Foundations of Physics, Vol. 7, Nos. 11/12, 1977

Generalized Two-Level Quantum Dynamics. I. Representations of the Kossakowski Conditions

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Received June 9, 1976

This communication is part I of a series of papers which explore the theoretical possibility of generalizing quantum dynamics in such a way that the predicted motions of an isolated system would include the irreversible (entropy-increasing) state evolutions that seem essential if the second law of thermodynamics is ever to become a theorem of mechanics. In this first paper, the general mathematical framework for describing linear but not necessarily Hamiltonian mappings of the statistical operator is reviewed, with particular attention to detailed representations of the Kossakowski conditions for the case of a two-level system.

1. GENERAL INTRODUCTION

For more than a century it has been evident that two fundamental theories of physics—mechanics and thermodynamics—are incompatible with one another. Whether the mechanics is classical or quantal, it is a matter of simple, unassailable logic that the Gibbs–von Neumann entropy formula is invariant under all Hamiltonian motions, and hence that some cherished construct of theoretical physics must eventually be modified before the second law of thermodynamics can become a theorem of mechanics. This is of course the famous problem of irreversibility.

The situation is somewhat reminiscent of the historic contradiction between Newtonian mechanics and Maxwellian optics, which was finally resolved by the special theory of relativity. Something had to be altered in one or both of those theories. As is well known, it turned out to be the Galilean kinematics that Einstein discarded, with the result that mechanics

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was dramatically revised, while electromagnetic field theory remained unscathed.

Similarly, in the modern irreversibility problem it seems obvious that something must be altered in either thermodynamics or quantum mechanics, or both; and there have indeed been many proposals to alleviate the dilemna, ranging from blind refusals to acknowledge the difficulty to proud assertions that the problem has been solved. Although it is not our current objective to offer a comprehensive review of the situation, we shall briefly mention several approaches that have been suggested in order to establish the context of our present investigations.

According to one viewpoint, Hamiltonian quantum mechanics is to be regarded as sacrosanct, so that any change in physical theory designed to accommodate the second law of thermodynamics must occur somewhere within thermodynamics and its physical interpretation. Included within this category are (a) the informational explanation,[1,2] wherein the entropy becomes subjective or "anthropomorphic" and its increase merely reflects the inevitable growth of obsolescence of past knowledge, (b) the random external field hypothesis,[3,4] according to which thermodynamically closed systems are actually mechanically open subsystems driven to higher levels of entropy by their surroundings, and (c) the theories of the prolific "Brussels school,"[5] which has an entropy expression of its own to replace the invariant formula of ordinary statistical thermodynamics. We regard each of these attemtps to deduce irreversibility as unsatisfactory, for these reasons, respectively: (a) Even though we admire the potency of information theory for systematic guessing of undetermined states and believe it to be a necessity in the practice of statistical physics,[6] we believe nevertheless that the second law is an objective physical principle which would be valid even if the quantum states were completely determined; in other words, the thermodynamic entropy of a closed system will rise irreversibly even if the sequence of exact quantum states is *known* and the information-theoretic entropy is therefore zero. (b) About twenty years ago, one of us (W.B.) was among the first to advocate the view that the quantal uncertainties of the enclosure material drive up the entropy of the enclosed substance; there are recent developments[7] along this line in which the "enclosure" becomes the astrophysical universe itself, constrained by cosmological boundary conditions, which are regarded as the ultimate source of the asymmetry exhibited by the second law. We are not prepared to comment conclusively on the cosmological version of this approach; however, the basic flaws in any version involving a bounded enclosure are that in Hamiltonian motion the composite system of enclosure plus substance will have its total entropy still invariant and that, since the overall motion is quasiperiodic,[8] the subentropy of the substance alone cannot display any permanent tendency to increase. (c) The Brussels entropy can only increase for quantum systems characterized by exotic mathematical properties which are associated only with the so-called thermodynamic limit ($N \to \infty$, $V \to \infty$, N/V finite). Though we would not deny the efficacy of this limit concept in the practical computation of intensive parameters, we cannot accept the notion that the second law could be applicable only to such obviously fictitious systems.

