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On the exponential of matrices in $su(4)$

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Abstract

This paper provides explicit techniques to compute the exponentials of a variety of anti-Hermitian matrices in dimension 4. Many of these formulae can be written down directly from the entries of the matrix. Whenever any spectral calculations are required, these can be done in closed form. In many instances only 2×2 spectral calculations are required. These formulae cover a wide variety of applications. Conditions on the matrix which render it to admit one of three minimal polynomials are also given. Matrices with these minimal polynomials admit simple and tractable representations for their exponentials. One of these is the Euler–Rodrigues formula. The key technique is the relation between real 4×4 matrices and the quaternions.

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1. Introduction

Finding the exponential of a 4×4 anti-Hermitian matrix explicitly is a problem which is of importance to quantum physics and its applications, especially to quantum optics, quantum information processing and computation. The problem of computing the solution to

$$\dot{V}(t) = \mathrm{i}H(t)V(t), \qquad V(0) = I_4, \qquad V \in U(4) \tag{1.1}$$

with $H(t)$ a 4×4 Hermitian matrix, arises in the study of four-level (or two-qubit) systems. Here $U(4)$ stands for the group of 4×4 unitary matrices, i.e., 4×4 complex matrices whose inverse is their own transpose conjugate. The solution to this problem can be reduced to the problem of computing the exponential $\exp(\mathrm{i}\gamma(t)\tilde{H})$ with $\tilde{H}$ a 4×4 Hermitian matrix, typically different from $H(t)$, and $\gamma(t)$ some function. This reduction is achieved via either a passage to a rotating frame, approximations such as the rotating wave approximation, or techniques such as the Wei–Norman expansion or the Magnus expansion, or a combination thereof, [15, 20, 22]. Further, in the context of controlling four-level quantum systems, it is known that the unitary generators obtainable by allowing arbitrary time-varying external fields are precisely those obtainable by using only piecewise constant fields. This is the 'controllability with admissible controls is equivalent to controllability with piecewise constant controls' result of [11], valid for any compact Lie group. Now determining the unitary generator after the application of a constant field to a four-level system is a matter of exponentiating 4×4 anti-Hermitian matrices. Further impetus to this question is provided by the issue of universality in quantum computation. Indeed, in quantum computation, due to various universality-type results, it is known that to synthesize any quantum circuit it suffices to realize unitary matrices which are the tensor products of the identity matrix and unitary matrices which have either size 2 or 4 (see, for instance, [4]). This, in turn, is equivalent to generating unitary matrices of size 2 or 4 *selectively* (this is essentially what the identity matrices in the tensor product amount to—the identity refers to the fact that the external interaction which seeks to address certain levels or qubits does not disturb the other qubits, i.e., the addressing of the target qubits or levels is selective). In particular, this requires the *accurate computation* of exponential of anti-Hermitian matrices of sizes 2 or 4.

The purpose of this paper, keeping the above goal in mind, is twofold. First, we point out that the formulae in [19] extend in a straightforward manner to provide explicit closed-form formulae for the exponentials of a variety of matrices in $su(4)$—the Lie algebra of 4×4 anti-Hermitian matrices with null trace. These formulae already cover a wide variety of physical applications. Secondly, we characterize when a matrix in $su(4)$ admits either a quadratic minimal polynomial or a Euler–Rodrigues-type formula for its exponential. In either instance the exponential of the matrix has a particularly simple representation.

It is obvious that there is no loss of generality in assuming that the matrix being exponentiated has zero trace. It is noted further that, in most instances, in the problem of exponentiating $\gamma(t)\tilde{H}, \tilde{H} \in su(4)$, one can assume γ to be constant. To illustrate this consider the well-known formula $\exp(\mathrm{i}a(t)I_2 \otimes \sigma_x + \mathrm{i}b(t)I_2 \otimes \sigma_y + \mathrm{i}c(t)I_2 \otimes \sigma_z) = \cos(\lambda(t))I_4 + \frac{\sin(\lambda(t))}{\lambda(t)}(\mathrm{i}a(t)I_2 \otimes \sigma_x + \mathrm{i}b(t)I_2 \otimes \sigma_y + \mathrm{i}c(t)I_2 \otimes \sigma_z), \lambda(t) = \sqrt{a(t)^2 + b(t)^2 + c(t)^2}$. This formula would not suffer any modifications, beyond $\lambda(t)$ being autonomous, if each of $a(t), b(t), c(t)$ were constant. In particular, all the results of section 3 extend verbatim to the case where $\gamma(t)$ is not constant.

The formulae provided in this paper rely on an associative algebra isomorphism between $H \otimes H$ and $gl(4, R)$. Here H stands for the skew-field of the quaternions (i.e., H behaves very much like a field except that the multiplication in it is not commutative, see [12] for details) while $gl(4, R)$ represents 4×4 real matrices—the Lie algebra of the general linear Lie group, $GL(4, R)$. This isomorphism, known from the theory of Clifford algebras [12], has only recently been used in concrete (numerical) linear algebra questions. To the best of our knowledge the innovative work of [6, 9, 13, 14] on the eigenvalue problem for a variety of structured real matrices is the first such instance.

In [19], the same isomorphism was used to compute closed-form formulae for exponentials of structured real matrices. This is indeed the point of departure for this paper. Given the close relationship between the quaternions and the Pauli matrices, it seems plausible that the basis for $gl(4, R)$ provided by the aforementioned associative algebra isomporphism is essentially the basis for $u(4)$ provided by the various Kronecker products of the Pauli matrices and I_2. It is tempting to believe that this correspondence is as elementary as assigning, for instance, the elements $\mathrm{i} \otimes 1, j \otimes 1, k \otimes 1$ in $H \otimes H$ to the matrices $\sigma_x \otimes I_2, \sigma_y \otimes I_2, \sigma_z \otimes 1$ etc; however, a moment's reflection shows that it cannot be this simple. For instance, the matrix $\sigma_x \otimes I_2$ is a real symmetric matrix, since σ_x and I_2 are real symmetric, and the Kronecker product of two real symmetric matrices is also real symmetric. On the other hand, the matrix associated with the quaternion tensor $\mathrm{i} \otimes 1$ is real antisymmetric. Indeed, a 4×4 matrix is real anti-symmetric iff its quaternion tensor representation is $p \otimes 1 + 1 \otimes q$, with p, q both purely imaginary quaternions (i.e, quaternions whose real parts are null) [6, 9, 13, 14]. In light of this, it is a pleasant circumstance that the aforementioned plausible connection is indeed valid. The precise correspondence is presented in the next section.

