Coupled cluster method in Hamiltonian lattice field theory

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The coupled cluster or $\exp(S)$ form of the eigenvalue problem for a 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. [S0556-2821(97)02705-7]

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I. 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 [1] (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 [2], the $\exp(-tH)$ method [3], or variational techniques [4]. 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 Green's function Monte Carlo method [5]).

This also holds for the coupled cluster $[\exp(S)]$ method which attracted special attention in recent years [6–9]. (Some encouraging results within this framework were obtained recently [10].) Here the basic idea is to incorporate manifestly the correct volume dependences of observables by writing the ground state in the form $\psi_0 = e^S$ and putting $\psi = F\psi_0$ for excited states. The ''Schrödinger'' equation for the functions S and F can be formulated rigorously [6] and it is tempting to define approximations by a suitable truncation of a loop space expansion of these quantities [6,7,10].

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 a 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 Sec. II. The group of the link variables, the local lattice gauge group, and the lattice Euclidean group will play a role.

As discussed in Sec. III, 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 wave function related to the ground state function S and to the ''excitation operator'' F.

This structure has been used in Refs. [6,7,10] 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 wave functions 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 and handling such a basis in an effective way is addressed in the Secs. IV–VI. There exist two strategies for the construction of such basis systems.

(1) Section IV. 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. [11]. An application is the ''exact linked cluster expansion'' discussed in Ref. [12].

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) Section V. 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 wave functions is in general nonorthogonal and *overcomplete*.

In Refs. [6–8] the problem of having linear dependences was solved 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 wave functions generated from up to fourth order plaquette polynomials have been possible up to now.

In Sec. V 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 D-loop functions can, up to a normalization factor, be uniquely characterized by the eigenvalue pattern of a certain set of commuting Casimir operators.

(2) The same Casimir operators may be used to generate suitable subsets of character functions. Hereby, also the matrix elements of these operators are determined.

Diagonalizing these (in general small) Casimir operator matrices in the space of character functions yields then the mapping on the D-loop states.

This solves the problem of linear dependences among the character 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.

(3) Section VI. The characteristic coupled cluster matrix elements are easily computed within the (nonorthogonal and overcomplete) character functions. Using the mapping to the D-loop basis, the final calculation of the Kogut-Susskind eigenvalue problem can be done with respect to this orthogonal basis.

Our procedure yields the usual ordering for the basis functions [6–10] connected with a Lanczos idea. The problem of choosing a truncation based on this ordering is outlined in the last section, Sec. VII. Here, we also discuss the general limitations of a truncated calculation in the sense of a scaling window.

The Appendix contains a complete description of the construction of the mapping between the D-loop functions and the character functions for the example of the SU(2) Kogut-Susskind theory in two dimensions up to the third order. Also the corresponding ingredients for the computation of the coupled cluster matrix elements are given. These examples are important for the clarification of our considerations.

Numerical calculations within the presented framework generalizing the previous attempts [6–10] are on the way and will be published in the future [17].

II. 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

$$\mathcal{H}=\{\Psi(U_1,\ldots U_N)\}, \tag{1}$$

where the quantities U_l ($l=1,\ldots,N$) 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 as 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

$$D^{j_1}_{m_1,m_1'}(U_1)D^{j_2}_{m_2,m_2'}(U_2)\cdots D^{j_N}_{m_N,m_N'}(U_N). \tag{2}$$

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

$$G_{\rm loc}=[\mathrm{SU}(n)]^M, \tag{3}$$

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

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

$$[\rho(g)\Psi](U_1,\ldots,U_N)=\Psi(U_1^g,\ldots,U_N^g), \tag{4}$$

where the link variables are transformed like parallel transporters,

$$U_l^g=g(x)U_l g^{-1}(x+\epsilon e_j), \tag{5}$$

if the link $l=(x,e_j)$ connects the sites x and $x+\epsilon e_j$ (ϵ is the lattice spacing, and e_j is a positive unit vector in the 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 ρ, i.e., by the gauge-invariant states

$$\mathcal{H}_{\rm phys}=\{\Psi\in\mathcal{H}\,|\,\rho(g)\Psi=\Psi \ \text{ for all } \ g\in G_{\rm loc}\}. \tag{6}$$

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

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 Euclid-

ean group is a discrete remnant of the standard continuum Euclidean group and is defined as follows:

Let

$$R^D_{\rm latt}=\left\{ x=\epsilon\sum_{j=1}^{D} n_j e_j \,\middle|\, n_j=\text{integer}\right\} \tag{7}$$

be the set of lattice sites of an infinite lattice. The lattice translation group $G_{\rm lt}$ is then isomorphic to $R^D_{\rm latt}$ and given by the mapping of $R^D_{\rm latt}$:

$$x\to x+a \tag{8}$$

for any $a\in R^D_{\rm latt}$. The lattice rotation group $G_{\rm LR}$ is the restriction of the group $O(D)$ leaving $R^D_{\rm latt}$ invariant. We call $G_{\rm LR}$ 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 lattice Euclidean group G_E is then the semidirect product $G_E=G_{\rm LR}\otimes_s G_{\rm LT}$ defined for $u=(R,a)\in G_E$ by the mapping of $R^D_{\rm latt}$:

$$x\to ux=Rx+a. \tag{9}$$

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 $x+\epsilon e_j$ $(x\in R^D_{\rm latt})$ 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

$$\lambda\to u\lambda=(ux,Rc_j). \tag{10}$$

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 $U\to U^{-1}$ if the link in question is reoriented: If Ψ 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

$$[T(u)\Psi](U_{n_1},\ldots,U_{n_r})=\Psi(U^{\sigma_1}_{l_1},\ldots,U^{\sigma_r}_{l_r}). \tag{11}$$

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 $\mathcal{H}_{\rm phys}$ corresponding to specific irreducible representations of G_E.

For translations we have a ''lattice momentum projection''

$$\Pi_{\rm LT}(p)=\sum_{a\in R^D_{\rm latt}} e^{-ia_jp_j}T(R=1,a), \tag{12}$$

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

If $d^\Gamma_{\nu,\nu'}$ denote the D functions for the irreducible representations (including inversions) of the cubic group $G_{\rm LR}$ [13], a projection on ''lattice angular momentum'' Γ is given by

$$\Pi_{\rm LR}(\Gamma;\nu,\nu')=\sum_{R\in G_{\rm LR}} d^\Gamma_{\nu\nu'}(R)T(R,a=0). \tag{13}$$

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

$$T(1,a)\Pi_{\rm LT}(p)\Psi=e^{ip_ja_j}\Pi_{\rm LT}(p)\Psi,$$

$$T(R,0)\Pi_{\rm LR}(\Gamma;\nu,\nu')\Psi=\sum_{\nu''} d^\Gamma_{\nu,\nu''}(R)\Pi_{\rm LR}(\Gamma;\nu'',\nu')\Psi. \tag{14}$$

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

$$\Psi^{\Gamma p}_{\nu\nu'}=\Pi_{\rm LT}(p)\Pi_{\rm LR}(\Gamma,\nu\nu')\Psi, \tag{15}$$

the relations

$$T(1,a)\Psi^{\Gamma p}_{\nu\nu'}=e^{ip_ja_j}\Psi^{\Gamma p}_{\nu\nu'},$$

$$T(R,0)\Psi^{\Gamma,p}_{\nu\nu''}=\sum_{\nu'} d^\Gamma_{\nu\nu''}(R)\Psi^{\Gamma,Rp}_{\nu''\nu'}. \tag{16}$$

The basic problem of a ''lattice Yang-Mills theory'' is then to find in $\mathcal{H}_{\rm phys}$ (approximate) eigenfunctions of the type $\Psi^{\Gamma p}_{\nu\nu'}$ of the Kogut-Susskind Hamiltonian [1] $H_{\rm KS}=(g^2/2\epsilon)H$ with

$$H=E_{la}E_{la}-xV,\quad V=\sum_{\square}\chi_\square,\quad x=\frac{2}{g^4}, \tag{17}$$

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

$$\chi_\square:=\mathrm{tr}U^{\sigma_1}_{l_1}U^{\sigma_2}_{l_2}U^{\sigma_3}_{l_3}U^{\sigma_4}_{l_4}, \tag{18}$$

when $\square=(l_1,\sigma_1,\ldots,l_4,\sigma_4)$. The ''color-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

$$[E_{la},U_{l'}]=\delta_{ll'}\lambda^aU_l, \tag{19}$$

where the SU(n) generators λ^a are normalized according to $\mathrm{tr}\lambda^a\lambda^b=\delta^{ab}/2$.