A second logical alternative for unifying mechanics and thermodynamics is to accept the premises of the latter as facts which contemporary quantum mechanics fails to predict, and to seek therefore some refinement of mechanics which would enable it to describe irreversible processes in a direct rational manner. This point of view is certainly the minority position, but it has been suggested before and to some extent developed by Sudarshan[9–12] and his colleagues, and by Kossakowski[13,14] and Ingarden.[15,16]

The present series of papers investigates all possible linear dynamical postulates applicable to the simplest imaginable model, the two-level quantum system. The idea is to explore the theoretical possibility of generalizing quantum mechanics so that it can easily describe both reversible and irreversible (entropy-increasing) motions. The remainder of the present communication (part I of the series) establishes the mathematical framework for discussing linear generalizations of quantum dynamics, with particular attention to the two-level system. In part II we shall classify in a geometrically visualizable manner all possible motions that can be linearly generated for a two-level system. Finally, in part III we shall consider the thermodynamically interesting class of energy-conserving, entropy-increasing motions.

2. OPERATOR SPACE FORMALISM

Let the system of interest be characterized by a Hilbert space $\mathscr{H}$, the self-adjoint operators on $\mathscr{H}$ corresponding as usual to the physical observales associated with the system. Let $\{| \alpha_n\rangle\}$, a complete orthonormal set spanning $\mathscr{H}$, be chosen as a representation so that any observable B can be written as

$$B = \sum_{mn} | \alpha_m\rangle B_{mn} \langle\alpha_n | \tag{1}$$

where B_{mn} are c-numbers with $B_{mn} = B_{nm}^*$. When B operates on any vector $| \beta\rangle$ in $\mathscr{H}$ we have a new vector

$$| \beta'\rangle = B | \beta\rangle = \sum_{mn} B_{mn} \langle\alpha_n | \beta\rangle | \alpha_m\rangle \tag{2}$$

The preparation, or quantum state, of the system is represented by a statistical operator

$$\rho = \sum | \alpha_m\rangle \rho_{mn} \langle\alpha_n | \tag{3}$$

where $\rho_{mn} = \rho_{nm}^*$, $\operatorname{Tr} \rho = 1$, and the ρ_{nm} are elements of a positive-semi definite matrix. The mean value of the observable B as measured over the ensemble described by ρ is given by the basic interpretive formula

$$\langle B \rangle = \operatorname{Tr}(B\rho) \tag{4}$$

We adopt the Schrödinger picture, in which the observables are independent of time while the statistical operator evolves with time, so that the expectation value evolves with rate of change

$$(d/dt)\langle B \rangle = \operatorname{Tr}(B\, d\rho/dt) \tag{5}$$

The general dynamical problem then is to describe the time dependence of the statistical operator. Thus, given $\rho(0)$ at time zero, we wish to find a linear law which determines $\rho(t)$ at a later time t. [The restriction to linear mappings is suggested by the fact that any mixed quantal ensemble may be subdivided into or composed from distinct subensembles which are assumed to evolve independently. Thus, if $\rho_1(0) \to \rho_1(t)$, $\rho_2(0) \to \rho_2(t)$, then by hypothesis $\rho(0) = W_1\rho_1(0) + W_2\rho_2(0) \to \rho(t) = W_1\rho_1(t) + W_2\rho_2(t)$.] This essentially means that we wish to find a linear superoperator $\mathscr{T}(t)$ which, when operating on $\rho(t_1)$, produces $\rho(t_2)$:

$$\mathscr{T}(t_2, t_1)\, \rho(t_1) = \rho(t_2) \tag{6}$$

This is closely analogous to the behavior of the operator B on the vector $| \beta \rangle$ in (2), which prompts one to set up a new linear vector space $\mathscr{A}$ whose elements are the operators on $\mathscr{H}$. We shall wish to decide arbitrarily on sets of operators of $\mathscr{H}$ that can serve as the basis, or "quorum,"[6] for $\mathscr{A}$. The most obvious choice is the dyadic set