It is worth mentioning that the results presented here can also be used to exponentiate matrices in $su(3)$. Indeed, one has to just embed such a matrix as a principal submatrix in a 4×4 matrix, with the rest of the 4×4 matrix consisting of zero entries. A different application would be to exponentiate matrices in $so(6, R)$, the Lie algebra of 6×6 real anti-symmetric or skew-symmetric matrices. $SU(4)$ is a double cover of $SO(6, R)$, [12]. By making this covering homomoprhism explicit, one can reduce the problem of exponentiation in $so(6, R)$ to finding exponentials in $su(4)$.

The balance of this paper is organized as follows. In the next section, the relation between the $H \otimes H$ basis for $gl(4, R)$ and the Pauli tensor product basis, i.e., the matrices consisting of all possible Kronecker products of $I_2, \sigma_x, \sigma_y, \sigma_z$ amongst themselves, is made explicit. The same section also establishes notation used throughout this paper. Section 3 presents $su(4)$ analogues of the results of [19]. In particular, several illustrations drawn from important applications are given. Section 4 presents conditions which ensure that an $su(4)$ matrix either has a quadratic minimal polynomial or admits a Euler–Rodrigues' formula. The same section also presents conditions equivalent to an $su(4)$ matrix to stem from a normal matrix (i.e., if $X = B + \mathrm{i}C$, then $BC = CB$, where B, C are the skew-symmetric (antisymmetric) and symmetric parts of $X \in su(4)$, respectively). The final section offers conclusions.

2. Notation and preliminary observations

The following definitions and notation will be frequently met in this work.

- $gl(n, R)$ represents the algebra of real $n \times n$ matrices. This is, of course, the Lie algebra of the Lie groups of real invertible matrices. For more on the notions of Lie groups and Lie algebras we refer the readers to [8].
- $SU(n)$ represents the Lie group of $n \times n$ unitary matrices of determinant 1, i.e., $n \times n$ matrices with complex entries, whose inverses are their own transpose conjugates. $su(n)$ represents the corresponding Lie algebra of $n \times n$ skew-Hermitian, traceless matrices. $su(2) \otimes su(2)$ is the Lie algebra spanned by matrices of the form $I_2 \otimes U + V \otimes I_2$, $U, V \in su(2)$. Note that it is customary to use the terminology 'anti-Hermitian' for skew-Hermitian matrices.
- R_n represents the matrix with 1 on the anti-diagonal and zeros elsewhere. Any $n \times n$ matrix A satisfying $A^T R_n + R_n A = 0$ is said to be *perskewsymmetric*. *Persymmetric* matrices are those matrices, X, which satisfy $X^T R_n = R_n X$. Such matrices are symmetric about the anti-diagonal.
- J_{2n} is the $2n \times 2n$ matrix which, in block form, is given by $J_{2n} = \begin{pmatrix} 0_n & I_n \\ -I_n & 0_n \end{pmatrix}$. Matrices, Z, satisfying $Z^T J_{2n} = J_{2n} Z$ are called *skew-Hamiltonian* (sometimes anti-Hamiltonian). The term 'Hamiltonian' will not typically be used in the sense of quantum mechanics, unless specified to the contrary (i.e., it will not be used to mean a Hermitian matrix).
- Throughout H will denote the field (more precisely the division algebra) of the *quaternions*, while P stands for the *purely imaginary* quaternions, tacitly identified with R^3. *Further, in this paper the symbol* i *will be used for both the corresponding complex number and the corresponding quaternion.* The context should make it clear which of the two is implied. Thus, for instance, in $\mathrm{i}M_{i \otimes j}$, the first i stands for the complex number i, while the second i (in the subscript) stands for the quaternion.

Remark 2.1.

(i) Throughout this paper, use of the following observation will be made. Let X be an $n \times n$ matrix satisfying $X^2 + c^2 I_n = 0, c \neq 0$. Then $\mathrm{e}^X = \cos(c) I_n + \frac{\sin(c)}{c} X$. Here c^2 is allowed to be complex, and c is then taken to be $\sqrt{r}\,\mathrm{e}^{\mathrm{i}\frac{\theta}{2}}$, with $c^2 = r\,\mathrm{e}^{\mathrm{i}\theta}, \theta \in [0, 2\pi)$.

(ii) The fact that any matrix which satisfies $X^3 = -c^2 X, c \neq 0$, satisfies $\mathrm{e}^X = I + \frac{\sin(c)}{c} X + \frac{1-\cos(c)}{c} X^2$ (Euler–Rodrigues's formula) will also be used. Once again c^2 is permitted to be complex. Note that any matrix which satisfies $X^2 + c^2 I_n = 0, c \neq 0$, automatically satisfies $X^3 = -c^2 X, c \neq 0$. For such matrices the exponential formula in (i) is better to work with than the Rodrigues' formula. Therefore, in this paper we will allude to a matrix admitting a Euler–Rodrigues formula only if its minimal polynomial is of the form $x^3 + c^2 x$.

(iii) Explicit formulae for e^A can be produced if the minimal polynomial of A is known and it is low in degree (cf [1] where such formulae are written down from the characteristic polynomial). However, since the corresponding explicit formulae for e^A are more complicated than those corresponding to (i) and (ii), they will not be pursued here.

$H \otimes H$ **and** $gl(4, R)$. The algebra isomorphism between $H \otimes H$ and $gl(4, R)$, which is central to this work, is the following.

- Associate with each product tensor $p \otimes q \in H \otimes H$, the matrix, $M_{p \otimes q}$, of the map which sends $x \in H$ to $px\bar{q}$, identifying R^4 with H via the basis $\{1, i, j, k\}$. Thus, if $p = p_0 + p_1 i + p_2 j + p_3 k$; $q = q_0 + q_1 i + q_2 j + q_3 k$, then

$$M_{p \otimes q} = [x \mid y \mid u \mid v],$$

with x, y, u, v, the columns of the matrix $M_{p \otimes q}$, given by the vectors in R^4 representing the quaternions $p\bar{q}, pi\bar{q}, pj\bar{q}, pk\bar{q}$ respectively. Here, $\bar{q} = q_0 - q_1 i - q_2 j - q_3 k$.

- Extend this to the full tensor product by linearity, This yields an algebra isomorphism between $H \otimes H$ and $gl(4, R)$. In particular, a basis for $gl(4, R)$ is provided by the 16 matrices $M_{e_x \otimes e_y}$ as e_x, e_y run through $1, i, j, k$.

This connection, which is known from the theory of Clifford algebras, has been put to great practical use in solving eigenvalue problems for structured matrices by Mackey *et al* [6, 9, 13, 14]. It can also be used for finding exponentials, e^A, $A \in gl(4, R)$ [19].

