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Evolution matrix in a coherence vector formulation for quantum Markovian master equations of N-level systems

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Abstract. Quantum Markovian master equations in N dimensions are systematically transformed into vector form by using the Lie algebra of the special unitary group SU(N). Density operators are represented through coherence vectors and the infinitesimal Kossakowski generator of completely positive quantum dynamical semigroups appears as a real evolution matrix that is not completely diagonalisable, in general. A complete classification of the spectrum of the latter and its Jordan canonical form, together with all types of associated stationary states, is given in detail. The results of this analysis are particularly suited for computations in practical applications.

1. Introduction

In the quantum theory of irreversible processes considerable progress has been made in recent years by introducing the concept of completely positive quantum dynamical semigroups (Kossakowski 1972a, b, Gorini *et al* 1976, 1978). It guarantees that the time evolution of an open system preserves the basic quantum mechnical properties of density operators as required by the von Neumann conditions. In particular, for N-level systems the structure of quantum Markovian master equations is therefore completely known and is, of course, of considerable value for a wide range of potential applications in any kind of spectroscopy. Surprisingly, very little has been done (Pöttinger and Lendi 1984, 1985, Lendi 1986) and preference seems to be given to inventing purely phenomenological equations. This may partly be due to the fact that the theory is usually not formulated in a way that is easily accessible to practical applications.

The aim of this paper is to provide such a formulation by introducing the coherence vector concept and to show, in a systematic way, how to transform a rather complicated matrix equation to a linear inhomogeneous first-order differential equation for this coherence vector. The complete classification of the spectral properties of the associated evolution matrix is then of central importance, as shown in § 3. Finally, we give an explicit analysis of the different possible types of final destination states in § 4. For further theoretical details and applications to spectroscopic problems the reader is referred to the fourthcoming publication of Kossakowski *et al* (1986).

2. The Kossakowski generator as evolution matrix

Quantum Markovian master equations for N-level systems are given by a matrix

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differential equation for an $(N \times N)$ density matrix ρ_t in the form

$$\dot{\rho}_t = \mathscr{L}\rho_t \tag{2.1}$$

where $\mathscr{L}$ is the infinitesimal generator of a completely positive quantum dynamical semigroup of time translations

$$\Lambda_t = \exp(\mathscr{L}t) \qquad t \geqslant 0. \tag{2.2}$$

The basic structure theorem (Gorini *et al* 1976) states that $\mathscr{L}$ can generally be represented in a so-called Kossakowski-normal form

$$\mathscr{L}\rho_t = -\mathrm{i}[H, \rho_t] + \tfrac{1}{2}\sum_{i,k=1}^{N^2-1} a_{ik}\{[F_i, \rho_t F_k^*] + [F_i\rho_t, F_k^*]\} \tag{2.3}$$

where

$$H = H^* \qquad \mathrm{Tr}(H) = 0 \tag{2.4}$$

$$A = \{a_{ik}\}_1^M \qquad A = A^* \geqslant 0 \tag{2.5}$$

$$\mathrm{Tr}(F_i) = 0 \qquad \mathrm{Tr}(F_i F_k^*) = \delta_{ik} \qquad 1 \leqslant i, k \leqslant M \tag{2.6}$$

with the abbreviation

$$M = N^2 - 1. \tag{2.7}$$

Recall that the time evolution

$$\Lambda_t\colon \rho_t = \Lambda_t\rho_0 \tag{2.8}$$

has the property of strictly preserving the von Neumann conditions

$$\rho_t = \rho_t^* \qquad \rho_t > 0 \qquad \mathrm{Tr}(\rho_t) = 1 \qquad t \geqslant 0 \tag{2.9}$$

with the convention of denoting by $\rho > 0$ a matrix with associated positive quadratic form.