$$\{Q_{nm}\} \equiv \{| \alpha_n \rangle \langle \alpha_m |\} \tag{7}$$

Any operator B then can be written as

$$B = \sum_{nm} B_{nm} Q_{nm} \tag{8}$$

We shall write $| Q_{nm})$ for the vector in $\mathscr{A}$ corresponding to the operator Q_{nm} on $\mathscr{H}$, and define a scalar product in $\mathscr{A}$ by

$$(A \mid B) = \operatorname{Tr}(A^\dagger B) \tag{9}$$

so that

$$(Q_{nm} \mid Q_{jk}) \equiv \operatorname{Tr}(Q_{nm}^\dagger Q_{jk}) = \delta_{nj}\, \delta_{mk} \tag{10}$$

and

$$(A \mid B) = \sum_{nm} A_{mn}^* B_{nm} \tag{11}$$

if

$$| A) = \sum_{nm} A_{nm} \mid Q_{nm})$$

3. GENERALIZED DYNAMICAL POSTULATE

Any superoperator on $\mathscr{A}$ has the form

$$\mathscr{T} = \sum_{mnjk} \mid Q_{mn}) \, \mathscr{T}_{mn,jk} \, (Q_{jk} \mid \tag{12}$$

while the statistical operator becomes a vector

$$| \rho) = \sum_{mn} \rho_{mn} \mid Q_{mn}) \tag{13}$$

Hence in this representation the law of evolution (6) becomes

$$\rho_{mn}(t_2) = \sum_{jk} \mathscr{T}_{mn,jk}(t_2 \, , t_1) \, \rho_{jk}(t_1) \tag{14}$$

Returning to the more general notation, we shall postulate that the evolution superoperator $\mathscr{T}$ for an isolated system depends only on the difference $(t_2 - t_1)$ and

$$\mathscr{T}(t_n - t_k) \, \mathscr{T}(t_k - t_l) = \mathscr{T}(t_n - t_l) \tag{15}$$

with

$$\mathscr{T}(0) = 1_{\mathscr{A}} \tag{16}$$

the identity in $\mathscr{A}$. In other words, just as in ordinary quantum dynamics we continue to assume that time is homogeneous and evolution is transitive. This postulate amounts to the statment that there exists a superoperator $\mathscr{L}$ on $\mathscr{A}$, the generator of temporal evolution, such that

$$\mathscr{T}(t_2 - t_1) = e^{(t_2 - t_1)\mathscr{L}} \tag{17}$$

If the matrix $\mathscr{T}_{mn,jk}$ in (12) has an inverse, it is possible to invert (14). Thus, writing (14) in the form

$$\rho(t_2) = e^{(t_2 - t_1)\mathscr{L}} \rho(t_1) \tag{18}$$

we also have

$$\rho(t_1) = e^{-(t_2 - t_1)\mathscr{L}} \rho(t_2) \tag{19}$$

Equation (19) would imply that, given a statistical operator at time t_2, we can compute the state from which it must have evolved at an earlier time t_1;

but the essence of thermodynamic irreversibility is that once entropy is maximized, such a retrodictive computation must be impossible. Therefore, to obtain irreversible motion, we must have some evolution superoperators that do not possess an inverse.

Setting $t_2 = t$ and differentiating (18), we express the law of evolution as a differential equation

$$\partial\rho(t)/\partial t = \mathscr{L}e^{(t-t_1)\mathscr{L}}\rho(t_1) = \mathscr{L}\rho(t) \tag{20}$$

If there exists an operator H on $\mathscr{H}$ such that

$$\mathscr{L}\rho = (1/i)[H, \rho] \tag{21}$$

then (20) becomes the familiar Liouville–von Neumann equation of motion for the statistical operator, which has no capacity for describing irreversible motion. However, we do not intend to restrict the Liouville superoperator, or *Liouvillian*, $\mathscr{L}$ to the Hamiltonian form. In the dyadic representation of $\mathscr{A}$ the equation of motion can also be written

$$\sum_{mn} \frac{\partial\rho_{mn}}{\partial t} \mid Q_{mn}) = \sum_{mnjk} \mathscr{L}_{mn,jk}\rho_{jk} \mid Q_{mn}) \tag{22}$$

or

$$\dot{\rho}_{mn} = \sum_{jk} \mathscr{L}_{mn,jk}\rho_{jk} \tag{23}$$

where

$$\mathscr{L}_{mn,jk} \equiv (Q_{mn} \mid \mathscr{L} \mid Q_{jk}) \tag{24}$$

The main objective now is to investigate the conditions that must be met by the matrix $\mathscr{L}_{mn,jk}$ to qualify as an acceptable generator of dynamic evolution.