Remark 2.2. *Canonical form for* $X \in su(4)$. Let $= \mathrm{i}H$, with H Hermitian and traceless. Then

$$H = \sum_{i=1}^{3} \alpha_i I_2 \otimes \sigma_i + \sum_{i=1}^{3} \beta_i \sigma_i \otimes I_2 + \sum_{j=1}^{3} \sum_{k=1}^{3} \gamma_{jk} \sigma_j \otimes \sigma_k, \qquad \alpha_i, \beta_i, \gamma_{jk} \in R. \tag{2.2}$$

It is well known that via conjugation by a local unitary transformation (i.e., conjugation via a $U \in SU(2) \otimes SU(2)$) H can be put into the form

$$\sum_{i=1}^{3} a_i I_2 \otimes \sigma_i + \sum_{i=1}^{3} b_i \sigma_i \otimes I_2 + \sum_{i=1}^{3} c_i \sigma_i \otimes \sigma_i \tag{2.3}$$

with $a_i, b_i, c_i \in R$. We will use this canonical form at some points in section 4 (but not in section 3). Furthermore, this local unitary transformation is determined by finding the singular value factorization of the real 3×3 matrix (γ_{jk}) [2]. But this amounts to finding the spectral factorization of a real 3×3 symmetric matrix—which can be performed in closed form [3].

Relation to the Pauli tensor product basis. As mentioned in the introduction, the above basis for $gl(4, R)$ is closely related to the basis $\sigma_i \otimes \sigma_j, i, j = 1, \ldots, 4$ (with $\sigma_0 = I_2, \sigma_1 = \sigma_x, \sigma_2 = \sigma_y, \sigma_3 = \sigma_k$). The precise relation is tabulated below.

Pauli tensor basis	Quaternion tensor basis
$I_2 \otimes I_2$	$M_{1\otimes 1}$
$\sigma_x \otimes I_2$	$M_{\mathrm{i}\otimes k}$
$\sigma_y \otimes I_2$	$-\mathrm{i}M_{1\otimes j}$
$\sigma_z \otimes I_2$	$M_{\mathrm{i}\otimes i}$
$I_2 \otimes \sigma_x$	$M_{k\otimes j}$
$I_2 \otimes \sigma_y$	$\mathrm{i}M_{\mathrm{i}\otimes 1}$
$I_2 \otimes \sigma_z$	$M_{j\otimes j}$
$\sigma_x \otimes \sigma_x$	$M_{j\otimes i}$
$\sigma_x \otimes \sigma_y$	$-\mathrm{i}M_{1\otimes k}$
$\sigma_x \otimes \sigma_z$	$-M_{k\otimes i}$
$\sigma_y \otimes \sigma_x$	$-\mathrm{i}M_{1\otimes k}$
$\sigma_y \otimes \sigma_y$	$M_{\mathrm{i}\otimes j}$
$\sigma_y \otimes \sigma_z$	$\mathrm{i}M_{j\otimes 1}$
$\sigma_z \otimes \sigma_x$	$-M_{j\otimes k}$
$\sigma_z \otimes \sigma_y$	$-\mathrm{i}M_{1\otimes i}$
$\sigma_z \otimes \sigma_z$	$M_{k\otimes k}$

3. Some closed form formulae for exponentials in $su(4)$

In this section, we provide closed form formulae for the exponentials of several matrices in $su(4)$, *without resorting to the canonical form in equation* (2.3). These formulae are based on expressing the matrix in question as a sum of commuting summands, each of which satisfies the condition in (i) of remark 2.1. These formulae can be divided into two classes: (i) those which can be directly written down from the entries of the matrix; (ii) those that require the spectral factorization of an associated real 3×3 symmetric matrix. This latter spectral factorization can be achieved in closed form [3]. In particular, for several cases only a 2×2 spectral factorization is needed. These will be pointed out. Since most of these formulae are the $su(4)$ analogues of the results in [19], proofs will be provided only for cases not considered in [19]. In the interests of brevity, we have not considered analogues of every possible result in [19].

Remark 3.1. Consider $X \in su(4)$, written as $X = B + iC$, with B, C real. Suppose it is skew-Hamiltonian, for instance. Then a simple calculation reveals that the real matrices B, C are skew-Hamiltonian as well. Hence so is the real matrix $B + C$. This observation yields the $H \otimes H$ representation of such an $X \in su(4)$. The basic properties used in exponentiating the corresponding real matrix $B + C$ in [19] was that it could be expressed as the sum of commuting summands, each of which is annihilated by a polynomial of the type in (i) of remark 2.1. Now these properties are not vitiated by the presence of the imaginary unit i in X. Therefore, their exponentials are similarly found. The only difference is that the hyperbolic trigonometric functions in the formula for e^{B+C} will now be replaced by their ordinary trigonometric equivalents. Similar arguments hold if X is perskewsymmetric etc.

3.1. Exponentials directly from the entries

Below a list of three families of matrices in $su(4)$, whose exponentials can be directly found from their $H \otimes H$ representations, is presented.

(i) *Symmetric, tridiagonal,* $S_{ii} = 0$. Consider

$$S = \mathrm{i}\begin{pmatrix} 0 & \alpha & 0 & O \\ \alpha & 0 & \beta & 0 \\ 0 & \beta & 0 & \gamma \\ 0 & 0 & \gamma & 0 \end{pmatrix}.$$

Since such matrices arise in several applications, it is interesting to note that they can be easily exponentiated. Indeed, such an S has the following representation:

$$S = \mathrm{i}[M_{p\otimes i} + M_{q\otimes j} + M_{r\otimes k}] = X + Y + Z,$$

with $p = \left(0, \frac{\beta}{2}, 0\right)$, $q = \left(\frac{\beta}{2}, 0, \frac{\gamma+\alpha}{2}\right)$, $r = \left(0, \frac{\gamma-\alpha}{2}, 0\right)$, $\alpha, \beta, \gamma \in R$. In terms of the Pauli tensor basis, S is $\mathrm{i}\frac{\beta}{2}(\sigma_x \otimes \sigma_x) + \mathrm{i}\frac{\beta}{2}\sigma_y \otimes \sigma_y + \mathrm{i}\frac{\gamma-\alpha}{2} I_2 \otimes \sigma_x + \mathrm{i}\frac{\alpha-\gamma}{2}\sigma_z \otimes \sigma_x$. Now note that Y commutes with both X and Z, while X and Z anticommute. Further each squares to a negative constant times the identity. So e^S is given by

$$\mathrm{e}^S = \left[\cos(\lambda_1) I_4 + \mathrm{i}\frac{\sin(\lambda_1)}{\lambda_1}(M_{p\otimes i} + M_{r\otimes k})\right]\left[\cos(\lambda_2) I_4 + \mathrm{i}\frac{\sin(\lambda_2)}{\lambda_2} M_{q\otimes j}\right].$$

In terms of the Pauli matrices this becomes

$$\mathrm{e}^S = \left[\cos(\lambda_1) I_4 + \mathrm{i}\frac{\sin(\lambda_1)}{\lambda_1}\left(\frac{\beta}{2}(\sigma_x \otimes \sigma_x) + \frac{\alpha-\gamma}{2}\sigma_z \otimes \sigma_x\right)\right]$$
$$\times\left[\cos(\lambda_2 I_4 + \mathrm{i}\frac{\sin(\lambda_2)}{\lambda_2}\left(\frac{\beta}{2}\sigma_y \otimes \sigma_y + \frac{\gamma+\alpha}{2} I_2 \otimes \sigma_x\right)\right]$$

with $\lambda_1 = \frac{1}{2}\sqrt{\beta^2 + (\gamma-\alpha)^2}$, $\lambda_2 = \frac{1}{2}\sqrt{\beta^2 + (\gamma+\alpha)^2}$.