Without loss of generality one may choose a complete orthonormalised set of Hermitian matrices:

$$\{F_i\}_1^M \qquad F_i = F_i^* \tag{2.10}$$

to fulfil (2.6) and a particularly simple choice is offered by the infinitesimal generators of the special unitary group $\mathrm{SU}(N)$, whose systematic construction will be briefly summarised. Start with the simple $(N \times N)$ matrices $P^{(i,k)}$ whose elements $P_{\mu\nu}^{(i,k)}$ are all zero except for one:

$$P_{\mu\nu}^{(i,k)} = \delta_{\mu i}\delta_{\nu k} \qquad (1 \leqslant i, k, \mu, \nu \leqslant N). \tag{2.11}$$

Next, by taking linear combinations for $i \neq k$,

$$S^{(i,k)} = \frac{1}{\sqrt{2}}(P^{(i,k)} + P^{(k,i)}) \qquad i < k \tag{2.12}$$

$$J^{(i,k)} = \frac{\mathrm{i}}{\sqrt{2}}(P^{(i,k)} - P^{(k,i)}) \qquad i < k. \tag{2.13}$$

$N(N-1)$ Hermitian and traceless matrices are constructed. The projectors $P^{(k,k)}$ are finally used to build up $N-1$ further matrices through

$$D^{(l)} = \frac{1}{[l(l+1)]^{1/2}}\left(\sum_{k=1}^{l} P^{(k,k)} - lP^{(l+1,l+1)}\right) \qquad (1 \leqslant l \leqslant N-1). \tag{2.14}$$

Thus there is a set $M = \{S^{(i,k)}, J^{(i,k)}, D^{(l)}\}$ of $M = N^2 - 1$ matrices which are orthonormalised with respect to the trace metric due to the relation following from (2.11):

$$\mathrm{Tr}(P^{(i,k)}P^{(m,n)}) = \delta_{in}\delta_{km}. \tag{2.15}$$

Its completeness follows from standard arguments of linear algebra. Consequently, any Hermitian $(N \times N)$ matrix $X = X^*$ can be represented in a unique way by

$$X = \frac{1}{N}\mathrm{Tr}(X)\mathbb{1}_N + \sum_{k=1}^{M} x_k F_k \qquad x_k \in \mathbb{R} \tag{2.16}$$

($\mathbb{1}_N$ is the unit matrix in N dimensions) by taking for $\{F_k\}_1^M$ the set $\mathcal{M}$, for instance, the numbering being a matter of convenience. Since these F_k can be shown to be infinitesimal generators of unitary transformations in N dimensions with determinant equal to one (Lichtenberg 1970, Georgi 1982) they form the Lie algebra of SU(N) with

$$[F_i, F_k] = \mathrm{i}\sum_{l=1}^{M} f_{ikl}F_l \qquad f_{ikl} \in \mathbb{R} \tag{2.17}$$

$$\{F_i, F_k\} = \frac{2}{N}\delta_{ik} + \sum_{l=1}^{M} d_{ikl}F_l \qquad d_{ikl} \in \mathbb{R} \tag{2.18}$$

where $\{\cdot, \cdot\}$ denotes an anticommutator and the f and d are completely antisymmetric or symmetric structure constants (with respect to interchange of any pair of indices).

We are now in position to proceed to the construction of the evolution matrix G. For this purpose, the time-dependent density matrix ρ_t is decomposed into

$$\rho_t = \frac{1}{N}\mathbb{1}_N + \sum_{i=1}^{M} v_i(t)F_i \tag{2.19}$$

where the $v_i(t)$ are real-valued functions of time with

$$v_i(t) = \mathrm{Tr}(\rho_t F_i) \tag{2.20}$$

and bounded by certain restrictions to be discussed in the next section. Thus time evolution of ρ_t is given by transformations of a so-called coherence vector

$$\boldsymbol{v}(t) = (v_1(t), v_2(t), \ldots, v_M(t))^{\mathrm{T}} \in \mathbb{R}^{(M)} \tag{2.21}$$

in a real M-dimensional vector space, and the differential equation equivalent to the quantum Markovian master equation (2.1)

$$\dot{\boldsymbol{v}}(t) = G\boldsymbol{v}(t) + \boldsymbol{k} \tag{2.22}$$

is of the simplest linear inhomogeneous evolution type with real matrix elements g_{ik} of G and real $\boldsymbol{k}$, of course. According to Hamiltonian and non-Hamiltonian contributions to the Kossakowski generator $\mathcal{L}$ in (2.3) we decompose