4. THE KOSSAKOWSKI CONDITIONS

An elegant theorem due to Kossakowski[14] enunciates the necessary and sufficient conditions that the Liouvillian be an acceptable dynamical evolution generator, which means that $e^{t\mathscr{L}}\rho$ must be a statistical operator if ρ is a statistical operator; i.e., if ρ has the form (3), then so must $e^{t\mathscr{L}}\rho$. We shall state the theorem without proof:

Let $\{P_n\}$ be orthogonal projectors (elements of $\mathscr{A}$) onto a complete set of finite subspaces of $\mathscr{H}$; i.e., $\{P_n\}$ gives a resolution of the identity in $\mathscr{H}$:

$$P_nP_m = \delta_{nm} P_n, \qquad \operatorname{Tr} P_n < \infty, \qquad \sum_n P_n = 1 \tag{25}$$

Then $\mathscr{L}$ generates a dynamical evolution if and only if for all possible sets $\{P_n\}$

$$(P_n \mid \mathscr{L} \mid P_n) \leqslant 0; \qquad (P_n \mid \mathscr{L} \mid P_m) \geqslant 0; \qquad n \neq m \tag{26}$$

and

$$\sum_n (P_n \mid \mathscr{L} \mid P_m) = 0, \qquad \text{for every } m \tag{27}$$

[Note that the subset of operators $\{Q_{nn}\}$ from (7) is a particularly simple example of a $\{P_n\}$.]

Because all possible sets $\{P_n\}$ are involved in the theorem, we shall need below a lemma concerning the transformations induced in $\mathscr{A}$ by transformations in $\mathscr{H}$. The unitary transformation in $\mathscr{H}$

$$\{\mid \alpha_n\rangle\} \to \{\mid \alpha_n'\rangle\} = \left\{\sum_k \mid \alpha_k\rangle\langle\alpha_k \mid \alpha_n'\rangle\right\} \tag{28}$$

induces $\{Q_{mn}\} \to \{Q'_{mn}\}$, where

$$Q_{mn} = \mid \alpha_m\rangle\langle\alpha_n \mid = \sum_{kj} \mid \alpha_k'\rangle\langle\alpha_k' \mid \alpha_m\rangle\langle\alpha_n \mid \alpha_j'\rangle\langle\alpha_j' \mid \tag{29}$$

so that

$$\mid Q_{mn}) = \sum_{kj} \langle\alpha_k' \mid \alpha_m\rangle\langle\alpha_n \mid \alpha_j'\rangle \mid Q'_{kj}) \tag{30}$$

and

$$(Q'_{kj} \mid Q_{mn} = \langle\alpha_k' \mid \alpha_m\rangle\langle\alpha_n \mid \alpha_j'\rangle \tag{31}$$

Finally, from

$$\mathscr{L}'_{fg,ij} = (Q'_{fg} \mid \mathscr{L} \mid Q'_{ij}), \qquad \mathscr{L}_{mn,kl} = (Q_{mn} \mid \mathscr{L} \mid Q_{kl}) \tag{32}$$

we have the desired lemma:

$$\mathscr{L}'_{fg,ij} = \sum_{mnkl} (Q'_{fg} \mid Q_{mn})(Q_{mn} \mid \mathscr{L} \mid Q_{kl})(Q_{kl} \mid Q'_{ij}) \tag{33}$$

$$= \sum_{mnkl} \langle\alpha_f' \mid \alpha_m\rangle\langle\alpha_n \mid \alpha_g'\rangle\langle\alpha_k \mid \alpha_i'\rangle\langle\alpha_j' \mid \alpha_l\rangle \, \mathscr{L}_{mn,kl} \tag{34}$$