III. 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 ϕ and diagonalize H restricted to the finite-dimensional space spanned by $(\phi, H\phi, H^2\phi, \ldots, H^n\phi)$. 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 ground state energy E_0 and excitation energies $E-E_0$ of H_{KS} have the behavior

$$E_0 \propto N, \quad E-E_0 \propto 1. \tag{20}$$

Also the ground state wave function 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*

$$\Psi_0(U) = \exp[S(U)] \tag{21}$$

$[U=(U_1,..,U_N)]$ for the ground state and

$$\Psi(U) = F(U)\exp[S(U)] \tag{22}$$

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 Ψ_0.

The validity of these volume dependences 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 nonlinear equation

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

for S and in the linear equation

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

for the excitation operator F.

Here, we use the abbreviation

$$\mu = (l,a) \tag{25}$$

for link-color quantum number and the notation

$$f_\mu = [E_{la}, f], \quad f_{\mu\mu} = [E_{la}, [E_{la}, f]] \tag{26}$$

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 Eq. (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,Γ,ν,ν') [see Eq. (15)]. We then write F and S in the form (S has to have trivial quantum numbers)

$$F(p,\Gamma,\nu,\nu') = \Pi_{\mathrm{LT}}(p)\Pi_{\mathrm{LR}}(\Gamma;\nu,\nu')F_{\mathrm{int}}(p,\Gamma,\nu,\nu'),$$

$$S = \Pi_0 S_{\mathrm{int}}, \quad \Pi_0 = \Pi_{\mathrm{LT}}(0)\Pi_{\mathrm{LR}}(0,0,0). \tag{27}$$

If $F\Psi_0$ corresponds in the continuum limit to a *bound state*, we expect that F_{int} may be chosen to describe a *localized* state. This is analogous to nonrelativistic 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_{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 Secs. IV and V.

We call the basis

$$\chi^\alpha(U_{l_1}, \ldots, U_{l_{m_\alpha}}), \quad \alpha = 1,2,3, \ldots, \tag{28}$$

and impose the following conditions: (1) χ^α should be gauge invariant; (2) χ^α should be ''linked'' (see Sec. V for the precise definition); a main consequence is that m_α is finite for any α, though not limited; (3) χ^α should be ''standardized''; i.e., the equation

$$T(u)\chi^\alpha = \lambda\chi^\beta (u \in G_E) \tag{29}$$

should only have solutions for $\alpha=\beta$; (4) χ^α should be a strong coupling eigenfunction, i.e.,

$$\sum_a E_{l,a}E_{l,a}\chi^\alpha = \epsilon_{\alpha,l}\chi^\alpha. \tag{30}$$

It will be convenient to specify χ^1 as the ''plaquette function'' by putting [see Eq. (17)]

$$\Pi_0\chi^1 = 4(D-1)V \tag{31}$$

and to distinguish the constant function via

$$\chi^0 = 1. \tag{32}$$

χ^0 fulfills the relation

$$\Pi_0\chi^0 = s_0 N\chi^0, \tag{33}$$

where the symmetry factor $s_0 = |G_{\mathrm{LR}}|$ is equal to 8 and 48 for $D=2$ and 3, respectively.

Simplifying Eq. (27) by writing $F=\Pi F_{\rm int}$ and introducing the functions $\widetilde{S}(S)$ and $\widetilde{F}(S,F)$ by

$$(\Pi_0 S_{\rm int})_\mu(\Pi_0 S_{\rm int})_\mu=\Pi_0\widetilde{S},\quad (\Pi F_{\rm int})_\mu(\Pi_0 S_{\rm int})_\mu=\Pi\widetilde{F}, \tag{34}$$

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

$$(S_{\rm int})_{\mu\mu}+\widetilde{S}-\frac{x}{4(D-1)}\chi^1=\frac{E_0}{s_0 N},$$

$$(F_{\rm int})_{\mu\mu}+2\widetilde{F}=(E-E_0)F_{\rm int}. \tag{35}$$

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 $|S_{\rm int}|,|F_{\rm int}|\propto 1$, we have also $|\widetilde{S}|,|\widetilde{F}|\propto 1$.

The norm relations for $S_{\rm int}$ and $F_{\rm int}$ are fulfilled because of their localized nature; those for $\widetilde{S},\widetilde{F}$ 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

$$\sum_\alpha=\sum_{\alpha=1,2,\ldots},\quad \sum_\alpha{}'=\sum_{\alpha=0,1,2,\ldots}, \tag{36}$$

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

$$S_{\rm int}(U)=\sum_\alpha S_\alpha\chi^\alpha(U),$$

$$F_{\rm int}(p,\Gamma,\nu,\nu';U)=\sum_\alpha{}' F_\alpha(p,\Gamma,\nu,\nu')\chi^\alpha(U). \tag{37}$$

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

$$\epsilon_\alpha S_\alpha+\sum_{\beta,\gamma}C_\alpha^{\beta\gamma}S_\beta S_\gamma=\frac{x}{4(D-1)}\delta_{\alpha 1}+\frac{E_0}{s_0 N}\delta_{\alpha 0}, \tag{38}$$

$$\epsilon_\alpha F_\alpha(p,\Gamma,\nu,\nu')$$

$$+2\sum_{\beta,\gamma,\nu_1}{}' C_\alpha^{\beta\gamma}(p,\Gamma,\nu_1,\nu')S_\beta F_\gamma(p,\Gamma,\nu,\nu_1)$$

$$=(E-E_0)F_\alpha(p,\Gamma,\nu,\nu'),$$

$$\epsilon_\alpha=\sum_l \epsilon_{\alpha,l}. \tag{39}$$

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 $\widetilde{S}$ and $\widetilde{F}$, respectively, which are obtained as follows.

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

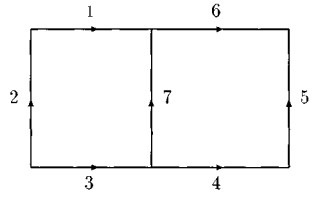

FIG. 1. Link pattern of the D-loop functions (42). The numbers indicate the enumeration of the link angular momenta $(J_1,\ldots,J_7)$.

$$\sum_{u\in G_E}\chi^\beta T(u)\chi^\gamma=\sum_{\alpha,u}{}' c_{\alpha,u}^{\beta\gamma}T(u)\chi^\alpha\quad(\beta,\gamma\neq 0) \tag{40}$$

for all cases where the functions χ^β and $T(u)\chi^\gamma$ *have a common link variable*. This yields, then,

$$C_\gamma^{\alpha\beta}(p,\Gamma,\nu,\nu')=\tfrac{1}{2}(\epsilon_\gamma-\epsilon_\alpha-\epsilon_\beta)$$

$$\times\sum_{u=(R,a)}c_{\gamma,R,a}^{\alpha\beta}d_{\nu\nu'}^{\Gamma}(R^{-1})e^{-ip_j a_j},$$

$$C_\gamma^{\alpha\beta}=C_\gamma^{\alpha\beta}(0,0,0,0). \tag{41}$$

A proof hereof is given in the Appendix (subsection 1). The linked cluster theorem guaranteeing the correct volume dependences of the relevant quantities discussed above is now given by the fact that, due to the localized nature of the functions χ^α, the right-hand side (RHS) sums in Eqs. (40) and (41) run only over a finite number of terms.