$$G = Q + R \tag{2.23}$$

and also (see (2.4))

$$H = \sum_{n=1}^{M} h_n F_n \qquad h_n \in \mathbb{R} \tag{2.24}$$

and find, by using (2.17)-(2.21), the general formulae for the matrix elements q_{ik} of Q, r_{ik} of R and the components k_i of $\boldsymbol{k}$,

$$q_{ik} = -\sum_{n=1}^{M} h_n f_{nik} \tag{2.25}$$

$$r_{ik} = -\tfrac{1}{4} \sum_{\substack{l,m,n=1 \\ (l \leq m)}}^{M} (2-\delta_{lm}) \operatorname{Re}(a_{lm})\{f_{lni}f_{mnk} + f_{mni}f_{lnk}\} + \tfrac{1}{2} \sum_{\substack{l,m,n=1 \\ (l<m)}}^{M} \operatorname{Im}(a_{lm})\{f_{mni}d_{lnk} - f_{lni}d_{mnk}\} \tag{2.26}$$

$$k_i = -\frac{2}{N} \sum_{\substack{l,m=1 \\ (l<m)}}^{M} \operatorname{Im}(a_{lm}) f_{lmi} \tag{2.27}$$

with $\operatorname{Re}(\cdot)$ and $\operatorname{Im}(\cdot)$ the real and imaginary parts of a quantity. The important symmetry relations are as follows:

$$Q^{\mathrm{T}} = -Q \tag{2.28}$$

$$R^{\mathrm{T}} = R \qquad \text{for arbitrary } A \text{ iff } N = 2 \tag{2.29}$$

$$R^{\mathrm{T}} = R \qquad \text{for } 3 \leq N < \infty \text{ iff } A = A^{\mathrm{T}}. \tag{2.30}$$

In all other cases R has no definite symmetry. This shows that, in general, the evolution matrix G is of no definite symmetry either, with the consequence that the solutions of (2.22) may be complicated and have to be analysed carefully. Before we do that (in § 3) it is worthwhile to mention the case of purely reversible dynamics characterised by

$$A = 0 (R = 0, \boldsymbol{k} = 0) \rightarrow G^{\mathrm{T}} = -G \tag{2.31}$$

such that the Frobenius norm

$$\|\rho_t\|^2 = \operatorname{Tr}(\rho_t^2) \tag{2.32}$$

or, equivalently, the otherwise time-dependent length $\eta(t)$ of the coherence vector,

$$\eta^2(t) = \sum_{k=1}^{M} v_k^2(t) \qquad \|\rho_t\|^2 = \frac{1}{N} + \eta^2(t) \tag{2.33}$$

becomes a constant of motion due to the skew symmetry of G. This is the reason why, for classical dynamical systems, the original non-linear equations are transformed, whenever possible, to the above linear quantum-like structure and then a complete set of constants of motion can be found (Lax 1968, Moser 1980).

3. The spectrum of G and general solutions

Since G is asymmetric its eigenvalues λ_k are, in general, complex quantities and we denote by $\sigma[G]$ the whole spectrum:

$$\sigma[G] = \{\lambda_k = \mu_k + \mathrm{i}\nu_k\}_1^M \qquad \mu_k, \nu_k \in \mathbb{R} \tag{3.1}$$

which must be subjected to restrictions following from the von Neumann conditions (2.9). In fact, the latter imply that

$$0 \leq \eta(t) \leq (1 - 1/N)^{1/2} \qquad t \geq 0 \tag{3.2}$$

and, trivially, the solutions of (2.22) must therefore be bounded for all times. The second important property of G is its asymmetry with the somewhat uncomfortable consequence that it may not be completely diagonalisable. In such a case we denote by $J[\lambda_k\,;\,d_k]$ the Jordan block associated with an eigenvalue λ_k of multiplicity d_k and by $\mathbb{R}^{(d_k)}_{\lambda_k} \subseteq \mathbb{R}^{(M)}$ the corresponding subspace. The spectrum σ, together with the Jordan normal form of G, is then classified in terms of three subsets:

$$\sigma[G] = \sigma^{(s)} \cup \sigma^{(d)} \cup \sigma^{(0)} \tag{3.3}$$

each of them giving rise to a qualitatively different solution of the evolution equation:

$$\sigma^{(s)} = \{\lambda_k\}_1^K \qquad \mu_k \leqslant 0,\ \nu_k \text{ arbitrary (but } \nu_k \neq 0 \text{ for } \mu_k = 0). \tag{3.4}$$

