SU(3) matrix functions

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1. Introduction

Lattice QCD simulation algorithms require the SU(3) exponential function to be evaluated very many times (at least four times per lattice point and update cycle). As already noted by Morningstar and Peardon [1], the Cayley–Hamilton theorem allows such matrix functions to be represented and computed economically.

In this note, the representation is worked out in some detail, the emphasis being on its regularity properties and suitability for numerical purposes. An efficient and numerically stable algorithm for the calculation of the exponential function and its derivatives is then described.

2. The Cayley–Hamilton theorem

2.1 Characteristic equation

Let X be an element of the Lie algebra $\mathfrak{su}(3)$ of SU(3) (see appendix A for the SU(3) conventions used). Since X is traceless, the characteristic polynomial

$$\det(\lambda - X) = \lambda^3 - \tfrac{1}{2}\mathrm{tr}(X^2)\lambda - \det X \tag{2.1}$$

depends on only two real parameters

$$t = -\tfrac{1}{2}\mathrm{tr}(X^2), \qquad d = i\det X. \tag{2.2}$$

Both t and d are polynomial invariants of X, i.e. they are invariant under the adjoint action $X \to UXU^{-1}$ of $U \in \mathrm{SU}(3)$.

The Cayley–Hamilton theorem asserts that the matrix X satisfies the characteristic equation

$$X^3 + tX + id = 0. \tag{2.3}$$

For diagonalizable matrices like X, the statement is nearly trivial, because the eigenvalues of X are the roots of the characteristic polynomial.

2.2 Range of the invariant parameters

In the following, a detailed understanding of the relation between $X \in \mathfrak{su}(3)$ and the invariant parameters t and d will be helpful.

Lemma 2.1. *The image of* $\mathfrak{su}(3)$ *in the plane of the parameters (2.2) is the closed region defined by the inequalities*

$$t \geq 0, \qquad d^2 \leq \tfrac{4}{27} t^3. \tag{2.4}$$

Proof: The eigenvalues ix_1, ix_2, ix_3 of a given matrix $X \in \mathfrak{su}(3)$ are purely imaginary and may be ordered so that $|x_1|$ is greater or equal than the magnitude of the other eigenvalues. Since X is traceless, there exists a real number r in the range $0 \leq r \leq 1$ such that

$$x_2 = -x_1 r, \qquad x_3 = -x_1(1-r). \tag{2.5}$$

The parameters (2.2) are then given by

$$t = x_1^2\{1 - r(1-r)\}, \qquad d = x_1^3 r(1-r). \tag{2.6}$$

In particular, $t \geq 0$ and

$$d^2 = t^3 \frac{u^2}{(1-u)^3}, \tag{2.7}$$

where $u = r(1-r)$. The right-hand side of this equation is monotonically increasing with u and therefore assumes its maximum at the endpoint $u = \frac{1}{4}$ of the range of u. For all $X \in \mathfrak{su}(3)$, the parameters t and d thus satisfy the bounds (2.4).

It remains to be shown that each point (t, d) in the domain (2.4) is related to the eigenvalues of a matrix $X \in \mathfrak{su}(3)$ through eqs. (2.5) and (2.6). If $d = 0$ the choice

$$x_1 = \sqrt{t}, \qquad x_2 = -x_1, \qquad x_3 = 0, \tag{2.8}$$

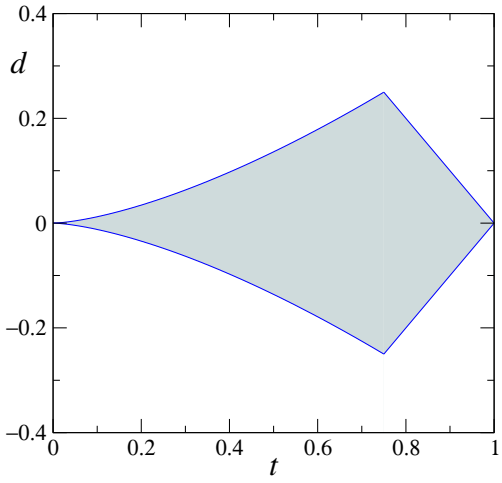

Fig. 1. Image of the ball $\|X\|_2 \leq 1$ in the plane of the invariant parameters (2.2).