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

The important task is now to compute the matrix elements $c_{\alpha u}^{\beta\gamma}$, for which one needs an efficient and systematic way to set up and handle the basis elements χ^α.

IV. *D*-LOOP BASIS

An orthogonal basis of functions χ^α 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 χ^α (α fixed) depends on the link variables $(U_{l_1},\ldots,U_{l_r})$. 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 four-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 two-point vertex and by the condition that the coupling $J_a+J_b\to J_c$ should be possible if (l_a,l_b,l_c) form a three-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 $[\alpha=(J_1,J_4,J_7)]$

$$\chi^{\alpha}=\sum_{M_1,\ldots,M_{10}} D^{J_1}_{M_1,M_2}(U_1)D^{J_1}_{M_2,M_3}(U_2)D^{J_1}_{M_3,M_8}(U_3^{-1}) \times\begin{pmatrix} J_1,J_7,J_4 \\ M_8,M_{10},M_4 \end{pmatrix} D^{J_7}_{M_7,M_{10}}(U_7)\begin{pmatrix} J_1,J_7,J_4 \\ M_1,M_7,M_9 \end{pmatrix} \times D^{J_4}_{M_4,M_5}(U_4^{-1})D^{J_4}_{M_5,M_6}(U_5^{-1})D^{J_4}_{M_6,M_9}(U_6). \quad (42)$$

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

In view of the construction of a mapping between this basis and the character functions (see below), it is convenient to rephrase the characterization of these states in the following way. For any $\chi^{\alpha}=\chi^{\alpha}(U_{l_1},\ldots,U_{l_{r_\alpha}})$ (α fixed) there exists a characteristic (finite) set of commuting operators $(A_1,\ldots,A_{M_\alpha})$ with the property that

$$A_\lambda\chi^{\alpha}=a_\lambda\chi^{\alpha} \quad (43)$$

and such that the state χ^{α} is *uniquely* characterized by the eigenvalues $(a_1,\ldots,a_{M_\alpha})$.

In the case SU(2) and $D=2$, these operators are given by a combination of the two sets

$$\sum_a E_{\lambda a}E_{\lambda a}, \quad \lambda=l_1,\ldots,l_{r_\alpha}, \quad (44)$$

and all operators

$$\sum_a (E_{ba}+E_{ca})(E_{ba}+E_{ca}), \quad (45)$$

which fulfill the condition that (b,c) are ingoing links of a four-point vertex in the link set related to χ^{α}.

The more general case may be extracted from Refs. [11,12]. Important for our purpose is that each A_λ is a Casimir operator of the local lattice gauge group $G_{\rm loc}$, 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 (43). In addition, suitable permutation operators have to be included if the SU(3) Clebsch-Gordan decompositions generalizing Eq. (42) have the property that the same irreducible representations occur several times. [For SU(2), an example for the definition of such a permutation operator is given in the Appendix (subsection 3).]

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.

V. THE SET OF CHARACTER FUNCTIONS

An alternative for the construction of a basis avoiding the explicit handling of SU(n) couplings and allowing an easy computation of the coupled cluster matrix elements 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 think that this is indeed the most convenient starting point for defining the basis and we will pursue this idea in detail in this paper.

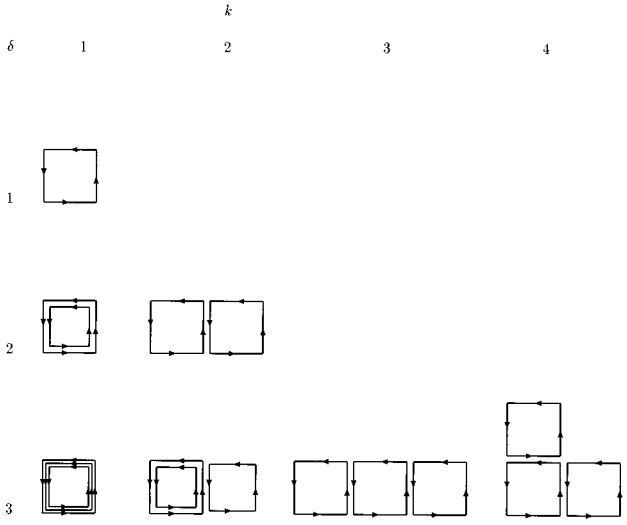

FIG. 2. Loop structure of the generic character functions $\Lambda_G^{\delta,k}$ [see Eq. (49)] up to order $\delta=3$ for SU(2).

We will define this method here systematically 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 simple way of eliminating linear dependences.

The basic idea of Refs. [6–10] is to work with the general set of loop space functions given by the algebra of all characters related to closed lattice loops, i.e., to work with linear combinations of functions of the type

$$\prod_{j=1}^{r} \mathrm{tr}(U^{\sigma_{j1}}_{l_{j1}}\cdots U^{\sigma_{jm_j}}_{l_{jm_j}}), \quad (46)$$

which are defined in terms of loops $L_1,\ldots,L_r$ given by certain sets of generalized connected links:

$$L_j=(l_{j1},\sigma_{j1},\ldots,l_{jm_j},\sigma_{jm_j}). \quad (47)$$

The simplest example is the plaquette function (18); more examples will be given below, especially also in Figs. 2 and 4 and in the Appendix (subsection 2).

The clear merit of these functions is that they are manifestly gauge invariant and that a product decomposition of the type (40) can be easily worked out; their deficiency is that they are neither orthogonal nor linear independent.

In Refs. [6–10] linear-independent subsets were selected by using the Cayley-Hamilton relationship which yielded nonorthogonal basis elements which were no strong coupling eigenstates [i.e., Eq. (30) was not fulfilled which invalidates the possibility of leaving out in Eq. (40) the derivatives present in the original coupled cluster equations (23) and (24); see the Appendix (subsection 1)].

Here we will follow a new and hopefully more systematic strategy by relating the character functions (46) to the D-loop basis of Sec. IV (which are strong coupling eigen-

states) by diagonalizing simultaneously the commuting operators A_λ [Eq. (43)]. This is possible because the matrix elements of these operators, being of the type of second (or perhaps third) order derivative [see Eqs. (44) and (45)], may be computed with respect to the character functions using the commutation rules (19), the product rule of differentiation, and the standard property of the SU(n) generators λ^a:

$$\sum_a \lambda^a_{ij}\lambda^a_{i'j'} = \frac{1}{2}\left(\delta_{ij'}\delta_{ji'} - \frac{1}{n}\delta_{ij}\delta_{i'j'} \right). \tag{48}$$

We describe now this construction of the D-loop basis in terms of the character functions in detail and start with the introduction of a systematic *ordering* of the character functions (46) related to a Lanczos iteration of the product decomposition in Eq. (40) (see [6–8]).

A. Generic functions

First, we introduce the set of ''generic'' functions

$$\Lambda_G^{\delta,k}\ \delta = 1,2,\ldots\ k = 1,..,n_\delta, \tag{49}$$

of δ-fold *linked, standardized plaquette products*.

δ is the ''order'' of the function $\Lambda_G^{\delta,k}$. In first order we have $n_1 = 1$ and the character (49) is the plaquette function $\Lambda_G^{1,1} = \chi^1$.

Generally, we have the structure that for each (δ,k), $\delta \geqslant 2$, there exist Euclidean group elements $u_2, \ldots, u_\delta$ [depending on (δ,k)] such that $\Lambda_G^{\delta,k} = \chi^1 T(u_2)\chi^1 \ldots T(u_\delta)\chi^1$.