If $\lambda_{k'} = \lambda_{k''} = \cdots$ ($d_{k'}$-fold)then G is diagonalisable in $\mathbb{R}^{(d_{k'})}_{\lambda_{k'}}$;

$$\sigma^{(d)} = \{\lambda_l\}_{K+1}^L \qquad \mu_l < 0,\ \nu_k \text{ arbitrary.} \tag{3.5}$$

Only $d_{l'}$-fold (>1) sequences $\lambda_{l'} = \lambda_{l''} = \cdots$ and G is non-diagonalisable in $\mathbb{R}^{(d_{l'})}_{\lambda_{l'}}$ with Jordan block $J[\lambda_{l'}\,;\,d_{l'}]$;

$$\sigma^{(0)} = \{\lambda_m\}_{L+1}^M \qquad \lambda_m = 0. \tag{3.6}$$

G is diagonalisable in $\mathbb{R}_0^{(M-L-1)}$.

In correspondence to (3.3)-(3.6), the complete solution of the homogeneous part of (2.22):

$$\dot{\boldsymbol{u}}(t) = G\boldsymbol{u}(t) \tag{3.7}$$

is given by

$$\boldsymbol{u}(t) = \boldsymbol{u}^{(s)}(t) + \boldsymbol{u}^{(d)}(t) + \boldsymbol{u}^{(0)} \tag{3.8}$$

together with the constants for the initial condition,

$$\boldsymbol{s} = (s_1, s_2, \ldots, s_M)^{\mathrm{T}} \tag{3.9}$$

where

$$\boldsymbol{u}^{(s)}(t) = \sum_{\substack{k=1 \\ (\lambda_k \in \sigma^{(s)})}}^{K} s_k \exp(\lambda_k t)\boldsymbol{x}^{(k)} \tag{3.10}$$

$$\boldsymbol{u}^{(d)}(t) = \sum_{\substack{l=\{K+1\} \\ (\lambda_l \in \sigma^{(d)})}}^{\{L\}} \exp(\lambda_l t)\left(\sum_{q=1}^{d_l} s_q \boldsymbol{p}_q^{(l)}(t)\right) \tag{3.11}$$

$$\boldsymbol{u}^{(0)} = \sum_{m=L+1}^{M} s_m \boldsymbol{x}^{(m)} \tag{3.12}$$

and where the special summation from $l = \{K+1\}$ until $\{L\}$ in the second summand indicates that l runs only over the indices l' of different Jordan blocks $J[\lambda_{l'}, d_{l'}]$. Furthermore, $\{\boldsymbol{x}^{(k)}\}_1^K$ and $\{\boldsymbol{x}^{(m)}\}_{L+1}^K$ are right-eigenvectors of G and the components of the vectors $\boldsymbol{p}_q^{(l)}(t)$ are polynomials at most of degree $(q-1)$ in t

$$\boldsymbol{p}_q^{(l)}(t) = \sum_{n=0}^{q-1} \frac{t^n}{n!}(G - \lambda_l \mathbb{1}_N)^n \boldsymbol{y}_q^{(l)} \tag{3.13}$$

the constant vector $\boldsymbol{y}_q^{(l)}$ being a solution of

$$(G - \lambda_l \mathbb{1}_N)^q \boldsymbol{y}_q^{(l)} = 0. \tag{3.14}$$

The detailed proofs follow from standard algebra (Gantmacher 1958). Note that the constants (3.9) are obtained from the initial condition $\boldsymbol{u}(o)$ through