satisfies all conditions. In all other cases, there is a unique value of $u \in [0, \frac{1}{4}]$ such that eq. (2.7) holds. One may then set

$$x_1 = \mathrm{sign}(d)\sqrt{\frac{t}{1-u}} \tag{2.9}$$

and define x_2 and x_3 through eq. (2.5), where $r(1-r) = u$. As can be easily verified, this choice of x_1, x_2, x_3 satisfies both (2.5) and (2.6). □

With little additional work, one can show that t and d are in fact the only invariants of X. A more complete statement is summarized by the following lemma.

Lemma 2.2. *Up to permutations, the eigenvalues of $X \in \mathfrak{su}(3)$ are uniquely determined by the invariants t and d. Moreover, X has degenerate eigenvalues if and only if the point (t, d) is on the boundary of the domain (2.4).*

Another useful result is

Lemma 2.3. *The image in the (t, d)-plane of the set of all $X \in \mathfrak{su}(3)$ with norm $\|X\|_2 \leq M$ is the domain characterized by the bounds (2.4) and the inequality*

$$|d| \leq M(M^2 - t). \tag{2.10}$$

Proof: Equation (2.6) implies $x_1^2 \geq t$ and $|d| = |x_1|(x_1^2 - t)$. The Lemma then follows from the fact that $|x_1| = \|X\|_2$. □

For illustration, the image of the ball $\|X\|_2 \leq 1$ is shown in fig. 1. Lemma 2.3 implies that $\|X\|_2$ is the unique solution $x \geq \sqrt{t}$ of the equation $x(x^2 - t) = |d|$. Explicitly,

$$\|X\|_2 = \sqrt{\frac{4t}{3}} \cos\phi, \qquad \phi = \frac{1}{3} \arccos\varrho, \qquad \varrho = \sqrt{\frac{27d^2}{4t^3}} \tag{2.11}$$

($0 \leq \varrho \leq 1$ in view of Lemma 2.1 and ϕ is consequently in the range $0 \leq \phi \leq \pi/6$).

3. Matrix functions

3.1 Cayley–Hamilton representation

Let $f(\lambda)$ be an arbitrary function that is defined and holomorphic in an open neighbourhood of the imaginary axis $\operatorname{Re}\lambda = 0$ in the complex plane. For any $X \in \mathfrak{su}(3)$, a 3×3 matrix $f(X)$ may then be defined through

$$f(X) = \oint \frac{\mathrm{d}\lambda}{2\pi i} \frac{f(\lambda)}{\lambda - X}, \tag{3.1}$$

where the integration contour encircles the spectral range of X (see fig. 2). Evidently,

$$f(X)v = f(\zeta)v \tag{3.2}$$

if v is an eigenvector of X with eigenvalue ζ, i.e. the definition (3.1) coincides with the usual definition of functions of a diagonalizable matrix.

Using the characteristic equation (2.3), it is now straightforward to check that

$$(\lambda - X)^{-1} = (\lambda^2 + t + \lambda X + X^2)(\lambda^3 + t\lambda + id)^{-1}. \tag{3.3}$$

When inserted in eq. (3.1), this leads to the representation

$$f(X) = f_0 + f_1 X + f_2 X^2 \tag{3.4}$$

where

$$f_k = \oint \frac{\mathrm{d}\lambda}{2\pi i} \frac{\rho_k}{\lambda^3 + t\lambda + id} f(\lambda), \qquad \{\rho_0, \rho_1, \rho_2\} = \{\lambda^2 + t, \lambda, 1\}. \tag{3.5}$$

