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Evolution and decoherence in finite level systems

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Abstract

Forms of dynamics of open finite level systems is formulated. We give a presentation of stochastic dynamics of such systems in terms of maps. Completely positive maps are classified and parametrized. If the system is coupled to a companion system, the contraction of the unitary evolution of the combined system leads to a completely positive map of the system density matrix. The inverse problem of embedding a stochastic map in a unitary map of the combined system is posed and solved. This construction is *not* unique. Dephasing and decoherence stem from the same mechanism. The decoherence induced may be viewed in terms of the distance between the diagonal forms of the initial density matrix and the final: $D = \sum_i |\lambda'_i - \lambda_i|$. The unitary factor of the evolution does not contribute to the decoherence so defined. A model is given for the stochastic evolution of a qubit coupled to a qubit. This yields a completely positive map for the original qubit. A triangle inequality constraint obtains for the three relaxation times; and it is due to the complete positivity of the map. Some comments are made about bipartite entangled systems in relation to maps.

1. Stochastic dynamics of open systems

Given an isolated quantum system with a finitely many dimensional state space represented by an $n \times n$ density matrix ρ with properties

$$x_r^* \rho_{rs} x_s \geqslant 0; \quad tr(\rho) = 1; \quad \rho^\dagger = \rho$$

the dynamical evolution is by a suitable unitary transformation

$$\rho(t_2) = U(t_2, t_1)\rho(t_1)U^\dagger(t_2, t_1).$$

If there were a Hamiltonian H which is time independent

$$U(t_2, t_1) = \exp(-\mathrm{i}Ht).$$

If the Hamiltonian were time dependent this is modified to read

$$U(t_2, t_1) = T\left\{ \exp\left(-\mathrm{i} \int_{t_1}^{t_2} H(t)' \mathrm{d}t' \right) \right\},$$

where T is the time ordering. If the system is interacting with external fields which are constant or time dependent, this result obtains. All that is needed is that the external fields do not manifest any back reaction.

If we were to take into account the back reaction this is no longer possible. The time evolution is still linear. The most general form of such a dependence is by a dynamical map [1]:

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$$\rho_{rs}(t_1) \to B_{rr',s's}(t_2,t_1)\rho_{r's'}(t_1).$$

The standard properties of ρ are met if and only if the following relations hold for B:

$$B^*_{rr',s's} = B_{ss',rr'} \quad \text{(hermiticity)},$$

$$\Sigma_r B_{rr',s'r} = \delta_{r's'} \quad \text{(normalization)},$$

and

$$\sum_{rr'ss'} x_{r'}x^*_{s'}y^*_r y_s B_{rs,s'r'} \geqslant 0 \quad \text{(positivity)}.$$

The Hermitian super matrix B is not necessarily positive. If it is, then B is said to be completely positive [2].

$$z^*_{rr'}z_{ss'}B_{rr',s's} \geqslant 0 \quad \text{(complete positivity)}.$$

2. Completely positive maps: extreme maps

A completely positive map is of the form

$$\rho_{rs} \to \sum_{r's'} \zeta_{rr'}(v)\zeta^*_{ss'}(v)\lambda(v)\rho_{r's'},$$

where the ζ, λ are the eigenvectors and the eigenvalues (all positive) of B. We may absorb the eigenvalues into the eigenvectors and write this in the form

$$\rho \to \sum_{r's'} C_{rr'}(v)\rho_{r's'}C^\dagger_{s's} \equiv C(v)\rho C^\dagger(v); \quad \sum_v C(v)C^\dagger(v) = 1.$$

We note that unitary evolution is of this form with one single nonzero eigenvalue:

$$\rho \to U\rho U^\dagger; \quad U \equiv C(1).$$

Let us now consider noncoherent evolutions:

Start with a coupled system which includes the system of interest S in interaction with another system R. The density matrices of the combined system may be written in terms of (positively entangled) state vectors Ψ_{ra} in the form

$$\mathscr{R} = \mathscr{R}_{ar,bs}.$$

The unentangled state vectors would be Kronecker products:

$$\Psi_{ra} = \psi_r\varphi_a.$$

More generally

$$\Psi_{ra} = \sum_\mu s(\mu)\varphi_a(\mu)\psi_r(\mu); \quad \sum_\mu s^*(\mu)s(\mu) = 1.$$