(ii) *Perskewsymmetric* X. Such an $X \in su(4)$ satisfies, in addition, $X^T R = -RX$. Such matrices are expressible in the form

$$\mathrm{i}[p_1\sigma_z \otimes I_2 + p_2\sigma_x \otimes \sigma_z + \alpha\sigma_y \otimes \sigma_z + q_1 I_2 \otimes \sigma_z + q_2\sigma_z \otimes \sigma_x + \beta\sigma_z \otimes \sigma_y].$$

Their exponential is given by

$$\left[\cos(\lambda_1) I_4 + \mathrm{i}\frac{\sin(\lambda_1)}{\lambda_1}(p_1\sigma_z \otimes I_2 + p_2\sigma_x \otimes \sigma_z + \alpha\sigma_y \otimes \sigma_z)\right]$$
$$\times\left[\cos(\lambda_2) I_4 + \mathrm{i}\frac{\sin(\lambda_2)}{\lambda_2}(q_1 I_2 \otimes \sigma_z + q_2\sigma_z \otimes \sigma_x + \beta\sigma_z \otimes \sigma_y)\right]$$

with $\lambda_1 = \sqrt{\|p\|^2 + \alpha^2}$, $\lambda_2 = \sqrt{\|q\|^2 + \beta^2}$

(iii) *Skew-Hamiltonian* X. These matrices satisfy, in addition, $X^T J = JX$. Such matrices are associated with time-reversal symmetries [8]. More specifically, a Hamiltonian (in the usage of quantum mechanics), H, i.e., a Hermitian H, is associated with time-reversal symmetry if $H^T J = JH$. Clearly if H satisfies this additional condition, so does $X = \mathrm{i}H$. Such matrices are expressible in the form

$$\mathrm{i}[bI_4 + p_1\sigma_y \otimes \sigma_y + p_2 I_2 \otimes \sigma_z + p_3 I_2 \otimes \sigma_x + c\sigma_z \otimes \sigma_y + d\sigma_x \otimes \sigma_y].$$

Their exponential is given by

$$\mathrm{e}^{\mathrm{i}b}\left[\cos(\lambda) I_4 + \mathrm{i}\frac{\sin(\lambda)}{\lambda}(p_1\sigma_y \otimes \sigma_y + p_2 I_2 \otimes \sigma_z + p_3 I_2 \otimes \sigma_x + c\sigma_z \otimes \sigma_y + d\sigma_x \otimes \sigma_y)\right],$$

$$\lambda = \sqrt{\|p\|^2 + c^2 + d^2}.$$

3.2. The purely imaginary case

The following algorithm for exponentiating a matrix $X \in su(4)$, which is simultaneously symmetric (equivalently purely imaginary), follows directly from the corresponding algorithm for exponentiating purely real symmetric matrices in [19]. The only difference is that the cosh(), sinh() in [19] will be replaced by cos(), sin(). Note that such an S will not have any terms in equation (2.2) corresponding to members of the Pauli tensor basis, which contain *precisely one* σ_y term.

- Represent the given symmetric $S \in su(4)$ as the matrix as $\mathrm{i}[M_{p\otimes i} + M_{q\otimes j} + M_{r\otimes k}]$, $p, q, r \in P$.
- Identifying the pure quaternions p, q, r with vectors in R^3, find the spectral factorization of the real 3×3 symmetric matrix $X^T X$, where $X = [p \mid q \mid r]$. Thus $X^T X = \sum_{1=}^{3} \sigma_i^2 v_i v_i^T$.
- Compute $u_i = X v_i$. (Note that u_i are almost the left singular vectors. The only difference is $\|u_i\| = \sigma_i$.) Then $S = \mathrm{i}\sum_{i=1}^{3} M_{u_i\otimes v_i}$. Hence,

$$\mathrm{e}^S = \prod_{i=1}^{3}\left(\cos(\sigma_i) I_4 + \mathrm{i}\frac{\sin(\sigma_i)}{\sigma_i} M_{u_i\otimes v_i}\right). \tag{3.4}$$

Definition 3.1 (Bisymmetric type)**.** *For several important examples only a* 2×2 *spectral factorization is needed (which is extremely easy to write). Since the archtypical example is provided by a matrix in* $su(4)$ *which is, in addition, bisymmetric (i.e., simultaneously symmetric and persymmetric), we will, to avoid circumlocution, call all such matrices of the bisymmetric type.*

3.3. Illustrative examples

We provide some important illustrations of the formulae developed in this section.

Illustration 1. *Rabi oscillations in four-level systems.* In [7] a detailed calculation, via a calculation of eigenvectors and eigenvalues, is provided to calculate the evolution of a four-level system, being irradiated by three laser fields, under the rotating wave approximation and under resonance. Specifically, they consider a four-level system with energy levels $\{E_k, k = 1, \ldots, 3\}$ which satisfy $E_1 - E_0 > E_2 - E_1 > \cdots > E_3 - E_2$. This system is irradiated by three laser fields with frequencies $\omega_k = E_k - E_{k-1}, k = 1, \ldots, 3$. After passage to a rotating frame, and under the assumptions of resonance and the rotating wave approximation, the unitary generator in the rotating frame satisfies

$$\mathrm{i}\dot{\tilde{U}} = (E_0 I_4 + C)\tilde{U} \tag{3.5}$$

with

$$C = \begin{pmatrix} 0 & g_1 & 0 & 0 \\ g_1 & 0 & g_2 & 0 \\ 0 & g_2 & 0 & g_3 \\ 0 & 0 & g_3 & 0 \end{pmatrix}.$$