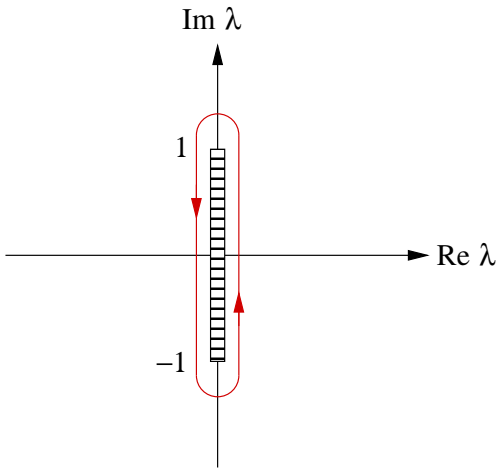

Fig. 2. The contour integral (3.1) runs around a loop in the complex λ-plane which tightly encloses the spectral range of X.

Since the denominator in these integrals coincides with $\det(\lambda - X)$, the integration contour avoids the poles of the integrand and the coefficients f_0, f_1, f_2 are therefore well-defined functions of t and d. Moreover, they extend to holomorphic functions in a complex neighbourhood of the domain (2.4).

3.2 Alternative expressions for f_k

The coefficients f_k can be worked out in terms of the (purely imaginary) eigenvalues $\lambda_1, \lambda_2, \lambda_3$ of X. Noting

$$\lambda^2 + t = \tfrac{2}{3}t + \tfrac{1}{3}\sum_{k<l}(\lambda - \lambda_k)(\lambda - \lambda_l), \tag{3.6}$$

$$\lambda = \tfrac{1}{3}\sum_{k}(\lambda - \lambda_k), \tag{3.7}$$

$$\lambda^3 + t\lambda + id = (\lambda - \lambda_1)(\lambda - \lambda_2)(\lambda - \lambda_3), \tag{3.8}$$

the integrands in eq. (3.5) can be reduced to pole terms with up to 3 poles. Using the residue theorem, the integration over λ then leads to fully explicit expressions for f_0, f_1 and f_2. These expressions are however not manifestly regular if some of the eigenvalues coincide and are therefore of limited use.

When the Feynman parameter formula

$$\frac{1}{r_1 r_2 \dots r_n} = \Gamma(n) \int_0^1 \mathrm{d}s_1 \dots \mathrm{d}s_n \, \delta\big(1 - \textstyle\sum_k s_k\big) \frac{1}{\big(\sum_k s_k r_k\big)^n} \tag{3.9}$$

is first applied, one instead obtains the expressions

$$f_0 = \tfrac{1}{3} \sum_k f(\lambda_k) + \tfrac{2}{3} t f_2, \tag{3.10}$$

$$f_1 = \tfrac{1}{3} \sum_{k<l} \int_0^1 \mathrm{d}s_1 \, f'(s_1 \lambda_k + (1-s_1)\lambda_l), \tag{3.11}$$

$$f_2 = \int_0^1 \mathrm{d}s_1 \int_0^{1-s_1} \mathrm{d}s_2 \, f''(s_1\lambda_1 + s_2\lambda_2 + (1-s_1-s_2)\lambda_3). \tag{3.12}$$

The integrals in these formulae run over the spectral range of X and are manifestly singularity-free for all X.

3.3 Uniqueness of the Cayley–Hamilton representation

The presence of the singularities alluded to above is related to a non-uniqueness of the Cayley–Hamilton representation as stated by the following lemma.

Lemma 3.1. *For a fixed matrix $X \in \mathfrak{su}(3)$, the coefficients f_0, f_1, f_2 are uniquely determined through eq. (3.4) if and only if the eigenvalues of X are non-degenerate.*

Proof: Equation (3.4) is equivalent to the Vandermonde system

$$f(\lambda_k) = f_0 + f_1 \lambda_k + f_2 \lambda_k^2, \qquad k = 1, 2, 3, \tag{3.13}$$

where, as above, $\lambda_1, \lambda_2, \lambda_3$ denote the eigenvalues of X. Such systems are known to have a unique solution if and only if the eigenvalues are pairwise different. □

The coefficients given by eq. (3.5) are a particular choice of f_0, f_1, f_2, which is distinguished by the fact that the coefficients are continuous (actually even differentiable) functions of t and d. With this additional requirement, the Cayley–Hamilton representation becomes unique.