5. THE TWO-LEVEL QUANTUM SYSTEM

We turn from the general theorem to a particular application—a system whose observables have only two eigenvalues. Associated with the two-dimensional Hilbert space $\mathscr{H}_2$ are only two classes of $\{P_n\}$: (i) sets of two one-dimensional projectors like $|\alpha_1\rangle\langle\alpha_1|$ and $|\alpha_2\rangle\langle\alpha_2|$, and (ii) one two-dimensional projector, the identity in $\mathscr{H}_2$,

$$1 = |\alpha_1\rangle\langle\alpha_1| + |\alpha_2\rangle\langle\alpha_2|$$

All pairs in class (i) are connected by unitary transformations. In $\mathscr{H}_2$ the Kossakowski conditions (26) and (27) for class (i) projections are therefore

$$\begin{aligned} (P_1 | \mathscr{L} | P_1) \leqslant 0, \qquad (P_1 | \mathscr{L} | P_2) \geqslant 0 \\ (P_2 | \mathscr{L} | P_1) \geqslant 0, \qquad (P_2 | \mathscr{L} | P_2) \leqslant 0 \end{aligned} \tag{35}$$

and

$$\begin{aligned} (P_1 | \mathscr{L} | P_2) + (P_2 | \mathscr{L} | P_2) = 0 \\ (P_1 | \mathscr{L} | P_1) + (P_2 | \mathscr{L} | P_1) = 0 \end{aligned} \tag{36}$$

where P_1, P_2 are arbitrary orthogonal one-dimensional projectors on $\mathscr{H}_2$. In the notation of (32) these read

$$\mathscr{L}_{11,11} \leqslant 0, \qquad \mathscr{L}_{22,22} \leqslant 0, \qquad \mathscr{L}_{11,22} \geqslant 0, \qquad \mathscr{L}_{22,11} \geqslant 0 \tag{37}$$

$$\mathscr{L}_{11,22} + \mathscr{L}_{22,22} = 0, \qquad \mathscr{L}_{11,11} + \mathscr{L}_{22,11} = 0 \tag{38}$$

and these equations are to be true for all orthonormal pairs $\{\alpha_n\}$ in $\mathscr{H}_2$.

The class (ii) of projections has only one member, the identity; the corresponding implication of statements (26) and (27) is

$$(1 | \mathscr{L} | 1) = 0 \tag{39}$$

from which we have

$$\begin{aligned} 0 &= \sum_{mnkj} (1 | Q_{mn}) \mathscr{L}_{mn,kj} (Q_{kj} | 1) \\ &= \sum_{mnkj} \mathscr{L}_{mn,kj} \operatorname{Tr} Q_{mn} \cdot \operatorname{Tr} Q_{kj} \\ &= \sum_{mnkj} \mathscr{L}_{mn,kj}\, \delta_{mn}\, \delta_{kj} = \sum_{mk} \mathscr{L}_{mm,kk} \end{aligned}$$

which is an identity if (38) is satisfied. The entire set of necessary and sufficient conditions is therefore contained in (37) and (38).

To investigate the effect of a change of representation, we note that the most general unitary transformation in $\mathscr{H}_2$ is represented by the unitary matrix

$$u = \begin{pmatrix} a & b \\ -b^* e^{i\phi} & a^* e^{i\phi} \end{pmatrix}, \qquad |a|^2 + |b|^2 = 1, \quad \phi \text{ real} \tag{40}$$

When this transformation is used to generate a new pair of projections from the two initially chosen, the arbitrary phase ϕ is redundant. The components of u may be written as

$$u_{mn} = \langle \alpha_n \mid \alpha_m' \rangle \tag{41}$$

so that (28) becomes

$$\begin{pmatrix} \mid \alpha_1' \rangle \\ \mid \alpha_2' \rangle \end{pmatrix} = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \begin{pmatrix} \mid \alpha_1 \rangle \\ \mid \alpha_2 \rangle \end{pmatrix} \tag{42}$$

