SU(3) matrix functions

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1. Introduction

The use of the Wilson flow as an accelerator for the HMC algorithm along the lines of ref. [1] requires a reliable and reasonably fast program for the SU(3) exponential function and its derivatives up to the second order. As already noted by Morningstar and Peardon [2], the Cayley–Hamilton theorem allows such matrix functions to be represented in an economical way.

In the present note, the representation is worked out in some detail, the emphasis being on its regularity properties and suitability for numerical purposes. The SU(3) notation used is summarized in appendix A.

2. The Cayley–Hamilton theorem

2.1 Characteristic equation

Let X be an arbitrary element of the Lie algebra $\mathfrak{su}(3)$ of SU(3). 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

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

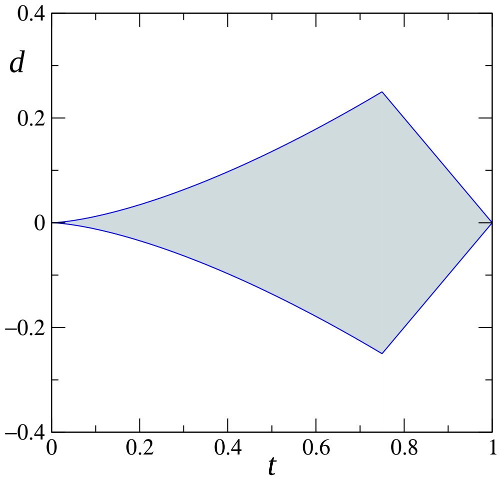

Fig. 1. Image of the ball $\|X\|_2 \leq 1$ in the plane of the invariant parameters (2.2).

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). $\square$

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 subset 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: From eq. (2.6) one infers that $t \leq x_1^2$ and

$$|d| = |x_1|(x_1^2 - t). \tag{2.11}$$

The bound (2.10) follows from this equation and the fact that $|x_1| = \|X\|_2$. □

For illustration, the image of the ball $\|X\|_2 \leq 1$ is shown in fig. 1. Whether a given matrix $X \in \mathfrak{su}(3)$ has norm less than or equal to some value M can, incidentally, easily be checked by calculating t and d and by verifying that the bound (2.10) holds.

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 $\mathrm{Re}\,\lambda = 0$ 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

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

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

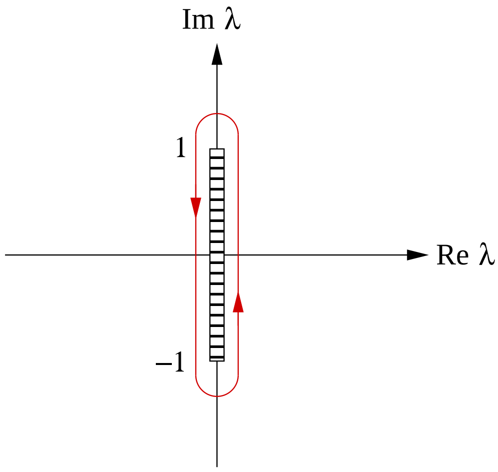

Fig. 2. The contour integral (3.1) runs around a loop in the complex λ-plane which tightly encloses the spectral range of X.

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

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

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. $\square$

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

4.1 Differentiation of the Cayley–Hamilton representation

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.

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

$$\partial^a f(X) = \partial^a f_0 + \partial^a f_1 X + \partial^a f_2 X^2 + f_1 T^a + f_2(T^a X + X T^a). \tag{4.1}$$

The second-order derivative is similarly given by

$$\begin{aligned}\partial^a \partial^b f(X) = {} & \partial^a \partial^b f_0 + \partial^a \partial^b f_1 X + \partial^a \partial^b f_2 X^2 \\ & + \partial^a f_1 T^b + \partial^b f_1 T^a + \partial^a f_2(T^b X + X T^b) + \partial^b f_2(T^a X + X T^a) \\ & + f_2(T^a T^b + T^b T^a).\end{aligned} \tag{4.2}$$