Here g_i are the amplitudes of the three laser fields. Thus $\tilde{U}(t) = \mathrm{e}^{-\mathrm{i}E_0 t}\exp(-\mathrm{i}Ct)$. In [7], $\exp(-\mathrm{i}Ct)$ is calculated by a direct calculation of the eigenvalues and eigenvectors of the matrix $-\mathrm{i}C$. Now, $-\mathrm{i}C$ is precisely a symmetric, tridiagonal matrix with a zero diagonal—i.e., of the type considered in item (1) of the list in the previous subsection. Thus, $\exp(-\mathrm{i}Ct)$

may be found directly and is equal to

$$e^{-iCt} = \left[\cos(\lambda_1)I_4 + i\frac{\sin(\lambda_1)}{\lambda_1}(\beta(\sigma_x \otimes \sigma_x) + (\alpha - \gamma)\sigma_z \otimes \sigma_x)\right] \times \left[\cos\left(\lambda_2 I_4 + i\frac{\sin(\lambda_2)}{\lambda_2}(\beta\sigma_y \otimes \sigma_y + (\gamma + \alpha)I_2 \otimes \sigma_x\right)\right],$$

with $\alpha = -\frac{1}{2}g_1 t$, $\beta = -\frac{1}{2}g_2 t$, $\gamma = -\frac{1}{2}g_3 t$, $\lambda_1 = \sqrt{\beta^2 + (\alpha - \gamma)^2}$, $\lambda_2 = \sqrt{\beta^2 + (\gamma + \alpha)^2}$.

A laborious but straightforward calculation confirms that the matrix entries provided by the above representation of $\exp(-iCt)$ coincide with those in [7].

Illustration 2. *Josephson junction.* In [21, 23] the following system is considered:

$$i\dot{U} = HU, U(0) = I_4$$

with

$$H = \begin{pmatrix} E_{00} & -\frac{1}{2}E_{J1} & -\frac{1}{2}E_{J2} & 0 \\ -\frac{1}{2}E_{J1} & E_{10} & 0 & -\frac{1}{2}E_{J2} \\ -\frac{1}{2}E_{J2} & 0 & E_{10} & -\frac{1}{2}E_{J1} \\ 0 & -\frac{1}{2}E_{J2} & -\frac{1}{2}E_{J1} & E_{00} \end{pmatrix}.$$

In [23] $E_{00}, E_{10}, E_{J1}, E_{J2}$ are taken to be constants reflecting current technology. Thus $U(t) = e^{-iHt}$. Now note that

$$-iH = -i\left[\tfrac{1}{2}(E_{00} + E_{10})I_4 - -\tfrac{1}{2}E_{J2}\sigma_x \otimes I_2 - \tfrac{1}{2}E_{J1}I_2 \otimes \sigma_x + \tfrac{1}{2}(E_{00} - E_{10})\sigma_z \otimes \sigma_z\right]. \tag{3.6}$$

In terms of the Pauli tensor basis this is $-i\left[\frac{1}{2}(E_{00} + E_{10})M_{1\otimes 1} - \frac{1}{2}E_{J2}M_{i\otimes k} - \frac{1}{2}E_{J1}M_{k\otimes j} + \frac{1}{2}(E_{00} - E_{10})M_{k\otimes k}\right]$. Hence, $e^{-iHt} = e^{-i(E_{00}+E_{10})t}\, e^{-i\tilde{H}t}$, with $-i\tilde{H} = -i[M_{p\otimes k} + M_{q\otimes j}]$, with the purely imaginary quaternions of the form $p = p_1 i + p_3 k, q = q_3 k$. Thus, the singular value factorization of the 2×2 matrix

$$\begin{pmatrix} p_1 & 0 \\ p_3 & q_3 \end{pmatrix}$$

has to be found. Thus, this is an example of the *bisymmetric type*. Specifically, the calculations proceed as follows: $\tilde{H} = -i\left[M_{u_1\otimes v_1} + M_{u_2\otimes v_2}\right]$ with $v_1 = \cos\theta i - \sin\theta k$, $v_2 = \sin\theta i + \cos\theta k$, Here $\tan(2\theta) = \frac{2p^Tq}{q^Tq - p^Tp}$. Further $u_1 = p_1\cos\theta i - (p_3 + q_3)\sin\theta k$, $u_2 = p_1\sin\theta i + (p_3 + q_3)\cos\theta k$. Then $\|v_i\| = 1, i = 1, 2$, while $\|u_1\| = \sigma_1 = \sqrt{q^Tq\cos^2\theta + r^Tr\sin^2\theta - q^Tr\sin(2\theta)}$, $\|u_2\| = \sigma_2 = \sqrt{q^Tq\sin^2\theta + r^Tr\cos^2\theta + q^Tr\sin(2\theta)}$. Hence,

$$e^{-i\tilde{H}t} = \left[\cos\sigma_1 I - i\frac{\sin\sigma_1}{\sigma_1}M_{u_1\otimes v_1}\right]\left[\cos\sigma_2 I - i\frac{\sin\sigma_2}{\sigma_2}M_{u_2\otimes v_2}\right]. \tag{3.7}$$

This reads, in terms of the Pauli matrices, as the following.

Illustration 3. *Scalar coupling Hamiltonian.* The matrix being exponentiated is $X = -iH = i[aI_4 + b\sigma_z \otimes I_2 + cI_2 \otimes \sigma_z + d\sigma_z \otimes \sigma_z + e\sigma_x \otimes \sigma_x + f\sigma_y \otimes \sigma_y]$. This is the so-called scalar coupling Hamiltonian, and is widely used in NMR spectroscopy. The corresponding $H \otimes H$ representation is given by

$$\begin{aligned} X &= -i[aM_{1\otimes 1} + bM_{i\otimes i} + cM_{j\otimes j} + dM_{k\otimes k} + eM_{j\otimes i} + fM_{i\otimes j}] \\ &= -i[aM_{1\otimes 1} + M_{p\otimes i} + M_{q\otimes j} + M_{r\otimes k}] \end{aligned}$$

with $p = (b, e, 0), q = (f, c, 0), r = (0, 0, d)$. Hence $e^{tX} = e^{iat}\exp -it(M_{p\otimes i} + M_{q\otimes j} + M_{r\otimes k})$. Thus, it remains to find the exponential of the purely imaginary symmetric matrix $-it(M_{p\otimes i} + M_{q\otimes j} + M_{r\otimes k})$. Now note that the real matrix $-t[p \mid q \mid r]$ is a block diagonal matrix, with the northwest block a real 2×2 matrix and the southeast block the 1×1 matrix $(-td)$. Hence, one needs to find only the singular value factorization of the real 2×2 matrix,