The system $R + S$ is considered closed and would evolve unitarily

$$\mathscr{R}_{ar,sb} \to \sum_{r',a';s',b'} V_{rr',aa'}\mathscr{R}_{r'a',s'b'}V^*_{ss',bb'}.$$

The state of the system S by itself is given by the density matrix

$$\rho_{rs}(t_2) = \sum_a \mathscr{R}_{ra,sa}(t_2) = \sum_a \sum_{r',s';a',b'} V_{rr',aa'}(t_2,t_1)\mathscr{R}_{r'a',s'b'}(t_1)V^*_{ss',ab'}(t_2,t_1).$$

This can be written in the form

$$\rho(t_2) = \sum_v C(v)\rho(t_1)C^\dagger(v)$$

with

$$\rho(t_1) = \mathrm{tr}_R\{\mathscr{R}(t_1)\}; \quad \rho(t_2) = \mathrm{tr}_R\{\mathscr{R}(t_2)\},$$

provided the initial state of the combined system is completely separable, that is

$$\mathscr{R}(t_1)_{ra,sb} = \tau_{ab}(t_1)\rho_{rs}(t_1).$$

If we were to work in a basis where $\tau_{ab}(t_1)$ is diagonal:

$$\tau_{ab}(t) = \sum_n k_n(t)\delta_{an}\delta_{bn}; \quad k_n(t) \geqslant 0; \ \sum k_n(t) = 1,$$

the expression for $\rho_{rs}(t_2)$ becomes

$$\begin{aligned}\rho_{rs} &\to \sum_n \sum_a \sum_{r',s';a',b'} V_{rr',aa'}(t_2,t_1)\rho_{r's'}(t_1)\{k_n(t_1)\delta_{a'n}\delta_{b'n}\}V^*_{ss',ab'}(t_2,t_1)\\ &= \sum_{n,a;r',s'} k_n(t_1)V_{rr',an}(t_2,t_1)\rho_{r's'}(t_1)V^*_{ss',an}(t_2,t_1).\end{aligned}$$

If we put

$$C_{rr'}(v,n) = V_{rr',vn},$$

the decoherent evolution may be written

$$\rho(t_2) = \sum_{v,n} k_n C(v,n)\rho(t_1)C^\dagger(v,n),$$

which is the convex combination of completely positive maps with any fixed value of n. The dynamical maps thus form a *convex set* of which the *extremal elements* are obtained by choosing the density matrix of R itself to be a projection. It is therefore of interest to study these extremal maps. A map

$$\rho \to \sum_n C(n)\rho C^\dagger(n); \quad \sum_n C^\dagger(n)C(n) = 1$$

is extremal if we cannot write it in the form

$$\sum_n \{\cos^2\theta C(1,n)\rho C^\dagger(1,n) + \sin^2\theta C(2,n)\rho C^\dagger(2,n)\}.$$

So the decoherent dynamical evolution may be separated into classes, depending upon the range of n [3]. The simplest maps are these extremal maps which are the building blocks of all completely positive maps.

3. Parametrization of extreme completely positive maps

For $n = 1$, $CC^\dagger = 1$ implies that C is unitary. So we start with the case $n = 2$.

$$\rho \to C(1)\rho C^\dagger(1) + C(2)\rho C^\dagger(2),$$

$$C^\dagger(1)C(1) + C^\dagger(2)C(2) = 1.$$

By a unitary transformation on the state space we could make $C(1)$ diagonal. Let us parametrize this in the form:

$$C(1) = \begin{pmatrix} \cos\theta_1 & 0 \\ 0 & \cos\theta_2 \end{pmatrix} = C^\dagger(1),$$

then

$$C(2)C^\dagger(2) = \begin{pmatrix} 1-\cos^2\theta_1 & 0 \\ 0 & 1-\cos^2\theta_2 \end{pmatrix} = \begin{pmatrix} \sin^2\theta_1 & 0 \\ 0 & \sin^2\theta_2 \end{pmatrix}.$$

The solution to this equation is

$$C(2) = \begin{pmatrix} \sin\theta_1 & 0 \\ 0 & \sin\theta_2 \end{pmatrix} U(2); \quad U(2)U^\dagger(2) = 1,$$

where $U(2)$ is any unitary operator. Thus the most general solutions for rank 2 is:

$$C(1) = V\begin{pmatrix} \cos\theta_1 & 0 \\ 0 & \cos\theta_2 \end{pmatrix} U(1), \quad C(2) = V\begin{pmatrix} \sin\theta_1 & 0 \\ 0 & \sin\theta_2 \end{pmatrix} U(2),$$

where $U(1)$, $U(2)$, V are arbitrary 2×2 unitary matrices. We shall show below that we need not consider any rank greater than the dimension of the density matrix.