$$\boldsymbol{s} = T^{-1}\boldsymbol{u}(0) \tag{3.15}$$

where T is a matrix with the linearly independent vectors $\boldsymbol{x}^{(k)}$, $\boldsymbol{y}_q^{(l)}$ and $\boldsymbol{x}^{(m)}$ as columns and, therefore, the inverse exists always. Finally, we recall that $\boldsymbol{u}(t)$ can always be written in real form since for any complex conjugate pair, e.g. $\lambda_k = \bar{\lambda}_{k+1} \in \sigma^{(s)}$, the corresponding two summands in (3.10) may be combined to give

$$\exp(\mu_k t)[s_k(\boldsymbol{w}^{(1)} \cos \nu_k t - \boldsymbol{w}^{(2)} \sin \nu_k t) + s_{k+1}(\boldsymbol{w}^{(1)} \sin \nu_k t + \boldsymbol{w}^{(2)} \cos \nu_k t)] \tag{3.16}$$

where

$$G\boldsymbol{w}^{(k)} = \lambda_k \boldsymbol{w}^{(k)} \qquad \boldsymbol{w}^{(k)} = \boldsymbol{w}^{(1)} + \mathrm{i}\boldsymbol{w}^{(2)}. \tag{3.17}$$

In the next section, the present results will be used to classify all stationary states of (2.1) or, equivalently, (2.22).

4. Relaxing semigroups

The question about existence and nature of final destination states for irreversible processes in open quantum systems is of particular interest in connection with the approach to equilibrium (Alicki 1976, Spohn and Lebowitz 1978). By equilibrium one usually means either a thermodynamic equilibrium or else any stationary state. Due to the linearity of the dynamical equations there are only stationary states for $t \to \infty$ but of quite different properties. In any case we introduce formally

$$\rho^{(\infty)} = \lim_{t \to \infty} \rho_t \tag{4.1}$$

or, equivalently in the coherence vector language,

$$\boldsymbol{v}^{(\infty)} = \lim_{t \to \infty} \boldsymbol{v}(t) \tag{4.2}$$

where $\boldsymbol{v}(t)$ is now the general solution of equation (2.22),

$$\boldsymbol{v}(t) = \boldsymbol{u}(t) + \boldsymbol{w} \tag{4.3}$$

with $\boldsymbol{u}(t)$ a solution of the homogeneous part (3.7) and $\boldsymbol{w}$ a particular solution obtained from

$$G\boldsymbol{w} + \boldsymbol{k} = 0. \tag{4.4}$$

Again, the spectral properties of G will lead to the distinction of three qualitatively different types of so-called relaxing semigroups Λ_t (equation (2.8)).

(i) A semigroup Λ_t is called uniquely relaxing if the limit (4.1) exists and is independent of any initial conditions ρ_0.

This means that $\rho^{(\infty)}$ is exclusively determined by the semigroup generator $\mathscr{L}(\mathscr{L}\rho^{(\infty)} = 0)$, or else by the evolution matrix G and the vector $\boldsymbol{k}$. Furthermore, this type of stationary state is an invariant state or a fixed point of the mapping Λ_t:

$$\rho^{(\infty)} = \Lambda_t \rho^{(\infty)}. \tag{4.5}$$

Since we have

$$\boldsymbol{u}(t) = \exp(Gt)\boldsymbol{u}(0) \qquad \boldsymbol{u}(0) = \boldsymbol{v}(0) - \boldsymbol{w} \tag{4.6}$$

equation (4.5) implies

$$\lim_{t\to\infty} \boldsymbol{u}(t) = 0 \tag{4.7}$$

and, according to (3.10)-(3.12), this is only possible for

$$\det(G) \neq 0. \tag{4.8}$$

Thus, one can identify

$$\boldsymbol{v}^{(\infty)} = \boldsymbol{w} \qquad \boldsymbol{w} = -G^{-1}\boldsymbol{k} \tag{4.9}$$

and the spectral properties of G are characterised by a restriction on (3.3):

$$\sigma[G] = \tilde{\sigma}^{(s)} \cup \sigma^{(d)} \tag{4.10}$$

where $\tilde{\sigma}^{(s)}$ differs from $\sigma^{(s)}$ in (3.4) by the stronger requirement $\mu_k < 0$. Although it would be desirable to relate the discussed properties of G to those of A in (2.3) this seems to be a rather inaccessible task in general and there is only one useful theorem known. This is due to Spohn (1976) who proved that a sufficient condition for Λ_t to be uniquely relaxing is given for a relaxation matrix A with n_0 zero eigenvalues if

$$2n_0 < M. \tag{4.11}$$

Note that this condition is not always necessary, however, and the details may be more subtle and admit unique relaxation even in cases where (4.11) is violated (Kossakowski *et al* 1986).