$$-t\begin{pmatrix} b & f \\ e & c \end{pmatrix} = [\tilde{p} \mid \tilde{q}].$$

Hence this is also of the *bisymmetric type*. The corresponding right singular vectors of $-t[p \mid q \mid r]$, written as quaternions, are $v_1 = \cos\theta i - \sin\theta j$, $v_2 = \sin\theta i + \cos\theta j$, $v_3 = k$, Here $\tan(2\theta) = \frac{2\tilde{p}^T\tilde{q}}{\tilde{q}^T\tilde{q}-\tilde{p}^T\tilde{p}} = \frac{2(bf+ec)}{f^2+c^2-b^2-e^2}$. Further $u_1 = -t(b\cos\theta i - f\sin\theta j)$, $u_2 = -t(e\sin\theta i + c\cos\theta j)$, $u_3 = -tdk$. Then $\|v_i\| = 1, i = 1,2,3$, while $\|u_1\| = \sigma_1 = t\sqrt{\tilde{p}^T\tilde{p}\cos^2\theta + \tilde{q}^T\tilde{q}\sin^2\theta - \tilde{p}^T\tilde{q}\sin(2\theta)}$, $\|u_2\| = \sigma_2 = t\sqrt{\tilde{p}^T\tilde{p}\sin^2\theta + \tilde{q}^T\tilde{q}\cos^2\theta + \tilde{p}^T\tilde{q}\sin(2\theta)}$, $\|u_3\| = td$. Hence,

$$\mathrm{e}^{-\mathrm{i}tX} = \mathrm{e}^{-\mathrm{i}at}\left[\cos(\sigma_1)I_4 + \frac{\sin(\sigma_1)}{\sigma_1}M_{u_1\times v_1}\right]\left[\cos(\sigma_2)I_4 + \frac{\sin(\sigma_2)}{\sigma_2}M_{u_2\times v_2}\right] \times\left[\cos(\sigma_3)I_4 + \frac{\sin(\sigma_3)}{\sigma_3}M_{u_3\times v_3}\right].$$

Remark 3.2. There are several other practical applications which lead to the problem of exponentiating $su(4)$ matrices of the bisymmetric type. Examples include superconducting circuits for solid-state quantum computation [18], J cross polarization experiments [17], Heisenberg Hamiltonians (under the assumption that only one of the three components of the magnetic field, assumed to be constant in time, is active during any period of time).

Remark 3.3. The number of matrices which can be easily exponentiated in this fashion can be expanded by combining the above observations together with some useful conjugations. Two classes of such conjugations immediately spring to mind. The first is obviously the class of local unitary transformations. Thus, for instance the matrix $X_1 = \mathrm{i}(a\sigma_z \otimes \sigma_z + b\sigma_y \otimes I_2 + cI_2 \otimes \sigma_y)$ is explicitly locally unitarily equivalent to $X_2 = \mathrm{i}(a\sigma_z \otimes \sigma_z + b\sigma_x \otimes I_2 + cI_2 \otimes \sigma_x)$. The former is not a symmetric matrix, while the latter is (in fact, it is of the bisymmetric type). However, e^{X_1} is easily found once e^{X_2} is. The second type of conjugation is via the so-called magic basis matrix (see [16], for instance). Explicitly, letting

$$V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 & \mathrm{i} \\ 0 & \mathrm{i} & 1 & 0 \\ 0 & \mathrm{i} & -1 & 0 \\ 1 & 0 & 0 & -\mathrm{i} \end{pmatrix}$$

it is known that $V(so(4,R))V^* = su(2)\otimes su(2)$. It is instructive to examine its effect on some of the other matrices considered here. Thus, for instance

- X, symmetric, tridiagonal with $X_{ii} = 0$ implies $VXV^* = \mathrm{i}\big[\frac{\beta}{2}\sigma_y \otimes I_2 + \frac{\beta}{2}\sigma_y \otimes \sigma_x + \frac{\gamma-\alpha}{2}\sigma_y \otimes \sigma_z + \frac{\alpha-\gamma}{2}\sigma_z \otimes \sigma_y\big]$. If one writes such a matrix explicitly, it is not clear that it too can be written as the sum of commuting summands, each of which is easily exponentiated.
- X, skew-Hamiltonian implies $VXV^* = \mathrm{i}[aI_2 \otimes I_2 + b\sigma_y \otimes \sigma_x + c\sigma_y \otimes \sigma_y + d\sigma_y \otimes \sigma_z + e\sigma_x \otimes I_2 + f\sigma_z \otimes I_2]$.
- X, perskewsymmetric implies $VXV^* = \mathrm{i}[a\sigma_x \otimes \sigma_x + b\sigma_x \otimes \sigma_z + cI_2 \otimes \sigma_y + d\sigma_y \otimes \sigma_y + e\sigma_z \otimes \sigma_y + f\sigma_x \otimes I_2]$.

Thus, all such matrices are readily exponentiated.

4. Euler–rodrigues formulae

In this section, we will find conditions which imply that a given $X \in su(4)$ admits one of three minimal polynomials. For such X the corresponding formulae for e^X are very handy. In particular, one of them is a Euler–Rodrigues-type formula, which explains the title of the section. Finally, we will provide conditions that an $su(4)$ matrix $X = B + iC$ is of the normal type, i.e., $BC = CB$. Note that, since X is a complex matrix, being of the normal type is not the same as being normal. For some of the results below, we will appeal to the canonical form for X in equation (2.3). This section will make use of the eigenvalue structure of matrices in $su(4)$. However, one does not need to determine the eigenvalues themselves.

Given an annihilating polynomial p for any matrix X, one can use p to find e^X. There are at least two manners in which to achieve this. One finds the zeros of p (but not the eigenvectors of X), and then proceeds to use any of a variety of methods (e.g, interpolation) to find e^X [10]. Alternatively one can express, via p, higher order powers of X in terms of lower orders and use this to establish formulae for e^X. In general, the representations of e^X obtained via either method are not always easy to work with. There are however three instances when either method produces the same representation and this is particularly easy to manipulate. Specifically, these are as follows.

(1) *Quadratic type I*: $p(x) = x^2 + c^2$. The corresponding formula for e^X is $e^X = \cos(c)I_n + \frac{\sin(c)}{c}X$.
(2) *Quadratic type II*: $p(x) = x^2 + 2\beta x + \gamma, \beta \neq 0$. Now $e^X = e^{-\beta}\big[\big(\cos\sigma + \frac{\beta\sin(\sigma)}{\sigma}\big)I + \frac{\sin\sigma}{\sigma}X\big]$, with $\sigma = \sqrt{\beta^2 - \gamma}$.
(3) *Cubic type I*: $p(x) = x^3 + c^2 x$. In this case, $e^X = I + \frac{\sin(c)}{c}X + \frac{1-\cos(c)}{c}X^2$.

Remark 4.1. The results to be presented here should be seen as a complement to those in the previous section. In section 3, only the first of the above minimal polynomials was used. There will be several $X \in su(4)$ which are amenable to the techniques of either section. Consider, for instance, $X = -iJ(t)(\sigma_x\sigma_x + \sigma_y\sigma_y + \sigma_z\sigma_z)$. This matrix arises in the study of quantum dots [5]. The corresponding p is $x^2 - 2iJx + 3J^2$. However, X is also the sum of three commuting terms, each of which is annihilated by a polynomial of the first type in the above list.