The classification of *all* dynamical maps, even for the 2×2 case is considerably more complicated [4].

For three level systems we can have both rank 2 and rank 3 decoherent evolutions. For rank 3 we have, as for 2×2 systems,

$$C(1) = V\begin{pmatrix} \cos\theta_1 & 0 & 0 \\ 0 & \cos\theta_2 & 0 \\ 0 & 0 & \cos\theta_3 \end{pmatrix} U(1).$$

Then we have the constraint

$$C^\dagger(2)C(2) + C^\dagger(3)C(3) = \begin{pmatrix} \sin^2\theta_1 & 0 & 0 \\ 0 & \sin^2\theta_2 & 0 \\ 0 & 0 & \sin^2\theta_3 \end{pmatrix} \equiv S^2$$

with

$$S = \begin{pmatrix} \sin\theta_1 & 0 & 0 \\ 0 & \sin\theta_2 & 0 \\ 0 & 0 & \sin\theta_2 \end{pmatrix}.$$

Write

$$C(2) = SD(2); \quad C(3) = SD(3),$$

then

$$SD^\dagger(2)D(2)S^\dagger + SD^\dagger(3)D(3)S^\dagger = S^2 = SS^\dagger$$

and consequently

$$D^\dagger(2)D(2) + D^\dagger(3)D(3) = 1.$$

Now we have already solved this problem for the 2×2 system,

$$D(2) = V'\begin{pmatrix} \cos\theta'_1 & 0 & 0 \\ 0 & \cos\theta'_2 & 0 \\ 0 & 0 & \cos\theta'_3 \end{pmatrix} U'(2),$$

$$D(3) = V'\begin{pmatrix} \sin\theta'_1 & 0 & 0 \\ 0 & \sin\theta'_2 & 0 \\ 0 & 0 & \sin\theta'_3 \end{pmatrix} U'(3)$$

and hence

$$C(2) = VSV'\begin{pmatrix} \cos\theta'_1 & 0 & 0 \\ 0 & \cos\theta'_2 & 0 \\ 0 & 0 & \cos\theta'_3 \end{pmatrix} U'(2)U(2),$$

$$C(3) = VSV'\begin{pmatrix} \sin\theta'_1 & 0 & 0 \\ 0 & \sin\theta'_2 & 0 \\ 0 & 0 & \sin\theta'_3 \end{pmatrix} U'(3)U(3).$$

This procedure could be extended to $N \times N$ matrices.

By making use of the equivalence between $C(n)$ and

$$\sum_m O_{nm}C(m); \quad \sum_n O_{nm}O_{nm'} = \delta_{mm'}; \quad O^\dagger = O$$

we can further simplify this to get $\sin\theta_1 = 0; \sin\theta_1' = 0$.

For a 3×3 system, we wish to prove that the extremal maps need to have the number of terms equal to or less than 3. We have already determined these. An extermal map cannot be expressed as a convex combination of two other maps.

If the $C(n)$ are such that there is a nontrivial relation of the form

$$\sum_{m,n} K_{mn}C(n)C^\dagger(m) = 0.$$

Then, consider the two maps:

$$\sum_{m,n}(\delta_{mn} \pm K_{mn})C(m)\rho C^\dagger(n).$$

Then the original map is the average of these. The only question is whether these two maps are completely positive maps, that is whether $\delta_{mn} \pm K_{mn}$ considered as matrices in m, n are nonnegative. Since K_{mn} can be as small as we want (by scaling) this can be obtained.

So for an extremal map, the matrices $C(n)C^\dagger(m)$ should be linearly independent. This requires that for extremal maps there can be *no more than N matrices* $C(n)$ so that $C(m)C^\dagger(n)$ are linearly independent. It may be directly verified that the generic solutions we have found for $N = 2$ and $N = 3$ satisfy this constraint.