For SU(2), all occurring plaquettes $T(u_r)\chi^1$ should have the *same orientation* because we have $\mathrm{tr}g = \mathrm{tr}(g^\dagger)$ in this case.

For $D=2$, we have, for SU(2), $n_\delta = 1,2,4$ and for SU(3), $n_\delta = 1,4,12$ up to third order. Figure 2 gives the corresponding loop patterns of the functions (49) for SU(2).

The relevance of this set of functions is twofold.

(i) They determine, using just combinatorics, the possible elements of the D-loop basis occurring at order δ. They are given by the geometry of the link patterns of the generic set and by the condition that the eigenvalues of the ''link'' Casimir operators (44) should be consistent with 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.

Figure 3 exemplifies the related elements of the D-loop basis for SU(2) and $D=2$ up to $\delta=3$. Hereby, the basis elements are characterized by their link patterns (in analogy to Fig. 1) and by the eigenvalue patterns of the relevant Casimir operators (43).

Note that this gives the D-loop basis functions the natural quantum numbers (δ,k,ν) where ν counts different states related to the same generic function $\Lambda_G^{\delta,k}$.

(ii) The functions (49) are generic in analogy to the ''maximum weights'' occurring in the representation theory of compact Lie groups in the following sense.

B. Casimir subspaces

The application of the relevant Casimir operators generates from the states $\Lambda_G^{\delta,k}$ (δ,k fixed) characteristic ''Casimir subspaces'' of finite (in general small) dimension $M(\delta,k)$; i.e., one can find character functions

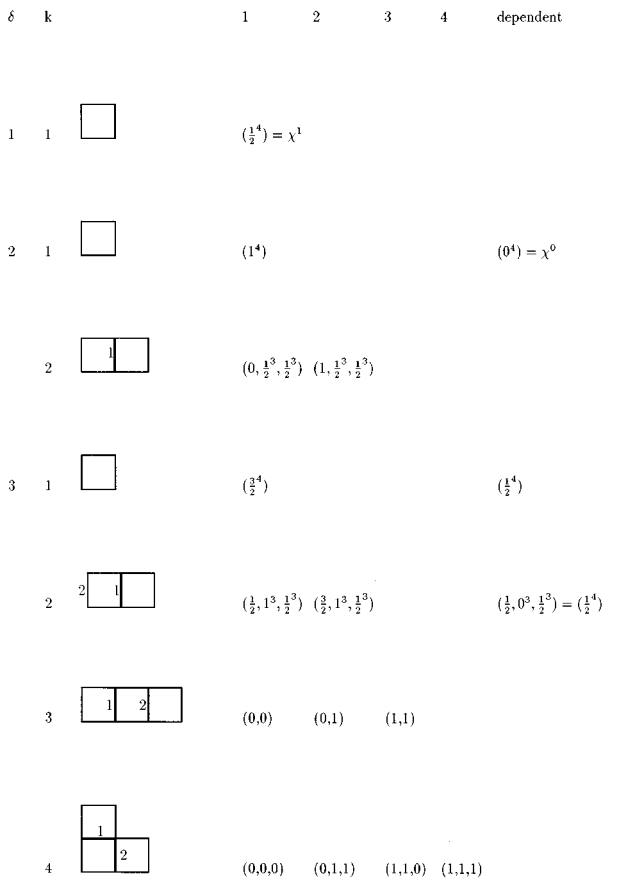

FIG. 3. SU(2) D-loop basis functions $\chi^{\delta,k,\nu}$ characterized by the link patterns and the related relevant Casimir eigenvalue patterns which are generated up the order $\delta=3$. If more than one unequal angular momentum occurs, the related links are enumerated in the link patterns and indicated in that order in the eigenvalue patterns. Angular momenta which correspond to unmarked links are placed behind the marked ones. Upper indices stand for the degeneracy of the 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 $\mathbf{j}_1+\mathbf{j}_2$ [Eq. (45)]. 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.

$$\Lambda^{\delta,k,\nu}, \quad \nu = 1,\ldots,M(\delta,k), \tag{50}$$

with $\Lambda^{\delta,k,1} = \Lambda_G^{\delta,k}$, spanning subspaces such that the evaluation of the relevant Casimir operators on these states mixes only the states with fixed (δ,k). (In principle, this is true for all Casimir operators of the local lattice gauge group, but only a finite set is relevant.) Consequently, with respect to the states (50) the relevant Casimir operators are reduced to $M\times M$ matrices

$$A_\lambda \Lambda^{\delta,k,\nu} = \sum_{\nu'=1}^{M(\delta,k)} A^\nu_{\nu'}(\lambda,\delta,k)\Lambda^{\delta,k,\nu'}. \tag{51}$$

Invoking the product rule and eliminating the resulting SU(n) generators with the help of Eq. (48) yields for the

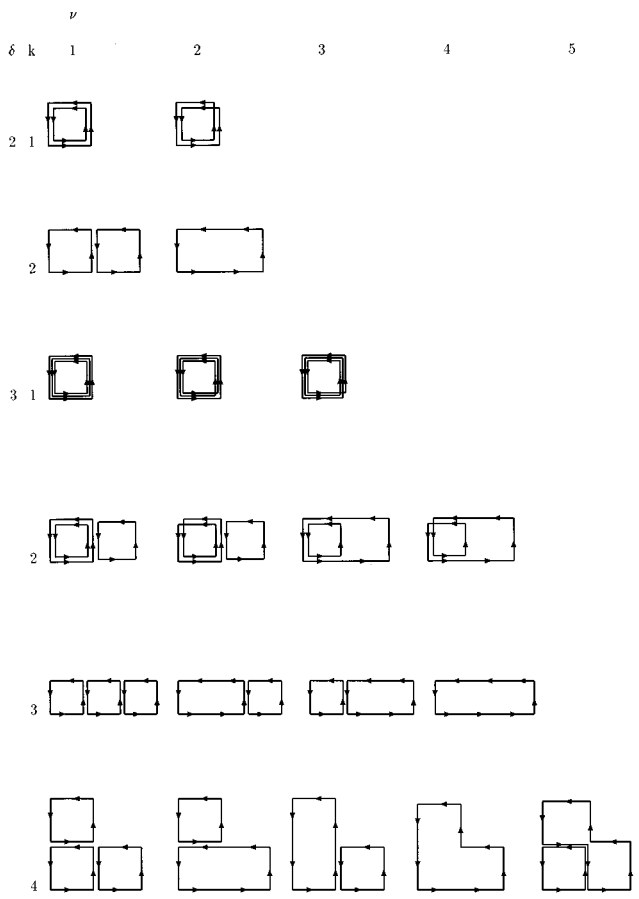

FIG. 4. Loop structure of the functions $\Lambda^{\delta,k,\nu}$ [see Eq. (50)] up to order $\delta=3$.

loop structure of the subspaces (50) (δ,k fixed) the simple geometrical condition that they are generated from the plaquette systems of the generic functions (49) 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. In the Appendix (subsection 2), the validity of the asserted property of the spaces (50) is demonstrated for these examples by working out the Casimir matrices (51).

Note that the sets (50) may also contain elements of lower order if they occur during the cutting and gluing procedure. Also a standardization is not introduced. This is convenient since this makes the ''Casimir matrices'' (51) especially simple. Note also that the range $M(\delta,k)$ of the quantum number ν in Eq. (51) is in general *larger* than the corresponding range of the D-loop basis states $\chi^{\delta,k,\nu}$.

