamma_1, \gamma_2, \gamma_3}^{\gamma; u, v, \gamma} \quad (u, v \in G_E)\) given by

\[
\Lambda^{\gamma} T(u) \Lambda^{\gamma} = \sum_{\gamma_3, v} \eta_{\gamma_3, u, v}^{\gamma_1, \gamma_2} T(v) \Lambda^{\gamma_3}
\]  

(66)

where we introduced the abbreviation \((\delta, k, \nu) = \gamma\). Here, the character functions \(\Lambda^{\gamma_1}\) and \(T(u) \Lambda^{\gamma_2}\) have to fulfill the restriction that they are linked, i.e. they should have a common link variable. Also the trivial function \(\Lambda^{0, 0, 0} = \chi^0\) should be left out.

The following structures simplify the determination of these \(\eta\)-coefficients:

a) There is only one non-vanishing term on the r.h.s. of (66). If \(\eta_{\gamma_3, u, v}^{\gamma_1, \gamma_2}\) is non-vanishing, it is equal to one. In this case we call the corresponding states \(\Lambda^{\gamma_1}, \Lambda^{\gamma_2}, \Lambda^{\gamma_3}\) non-trivially connected.

b) For each triple \(\Lambda^{\gamma_1}, \Lambda^{\gamma_2}, \Lambda^{\gamma_3}\) of non-trivially connected character functions we have a characteristic set of Euclidean group elements \(u_\lambda, v_\lambda\) such that

\[
\Lambda^{\gamma_1} T(u_\lambda) \Lambda^{\gamma_2} = T(v_\lambda) \Lambda^{\gamma_3} \quad ; \quad \lambda = 1, .., n(\gamma_1, \gamma_2, \gamma_3)
\]  

(67)
The determination of these elements \( u_\lambda, v_\lambda \) is now simplified by the following structure: Suppose we have found all solutions \( u_\lambda, v_\lambda \) for a non-trivially connected triple of generic functions

\[
\Lambda^{\delta_1,k_1}_G T(u_\lambda) \Lambda^{\delta_2,k_2}_G = T(v_\lambda) \Lambda^{\delta_1,k_1}_G
\]

(68)

If \( v_\lambda \) is suitably chosen, we have then for each \( \Lambda^{\delta_1,k_1,k_1} \) and \( \Lambda^{\delta_2,k_2,k_2} \) a function \( \Lambda^{\delta_3,k_3,k_3} \) so that they are non-trivially connected with the same set of Euclidean group elements as in (67) and this exhausts all possibilities.

Given the generic functions of the r.h.s. of (68) and \( \kappa_1, \kappa_2 \), the third character function \( \phi^{\delta_3,k_3} \) is then determined by finding just one pair \((uv)\) solving (65).

Up to third order \( \delta_3 = 3 \), a full computation of all \( \eta \)-coefficients in presented in Appendix A4.

6) The computation of the c-coefficients in (39).

Having solved the “combinatorial” problem of determining the coefficients of (66), one may compute the quantities \( c^{\alpha_1,\alpha_2}_{\alpha_3,u} \) by writing (66) in terms of the orthogonal and independent basis \( \chi^\alpha \) with the help of (60,61) and by applying the (Euclidean invariant) “total Casimir operator” \( \sum E_{ia} E_{ia} \) on both sides of the emerging equation. Writing \( \gamma(\alpha) = (\delta(\alpha), \bar{k}(\alpha), \bar{\nu}(\alpha)) \), we obtain as final result for the crucial coupled cluster matrix elements (39)

\[
c^{\alpha_1,\alpha_2}_{\alpha_3,u} = \left[ \sum_l (\epsilon_{\alpha_1,l} + \epsilon_{\alpha_2,l} - \epsilon_{\alpha_3,l}) \right] \sum_{\gamma_1,\gamma_2,\gamma_3} \sum_{\gamma_4 \text{ with } \alpha(\gamma_4) = \alpha_3} C^{\gamma_{\alpha_1}}_{\gamma_1} C^{\gamma_{\alpha_2}}_{\gamma_2} N(\gamma_4) \eta^{\gamma_1,\gamma_2}_{\gamma_3,u,v(\gamma_4)} D^{-1}_{\gamma_4}
\]