4. Derivatives of matrix functions

Matrix functions $f(X)$ are functions of the coordinates $X^1, \ldots, X^8$ of X with values in the space of complex 3×3 matrices (see appendix A). One is then interested in the derivatives of $f(X)$ with respect to the coordinates X^a.

4.1 Differentiation of the Cayley–Hamilton representation

If the associated partial differential operators are denoted by ∂_a, the differentiation of the Cayley–Hamilton representation (3.4) leads to the expression

$$\partial_a f(X) = f_1 T^a + f_2(T^a X + X T^a) + \sum_{k=0}^{2} \partial_a f_k X^k. \tag{4.1}$$

Since f_k depends on X only through the invariant parameters t and d, the derivatives of the coefficients in these equations can be expressed through

$$f_{k,t} = \frac{\partial f_k}{\partial t}, \qquad f_{k,d} = \frac{\partial f_k}{\partial d}, \tag{4.2}$$

Explicitly, they are given by

$$Y^a \partial_a f_k = -\mathrm{tr}\{XY\}\, f_{k,t} + i\,\mathrm{tr}\{X^2 Y\}\, f_{k,d} \tag{4.3}$$

for all $k = 0, 1, 2$ and $Y \in \mathfrak{su}(3)$.

4.2 Alternative expressions for $f_{k,t}$ and $f_{k,d}$

Starting from the representation (3.5), it is straightforward to show that

$$f_{0,t} = -d f_{2,d}, \tag{4.4}$$

$$f_{1,t} = -i f_{0,d} + i t f_{2,d}, \tag{4.5}$$

$$f_{2,t} = -i f_{1,d}. \tag{4.6}$$

The coefficients $f_{k,t}$ are thus obtained algebraically once the other coefficients $f_{k,d}$ are known.

Similarly to f_k, the derivatives of these coefficients can be represented through integrals of the form

$$f_{k,d} = \tfrac{2}{3}\delta_{k0}\, t f_{2,d} - i \int_0^1 \mathrm{d}s_1 \mathrm{d}s_2 \mathrm{d}s_3\, \delta(1 - s_1 - s_2 - s_3) \times \omega_{k,d}(s) f^{(k+3)}(s_1\lambda_1 + s_2\lambda_2 + s_3\lambda_3), \tag{4.7}$$

where the weights $\omega_{k,d}$ are given by

$$\omega_{0,d} = \tfrac{1}{3}, \tag{4.8}$$

$$\omega_{1,d} = \tfrac{1}{3}(s_1 s_2 + s_2 s_3 + s_3 s_1), \tag{4.9}$$

$$\omega_{2,d} = s_1 s_2 s_3. \tag{4.10}$$

These expressions are singularity-free, but involve high-order derivatives of the function $f(\lambda)$. Whether the differentiated Cayley–Hamilton representation is suitable for numerical evaluation thus depends on the behaviour of these derivatives.

5. Computation of the SU(3) exponential function

In this section, the Cayley–Hamilton formalism is applied to the exponential function $f(\lambda) = \mathrm{e}^{\lambda}$, the associated matrix function $f(X)$ being the SU(3) exponential function $\exp(X)$.

5.1 Numerical stability

Since the exponential function is differentiable and bounded along the imaginary axis, the coefficients (3.5) are well-behaved. In particular, if, say,

$$\|X\|_2 \leq 1, \tag{5.1}$$

there are no significant numerical cancellations in the Cayley–Hamilton representation (3.4). For larger matrices X the use of the latter may not be numerically safe, but the exponential can in this case be computed by evaluating $\exp(X/2^n)$ for some sufficiently large integer n and squaring that matrix n times.