C. *D* mapping

In order to relate the loop space functions (50) to the D-loop basis, one has to diagonalize the Casimir matrices (51), giving the eigenfunctions

$$\varphi^{\nu}(\delta,k)=\sum_{\nu'} C^{\nu}_{\nu'}(\delta,k)\Lambda^{\delta,k,\nu'}, \tag{52}$$

obeying

$$A_{\lambda}\varphi^{\nu}(\delta,k)=a_{\lambda}(\nu,\delta,k)\varphi^{\nu}(\delta,k). \tag{53}$$

For the SU(2), $D=2$ cases up to third order, this diagonalization is worked out in the Appendix (subsection 2). This yields examples for the following general structure of the mapping to the basis function χ^{α}.

With a suitable enumeration $\overline{\alpha(}\nu,\delta,k)$ one may identify

$$\varphi^{\nu}(\delta,k)=N(\nu,\delta,k)T(\overline{u(}\nu,\delta,k))\chi^{\overline{\alpha(}\nu,\delta,k)}. \tag{54}$$

Hereby, linear dependences are eliminated by the identification prescription

$$\overline{\alpha(}\nu,\delta,k)=\overline{\alpha(}\nu',\delta',k')\Leftrightarrow a_{\lambda}(\nu,\delta,k)=a_{\lambda}(\nu',\delta',k') \quad \text{for all } \lambda. \tag{55}$$

Also, one has to put $\varphi^{\nu}(\delta,k)=0$ if one of the eigenvalues $a_{\lambda}(\nu,\delta,k)$ is incompatible with the known possible eigenvalues of the Casimir operators [see the Appendix (subsection 2) for examples].

Of course, the equality of the eigenvalue patterns as in Eq. (55) guarantees the equality of the corresponding eigenfunctions only up to a (nonzero) factor $N(\nu,\delta,k)$ and up to a Euclidean transformation $T(\overline{u(}\nu,\delta,k))$.

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 1. Hence only the relative factors are needed; i.e., we may put $N(\nu,\delta,k)=1$ if the D-loop function $\chi^{\overline{\alpha(}\nu,\delta,k)}$ occurs for the first time when increasing the order δ. Also we may set for this first case $\overline{u(}\nu,\delta,k)=1$. As a result we may find for each number α an eigenfunction (52) characterized by $(\delta(\alpha),\overline{\nu(}\alpha),k(\alpha))$ defining an expansion of the elements of the D-loop basis in terms of the character functions

$$\chi^{\alpha}=\sum_{\nu'} C^{\overline{\nu(}\alpha)}_{\nu'}(\overline{\delta(}\alpha),\overline{k(}\alpha))\Lambda^{\overline{\delta(}\alpha),\overline{k(}\alpha),\nu'}. \tag{56}$$

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

$$\Lambda^{\delta,k,\nu}=\sum_{\nu'} D^{\nu}_{\nu'}(\delta,k)N(\nu',\delta,k)T(\overline{u(}\nu',\delta,k))\chi^{\overline{\alpha(}\nu',\delta,k)}. \tag{57}$$

See again the Appendix (subsection 2) for examples.

Equations (56) and (57) constitute a mapping between the D-loop basis and the character functions, called ''D mapping,'' in a form which is sufficient for the computation of the coupled cluster matrix elements (40).

We still have to give a recipe to compute the (relative) 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 [6–10]

$$\mathrm{tr}g^{\dagger}=\mathrm{tr}g \tag{58}$$

$$g^2=g\,\mathrm{tr}g-1 \quad [g\in \mathrm{SU}(2)] \tag{59}$$

and

$$\mathrm{tr}g^2=(\mathrm{tr}g)^2-2\mathrm{tr}g^\dagger, \tag{60}$$

$$g^3=g^2\mathrm{tr}g-g\mathrm{tr}g^\dagger+1 \quad [g\in \mathrm{SU}(3)]. \tag{61}$$

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 $\mathrm{tr}g^n g'$ with $n\geqslant 2$ [$n\geqslant 3$]. For this purpose, Eqs. (59) and (61), respectively, have to be iterated, yielding formulas of the type $g^n=ag^2+bg+c$ where a,b,c are polynomials in $\mathrm{tr}g$ and $\mathrm{tr}g^\dagger$. [For SU(2), $a=0$ and b,c become polynomials in $\mathrm{tr}g$ only.]

For SU(3) and $n=2$, also terms of the type $\mathrm{tr}g^2$ in Eq. (46) may be standardized with the help of Eq. (60). [See the Appendix (subsection 2) for examples.]

VI. COUPLED CLUSTER MATRIX ELEMENTS

The loop space character of the functions $\Lambda^{\delta,k,\nu}$ allows us to compute the coupled cluster matrix elements $c^{\alpha_1,\alpha_2}_{\alpha_3,u}$ in Eq. (40) in two steps.

A. Incorporation of the Euclidean group

The first step is to incorporate the Euclidean group in the product decomposition of Eq. (40) on the level of the (nonorthogonal and overcomplete) character functions (50) by computing the coefficients $\eta^{\gamma_1,\gamma_2}_{\gamma_3;u,v}$ $(u,v\in G_E)$ given by

$$\Lambda^{\gamma_1}T(u)\Lambda^{\gamma_2}=\sum_{\gamma_3,v}\eta^{\gamma_1,\gamma_2}_{\gamma_3;u,v}T(v)\Lambda^{\gamma_3}. \tag{62}$$

Here, we introduced the abbreviation $(\delta,k,\nu)=\gamma$, and the character functions Λ^{γ_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 $\Lambda^{0,1,1}=\chi^0$ should be left out on the left-hand side.

The following structures resulting directly from the loop space nature of the functions Λ^γ simplify the determination of these η coefficients [see the Appendix (subsection 4) for examples].

(a) There is only one nonvanishing term on the RHS of Eq. (62). If $\eta^{\gamma_1,\gamma_2}_{\gamma_3;u,v}$ is nonvanishing, it is equal to 1. In this case we call the corresponding states Λ^{γ_1}, Λ^{γ_2}, and Λ^{γ_3} *nontrivially connected*.

(b) For each triple Λ^{γ_1}, Λ^{γ_2}, and Λ^{γ_3} of nontrivially connected character functions we have a characteristic set of Euclidean group elements u_λ and v_λ such that

$$\Lambda^{\gamma_1}T(u_\lambda)\Lambda^{\gamma_2}=T(v_\lambda)\Lambda^{\gamma_3}, \quad \lambda=1,..,n(\gamma_1,\gamma_2,\gamma_3). \tag{63}$$

The determination of these elements u_λ and v_λ is now simplified by the following structure.

Suppose we have found all solutions u_λ and v_λ for a nontrivially connected triple of *generic functions*

$$\Lambda_G^{\delta_1,k_1}T(u_\lambda)\Lambda_G^{\delta_2,k_2}=T(v_\lambda)\Lambda_G^{\delta_1,k_1}. \tag{64}$$

If v_λ is suitably chosen, we have then for each $\Lambda^{\delta_1,k_1,\kappa_1}$ and $\Lambda^{\delta_2,k_2,\kappa_2}$ a function $\Lambda^{\delta_3,k_3,\kappa_3}$ so that they are nontrivially connected with the same set of Euclidean group elements as in Eq. (63) and this exhausts all possibilities.

Given the generic functions of the RHS of Eq. (64) and κ_1 and κ_2, the third character function $\phi^{\delta_3,k_3,\kappa_3}$ is then determined by finding *just one* pair (uv) solving Eq. (62).

Up to third order $\delta_3=3$, a full computation of all η coefficients is presented in the Appendix (subsection 4).