(69)

7 Discussion and conclusion

The coupled cluster formulation of Hamiltonian lattice QCD needs an efficient method to deal with suitable basis systems of loop space functions. Within this paper we have demonstrated that it possible to combine the merits of a D-function basis, used within the ELCE framework\[12\] with those of the character sets used within recent coupled cluster attempts\[7, 6\] without facing the respective deficiencies.

The merits are the orthogonality of the basis in the first case, the close relation to the Lanczos method and the easy computability of the coupled cluster matrix elements in the second case.

The deficiencies are the need of handling too many \( SU(n) \) recoupling coefficients for the computation of the Hamiltonian matrix elements when using D-functions, the non-orthogonality and linear dependence of the states when using the character functions.

Our combination is based upon the simple idea that the D-function basis may be characterized by the quantum numbers of a complete set of commuting operators. These operators are the Casimir operators of the local lattice gauge group (for the gauge group \( SU(3) \), also certain permutation operator have to be included) and our method relies on the fact that these commuting operators (where only a finite set is relevant for any specific case) may be evaluated as finite matrices with respect to the character functions. This allows the construction of a systematic mapping between the two frameworks.

Invoking the lattice Euclidean symmetry of the regularized gauge field theory and systematizing the action of this symmetry group, we were also able to formulate the coupled cluster lattice Hamiltonian eigenvalue problem for eigenstates with arbitrary lattice momentum and lattice angular momentum. The whole formulation may be done in the infinite volume limit.
For any concrete calculation of the spectrum, a truncation prescription has to be defined. This point has been much in dispute\cite{6, 7, 8, 10} because previously one had to make a (non-unique) choice of independent functions from the non-orthogonal set of character functions. Within our method we have a more natural definition because the orthogonal D-function basis is uniquely determined.

We want to stress that any truncated coupled cluster calculation will have the same limitations as any (finite volume) standard lattice Monte Carlo computation, namely that at best one has to hope for a scaling window indicating consistency with respect to the predicted renormalization group structure which has to be displayed by any observable when approaching the continuum limit. (This structure is still unclear within Ref.\cite{10} which gives the “best” coupled cluster results up to now.)

The reason for this expected scaling window in given by the fact that the truncation which has to be defined with respect to an expansion of the intrinsic wave functions of the vacuum and of the hadron, necessarily limits the possible lattice volume over which the physical states may extend. Consequently, when the physical lattice scale is set by choosing the coupling $g$, the method has to break down when the physical lattice volume, given by the truncation - or by the number of lattice points in the standard lattice Monte Carlo case - becomes smaller than the size of the hadron.

First attempts at doing concrete numerical calculations within the reported framework are on the way and will be reported in the future\cite{18}.

Finally we want to mention that our computational framework may, in principle, be easily extended to include Fermions. Especially, a formulation for Wilson Fermions within a quenched approximation yields equations whose treatment appear to be no more complicated than that for glueballs. Details of this structure will be reported elsewhere.

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### Appendix

#### A1. Proof of equation (37)

Introducing the abbreviation

$$D_{\nu,\nu'}^p(R, a) = d_{\nu,\nu'}^p(R)e^{ip\alpha_j}$$

the expansion of $F_\mu S_\mu$ according to (27) and (34) yields the relevant terms

$$(\Pi_\mu \rho \Pi_\mu \rho '(\Gamma; \nu, \nu') \chi^\alpha)_{\mu}(\Pi_0 \chi^\beta)_{\mu}$$

$$= \sum_{u_1, u_2 \in G_E} D_{\nu,\nu'}^p(u_1)(T(u_1)\chi^\alpha)_{\mu}(T(u_2)\chi^\beta)_{\mu}$$