The lemma (34) can then be written in terms of the parameters a and b, the coefficients of that transformation being a 16×16 matrix

$$U_{fg,ij;mn,kl}(a, b) = u_{fm}^* u_{gn} u_{ik} u_{jl}^* \tag{43}$$

Inspection of (34), (37), and (38) shows that the only rows of the U-matrix that are needed to determine whether a given $\mathscr{L}$ satisfies the Kossakowski conditions (37) and (38) have elements of the form $U_{ff,gg;mn,kl}(a, b)$. Thus the first condition in (37), namely $\mathscr{L}_{ff,ff} = 0$, for all orthonormal pairs $\{\mid \alpha_n \rangle\}$ in $\mathscr{H}_2$, is expressed as follows in terms of the U-matrix:

$$\mathscr{L}'_{ff,ff} = \sum_{mnkl} U_{ff,ff;mn,kl}(a, b)\, \mathscr{L}_{mn,kl} \leqslant 0, \qquad f = 1, 2 \tag{44}$$

$$\text{for every } a, b \text{ such that } \mid a \mid^2 + \mid b \mid^2 = 1$$

The second condition in (37) becomes

$$\mathscr{L}'_{ff,gg} = \sum_{mnkl} U_{ff,gg;mn,kl}(a,b)\, \mathscr{L}_{mn,kl} \geqslant 0, \qquad f \neq g \tag{45}$$

$$\text{for every } a, b \text{ such that } \mid a \mid^2 + \mid b \mid^2 = 1$$

Similarly, Eqs. (38) take the form

$$\sum_{f=1}^{2} \mathscr{L}'_{ff,gg} = \sum_{f=1}^{2} \sum_{mnkl} U_{ff,gg;mn,kl}(a, b)\, \mathscr{L}_{mn,kl} = 0, \qquad g = 1, 2 \tag{46}$$

$$\text{for every } a, b, \text{ such that } \mid a \mid^2 + \mid b \mid^2 = 1$$

Although these statements (44)–(46) do constitute necessary and sufficient conditions for a Liouvillian $\mathscr{L}$ to generate dynamical evolution for $\mathscr{H}_2$, it is not feasible to use these conditions to deduce an acceptable $\mathscr{L}$; rather, one must use less direct methods involving postulation of possible superoperators followed by an appeal to the conditions for either confirmation or rejection of the postulate.

6. HERMITIAN-QUORUM TREATMENT OF TWO-LEVEL SYSTEM

The form of the Kossakowski conditions for $\mathscr{H}_2$ given above was developed using the dyadic quorums $\{Q_{mn}\}$ as bases for the operator space $\mathscr{A}$. There are of course other possible choices, including in particular for the case of $\mathscr{H}_2$ the familiar Hermitian set containing the identity $\sigma_0 = 1$ and the three Pauli spin matrices $\boldsymbol{\sigma}$.

Let us adopt for convenience the set

$$\{\nu_\alpha\} \equiv \{1/\sqrt{2}, \boldsymbol{\sigma}/\sqrt{2}\} \equiv \{\nu_0, \boldsymbol{\nu}\}, \qquad \alpha = 0, 1, 2, 3 \tag{47}$$

which is readily seen to be an orthonormal basis for $\mathscr{A}$:

$$(\nu_\alpha \mid \nu_\beta) = \mathrm{Tr}(\nu_\alpha{}^\dagger \nu_\beta) = \mathrm{Tr}(\nu_\alpha \nu_\beta) = \delta_{\alpha\beta} \tag{48}$$

In terms of $\{\nu_\alpha\}$ the statistical operator ρ may be written as

$$\mid \rho) = (1/\sqrt{2}) \sum_\alpha s_\alpha \mid \nu_\alpha) \tag{49}$$

The properties of ρ as described in dyadic form by (3) require several necessary and sufficient constraints on the $\{s_\alpha\}$. Since $\mathrm{Tr}\,\rho = 1$,

$$s_0 = 1 \tag{50}$$

and since ρ is Hermitian,

$$s_\alpha = s_\alpha{}^* \tag{51}$$

Finally, in order to assure that ρ has only nonnegative eigenvalues, we must have

$$s_1{}^2 + s_2{}^2 + s_3{}^2 \leqslant 1 \tag{52}$$

In general, for any Hermitian operators A and B, we have

$$\mid A) = \sum_\alpha a_\alpha \mid \nu_\alpha), \qquad \mid B) = \sum_\beta b_\beta \mid \nu_\beta), \qquad (A \mid B) = \mathrm{Tr}(A^\dagger B) = \sum_\alpha a_\alpha b_\alpha \tag{53}$$

where the $\{a_\alpha\}$ and $\{b_\beta\}$ are real.