B. Computation of the c coefficients in Eq. (40)

Having solved the ''combinatorial'' problem of determining the coefficients of Eq. (62), one may compute the quantities $c^{\alpha_1,\alpha_2}_{\alpha,u}$ by writing Eq. (62) in terms of the orthogonal and independent basis $\underline{\chi^\alpha}$ with the help of Eqs. (56) and (57). Writing $\overline{\gamma(\alpha)}=(\delta(\alpha),k(\alpha),\overline{\nu(\alpha)})$ and recalling Eq. (54) for the definition of the function $\overline{u(\gamma)}$ we obtain, as a final result for the crucial coupled cluster matrix elements (40),

$$c^{\alpha_1,\alpha_2}_{\alpha_3,u}=\sum_{v\in G_E}\sum_{\gamma_1,\gamma_2,\gamma_3}\sum_{\gamma_4 \text{ with } \overline{\alpha(\gamma_4)}=\alpha_3} \times C^{\overline{\gamma(\alpha_1)}}_{\gamma_1}C^{\overline{\gamma(\alpha_2)}}_{\gamma_2}N(\gamma_4)\,\eta^{\gamma_1,\gamma_2}_{\gamma_3;u,v\,\overline{u(\gamma_4)}^{-1}}D^{\gamma_3}_{\gamma_4}. \tag{65}$$

VII. 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 is 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, and the nonorthogonality 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 previously [6–8,10]. Here we want to stress the following points in connection with this problem.

(1) In principle, several strategies have to be tried in order to find the ''best'' truncation. The ultimate criterium for the quality should be that higher orders become small. This makes higher order calculations most important.

(2) The prescription of Guo *et al.* [10] seems very promising. In our notation this truncation is defined by putting, in order δ,

$$c^{\alpha_1,\alpha_2}_{\alpha_3,u}=0 \quad \text{for} \quad \delta_1+\delta_2>\delta, \tag{66}$$

where $\alpha_j=\overline{\alpha(\delta_j,k_j,\nu_j)}$ $(j=1,2,3)$. This prescription limits the expansions (37) to the order δ. In Ref. [10], a rather successful, up to fourth order calculation was done with this truncation for a O^+ glueball with zero momentum.

(3) In nonrelativistic many-body theory, the standard truncation prescription is given by *projecting* the coupled cluster form of the eigenvalue equation on a suitable *finite set of orthogonal* Hilbert space states [15]. Hereby, the set of all states has to be ordered and the finite set used in the projection becomes larger and larger with increasing order, exhausting in the limit the whole Hilbert space.

This method is also well defined for the case of our Kogut-Susskind theory [9]. Within our formulation a natural choice for ordered sets of states would be the D-loop functions. Because of their orthogonality and because our formulation of the coupled cluster equations is in terms of an expansion in these D-loop functions, the computation of the projections (in terms of an N-fold Haar measure integral) is trivial. As a result we obtain in this case the truncation prescription, in order δ,

$$c^{\alpha_1,\alpha_2}_{\alpha_3,u}=0 \quad \text{for} \quad \delta_1,\ \delta_2,\ \text{or}\ \delta_3>\delta. \tag{67}$$

In Ref. [6] a similar method was introduced using, however, a *nonorthogonal* loop space basis. The experience of standard many-body theory is that the orthogonality is essential [15] so that Eq. (67), defined in terms of the D-loop basis, possibly improves the results of Ref. [6].

We want to stress that any truncated coupled cluster calculation (which is formululated in the infinte volume limit) 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. [10] which gives the ''best'' coupled cluster results up to now.)

The reason for this expected scaling window is 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 [16].

A systematic numerical analysis of these points is, of course, needed. Concrete calculations in this direction are on the way and will be reported in the future [17].

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 appears to be no more complicated than that for glueballs. Details of this structure will be reported elsewhere.

ACKNOWLEDGMENTS

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APPENDIX

1. Proof of Eq. (37)

Introducing the abbreviation

$$D^{p,\Gamma}_{\nu,\nu'}(R,a)=d^{\Gamma}_{\nu\nu'}(R)e^{ip_ja_j}, \tag{A1}$$

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

$$\begin{aligned}
&[\Pi_{\mathrm{LT}}(p)\Pi_{\mathrm{LR}}(\Gamma;\nu,\nu')\chi^\alpha]_\mu(\Pi_0\chi^\beta)_\mu \\
&\quad=\sum_{u_1,u_2\in G_E} D^{p,\Gamma}_{\nu,\nu'}(u_1)[T(u_1)\chi^\alpha]_\mu[T(u_2)\chi^\beta]_\mu \\
&\quad=\sum_{u_1,u_2\in G_E} D^{p,\Gamma}_{\nu,\nu'}(u_1)[T(u_1)\chi^\alpha]_\mu[T(u_1)T(u_1^{-1}u_2)\chi^\beta]_\mu \\
&\quad=\sum_{u_1} D^{p,\Gamma}_{\nu,\nu'}(u_1)T(u_1)\left[\sum_u \chi^\alpha_\mu(T(u)\chi^\beta)_\mu\right].
\end{aligned} \tag{A2}$$

The derivatives in the quantity $\Sigma_u\chi^\alpha_\mu[T(u)\chi^\beta]_\mu$ may be evaluated by using the ''total angular momentum'' $\mathbf{E}^2=\Sigma_\mu E_\mu E_\mu$ which commutes with any Euclidean operator $T(u)$. Invoking the product rule and the strong coupling eigenfunction properties (30) and (39) of the basis χ^α yields, with the definition (40),

$$\begin{aligned}
&\sum_{\mu,u\in G_E}\chi^\beta_\mu[T(u)\chi^\gamma]_\mu=\sum_{\alpha,u}{}' \tilde{c}^{\beta\gamma}_{\alpha,u}T(u)\chi^\alpha \\
&\tilde{c}^{\beta\gamma}_{\alpha,u}=\tfrac{1}{2}(\epsilon_\alpha-\epsilon_\beta-\epsilon_\gamma)c^{\beta\gamma}_{\alpha,u}.
\end{aligned} \tag{A3}$$

Hereby, the functions χ^β and $T(u)\chi^\gamma$ may be restricted to the cases where they display a common link variable because otherwise the derivatives yield zero. Inserting Eq. (A3) into Eq. (A2) gives the final result (41):

$$[\Pi_{\mathrm{LT}}(p)\Pi_{\mathrm{LR}}(\Gamma;\nu,\nu')\chi^{\alpha}]_{\mu}(\Pi_0\chi^{\beta})_{\mu}$$
$$=\sum_{u_1} D^{p,\Gamma}_{\nu,\nu'}(u_1)T(u_1)\sum_{u,\gamma}\tilde{c}^{\alpha,\beta}_{\gamma,u}T(u)\chi^{\gamma}$$
$$=\sum_{u,\gamma}\tilde{c}^{\alpha,\beta}_{\gamma,u}\sum_{u_1} D^{p,\Gamma}_{\nu,\nu_1}(u_1u)D^{p,\Gamma}_{\nu_1,\nu'}(u^{-1})T(u_1u)\chi^{\gamma}$$
$$=\sum_{\nu_1}\Pi_{\mathrm{LT}}(p)\Pi_{\mathrm{LR}}(\Gamma;\nu,\nu_1)\sum_{u,\gamma}\tilde{c}^{\alpha,\beta}_{\gamma,u}D^{p,\Gamma}_{\nu_1,\nu'}(u^{-1})\chi^{\gamma}. \tag{A4}$$

2. Examples for the *D* mapping

Within this subsection we will give the construction of ''Casimir matrices'' (51) for SU(2) and $D=2$ for some typical cases of subspaces (δ,k) taken from in Fig. 4. Subsequently, we will present the corresponding part of the D mapping resulting from a diagonalization.

Note that the D-loop basis is characterized by the quantum numbers (δ,k,ν); see Fig. 3. Concerning the character functions $\Lambda^{\delta,k,\nu}$, we leave out in the following the quantum numbers (δ,k) if they are fixed when discussing the corresponding specific subspace.