$$= \sum_{u_1, u_2 \in G_E} D_{\nu,\nu'}^p(u_1)(T(u_1)\chi^\alpha)_{\mu}(T(u_1)T(u_1^{-1}u_2)\chi^\beta)_{\mu}$$

$$= \sum_{u_1} D_{\nu,\nu'}^p(u_1)T(u_1)[\sum_u \chi^\alpha_{\mu}(T(u)\chi^\beta)_{\mu}]$$

$$= \sum_{u_1} D_{\nu,\nu'}^p(u_1)T(u_1)\sum_{u, \gamma} c^{\alpha,\beta}_{\gamma, u}T(u)\chi^\gamma$$
\[
\sum_{u,\nu} \sum_{\nu_2} D_{\nu \nu_2}^\nu (u_1 u) D_{\nu_1 \nu_1'}^\nu (u^{-1}) T(u_1 u) \chi_\gamma
\]

Here we assumed (39) and we arrived at the result (40).

\section*{A2. Examples for the D-mapping}

Within this appendix we will give the construction of “Casimir matrices” (55) for $SU(2)$ and $D = 2$ for some typical cases of subspaces $(\delta, k)$ taken from in Fig. 4. Subsequently, we will present the corresponding part of the D-mapping resulting from a diagonalization.

Note that also the D-loop basis is characterized by the same quantum numbers $(\delta, k)$, see Fig. 3.

$(\delta, k) = (2,1)$

Here, two parallel links with the same orientation occur. If a given link of this type is denoted by $U$, this case yields for the corresponding Casimir operator (48) a $2 \times 2$ matrix with respect to states of the type

\[
\Lambda^1 = tr(BU)tr(CU) \\
\Lambda^2 = tr(BUCU)
\]

For $(\delta, k) = (2,1)$, we have $B = C$ and $U$ may be any of the four links. A more general case is e.g. given by $U = U_2$ for $(\delta, k) = (3,2)$. (For enumeration see Fig 3). The evaluation of $A = E_a E_a$ yields

\[
A \Lambda^1 = \Lambda^1 + \Lambda^2 \\
A \Lambda^2 = \Lambda^1 + \Lambda^2
\]

The diagonalization gives the Casimir spectrum as an example of eqs. (56) and (57)

\[
\varphi^1 = \Lambda^1 + \Lambda^2 ; \ a(1) = 2 \\
\varphi^2 = \Lambda^1 - \Lambda^2 ; \ a(1) = 0
\]

For $A = B$ one may eliminate in the state $\varphi^2$ the function $(AU)^2$ via (61) yielding the identifications with the D-loop functions (see Fig. 3 for notations)

\[
\varphi^1 = \chi^{2,1} \\
\varphi^2 = 2 = 2\chi^0
\]

Note that we put the normalization factor $N(\nu, \delta, k)$ equal to one when the corresponding basis state $\chi^\alpha$ occurs for the first time. Within our examples, the Euclidean mapping $T(u)$ in (58) is the identity in most cases.

With the inversion

\[
\Lambda^1 = \frac{1}{2} \chi^{2,1} + \chi^0 \\
\Lambda^2 = \frac{1}{2} \chi^{2,1} - \chi^0
\]

these formulas give the D-mapping relevant for the subspace $(\delta, k) = (2,1)$. 
\((\delta, k) = (2, 2)\)

This case is of the type

\[
\Lambda^1 = \text{tr}(BU)\text{tr}(U^\dagger C)
\]
\[
\Lambda^2 = \text{tr}(BC)
\]

yielding

\[
A\Lambda^1 = 2\Lambda^1 - \Lambda^2
\]
\[
A\Lambda^2 = 0
\]

A diagonalization of (80) gives

\[
\varphi^1 = 2\Lambda^1 - \Lambda^2 ; a(1) = 2
\]
\[
\varphi^2 = \Lambda^2 ; a(1) = 0
\]

With the identification

\[
\varphi^1 = \chi^{2,2,1}
\]
\[
\varphi^2 = \chi^{2,2,2}
\]

and the inversion

\[
\Lambda^1 = \frac{1}{2}(\chi^{2,2,1} + \chi^{2,2,2})
\]
\[
\Lambda^2 = \chi^{2,2,2}
\]

this defines all the D-mapping ingredients for \((\delta, k) = (2, 2)\).