(ii) A semigroup Λ_t is called relaxing if the limit (4.1) exists but depends on the initial condition ρ_0.

Whereas in case (i) the stationary states could be obtained by setting $\dot{\boldsymbol{v}}(t) = 0$ ($\dot{\rho}_t = 0$) this is not so in this case since the limit (4.7) is different from zero:

$$\boldsymbol{u}^{(\infty)} = \lim_{t\to\infty} \boldsymbol{u}(t) \tag{4.12}$$

and, therefore, in contrast to (4.9) one has

$$\boldsymbol{v}^{(\infty)} = \boldsymbol{u}^{(\infty)} + \boldsymbol{w}. \tag{4.13}$$

As is clear from the spectral analysis in § 3, equation (4.12) with $\boldsymbol{u}^{(\infty)} \neq 0$ implies that G has at least one eigenvalue zero and thus the spectrum is characterised by

$$\sigma[G] = \tilde{\sigma}^{(s)} \cup \sigma^{(d)} \cup \sigma^{(0)}. \tag{4.14}$$

As a consequence, $\boldsymbol{w}$ in (4.3) or (4.13) cannot be obtained as in (4.9) but must be calculated from equation (4.4) which may have no solution at all if $\boldsymbol{k}$ is incompatible and then equation (2.22) has no bounded solution either. On the other hand, if $\boldsymbol{k}$ is compatible (4.4) has infinitely many solutions but let us consider this case in more detail. Denote by

$$r = \operatorname{rank}(G) \qquad \Delta = M - r \tag{4.15}$$

the rank and deficiency index of G and by $\boldsymbol{k}^{(\Delta)}$ a $\boldsymbol{k}$ vector whose components fulfil the Δ compatibility relations. The equation

$$G\boldsymbol{w} + \boldsymbol{k}^{(\Delta)} = 0 \tag{4.16}$$

admits a Δ-parametric set of solutions (infinitely many) but despite this there is only one solution $v(t)$ since in the latter the parameter dependence of $\boldsymbol{w}$ is exactly compensated by $\boldsymbol{u}(0)$ because the initial condition $\boldsymbol{v}(0) = \boldsymbol{u}(0) + \boldsymbol{w}$ must not depend on any of these parameters, of course. Note that (4.6) is always valid irrespective of the spectral properties of G and, therefore, $\boldsymbol{u}^{(\infty)}$ and $\boldsymbol{v}^{(\infty)}$ depend upon $\boldsymbol{v}(0)$ only. Finally, one can state that every initial condition $\boldsymbol{v}(0)$ (or ρ_0), together with the elements of G and a compatible $\boldsymbol{k}^{(\Delta)}$, uniquely determine the final state $\boldsymbol{v}^{(\infty)}$ (or $\rho^{(\infty)}$) and the fixed point property (4.5) is lost. Thus there are as many stationary states as there are initial conditions.

(iii) A semigroup Λ_t is called partially relaxing if the limit (4.1) does not exist but there is a decomposition of ρ_t in terms of two orthogonal projectors P and Q ($P+Q=\mathbb{1}_N$) such that

$$\lim_{t\to\infty} Q\rho_t Q = \rho^{[Q]} \tag{4.17}$$

$$P\rho_t P \xrightarrow[t\to\infty]{} \rho_t^{[P]}. \tag{4.18}$$

Here $\rho_t^{[P]}$ is a matrix whose non-zero elements are purely periodic functions of time. This is the case for a spectrum of G given by the general formula (3.3) but with the special requirement for $\sigma^{(s)}$ to necessarily contain eigenvalues λ_k with $\mu_k = 0$ whereas $\sigma^{(0)}$ may be empty or not. The relaxing part $\rho^{[Q]}$ can then be classified according to (i) or (ii) regarding the dependence on initial conditions.