$(\delta,k)=(2,1)$. Here, two parallel links with the same orientation occur. Only one of the four cases of link variables is relevant which we denote by U. Applying the cutting and gluing procedure to Λ^1 yields a two-dimensional space of the type

$$\Lambda^1=\mathrm{tr}(BU)\mathrm{tr}(BU),\quad \Lambda^2=\mathrm{tr}(BUBU). \tag{A5}$$

The evaluation of $A=E_aE_a$ is possible with the help of Eqs. (19) and (48), and the product rule of differentiation. A mixing of the states in Eq. (A5) arises because we have, for instance,

$$\sum_a [\mathrm{tr}(AU)]_a[\mathrm{tr}(BU)]_a=\frac{1}{2}(\mathrm{tr}AUBU)-\frac{1}{2n}\mathrm{tr}(AU)\mathrm{tr}(BU). \tag{A6}$$

The result of a detailed, but straightforward calculation is

$$A\Lambda^1=\Lambda^1+\Lambda^2,\quad A\Lambda^2=\Lambda^1+\Lambda^2. \tag{A7}$$

The diagonalization gives the Casimir spectrum as an example of Eqs. (52) and (53):

$$\varphi^1=\Lambda^1+\Lambda^2,\quad a(1)=2,$$
$$\varphi^2=\Lambda^1-\Lambda^2,\quad a(1)=0. \tag{A8}$$

Eliminating in the state φ^2 the function $(BU)^2$ via Eq. (59) yields the identifications with the D-loop functions (see Fig. 3 for the notation)

$$\varphi^1=\chi^{2,1},\quad \varphi^2=2=2\chi^0. \tag{A9}$$

Note that we put the normalization factor $N(\nu,\delta,k)$ equal to 1 when the corresponding basis state χ^{α} occurs for the first time. Within our examples, the Euclidean mapping $T(u)$ in Eq. (54) is the identity in most cases.

With the inversion

$$\Lambda^1=\tfrac{1}{2}\chi^{2,1}+\chi^0,\quad \Lambda^2=\tfrac{1}{2}\chi^{2,1}-\chi^0, \tag{A10}$$

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

$(\delta,k)=(2,2)$. In this case there is again only one relevant link variable, denoted by U, and the space (50) is of the type

$$\Lambda^1=\mathrm{tr}(BU)\mathrm{tr}(U^{\dagger}C),\quad \Lambda^2=\mathrm{tr}(BC). \tag{A11}$$

A corresponding, straightforward computation yields

$$A\Lambda^1=2\Lambda^1-\Lambda^2,\quad A\Lambda^2=0. \tag{A12}$$

A diagonalization of Eq. (A12) gives

$$\varphi^1=2\Lambda^1-\Lambda^2,\quad a(1)=2,\quad \varphi^2=\Lambda^2,\quad a(1)=0. \tag{A13}$$

With the identification

$$\varphi^1=\chi^{2,2,1},\quad \varphi^2=\chi^{2,2,2}, \tag{A14}$$

and the inversion

$$\Lambda^1=\tfrac{1}{2}(\chi^{2,2,1}+\chi^{2,2,2}),\quad \Lambda^2=\chi^{2,2,2}, \tag{A15}$$

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 subpace given by

$$\Lambda^1=(\mathrm{tr}g)^3,\quad \Lambda^2=\mathrm{tr}g\,\mathrm{tr}g^2,\quad \Lambda^3=\mathrm{tr}g^3, \tag{A16}$$

with $g=BU$. The product rule yields for the evaluation of the Casimir operator

$$A\Lambda^1=\tfrac{3}{4}\Lambda^1+3\Lambda^2,\quad A\Lambda^2=\Lambda^1+\tfrac{3}{4}\Lambda^2+2\Lambda^3,$$
$$A\Lambda^3=3\Lambda^2+\tfrac{3}{4}\Lambda^3. \tag{A17}$$

The eigenvectors and eigenvalues are

$$\varphi^1=\Lambda^1+3\Lambda^2+2\Lambda^3,\quad a(1)=\tfrac{15}{4},$$
$$\varphi^2=\Lambda^1-\Lambda^3,\quad a(2)=\tfrac{3}{4}$$
$$\varphi^3=\Lambda^1-3\Lambda^2+2\Lambda^3,\quad a(3)=-\tfrac{9}{4}. \tag{A18}$$

Using $\mathrm{tr}g^3=(\mathrm{tr}g)^3-3\mathrm{tr}g$ obtained from Eq. (59), this yields the identifications

$$\varphi^1=\chi^{3,1},\quad \varphi^2=3\chi^{1,1}. \tag{A19}$$

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

$$\varphi^3=0, \tag{A20}$$

yielding the linear dependence relation

$$\Lambda^2=\tfrac{1}{3}(\Lambda^1+2\Lambda^3)=(\mathrm{tr}g)^3-2\mathrm{tr}g, \tag{A21}$$

which is just the result for Λ^2 when eliminating g^2 by Eq. (59). The inversion (57) now reads

$$\Lambda^1=\tfrac{1}{6}\chi^{3,1}+2\chi^{1,1},\quad \Lambda^2=\tfrac{1}{6}\chi^{3,1},\quad \Lambda^3=\tfrac{1}{6}\chi^{3,1}-\chi^{1,1}, \tag{A22}$$

$(\delta,k)=(3,4)$. This case is interesting because it involves a four-point vertex; the dimension of the subspace (50) is 5. Calling the doubly occurring link variables U_1 and U_2 the generating character states are of the type

$$\Lambda^1=\mathrm{tr}(BU_1)\mathrm{tr}(U_1^\dagger CU_2)\mathrm{tr}(U_2^\dagger D),$$

$$\Lambda^2=\mathrm{tr}(BCU_2)\mathrm{tr}(U_2^\dagger D),$$

$$\Lambda^3=\mathrm{tr}(BU_1)\mathrm{tr}(U_1^\dagger CD),$$

$$\Lambda^4=\mathrm{tr}(BCD),$$

$$\Lambda^5=\mathrm{tr}(U_1^\dagger CU_2)\mathrm{tr}(BU_1U_2^\dagger D). \tag{A23}$$

Now we have three relevant Casimir operators, A_1 and A_2 as before of type (44) and $A_3=(E_{1a}+E_{2a})(E_{1a}+E_{2a})-A_1-A_2=2E_{1a}E_{2a}$ which is of the type (45). The related Casimir matrices are given by

$$A_1\Lambda^1=2\Lambda^1-\Lambda^2,\quad A_1\Lambda^2=0,\quad A_1\Lambda^3=2\Lambda^3-\Lambda^4,$$

$$A_1\Lambda^4=0,\quad A_1\Lambda^5=-\Lambda^4+2\Lambda^5, \tag{A24}$$

$$A_2\Lambda^1=2\Lambda^1-\Lambda^3,\quad A_2\Lambda^2=2\Lambda^2-\Lambda^4,\quad A_2\Lambda^3=0,$$

$$A_2\Lambda^4=0,\quad A_2\Lambda^5=-\Lambda^4+2\Lambda^5, \tag{A25}$$

$$A_3\Lambda^1=-2\Lambda^1+\Lambda^2+\Lambda^3-\Lambda^5,\quad A_3\Lambda^2=0,\quad A_3\Lambda^3=0,$$

$$A_3\Lambda^4=0,\quad A_3\Lambda^5=2\Lambda^4-4\Lambda^5. \tag{A26}$$

The simultaneous eigenfunctions are

$$\varphi^3=-2\Lambda^1+\Lambda^2+\Lambda^3-\Lambda^4+\Lambda^5,\quad a_1(1)=a_2(1)=2,$$

$$a_3(1)=-2,$$

$$\varphi^4=-2\Lambda^5+\Lambda^4,\quad a_1(2)=a_2(2)=2,\quad a_3(2)=-4,$$

$$\varphi^2=-2\Lambda^2+\Lambda^4,\quad a_1(3)=0,\quad a_2(3)=2,\quad a_3(3)=0,$$

$$\varphi^5=-2\Lambda^3+\Lambda^4,\quad a_1(4)=2,\quad a_2(4)=0,\quad a_3(4)=0,$$

$$\varphi^1=\Lambda^4,\quad a_1(5)=a_2(5)=a_3(5)=0, \tag{A27}$$

with the identifications

$$\varphi^\nu=\chi^{3,4,\nu},\quad \nu=1,2,3,4,\quad \varphi^5=T(P)\chi^{3,4,2}, \tag{A28}$$

where P describes the reflection (parity transformation) defined by $T(P)\Lambda^2=\Lambda^3$.