\((\delta, k) = (3, 1)\)

Here one has to deal with a three-dimensional subspace given by

\[
\Lambda^1 = (\text{tr} g)^3
\]
\[
\Lambda^2 = \text{tr} g \text{tr} g^2
\]
\[
\Lambda^3 = \text{tr} g^3
\]

with \(g = BU\). The product rule yields for the evaluation of the Casimir operator

\[
A\Lambda^1 = \frac{3}{4}\Lambda^1 + 3\Lambda^2
\]
\[
A\Lambda^2 = \Lambda^1 + \frac{3}{4}\Lambda^2 + 2\Lambda^3
\]
\[
A\Lambda^3 = 3\Lambda^2 + \frac{3}{4}\Lambda^3
\]

The eigenvectors and eigenvalues are

\[
\varphi^1 = \Lambda^1 + 3\Lambda^2 + 2\Lambda^3 ; a(1) = \frac{15}{4}
\]
\[
\varphi^2 = \Lambda^1 - \Lambda^3 ; a(2) = \frac{3}{4}
\]
\[
\varphi^3 = \Lambda^1 - 3\Lambda^2 + 2\Lambda^3 ; a(3) = -\frac{9}{4}
\]
Using \( \text{trg}^3 = (\text{trg})^3 - 3\text{trg} \) obtained from (63), this yields the identifications

\[
\begin{align*}
\varphi^1 &= \chi^{3,1} \\
\varphi^2 &= 3\chi^{1,1}
\end{align*}
\]

Since the eigenvalue \( a(3) \) is negative, we must have

\[
\varphi^3 = 0
\]

yielding the linear dependence relation

\[
\Lambda^2 = \frac{1}{3}(\Lambda^1 + 2\Lambda^3) = (\text{trg})^3 - 2\text{trg}
\]

which is just the result for \( \Lambda^2 \) when eliminating \( g^2 \) by (61). The inversion (64) now reads

\[
\begin{align*}
\Lambda^1 &= \frac{1}{6}\chi^{3,1} + 2\chi^{1,1} \\
\Lambda^2 &= \frac{1}{6}\chi^{3,1} \\
\Lambda^3 &= \frac{1}{6}\chi^{3,1} - \chi^{1,1}
\end{align*}
\]

\((\delta,k) = (3,4)\)

This case is interesting because it involves a 4-point vertex, the dimension of the subspace (54) is 5. Calling the doubly occurring link variables \( U_1, U_2 \) the generating character states are of the type

\[
\begin{align*}
\Lambda^1 &= \text{tr}(BU_1) \text{tr}(U_1^\dagger CU_2) \text{tr}(U_2^\dagger D) \\
\Lambda^2 &= \text{tr}(BCU_2) \text{tr}(U_2^\dagger D) \\
\Lambda^3 &= \text{tr}(BU_1) \text{tr}(U_1^\dagger CD) \\
\Lambda^4 &= \text{tr}(BCD) \\
\Lambda^5 &= \text{tr}(U_1^\dagger CU_2) \text{tr}(BU_1 U_2^\dagger D)
\end{align*}
\]