We begin with an explicit expression for the characteristic polynomial of an $X \in su(4)$ in canonical form.

Proposition 4.1. *Consider an $X \in su(4)$ in canonical form as given in equation (2.3). Let its characteristic polynomial be $x^4 + \mu x^2 + \nu x + \pi$. Then*

- $\mu = 2\sum_{i=1}^{3}\left(a_i^2 + b_i^2 + c_i^2\right)$
- $\nu = -8i\left(\sum_{i=1}^{3} a_i b_i c_i - \prod_{i=1}^{3} c_i\right)$.
- $\pi = \frac{1}{4}\big\{2\big(\sum_{i=1}^{3}\left(a_i^2 + b_i^2 + c_i^2\right)\big)^2 - 4\big[\big(\sum_{i=1}^{3}\left(a_i^2 + b_i^2 + c_i^2\right)\big)^2 + 4\sum_{i=1}^{3}\sum_{j=1}^{3} a_i^2 b_j^2$
$+ 4\sum_{i=1}^{3}\left(a_i^2 c_i^2 + b_i^2 c_i^2\right) + 2\sum_{i,j=1;i\neq j}^{3} c_i^2 c_j^2 - 4\sum_{i,j,k=1;i\neq j\neq k}^{3} a_i b_i c_j c_k\big]\big\}$.

Proof. These formulae follow from Newton's identities, which imply that the coefficients of the characteristic polynomial can be expressed in terms of the trace of suitable powers of X, in conjunction with $\mathrm{Tr}(X) = 0$. Further, $\mathrm{Tr}(X^i), i = 2, \ldots, 4$, were calculated by using the $H \otimes H$ representation of X and looking for the $1 \otimes 1$ term in X^i. It is worth emphasizing that the ease of quaternion multiplication renders it unnecessary to calculate X^3 or X^4 fully. Indeed, besides calculating the $1 \otimes 1$ term in X^3, one needs to find only those terms in X^3 which would yield a $1 \otimes 1$ term in X^4 (and quaternion multiplication facilitates this process).

We can now give a simple characterization of when X's minimal polynomial is of either *quadratic type I* or *cubic type I*. □

Proposition 4.2. *$X \in su(4)$ has (i) minimal polynomial $p(x) = x^2 + c^2$ iff $\nu = 0$ and $\mu^2 = 4\pi$; (ii) minimal polynomial $p(x) = x^3 + c^2 x$ iff $\nu = 0 = \pi$. Furthermore, in case (i) $c^2 = \frac{\mu}{2}$, while in case (ii) $c^2 = \mu$.*

Proof. First, in view of X's diagonalizability, $p(x) = x^2 + c^2$ is the minimal polynomial iff the characteristic polynomial has two distinct roots (which add up to zero) each repeated twice. Similarly, $p(x) = x^3 + c^2 x$ is the minimal polynomial iff the characteristic polynomial has two simple distinct roots (which add up to zero) and a double root equal to zero.

Suppose first that $\nu = 0$. Then the characteristic polynomial is a quadratic for x^2. The first case occurs precisely when this quadratic has a double root, i.e., when $\mu^2 = 4\pi$. Similarly, the second case occurs when one of the roots of this quadratic is nil, i.e., precisely when $\pi = 0$ in addition.

Conversely, suppose the minimal polynomial is $p(x) = x^2 + c^2$. Now using the characterization of the coefficients of the characteristic polynomial in terms of the elementary symmetric functions of the eigenvalues, it follows that $\nu = 0$ and $\mu^2 = 4\pi$. Similarly, if $p(x) = x^3 + c^2 x$ the same characterization yields $\nu = 0 = \pi$. □

Remark 4.2.

(i) Using these conditions it is easy to write down examples of $X \in su(4)$ which admit genuine Euler–Rodrigues formulae, i.e., X which have cubic type I minimal polynomials. For instance, $X = \mathrm{i}(I_2 \otimes \sigma_x + \sigma_x \otimes I_2 + \sigma_y \otimes \sigma_y + c\sigma_z \otimes \sigma_z)$, where c is any real solution of the quartic $c^4 + 14c^2 - 8c + 17 = 0$. This quartic admits at least two real solutions. Indeed, if all solutions were complex, then they must be of the form $a + \mathrm{i}b$, $a - \mathrm{i}b$, $-a + \mathrm{i}d$, $-a - \mathrm{i}d$, since there is no c^3 term. It is easy to see that if this is the case, then the coefficient of c^2 has to be necessarily negative. Note further that c, in this example, could easily be allowed to be time-varying.

(ii) It is noted in passing that one can write down the exponential of generic X which satisfy $\nu = 0$ (i.e., those cases for which neither of $\mu^2 = 4\pi$ nor $\pi = 0$ hold), since in this case all the eigenvalues of X are distinct and the corresponding interpolation-based formula [10] assumes a simple form.

Characterizing when X has a minimal polynomial of *quadratic type II* via coefficients of the characteristic polynomials does not seem fruitful. Therefore, we provide a different characterization. For this characterization we do not require that X be placed in the form of equation (2.3), though obviously the stated conditions would simplify for X in canonical form.

Proposition 4.3. *Let $X \in su(4)$ be expressed as $M_{p\otimes 1} + M_{1\otimes q} + \mathrm{i}[M_{r\otimes i} + M_{s\otimes j} + M_{t\otimes k}]$, with $p, \ldots, t$ purely imaginary quaternions. Denote by $C = [r \mid s \mid t]$. Then X admits $x^2 + 2\beta x + \gamma$, with $\beta \neq 0$, as its minimum polynomial iff there is a $\tilde{\beta} \in R$ satisfying the following conditions:*

$$\begin{aligned} C^T p &= \tilde{\beta} q \\ Cq &= \tilde{\beta} p \\ pq^T - \mathrm{Co}(C) &= \tilde{\beta} C, \end{aligned} \tag{4.8}$$

where $\mathrm{Co}(C)$ is the matrix of cofactors of C. If these conditions hold, then (i) $\gamma = -[\|p\|^2 + \|q\|^2 + \|r\|^2 + \|s\|^2 + \|t\|^2]$; (ii) $\beta = \mathrm{i}\tilde{\beta}$.

Proof. From a variety of viewpoints it should be clear that if $x^2+2\beta x+\gamma$ is to be the minimum polynomial of X, then necessarily β is purely imaginary, while γ is real. Using this fact, the above conditions stem from a direct calculation of X^2. □

Remark 4.3. The purpose of this remark is to identify some situations, under which the system of equations (4.8) admits solutions.