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

$$f_{k,t} = \frac{\partial f_k}{\partial t}, \qquad f_{k,d} = \frac{\partial f_k}{\partial d}, \tag{4.3}$$

$$f_{k,tt} = \frac{\partial^2 f_k}{\partial t^2}, \qquad f_{k,td} = \frac{\partial^2 f_k}{\partial t \partial d}, \qquad f_{k,dd} = \frac{\partial^2 f_k}{\partial d^2}. \tag{4.4}$$

Explicitly, they are then given by

$$\partial^a f_k = \tfrac{1}{2} X^a f_{k,t} + \tfrac{1}{2} Y^a f_{k,d}, \tag{4.5}$$

$$\begin{aligned}\partial^a \partial^b f_k = {} & \tfrac{1}{2}\delta^{ab} f_{k,t} + \tfrac{1}{2} d^{abc} X^c f_{k,d} \\ & + \tfrac{1}{4} X^a X^b f_{k,tt} + \tfrac{1}{4}(X^a Y^b + Y^a X^b) f_{k,td} + \tfrac{1}{4} Y^a Y^b f_{k,dd},\end{aligned} \tag{4.6}$$

where $Y^a = \frac{1}{2} d^{abc} X^b X^c$.

4.2 Relations among the derivatives of f_k

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

$$f_{0,t} = -df_{2,d}, \tag{4.7}$$

$$f_{1,t} = -if_{0,d} + itf_{2,d}, \tag{4.8}$$

$$f_{2,t} = -if_{1,d}. \tag{4.9}$$

Further differentiation then leads to the identities

$$f_{0,td} = -f_{2,d} - df_{2,dd}, \tag{4.10}$$

$$f_{1,td} = -if_{0,dd} + itf_{2,dd}, \tag{4.11}$$

$$f_{2,td} = -if_{1,dd}, \tag{4.12}$$

$$f_{0,tt} = idf_{1,dd}, \tag{4.13}$$

$$f_{1,tt} = 2if_{2,d} + tf_{1,dd} + idf_{2,dd}, \tag{4.14}$$

$$f_{2,tt} = -f_{0,dd} + tf_{2,dd}. \tag{4.15}$$

On the right of eqs. (4.7)–(4.15), only the derivatives $f_{k,d}$ and $f_{k,dd}$ with respect to d appear. Once these are computed, all other derivatives are thus given algebraically.

4.3 Alternative expression for $f_{k,d}$ and $f_{k,dd}$

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

$$\begin{aligned} f_{k,d} = \tfrac{2}{3}\delta_{k0}tf_{2,d} - i\int_0^1 &\mathrm{d}s_1\mathrm{d}s_2\mathrm{d}s_3\,\delta(1-s_1-s_2-s_3) \\ &\times \omega_{k,d}(s)f^{(k+3)}(s_1\lambda_1+s_2\lambda_2+s_3\lambda_3), \end{aligned} \tag{4.16}$$

$$\begin{aligned} f_{k,dd} = \tfrac{2}{3}\delta_{k0}tf_{2,dd} - \int_0^1 &\mathrm{d}s_1\mathrm{d}s_2\mathrm{d}s_3\,\delta(1-s_1-s_2-s_3) \\ &\times \omega_{k,dd}(s)f^{(k+6)}(s_1\lambda_1+s_2\lambda_2+s_3\lambda_3), \end{aligned} \tag{4.17}$$

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

$$\omega_{0,d} = \tfrac{1}{3}, \tag{4.18}$$

$$\omega_{1,d} = \tfrac{1}{3}(s_1 s_2 + s_2 s_3 + s_3 s_1), \tag{4.19}$$

$$\omega_{2,d} = s_1 s_2 s_3, \tag{4.20}$$

$$\omega_{0,dd} = \tfrac{1}{3}(s_1 s_2 s_3^2 + s_2 s_3 s_1^2 + s_3 s_1 s_2^2), \tag{4.21}$$

$$\omega_{1,dd} = \tfrac{1}{6}(s_1 s_2^2 s_3^2 + s_2 s_3^2 s_1^2 + s_3 s_1^2 s_2^2), \tag{4.22}$$

$$\omega_{2,dd} = \tfrac{1}{4} s_1^2 s_2^2 s_3^2. \tag{4.23}$$

These expressions are free of any singularities, but the fact that the representations (4.16),(4.17) involve high-order derivatives of the function $f(\lambda)$ should not be overlooked. Whether the differentiated Cayley–Hamilton representation is sutiable for numerical evaluation therefore depends on the behaviour of these derivatives.