5.2 Power series expansion

The matrix function associated to the polynomial

$$p(\lambda) = \sum_{n=0}^{N} \frac{\lambda^n}{n!} \tag{5.2}$$

satisfies

$$\| \exp(X) - p(X) \|_2 \leq \frac{\|X\|_2^{N+1}}{(N+1)!} \tag{5.3}$$

and thus provides an accurate approximation to the exponential function already for moderate values of the degree N if $\|X\|_2 \leq 1$.

Starting from eq. (2.3), the coefficients of the Cayley–Hamilton representation

$$p(X) = p_0 + p_1 X + p_2 X^2 \tag{5.4}$$

can be shown to be polynomials in the invariants t and d. Moreover, recalling the regular expressions (3.10)–(3.12) and noting that the derivatives

$$p^{(\nu)}(\lambda) = \sum_{n=0}^{N-\nu} \frac{\lambda^n}{n!} \tag{5.5}$$

approximate the exponential function, it follows that the coefficients p_k rapidly converge to the exact coefficients f_k of the exponential function when $N \to \infty$. In particular, the latter could, in this way, be computed to any desired accuracy.

5.3 Recursive computation of p_k

The polynomial $p(X)$ is best evaluated following the so-called Horner scheme (see ref. [2], sect. 5.3, for example). This method generates a sequence $q_n(X)$ of polynomials recursively according to

$$q_N = c_N, \tag{5.6}$$

$$q_n = X q_{n+1} + c_n, \qquad n = N-1, N-2, \ldots, 0, \tag{5.7}$$

where the coefficients c_n are given by

$$c_n = \frac{1}{n!}. \tag{5.8}$$

The last polynomial in the sequence, $q_0(X)$, then coincides with $p(X)$.

Now if one passes to the Cayley–Hamilton representation

$$q_n(X) = q_{n,0} + q_{n,1}X + q_{n,2}X^2, \tag{5.9}$$

the recursion assumes the form

$$q_{N,0} = c_N, \qquad q_{N,1} = q_{N,2} = 0, \tag{5.10}$$

$$q_{n,0} = c_n - id q_{n+1,2},$$

$$q_{n,1} = q_{n+1,0} - t q_{n+1,2},$$

$$q_{n,2} = q_{n+1,1}, \qquad n = N-1, N-2, \ldots, 0, \tag{5.11}$$

and the desired coefficients are then

$$p_k = q_{0,k}, \qquad k = 0, 1, 2. \tag{5.12}$$

Note that the coefficients $q_{n,k}$ are complex. Each step of the recursion thus requires 4 multiplications, 3 additions and a few register moves.

5.4 Choice of the degree N

If an ISO C compiler and double-precision arithmetic are used, and if X and N are such that

$$\frac{\|X\|_2^{N+1}}{(N+1)!} \leq \texttt{DBL\_EPSILON}, \tag{5.13}$$

the exponential $\exp(X)$ is obtained to machine precision (`DBL_EPSILON` is a C macro defined in the standard include file `float.h`). On machines complying with the IEEE 754 standard for double-precision (64 bit) data and arithmetic, the bound (5.13) holds for all X satisfying $\|X\|_2 \leq 1$ if $N = 17$.

6. Differential of the SU(3) exponential function

The derivative of the exponential function in direction $Y \in \mathfrak{su}(3)$ is defined by

$$\mathrm{d}_Y \mathrm{e}^X = \frac{\mathrm{d}}{\mathrm{d}h} \mathrm{e}^{X+hY}\Big|_{h=0} \tag{6.1}$$

or equivalently through

$$\mathrm{d}_Y \mathrm{e}^X = Y^a \frac{\partial \mathrm{e}^X}{\partial X^a}. \tag{6.2}$$

As will become clear below, the product

$$Z(X,Y) = \mathrm{e}^{-X} \mathrm{d}_Y \mathrm{e}^X \tag{6.3}$$

is an $\mathfrak{su}(3)$-valued linear function of Y, which satisfies

$$\left(\mathrm{d}_Y \mathrm{e}^X\right) \mathrm{e}^{-X} = Z(-X,Y), \tag{6.4}$$

$$\|Z(X,Y)\|_2 \leq \|Y\|_2, \tag{6.5}$$

for all $X, Y \in \mathfrak{su}(3)$.