5. Conclusion

The coherence vector formulation is a systematic generalisation to N dimensions of common relaxation treatments that lead to the well known Bloch equations for two-level systems (Allen and Eberly 1975). Remarkably, already for $N=2$ one obtains more general equations than the usual Bloch equations and finds interesting connections to recent experiments (Lendi 1986, Kossakowski *et al* 1986).

The detailed spectral analysis of the evolution matrix G presented has been based on two basic properties, one requiring boundedness of solutions and the other its asymmetry. However, it has been supposed that asymmetry may imply non-diagonalisability and therefore a non-trivial Jordan canonical form although this is not a necessary consequence of asymmetry. Since it is unusual to deal with non-diagonalisable matrices in problems of real physical importance one might conjecture that, due to the special formula (2.26) involving structure constants of the Lie algebra, the matrix G also acquires some unrevealed structure such that it is diagonalisable despite its asymmetry. That there is no general mathematical proof for diagonalisability can, of course, be shown by giving a counterexample. In order to avoid too lengthy formulae and estimates involving all inequalities derived from the most important property (2.5) we quote it, as far as possible, numerically for $N=2$ ($M=3$). Consider, thus, a matrix G fulfilling all necessary requirements stated in § 3. For instance,

$$G = \frac{1}{2}\begin{pmatrix} -17 & -1 & 1 \\ 1 & -17 & 1 \\ 2 & 0 & -16 \end{pmatrix} \tag{5.1}$$

with the decomposition (2.23) given by

$$Q=\frac{1}{2}\begin{pmatrix}0 & -1 & -\frac{1}{2}\\ 1 & 0 & \frac{1}{2}\\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix} \qquad R=\frac{1}{2}\begin{pmatrix}-17 & 0 & \frac{3}{2}\\ 0 & -17 & \frac{1}{2}\\ \frac{3}{2} & \frac{1}{2} & -16\end{pmatrix}. \tag{5.2}$$

G is not completely diagonalisable with the Jordan canonical form

$$J[G]=\begin{pmatrix}-8 & 1 & 0\\ 0 & -8 & 0\\ 0 & 0 & -9\end{pmatrix}. \tag{5.3}$$

The constant vector $\boldsymbol{k}$ in (2.22) is chosen to be

$$\boldsymbol{k}=(k_1, k_2, k_3)^{\mathrm{T}}=-\sqrt{2}(1, 0, 1)^{\mathrm{T}}. \tag{5.4}$$

All one has to show is that the original relaxation matrix A in the Kossakowski generator $\mathscr{L}$ is positive semidefinite, indeed. For completeness, we give the inversion formulae as obtained from equations (2.26) and (2.27) by using $f_{123}=\sqrt{2}$ and $d_{123}=0$ (for the normalised Pauli matrices):

$$a_{11}=-\tfrac{1}{2}(r_{22}+r_{33}-r_{11}) \qquad a_{22}=-\tfrac{1}{2}(r_{11}+r_{33}-r_{22}) \tag{5.5}$$

$$a_{33}=-\tfrac{1}{2}(r_{11}+r_{22}-r_{33}) \qquad a_{12}=r_{12}-\mathrm{i}k_3/\sqrt{2} \tag{5.6}$$

$$a_{13}=r_{13}+\mathrm{i}k_2/\sqrt{2} \qquad a_{23}=r_{23}-\mathrm{i}k_1/\sqrt{2}. \tag{5.7}$$

Thus we find

$$A=\frac{1}{4}\begin{pmatrix}16 & 4\mathrm{i} & 3\\ -4\mathrm{i} & 16 & 1+4\mathrm{i}\\ 3 & 1-4\mathrm{i} & 18\end{pmatrix} \tag{5.8}$$

which is even a positive matrix since all leading minors are positive. Therefore, time evolution carries density operators into density operators and the semigroup is uniquely relaxing since $\det(G)\neq 0$. For further details and applications to problems in magnetic and optical resonance spectroscopy the reader is referred to Kossakowski *et al* (1986).

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