The evolution generator $\mathscr{L}$ can now be written in the form

$$\mathscr{L} = \sum_{\alpha\beta} \mid \nu_\alpha)\, \mathscr{L}_{\alpha\beta} (\nu_\beta \mid \tag{54}$$

and the generalized dynamical equation $\mathscr{L}\rho = \dot{\rho}$ then yields

$$\sum_\alpha \mathscr{L}_{\beta\alpha} s_\alpha = \sum_\alpha \dot{s}_\alpha\, \delta_{\beta\alpha} = \dot{s}_\beta \tag{55}$$

In terms of $\{\nu_\alpha\}$, the general form of a one-dimensional projector in $\mathscr{H}_2$ is

$$P_{\hat{n}} = (1/\sqrt{2})(\nu_0 + \hat{\mathbf{n}} \cdot \boldsymbol{\nu}), \qquad \hat{\mathbf{n}} \cdot \hat{\mathbf{n}} = 1 \tag{56}$$

Using (56) one may therefore apply the general theorem (26)–(27) directly in order to obtain the restrictions on $\mathscr{L}_{\beta\alpha}$ necessary and sufficient to assure that (56) will have no solutions $s_\beta(t)$ that violate (50)–(52) at any time. However, since Kossakowski[17] has already taken this abstract appraoch to the $\mathscr{H}_2$ case as a means of illustrating his general theorem, we shall not repeat that derivation here.

Instead, we shall derive the necessary and sufficient conditions on $\mathscr{L}_{\beta\alpha}$ in a more straightforward manner, which will indicate the geometrical origin of the Kossakowski inequalities.

From (50) it follows that $\dot{s}_0 = 0$, so we must restrict $\mathscr{L}_{\beta\alpha}$ by

$$\mathscr{L}_{00} + \sum_{n=1}^{3} \mathscr{L}_{0n} s_n = 0 \tag{57}$$

which must be true for all sets $\{s_n\}$ satisfying (52). This implies

$$\mathscr{L}_{00} = \mathscr{L}_{0n} = 0, \qquad n = 1, 2, 3 \tag{58}$$

Writing (55) in the form $ds_\beta = \sum_\alpha \mathscr{L}_{\beta\alpha} s_\alpha \, dt$ and recalling that the s_α are all real, and must remain real throughout the evolution, we conclude immediately that all the coefficients $\mathscr{L}_{\beta\alpha}$ must be real. These findings can be summarized by writing the matrix form of $\mathscr{L}$ as

$$(\mathscr{L}_{\beta\alpha}) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \mathscr{L}_{10} & \mathscr{L}_{11} & \mathscr{L}_{12} & \mathscr{L}_{13} \\ \mathscr{L}_{20} & \mathscr{L}_{21} & \mathscr{L}_{22} & \mathscr{L}_{23} \\ \mathscr{L}_{30} & \mathscr{L}_{31} & \mathscr{L}_{32} & \mathscr{L}_{33} \end{pmatrix} \tag{59}$$

where all components[2] are real. It remains to discuss the further restrictions on these components required to ensure that as ρ evolves, it continues to have only nonnegative eigenvalues.

Consider an auxiliary real three-space $\mathscr{S}$ whose points $\mathbf{s}$ have coordinates (s_1, s_2, s_3). The elements $\mathbf{s}$ that lie on and within the unit sphere are in one-to-one correspondence with the statistical operators, through (49). From the dynamical evolution equation $\mathscr{L}\rho = \dot{\rho}$ we obtain

$$(\rho \mid \mathscr{L} \mid \rho) = (\rho \mid \dot{\rho}) = \tfrac{1}{2} \sum_n s_n \dot{s}_n = \tfrac{1}{2} \mathbf{s} \cdot \dot{\mathbf{s}} \tag{60}$$

[2] The transformation relating the elements $\mathscr{L}_{\beta\alpha}$ of (59) to the dyadic matrix elements $\mathscr{L}_{mn,kl}$ defined in (32) is given in the appendix.