The inverse constructon of embedding a stochastic map in the unitary evolution is not unique. Neither the *dimension* nor the *details* of the unitary map of the extended system *is unique*, claims to the contrary not withstanding! (The "Kraus" terms was introduced by us in 1960!) The $C(n)$ are *not unique* in so far as we have the possibility of making the linear transformation

$$C(n) \to M(n, n')C(n')$$

with $M(n, n')$ being a unitary matrix, not necessarily unimodular. Further, since no more than N^2 such matrices are linearly independent this is the largest number of terms in a *generic* map $C(n)$. We have already shown that this number may not exceed N for an *extremal* map.

There is a loss of relative phase information between certain decompositions of the component states. From a pure state density matrix

$$\rho = \psi\psi^\dagger,$$

we get, after the stochastic map

$$\rho \to \rho' = \sum_n \varphi_n\varphi_n^\dagger$$

with

$$\varphi_n = C(n)\psi.$$

Here even the relative phases of φ_n are lost since $C(n)$ maybe replaced by $e^{i\alpha_n}C(n)$ without changing the map. Thus stochasticity involves both dephasing and linear combinations of amplitudes.

There exists a method of "purification" [5] which replaces the impure matrix ρ' by a *pure* matrix $\rho'\prime$ but this is a *nonlinear* transformation even though it is a one-to-one map. This is specified by an arbitrary positive herlmitian matrix L and

$$\rho'' = \sum_{a,b} \frac{\rho(a)L\rho(b)}{\sqrt{\mathrm{tr}[\rho(a)L]\mathrm{tr}[\rho(b)L]}}; \quad \rho = \sum_a \lambda_a\rho(a), \;\; \rho(a)\rho(b) = \delta_{a,b}\rho(a).$$

This may be also looked on as a *phase coherent addition* of pure states.

4. Back reaction and stochasticity

We have shown that when the external reservoir R *reacts* back on the system S, a pure state will evolve into an impure state. This evolution may be thought of as the phases between components of a state vector becoming

decoherent. It is *not* the external (time dependent) reservoir influencing the system that causes decoherence, it is the *reaction* of the reservoir. It is also interesting to recognize that the reservoir need not be very large. For an extremal map, it need be no more than the dimension of the density matrix. So a 2×2 system coupled to another 2×2 system can reproduce *any* extremal dynamical map. Consider an interaction

$$H = \sigma_j C_{jk} \tau_k.$$

By suitable $U(2)$ transformations on σ and τ we could render it into the standard form

$$H = \gamma_1 \sigma_1 \tau_1 + \gamma_2 \sigma_2 \tau_2 + \gamma_3 \sigma_3 \tau_3.$$

Since $\sigma_1\tau_1,\ \sigma_2\tau_2,\ \sigma_3\tau_3$ commute

$$\mathrm{e}^{-\mathrm{i}Ht} = \mathrm{e}^{-\mathrm{i}(\gamma_1\sigma_1\tau_1)t}\mathrm{e}^{-\mathrm{i}(\gamma_2\sigma_2\tau_2)t}\mathrm{e}^{-\mathrm{i}(\gamma_3\sigma_3\tau_3)t} = \{\cos(\gamma_1 t) - \mathrm{i}\sigma_1\tau_1 \sin(\gamma_1 t)\}\{\cos(\gamma_2 t) - \mathrm{i}\sigma_2\tau_2 \sin(\gamma_2 t)\}\{\cos(\gamma_3 t) - \mathrm{i}\sigma_3\tau_3 \sin(\gamma_3 t)\}.$$

Hence

$$\mathrm{e}^{-\mathrm{i}Ht}\sigma_1\mathrm{e}^{\mathrm{i}Ht} = \sigma_1 \mathrm{e}^{2\mathrm{i}t(\gamma_2\sigma_2\tau_2 + \gamma_3\sigma_3\tau_3)},$$

$$\mathrm{e}^{-\mathrm{i}Ht}\sigma_2\mathrm{e}^{\mathrm{i}Ht} = \sigma_2 \mathrm{e}^{2\mathrm{i}t(\gamma_3\sigma_3\tau_3 + \gamma_1\sigma_1\tau_1)},$$

$$\mathrm{e}^{-\mathrm{i}Ht}\sigma_3\mathrm{e}^{\mathrm{i}Ht} = \sigma_3 \mathrm{e}^{2\mathrm{i}t(\gamma_1\sigma_1\tau_1 + \gamma_2\sigma_2\tau_2)}.$$

When partial traces are taken with respect to τ we get

$$\sigma_1 \to \sigma_1 \cos(2t\gamma_2)\cos(2t\gamma_3) \quad \text{etc.}$$

This map therefore corresponds to spin relaxation in the 'principal directions' 1, 2, 3. For any fixed t these represent a contraction map.