5. Application to the exponential function

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

5.1 Numerical stability

Since the exponential function is unchanged when differentiated, and since its magnitude is 1 along the imaginary axis, the coefficients f_k and their derivatives are all well-behaved. In particular, if, say,

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

there are no significant numerical cancellations in the Cayley–Hamilton representations (3.4),(4.1) and (4.2).

In the following, it will be taken for granted that the matrices $X \in \mathfrak{su}(3)$ considered satisfy the bound (5.1). An algorithmic strategy will then be developed that allows the coefficients f_k and their derivatives to be computed rapidly.

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

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

and thus provides an accurate approximation to the exponential function already for moderate values of the degree N.

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 "alternative 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 p_k converges to f_k when N is taken to infinity. As a consequence, the coefficients f_k can be computed numerically by calculating p_k for a sufficiently large value of N. In view of the results obtained in sect. 4, the same applies to the derivatives of the coefficients.

5.3 Recursive computation of p_k

The polynomial $p(X)$ is best evaluated following the so-called Horner scheme (see ref. [3], 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

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

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

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

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

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. Moreover, since the recursion has depth 1, the coefficients do not need to be preserved except for the last calculated ones.

5.4 Computation of $p_{k,d}$ and $p_{k,dd}$

The recursions for the first derivative of the coefficients $q_{n,k}$ is

$$q_{N,0,d} = q_{N,1,d} = q_{N,2,d} = 0, \tag{5.12}$$

$$q_{n,0,d} = -iq_{n+1,2} - idq_{n+1,2,d},$$

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

$$q_{n,2,d} = q_{n+1,1,d}, \qquad n = N-1, N-2, \ldots, 0. \tag{5.13}$$

In these equations, the solution of the recursion (5.11) appears as an inhomogeneous contribution. The computation thus requires both recursions (5.11) and (5.13) to be solved simultaneously. At and of the loop, the calculation then yields the desired coefficients $p_k = q_{0,k}$ and $p_{k,d} = q_{0,k,d}$.

The same comments apply to the recursion

$$q_{N,0,dd} = q_{N,1,dd} = q_{N,2,dd} = 0, \tag{5.14}$$

$$q_{n,0,dd} = -2iq_{n+1,2,d} - idq_{n+1,2,dd},$$

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

$$q_{n,2,dd} = q_{n+1,1,dd}, \qquad n = N-1, N-2, \ldots, 0, \tag{5.15}$$

which calculates the second derivative $p_{k,dd} = q_{0,k,dd}$ of the coefficients p_k. In total the computation then requires only 14 multiplications and 11 additions per iteration.

5.5 Choice of the degree N

In order to obtain the coefficients p_k with the least possible inaccuracy, the degree of the polynomial should be such that the second derivative $p''(\lambda)$ approximates e^λ to machine precision. If an ISO C compiler and double-precision arithmetic are used, this condition will be met if N is set to the smallest integer such that

$$\frac{1}{(N-1)!} \leq \texttt{DBL\_EPSILON} \tag{5.16}$$

(`DBL_EPSILON` is defined in the standard include file *float.h*).

Since the "alternative expressions" for the derivatives $p_{k,d}$ and $p_{k,dd}$ involve the derivatives of $p(\lambda)$ up to the 8th order, N must satisfy the more stringent bound

$$\frac{1}{(N-7)!} \leq \texttt{DBL\_EPSILON} \tag{5.17}$$

if also these coefficients are to be obtained to the highest possible precision.

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

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

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

References

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