6.1 Integral representation and series expansion

Partial integration shows that

$$\int_0^1 \mathrm{d}s\, \mathrm{e}^{(1-s)X} hY \mathrm{e}^{s(X+hY)} = \mathrm{e}^{X+hY} - \mathrm{e}^X \tag{6.6}$$

and differentiation with respect to h then leads to the integral representation

$$\mathrm{d}_Y \mathrm{e}^X = \int_0^1 \mathrm{d}s\, \mathrm{e}^{(1-s)X} Y \mathrm{e}^{sX}. \tag{6.7}$$

The properties (6.4) and (6.5) of the differential $Z(X,Y)$ are an immediate consequence of this representation and the fact that $\|\mathrm{e}^{sX}\|_2 = 1$.

Multiplying X by a real parameter r and expanding the expression on the right of eq. (6.7) in its Taylor series at $r = 0$ yields the series

$$\mathrm{d}_Y \mathrm{e}^X = \sum_{n=0}^{N-1} \frac{1}{(n+1)!} \sum_{k=0}^{n} X^k Y X^{n-k} + r_N(X,Y) \tag{6.8}$$

at $r = 1$, the remainder being bounded by

$$\|r_N(X,Y)\|_2 \leq \frac{\|X\|_2^N}{N!}\|Y\|_2. \tag{6.9}$$

The expansion (6.8) is thus rapidly convergent and therefore suitable for numerical evaluation.

The series actually coincides with the derivative $Y^a\partial_a p(X)$ of the polynomial $p(X)$ introduced in subsect. 5.2, which approximates the exponential function $\exp(X)$. Following the lines of sect. 4, the derivatives of the SU(3) exponential function can thus be obtained by differentiating the Cayley–Hamilton representation (5.4) of the polynomial $p(X)$.

6.2 Recursive computation of the coefficients $p_{k,d}$

Recalling the discussion in sect. 4, the derivatives of the polynomial $p(X)$ are given by

$$\begin{aligned} Y^a\partial_a p(X) &= p_1 Y + p_2(XY + YX) \\ &\quad - \sum_{k=0}^{2} \left\{ \mathrm{tr}(XY)\, p_{k,t} + \mathrm{Im}\,\mathrm{tr}(X^2Y)\, p_{k,d} \right\} X^k. \end{aligned} \tag{6.10}$$

Since the coefficients $p_{k,t}$ are related to $p_{k,d}$ through eqs. (4.4)–(4.6), it suffices to compute the latter.

A recursion producing these derivatives of the coefficients p_k is obtained by differentiating eqs. (5.10),(5.11) with respect to d. Explicitly, setting

$$r_{n,k} = \frac{\partial q_{n,k}}{\partial d}, \tag{6.11}$$

the differentiated recursion relations are

$$r_{N,0} = r_{N,1} = r_{N,2} = 0, \tag{6.12}$$

$$\begin{aligned} r_{n,0} &= -iq_{n+1,2} - idr_{n+1,2}, \\ r_{n,1} &= r_{n+1,0} - tr_{n+1,2}, \\ r_{n,2} &= r_{n+1,1}, \qquad n = N-1, N-2, \ldots, 0. \end{aligned} \tag{6.13}$$

Since the coefficients $q_{n+1,2}$ appear in these equations, the recursion (5.11) must be solved simultaneously and the process then yields both $p_k = q_{0,k}$ and $p_{k,d} = r_{0,k}$.