5. Dynamical semigroups

The time evolution discussed in the previous section is always a contraction, but these evolutions *do not* satisfy a semigroup property though they are contraction maps:

$$B(t_1)B(t_2) \neq B(t_1 + t_2).$$

But we could consider this evolution for a *short* time t_0 and then recouple S to *another copy* of R and then contract. This would lead to an iteration of $B(t_0)$ so that after nt_0,the evolution matrix is

$$[B(t_0)]^n = A(n),$$

$$A(0) = 1; \quad A(n_1)A(n_2) = A(n_1 + n_2),$$

thus yielding a *discrete semigroup*. Such a modality is appropriate for the system encountering one reservoir R_1, decoupling from it, recoupling to another similar reservoir R_2, and so on. For example a system undergoing successive interactions with a stream of particles would have such a stochastic evolution for times large compared with t_0.

For the model of a 2×2 systems S in successive interactions with a sequence of identical but distinct 2×2 reservoirs at intervals t_0 the evolution matrix is diagonal in the polarization components:

$$B(t_0)\cdot\left(\frac{1+\vec{\sigma}.\vec{a}}{2}\right) = \frac{1}{2}\{1 + \sigma_1 a_1 \cos(2t_0\gamma_2)\cos(2t_0\gamma_3) + \sigma_2 a_2 \cos(2t_0\gamma_3)\cos(2t_0\gamma_1) + \sigma_3 a_3 \cos(2t_0\gamma_1)\cos(2t_0\gamma_2)\}$$

which may be approximated by

$$\begin{aligned} B(t_0)\cdot\left(\frac{1+\vec{\sigma}.\vec{a}}{2}\right) &= \frac{1}{2}\left\{1 + [1 - (\gamma_2^2 + \gamma_3^2)t_0^2]\sigma_1 a_1 + [1 - (\gamma_3^2 + \gamma_1^2)t_0^2]\sigma_2 a_2 + [1 - (\gamma_1^2 + \gamma_s^2)t_0^2]\sigma_3 a_3\right\} \\ &\simeq \frac{1}{2}\left[1 + \mathrm{e}^{-(\gamma_2^2+\gamma_3^2)t_0^2}\sigma_1 a_1 + \mathrm{e}^{-(\gamma_3^2+\gamma_1^2)t_0^2}\sigma_2 a_2 + \mathrm{e}^{-(\gamma_1^2+\gamma_2^2)t_0^2}\sigma_3 a_3\right] \simeq \frac{1}{2}\left[1 + \mathrm{e}^{-\zeta_1}a_1\sigma_1 + \mathrm{e}^{-\zeta_2}a_2\sigma_2 + \mathrm{e}^{-\zeta_3}a_3\sigma_3\right] \end{aligned}$$

so

$$A(n)\left(\frac{1+\vec{\sigma}.\vec{a}}{2}\right)=\frac{1}{2}\left[1+\mathrm{e}^{-in\zeta_1}a_1\sigma_1+\mathrm{e}^{-n\zeta_2}a_2\sigma_2+\mathrm{e}^{-n\zeta_3}a_3\sigma_3\right].$$

The relaxation parameters ζ_1, ζ_2, ζ_3 satisfy the inequalities

$$\zeta_1+\zeta_2>\zeta_3,\quad \zeta_2+\zeta_3>\zeta_1,\quad \zeta_3+\zeta_1>\zeta_2.$$

While we have derived this result only for a special model of the interaction, the *Complete Positivity* of the Kossakowski semigroup [6] generator leads to the same triangle inequality for the relaxation rates.