No acceptable dynamical evolution can permit the end point of **s** to travel outside the unit sphere; therefore, whenever that point is on the unit sphere, we must have $\mathbf{s} \cdot \mathbf{s} \leqslant 0$. Hence from (60) we deduce that a necessary and sufficient condition for maintaining positivie-semidefiniteness of $\rho(t)$ in all motions generated by $\mathscr{L}$ is that $\mathscr{L}$ satisfy

$$(\rho \mid \mathscr{L} \mid \rho) \leqslant 0 \tag{61}$$

for every ρ whose corresponding **s** lies on the unit sphere. Comparing (49) and (56), we see immediately that (61) is equivalent to the assertion that

$$(P \mid \mathscr{L} \mid P) \leqslant 0 \qquad \text{for every projector } P \tag{62}$$

which is just the first Kossakowski inequality in (26). The form (59) and the condition (62) together are equivalent to the results obtained by Kossakowski[17] when he applied his general theorem (26)–(27) to the two-level system; our derivation from first principles therefore affirms his conclusion.

In part II we shall analyze in detail the various possible motions that can be generated by Liouvillians satisfying (59) and (62).

APPENDIX

We can obtain the Liouvillian matrix elements in the Hermitian quorum

$$\mathscr{L}_{\alpha\beta} = (\nu_\alpha \mid \mathscr{L} \mid \nu_\beta)$$

from the dyadic representation $\mathscr{L}_{mn,kl}$ by expressing the $\{\nu_\alpha\}$ in the form

$$\nu_{\alpha jk} = (1/\sqrt{2})\, \sigma_{\alpha jk}$$

where $\sigma_{\alpha jk}$ is the dyadic form of the Pauli spin σ_α. For example, $\mid \sigma_y)$ is represented by the column vector $(0, -i, +i, 0)$; $(\sigma_y \mid$ by the row vector $(0, +i, -i, 0)$. The resulting transformation is

$$\begin{aligned}
2\mathscr{L}_{10} &= L_{1211} + L_{1222} + L_{2111} + L_{2122} \\
2\mathscr{L}_{20} &= i(L_{1211} + L_{1222} - L_{2111} - L_{2122}) \\
2\mathscr{L}_{30} &= L_{1111} + L_{1122} - L_{2211} - L_{2222} \\
2\mathscr{L}_{11} &= L_{1212} + L_{1221} + L_{2112} + L_{2121} \\
2\mathscr{L}_{22} &= L_{1212} - L_{1221} - L_{2112} + L_{2121} \\
2\mathscr{L}_{33} &= L_{1111} - L_{1122} - L_{2211} + L_{2222} \\
2\mathscr{L}_{12} &= -i(L_{1212} - L_{1221} + L_{2112} - L_{2121})
\end{aligned}$$

$$
\begin{aligned}
2\mathscr{L}_{21} &= i(L_{1212} + L_{1221} - L_{2112} - L_{2121}) \\
2\mathscr{L}_{13} &= L_{1211} - L_{1222} + L_{2111} - L_{2122} \\
2\mathscr{L}_{31} &= L_{1112} + L_{1121} - L_{2212} - L_{2221} \\
2\mathscr{L}_{23} &= i(L_{1211} - L_{1222} - L_{2111} + L_{2122}) \\
2\mathscr{L}_{32} &= -i(L_{1112} - L_{1121} - L_{2212} + L_{2221}) \\
2\mathscr{L}_{00} &= L_{1111} + L_{1122} + L_{2211} + L_{2222} \\
2\mathscr{L}_{01} &= L_{1112} + L_{1121} + L_{2212} + L_{2221} \\
2\mathscr{L}_{02} &= i(L_{1112} - L_{1121} + L_{2212} - L_{2221}) \\
2\mathscr{L}_{03} &= L_{1111} - L_{1122} + L_{2211} - L_{2222}
\end{aligned}
$$

This transformation can easily be reversed.

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