6.3 Miscellaneous remarks

If the derivatives $\mathrm{d}_Y \mathrm{e}^X$ are to be computed to machine precision, N and X must be such that

$$\frac{\|X\|_2^N}{N!} \leq \texttt{DBL\_EPSILON}, \tag{6.14}$$

i.e. the degree N must be increased by 1 with respect to the one required in the case of the exponential function. Most of the computer time spent for the evaluation of the derivatives of the exponential function is however consumed by the 3×3 matrix operations in eq. (6.10).

If X has norm larger than 1, say $2^{n-1} < \|X\|_2 \leq 2^n$, repeated application of the identity

$$Z(X,Y) = \frac{1}{2}\left\{Z(X/2,Y) + U^{-1}Z(X/2,Y)U\right\}, \qquad U = \exp(X/2), \tag{6.15}$$

allows $Z(X,Y)$ to be expressed through $Z(X/2^n,Y)$ at the expense of $3n-1$ additional 3×3 matrix products.

Appendix A

A.1 Group generators

The Lie algebra $\mathfrak{su}(3)$ of SU(3) may be identified with the space of all anti-Hermitian traceless 3×3 matrices. With respect to a basis T^a, $a = 1, \ldots, 8$, of such matrices, the elements $X \in \mathfrak{su}(3)$ are given by

$$X = X^a T^a, \tag{A.1}$$

where $(X^1, \ldots, X^8) \in \mathbb{R}^8$ (repeated group indices are automatically summed over).

The generators T^a are assumed to satisfy the normalization condition

$$\mathrm{tr}\{T^a T^b\} = -\tfrac{1}{2}\delta^{ab}. \tag{A.2}$$

The structure of the Lie algebra is then encoded in the commutators

$$[T^a, T^b] = f^{abc} T^c, \tag{A.3}$$

while the completeness of the generators implies

$$\{T^a, T^b\} = -\tfrac{1}{3}\delta^{ab} + i d^{abc} T^c, \tag{A.4}$$

$$T^a_{\alpha\beta} T^a_{\gamma\delta} = -\tfrac{1}{2}\left\{\delta_{\alpha\delta}\delta_{\beta\gamma} - \tfrac{1}{3}\delta_{\alpha\beta}\delta_{\gamma\delta}\right\}. \tag{A.5}$$

It follows from these equations that the structure constants f^{abc} and the tensor d^{abc} are both real. Moreover, f^{abc} is totally anti-symmetric in the indices and d^{abc} totally symmetric and traceless.

A.2 Matrix norms

The natural scalar product in $\mathfrak{su}(3)$ is

$$(X, Y) = X^a Y^a = -2\,\mathrm{tr}\{XY\}. \tag{A.6}$$

In particular, $\|X\| = (X, X)^{1/2}$ is a possible definition of the norm of $X \in \mathfrak{su}(3)$.

Another useful matrix norm derives from the square norm

$$\|v\|_2 = \{|v_1|^2 + |v_2|^2 + |v_3|^2\}^{1/2} \tag{A.7}$$

of complex colour vectors v. If A is any complex 3×3 matrix, one defines

$$\|A\|_2 = \max_{\|v\|_2 = 1} \|Av\|_2. \tag{A.8}$$

This norm satisfies

$$\|A + B\|_2 \le \|A\|_2 + \|B\|_2, \qquad \|AB\|_2 \le \|A\|_2 \|B\|_2, \tag{A.9}$$

for all matrices A, B. Moreover, if A is Hermitian or anti-Hermitian, $\|A\|_2$ is equal to the maximum of the absolute values of its eigenvalues.

References

[1] C. Morningstar, M. Peardon, *Analytic smearing of SU(3) link variables in lattice QCD*, Phys. Rev. D69 (2004) 054501

[2] W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, *Numerical Recipes in FORTRAN*, 2nd ed. (Cambridge University Press, Cambridge, 1992)