Now we have three relevant Casimir operators, \( A_1 \) and \( A_2 \) as before of type (48) and \( A_3 = (E_{1a} + E_{2a})(E_{1a} + E_{2a}) - A_1 - A_2 = 2E_{1a}E_{2a} \) which is of the type (49). The related Casimir matrices are given by

\[
\begin{align*}
A_1\Lambda^1 &= 2\Lambda^1 - \Lambda^2 \\
A_1\Lambda^2 &= 0 \\
A_1\Lambda^3 &= 2\Lambda^3 - \Lambda^4 \\
A_1\Lambda^4 &= 0 \\
A_1\Lambda^5 &= -\Lambda^4 + 2\Lambda^5 \\
A_2\Lambda^1 &= 2\Lambda^1 - \Lambda^3 \\
A_2\Lambda^2 &= 2\Lambda^2 - \Lambda^4 \\
A_2\Lambda^3 &= 0 \\
A_2\Lambda^4 &= 0 \\
A_2\Lambda^5 &= -\Lambda^4 + 2\Lambda^5
\end{align*}
\]
\[ A_3 \Lambda^1 = -2 \Lambda^1 + \Lambda^2 + \Lambda^3 - \Lambda^5 \]  
\[ A_3 \Lambda^2 = 0 \]  
\[ A_3 \Lambda^3 = 0 \]  
\[ A_3 \Lambda^4 = 0 \]  
\[ A_3 \Lambda^5 = 2 \Lambda^4 - 4 \Lambda^5 \]  

The simultaneous eigenfunctions are
\[ \varphi^3 = -2 \Lambda^1 + \Lambda^2 + \Lambda^3 - \Lambda^4 + \Lambda^5 \quad ; \quad a_1(1) = a_2(1) = 2 \quad a_3(1) = -2 \]
\[ \varphi^4 = -2 \Lambda^5 + \Lambda^4 \quad ; \quad a_1(2) = a_2(2) = 2 \quad a_3(2) = -4 \]
\[ \varphi^2 = -2 \Lambda^2 + \Lambda^4 \quad ; \quad a_1(3) = 0 \quad a_2(3) = 2 \quad a_3(3) = 0 \]
\[ \varphi^5 = -2 \Lambda^3 + \Lambda^4 \quad ; \quad a_1(4) = 2 \quad a_2(4) = 0 \quad a_3(4) = 0 \]
\[ \varphi^1 = \Lambda^4 \quad ; \quad a_1(5) = a_2(5) = a_3(5) = 0 \]  

with the identifications
\[ \varphi^\nu = \chi^{3,4,\nu} \quad \nu = 1, 2, 3, 4 \]
\[ \varphi^5 = T(P) \chi^{3,4,2} \]  

where \( P \) describes the reflection (parity transformation) defined in equation (96).

The inversion (64) reads
\[ \Lambda^1 = \frac{1}{4}(-2 \chi^{3,4,3} + \chi^{3,4,1} - \chi^{3,4,2} - T(P) \chi^{3,4,2} - \chi^{3,4,4}) \]  
\[ \Lambda^2 = \frac{1}{2}(\chi^{3,4,1} - \chi^{3,4,2}) \]
\[ \Lambda^3 = -\frac{1}{2}(T(P) \chi^{3,4,2} - \chi^{3,4,1}) \]
\[ \Lambda^4 = \chi^{3,4,1} \]
\[ \Lambda^5 = \frac{1}{2}(\chi^{3,4,1} - \chi^{3,4,4}) \]  

A3. The “local action” of the permutation group

We explain this structure for the “typical” example \((\delta, k) = (3, 4)\) discussed in the Appendix A2, a generalization for general cases is straightforward, but will not be displayed within the paper.

For \( SU(2) \), first the equivalence of the fundamental representation and its adjoint has to be invoked by introducing the skew symmetric \( 2 \times 2 \) matrix
\[ \epsilon = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \]

which has the property that \( \epsilon g^{-1} \epsilon^{-1} = \bar{g} \) for any \( g \in SU(2) \). Consequently, the modified link variable \( \bar{U} = U \epsilon \) obeys instead of (5) the “tensor product” transformation rule (written in terms of matrix elements)
\[ (\bar{U}_i^g)_{jk} = g(x)_{j'j} g(x + e_j)_{kk'} (\bar{U}_i)_{j'k'} \]  

(96)
Introducing the “modified loop group elements” specified according to the common (four point) lattice site of our example (see eq.(89))

\[
\alpha = BU_1 \epsilon \\
\beta = U_1^\dagger DU_2 \epsilon \\
\gamma = U_2^\dagger D \epsilon
\]  