(i) When C has rank 1, equation (4.8) always possesses solutions, i.e., it is always possible to find $p, q, \tilde{\beta}$ satisfying them for the given C. Such a C always possesses a representation of the form $C = uv^T$, with $u^Tu = v^Tv$ (it is easy to find such a representation). Picking $\tilde{\beta} = u^Tu = v^Tv$, $p = u\sqrt{\tilde{\beta}}$, $q = v\sqrt{\tilde{\beta}}$ we find that equation (4.8) is satisfied. This yields a systematic procedure to construct examples admitting a quadratic minimal polynomial of *type II*.

(ii) Conversely, starting with a non-zero p one can find q, C such that equation (4.8) always holds. The key to this is to observe that if C is invertible in proposition 4.3, then the conditions given in equation (4.8) can be written in a different form, to wit: $CC^Tp = \tilde{\beta}^2p, q = C^{-1}(\tilde{\beta}p); \tilde{\beta}(pp^T - CC^T) = \det(C)I$. This yields a method to construct more examples of X admitting a quadratic minimal polynomial of Type II. Pick a $p \neq 0$. Choose $\tilde{\beta} = \sqrt{1 + p^Tp}$, and pick a C satisfying $\det(C) = -\beta$ and $CC^T = I + pp^T$. Finally, set $q = C^{-1}(\tilde{\beta}p)$.

This can always be achieved by picking C to be a solution of the equation $CC^T = I + pp^T$ with a negative determinant, since $I + pp^T$ is positive definite and thus possesses a square root. For instance, one could multiply the easily determined unique positive definite square root of $I + pp^T$ by $\mathrm{diag}(1, 1, -1)$ to obtain a C with determinant $-\tilde{\beta}$. Further, $\det(CC^T) = 1 + p^Tp$ and obviously $CC^Tp = \tilde{\beta}^2p$. Indeed, the eigenvectors of $I + pp^T$ are p (with eigenvalue $1 + p^Tp = \tilde{\beta}^2$), and any two vectors orthogonal to p (corresponding to eigenvalue 1 with double multiplicity).

(iii) If precisely one of p or q is zero, then there is no solution to equation (4.8). When both are zero, there is a solution iff CC^T is proportional to the identity matrix, i.e., iff the vectors r, s and t are orthogonal and have the same length. Note that in this case $X = \mathrm{i}[M_1 + M_2 + M_3]$, with the M_i commuting, and each with a quadratic minimal polynomial of type I. Further, this is precisely the case wherein the canonical form X, as in equation (2.3), is $X = \mathrm{i}[c_1\sigma_x \otimes \sigma_x + c_2\sigma_y \otimes \sigma_y + c_3\sigma_z \otimes \sigma_z]$, with either $c_1 = c_2 = c_3$ (in the event $\det(C) > 0$) or $c_1 = c_2 = -c_3$ (in the event $\det(C) < 0$). However, one does not require passage to this canonical form for finding e^X.

(iv) Similar conditions can be written down one p, q, r, s, t for X to admit other minimal polynomials. We omit them in the interests of brevity.

Conditions for 'normality'. Next, given $X = B + \mathrm{i}C$, we characterize, when $[B, C] = 0$, i.e., when the real matrix $B + C$ is normal. The motivation should be obvious—it is possible to exponentiate both B and $\mathrm{i}C$ in closed form, and hence X. While the statement of this result uses the canonical form given by equation (2.3), much of the proof does not require it.

Proposition 4.4. *Let* $X = B + \mathrm{i}C = M_{p\otimes 1+1\otimes q} + \mathrm{i}M_{r\otimes i+s\otimes j+t\otimes k}$, $p, \ldots, t \in P$ *be in canonical form. Suppose, without loss of generality, that at least one of* p, q *is non-zero. Then* $[B, C] = 0$ *iff the following conditions hold:*

(i) $p \neq 0, q = 0$: $a_1 = a_3 = c_1 = c_3 = 0$

(ii) $p \neq 0, q \neq 0$: $a_1 = a_3 = b_1 = b_3 = 0$, $\left|\frac{b_2}{a_2}\right| = \left|\frac{c_1}{c_3}\right| = 1$

(iii) $p = 0, q \neq 0$: $b_1 = b_3 = c_1 = c_3 = 0$

Proof. For any $X \in su(4)$ (even those not in canonical form) a quick calculation reveals that $[B, C] = 2[p \times r \otimes i + p \times s \otimes j + p \times t \otimes k + r \otimes (q \times i) + s \otimes (q \times j) + t \otimes (q \times k)]$. If X is in the canonical form in equation (2.3), then we have

$$p = (-a_2, 0, 0); \quad q = (0, b_2, 0); \quad r = (b_3, c_1, 0); \quad s = (c_2, a_3, a_1); \quad t = (b_1, 0, c_3).$$

Hence $[B, C]$ is twice the matrix representation of $b_1b_2 i \otimes i + (c_3b_2 - c_1a_2)k \otimes i + a_1a_2 j \otimes j - a_2a_3 k \otimes j - b_3b_2 \mathrm{i} \otimes k + (a_2c_3 - c_1b_2) j \otimes k$. The conclusion follows from this. □

Remark 4.4. By applying the proof of the previous result to X not in canonical form, one can deduce other commutativity results. For instance, suppose Y is in canonical form, and one defines $Y_1 = \mathrm{i}\left(\sum_{i=1}^3 a_i I_2 \otimes \sigma_i + \sum_{i=1}^3 b_i \sigma_i \otimes I_2\right)$ and $Y_2 = \mathrm{i}\sum_{i=1}^3 c_i \sigma_i \otimes \sigma_i$. Then $[Y_1, Y_2] = 0$ iff (i) $\frac{c_3}{c_2} = \frac{b_1}{a_1}$; (ii) $\frac{c_3}{c_1} = \frac{b_2}{a_2}$ and (iii) $\frac{c_2}{c_1} = \frac{b_3}{a_3}$. To see this let $X = B + \mathrm{i}C = V^* Y V$, with V the magic basis matrix (see remark 3.3). Then $[Y_1, Y_2] = 0$ iff $B + C$ is normal. Note that while Y is in canonical form, X is not.

5. Conclusions

In this paper, closed form formulae are provided for exponentials of several important anti-Hermitian 4×4 matrices. These matrices cover many important applications. The basic technique is the isomorphism between real 4×4 matrices and $H \otimes H$. We believe that this connection is aptly suited to exploit the properties of $su(4)$ stemming from its direct sum decomposition into the real skew-symmetric (antisymmetric) matrices and the purely imaginary symmetric matrices. While no claim to the superiority of the representation of the exponential provided by this work is made, it is our hope that further research will yield more applications of these formulae.

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