The inversion (57) reads

$$\Lambda^1=\tfrac{1}{4}[-2\chi^{3,4,3}+\chi^{3,4,1}-\chi^{3,4,2}-T(P)\chi^{3,4,2}-\chi^{3,4,4}],$$

$$\Lambda^2=\tfrac{1}{2}(\chi^{3,4,1}-\chi^{3,4,2}),\quad \Lambda^3=-\tfrac{1}{2}(T(P)\chi^{3,4,2}-\chi^{3,4,1}),$$

$$\Lambda^4=\chi^{3,4,1},\quad \Lambda^5=\tfrac{1}{2}(\chi^{3,4,1}-\chi^{3,4,4}). \tag{A29}$$

3. Local action of the permutation group

We explain this structure for the ''typical'' example $(\delta,k)=(3,4)$ discussed in subsection 2, above, of this Appendix; a generalization for general cases is straightforward, but will not be displayed within this paper.

For SU(2), first the equivalence of the fundamental representation and its adjoint has to be invoked by introducing the skew-symmetric 2×2 matrix

$$\epsilon=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix},$$

which has the property that $\epsilon g^{-1}\epsilon^{-1}=\tilde{g}$ for any $g\in \mathrm{SU}(2)$. Consequently, the modified link variable $U=U\epsilon$ obeys instead of Eq. (5) the ''tensor product'' transformation rule (written in terms of matrix elements)

$$(\overline{U_l^g})_{jk}=g(x)_{jj'}g(x+e_j)_{kk'}(\overline{U_l})_{j'k'}. \tag{A30}$$

Introducing the ''modified loop group elements'' specified according to the common (four point) lattice site of our example [see Eq. (89)]

$$\alpha=BU_1\epsilon,\quad \beta=U_1^\dagger DU_2\epsilon,\quad \gamma=U_2^\dagger D\epsilon, \tag{A31}$$

the character states (A23) may be written as

$$\Lambda^\nu=d(\nu)^{j_1j_2j_3j_4j_4j_6}\alpha_{j_1j_2}\beta_{j_3j_4}\gamma_{j_5j_6}. \tag{A32}$$

Each d coefficient couples the tensor product of the six fundamental representations — defined ''locally,'' corresponding to the chosen four point vertex—to the trivial representation; i.e., introducing the related six angular momentum operators $\mathbf{s}(r)$, $r=1,\ldots,6$ (s_j are the Pauli spin matrices in our case) the states (A32) obey

$$\mathbf{s}_{\mathrm{total}}\Lambda^\nu=0,\quad \mathbf{s}_{\mathrm{total}}=\sum_{r=1}^{6}\mathbf{s}(r). \tag{A33}$$

Obviously, the ''total angular momentum'' $\mathbf{s}_{\mathrm{total}}$ is invariant with respect to any permutation of the six variables appearing as indices in Eq. (A32); i.e., we may simultaneously characterize the space (A23) by the representations of the permutation group S_6 which acts on the states (A32) by

$$d(\nu)^{j_1j_2j_3j_4j_4j_6}\to d(\nu)^{j_{\sigma(1)}j_{\sigma(2)}j_{\sigma(3)}j_{\sigma(4)}j_{\sigma(5)}j_{\sigma(6)}} \tag{A34}$$

$(\sigma\in S_6)$. One may use the decomposition of this representation for classifying the states in the space (A23). In its general form, however, the corresponding permutation operators do not commute with the Casimir operators (43) since they involve only ''reduced total angular momenta.'' In our case we have, e.g.,

$$A_1=[\mathbf{s}(2)+\mathbf{s}(3)]^2,\quad A_2=[\mathbf{s}(4)+\mathbf{s}(5)]^2,$$

$$A_3=[\mathbf{s}(2)+\mathbf{s}(3)+\mathbf{s}(4)+\mathbf{s}(5)]^2-A_1-A_2. \tag{A35}$$

Conveniently chosen subgroups of S_6, however, do commute. We may take, e.g., S_2 embedded in S_6 in different ways: If π is the nontrivial 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).

4. Examples for the incorporation of the Euclidean group

We restrict ourselves to SU(2) and $D=2$. A convenient enumeration of the up to third order relevant elements of the Euclidean group for $D=2$ is given by

$$[n,\mu,m,\sigma]=R^n t^\mu R^m P^\sigma, \quad m,n=0,1,2,3,$$
$$\sigma=0,1, \quad \mu=0,1,2,3,4,5,\ldots, \tag{A36}$$

where we 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 fulfills $T(R)\chi^1=\chi^1=\Lambda^{1,1,1}$.

The ''one-unit'' translation t is defined by the condition that $\Lambda_G^{2,2}=\chi^1 T(t)\chi^1$.

Taking into account $T(P)\chi^1=\chi^1$, we obtain in lowest order $\gamma_1=\gamma_2=(1,1,1)$ the nontrivially connected cases [n, m, and σ are arbitrary with the restriction (A36)]

$$\gamma_3=(2,1,1), \quad u=[n,0,m,\sigma], \quad v=[0,0,0,0],$$
$$\gamma_3=(2,2,1), \quad u=[n,1,m,\sigma], \quad v=[n,0,0,0]. \tag{A37}$$

Combining first and second orders on the RHS of Eq. (62) we have the generic alternatives $\gamma_1=(2,1,1);\gamma_2=(1,1,1)$:

$$\gamma_3=(3,1,1), \quad u=[n,0,m,\sigma], \quad v=[0,0,0,0],$$
$$\gamma_3=(3,2,1), \quad u=[n,1,m,\sigma], \quad v=[n,0,0,0]. \tag{A38}$$

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

$$\gamma_3=(3,2,1), \quad u=[0,0,m,\sigma], \quad v=[0,0,0,0],$$
$$u=[0,1,m,\sigma], \quad v=[0,1,2,0],$$
$$\gamma_3=(3,3,1), \quad u=[0,2,m,\sigma], \quad v=[0,0,0,0],$$
$$u=[2,0,m,\sigma], \quad v=[0,1,2,0], \quad \gamma_3=(3,4,1),$$
$$u=[1,1,m,\sigma],$$
$$v=[0,0,0,0], \quad u=[3,1,m,\sigma], \quad v=[0,0,3,0]. \tag{A39}$$

Here, the Euclidean elements v are chosen such that a nontrivial connection with *the same* pairs (u,v) is described for the γ triplets (2,1,2),(1,1,1),[(3,1,2) or (3,2,2)] for the two cases (A38) and (2,2,2),(1,1,1),[(3,3,2) or (3,4,2)] for the cases (A39).

The Euclidean elements (u,v) for the cases where γ_1 and γ_2 are exchanged may be obtained by the replacements $u\to u^{-1}, v\to u^{-1}v$ in the above formulas. This follows from $\Lambda^2 T(u^{-1})\Lambda^1=T(u^{-1})[\Lambda^1 T(u)\Lambda^2]=T(u^{-1}v)\Lambda^3$ if $\Lambda^1 T(u)\Lambda^2=T(v)\Lambda^3$.

This provides all nonvanishing η coefficients (62) up to the order $\delta_3=3$.

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