(97)

the character states (89) may be written as

\[
\Lambda^\nu = d(\nu)^{j_1 j_2 j_3 j_4 j_5 j_6} \alpha_{j_1 j_2} \beta_{j_3 j_4} \gamma_{j_5 j_6}
\]  

(98)

Each d-coefficient couples the tensor product of the six fundamental representations - - defined “locally” corresponding to the chosen the four point vertex - to the trivial representation, i.e., introducing the related six angular momentum operators \(s(r), r = 1, \ldots, 6\) (\(s_j\) are the Pauli spin matrices in our case) the states (98) obey

\[
s_{\text{total}} \Lambda^\nu = 0
\]  

(99)

Obviously, the “total angular momentum” \(s_{\text{total}}\) is invariant with respect to any permutation of the six variables appearing as indices in (98), i.e. we may simultaneously characterize the space (89) the representations of the permutation group \(S_6\) which acts on the states (98) by

\[
d(\nu)^{j_1 j_2 j_3 j_4 j_5 j_6} \rightarrow d(\nu)^{j_{\sigma(1)} j_{\sigma(2)} j_{\sigma(3)} j_{\sigma(4)} j_{\sigma(5)} j_{\sigma(6)}}
\]  

(100)

(\(\sigma \in S_6\)). One may use the decomposition of this representation for classifying the states in the space (89). In its general form, however, the corresponding permutation operators do not commute with the Casimir operators (47) since they involve only “reduced total angular momenta”. In our case we have e.g.

\[
A_1 = (s(2) + s(3))^2 \\
A_2 = (s(4) + s(5))^2 \\
A_3 = (s(2) + s(3) + s(4) + s(5))^2 - A_1 - A_2
\]  

(101)

Conveniently chosen subgroups of \(S_6\), however, do commute. We may take, e.g., \(S_2\) embedded in \(S_6\) in different ways: If \(\pi\) is the non-trivial element of \(S_2\), we may put

\(\pi(1, 2, 3, 4, 5, 6) = (1, 3, 2, 4, 5, 6)\) - yielding \(\chi^{3,4,1}\) and \(\chi^{3,4,2}\) as antisymmetric and \(\chi^{3,4,3}\) and \(\chi^{3,4,4}\) as symmetric representations -

or \(\pi(1, 2, 3, 4, 5, 6) = (1, 3, 2, 5, 4, 6)\) - yielding \(\chi^{3,4,1}\) and \(\chi^{3,4,3}\) as antisymmetric and \(\chi^{3,4,2}\) and \(\chi^{3,4,4}\) as symmetric representations.

Of course, for SU(2), this does not yield independent quantum numbers. With a suitable choice of the permutation subgroup, however, this may be the case for SU(3).

**A4. Examples for the incorporation of the Euclidean group**

We restrict ourselves to \(SU(2)\) and \(D = 2\). A convenient enumeration of the Euclidean group for \(D = 2\) is given by

\[
[n, \mu, m, \sigma] = R^n t^\mu R^m P^\sigma \quad ; \quad m, n = 0, 1, 2, 3 \\
\sigma = 0, 1 \\
\mu = 0, 1, 2, 3, 4, 5, \ldots
\]  

(102)
where the use the following conventions:

The parity transformation \( P \) is fixed by the condition \( T(P) \Lambda^{3,4,2} = \Lambda^{3,4,3} \)

The rotation \( R \) is given by the constraint that it has rotation angle \( \pi/2 \) and fulfils \( T(R) \chi^1 = \chi^1 = \Lambda^{1,1,1} \)

The “one-unit” translation \( t \) is defined by the condition that \( \Lambda^{2,2} = \chi^1 \ T(t) \chi^1 \).

Taking into account \( T(P) \chi^1 = \chi^1 \), we obtain in lowest order \( \gamma_1 = \gamma_2 = (1,1,1) \) the non-trivially connected cases \( (n,m,\sigma) \) are arbitrary with the restriction (96))

\[
\begin{align*}
\gamma_3 &= (2,1,1) \quad u = [n,0,m,\sigma] \quad v = [0,0,0,0] \\
\gamma_3 &= (2,2,1) \quad u = [n,1,m,\sigma] \quad v = [4-n,0,0,0]
\end{align*}
\]

Combining first and second order on the r.h.s. of equation (69) we have the following generic alternatives:

\( \gamma_1 = (2,1,1); \gamma_2 = (1,1,1): \)

\[
\begin{align*}
\gamma_3 &= (3,1,1) \quad u = [n,0,m,\sigma] \quad v = [0,0,0,0] \\
\gamma_3 &= (3,2,1) \quad u = [n,1,m,\sigma] \quad v = [4-n,0,0,0]
\end{align*}
\]

\( \gamma_1 = (2,2,1); \gamma_2 = (1,1,1): \)

\[
\begin{align*}
\gamma_3 &= (3,2,1) \quad u = [0,0,m,\sigma] \quad v = [0,0,0,0] \\
& \quad u = [0,1,m,\sigma] \quad v = [0,1,2,0] \\
\gamma_3 &= (3,3,1) \quad u = [0,2,m,\sigma] \quad v = [0,0,0,0] \\
& \quad u = [2,0,m,\sigma] \quad v = [0,1,2,0] \\
\gamma_3 &= (3,4,1) \quad u = [1,1,m,\sigma] \quad v = [0,0,0,0] \\
& \quad u = [3,1,m,\sigma] \quad v = [0,0,1,1]
\end{align*}
\]

Here, the Euclidean elements \( v \) are chosen such that a non-trivial connection with the same pairs \( (u,v) \) is described for the \( \gamma \)-tripletts

\((2,1,2),(1,1,1),[(3,1,2) \text{ or } (3,2,2)]\) for the two cases (103) and
\((2,2,2),(1,1,1),[(3,3,2) \text{ or } (3,4,2)]\) for the cases (104).

The Euclidean elements \( (u,v) \) for the cases where \( \gamma_1 \) and \( \gamma_2 \) are exchanged may be obtained by the replacements

\( u \rightarrow u^{-1}, v \rightarrow u^{-1}v \)

in the above formulas. This follows from \( \Lambda^2 T(u^{-1}) \Lambda^1 = T(u^{-1})(\Lambda^1 T(u) \Lambda^2) = T(u^{-1}) \Lambda^3 \) if

\( \Lambda^1 T(u) \Lambda^2 = T(v) \Lambda^3 \).

This provides all non-vanishing \( \eta \)-coefficients (66) up to the order \( \delta_3 = 3 \).

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Figure 1. Link pattern of the D-loop functions (41). The numbers indicate the enumeration of the link angular momenta \((J_1, \ldots, J_7)\).
Figure 2. Loop structure of the generic character functions $\Lambda^\delta_{\kappa}$ (see equation (53)) up to order $\delta = 3$ for SU(2).
**Figure 3.** $SU(2)$ D-loop basis functions $\chi^{\delta,k,\nu}$ characterized by the link patterns and the related possible Casimir eigenvalue patterns which are generated up the order $\delta = 3$. Non-equal angular momenta are enumerated in the link patterns and indicated in that order in the eigenvalue patterns. Upper indices stand for the degeneracy of these angular momenta.

For $\delta = 3$, $k = 3$ or 4 all angular momenta which are not specified are equal to $\frac{1}{2}$.

For $(\delta, k) = (3, 4)$, the third angular momentum is given by the “intermediate” coupling $j_1 + j_2$ (eq. (49)).

The last column gives the linear dependent D-loop functions emerging up to this order.

The orientation of the links is not marked, it may be taken analogously to Fig. 1.
Figure 4. Loop structure of the functions $\Lambda^{\delta,k,\nu}$ (see equation (54)) up to order $\delta = 3$. 