For a 2×2 system the density matrices correspond to solid sphere of unit radius. A map will make a linear transformation of the sphere into an ellipsoid contained within this sphere. By a suitable rotation we can reduce the ellipsoid to standard form. These extremal maps can be parameterized as we have have done (or otherwise). In the example that we sketched above the 1,2,3 axes are the principal axes of the ellipsoid and the ellipsoid has the same center as the sphere. More generally we can have an inhomogeneous transfer which displaces the center of the ellipsoid.

With 3×3 systems the density matrices correspond to the product of 2-spheres, $S^2\times S^4$. Any density matrix has 8 parameters but by suitable $SU(3)$ transformations can be made diagonal. A convenient way of parameterizing is as follows:

$$\rho=\frac{1}{3}\begin{pmatrix}1+x-\frac{1}{\sqrt{3}}y & 0 & 0\\ 0 & 1+2\sqrt{3}y & 0\\ 0 & 0 & 1-x-\frac{1}{\sqrt{3}}y\end{pmatrix}$$

and the two nontrivial invariants are

$$I_2=x^2+y^2,$$

$$I_3=\left(\frac{1}{3}y^2-x^2\right)\frac{2}{\sqrt{3}}y.$$

The allowed values of x and y are represented by the interior points of a triangle bounded by

$$y=-\frac{\sqrt{3}}{2},$$

$$x+\frac{1}{\sqrt{3}}y=1,$$

$$-x+\frac{1}{\sqrt{3}}y=1$$

with vertices $(3/2,-\sqrt{3}/2),(-3/2,-\sqrt{3}/2),(0,\sqrt{3})$ where $(I_1,I_2)=(3,0)$, the same for all three vertices. Any decoherent evolution should map all these points *into* the interior of the triangle, but *not linearly*.

6. Remarks concerning the extremal density matrices of bipartite systems

Some remarks about *entangled systems*: The natural evolution by unitary transformations can affect the entanglement and separability. But with a decoherent evolution a pure state of the entangled systems can (and will) become impure, unless one can neglect the back reaction. When it cannot be neglected the decoherence will manifest itself as an additional source of degradation of quantum information.

These evolutions are not unitary and they serve to change the eigenvalues of the density matrix, in contrast to a generic unitary evolution. In particular, a pure state becomes impure. But any linear transformation of the convex set into itself has at least one fixed point. This is the equilibrium state left invariant by the stochastic evolution. It need not be the most degenerate state. For example, for the "pin map."

$$\rho_{rs}\to\rho'_{rs}=(\rho_0)_{rs}\delta_{r's'}\rho_{r's'}$$

the equilibrium state is ρ_0 and all states are mapped on to it, including the most degenerate state $\rho=1/N$.

A measure of dephasing is the loss of coherence within the density matrix which takes a pure state into mixtures. A pure state with only one unit eigenvalue is degraded into a mixture with loss of relative phase information. The difference between the trace of the square of the resultant matrix and unity is a measure of the dephasing. A unitary

evolution, however complicated, cannot change the eigenvalues of a density matrix. The change in the eigenvalues under a map would give us a measure of the decoherence suffered by any density matrix. If we need to have a single parameter, this may be defined by the "distance"

$$D = \sum_{j=1}^{N} |\lambda_j - \mu_j|.$$

This distance is unaffected by any unitary transformation which forms part of the stochastic map. Once one has reached equilibrium there is no change in the eigenvalues and hence no distance even when there is a unitary transformation which keeps changing the specific result of the map.

There is a close connection between dynamical (stochastic) maps and the density matrix of a bi-partite system; and the tools we have developed for the study of maps can also be used to study bipartite systems of arbitrary finite dimensions.

The dynamical maps are specified by the hermitian matrix $\mathscr{B}_{aj,bk}$ which is nonnegative for completely positive maps [1]. The trace of a dynamical map is N rather than 1 for a bipartite density matrix $\mathscr{R}$:

$$\mathscr{B}_{aj,aj} = N,$$

$$\mathscr{R}_{aj,aj} = 1.$$

The mapping matrix satisfies an additional restriction

$$\mathscr{B}_{aj,ak} = \delta_{jk}.$$

$\mathscr{R}_{aj,bk}$ is always nonnegative and has an eigenvector decomposition

$$\mathscr{R}_{aj,bk} = \sum_r \mu(r)\zeta_{aj}(r)\zeta^*_{bk}(r)$$

which reduces to a single term when the density matrix is pure. Both $\{\mathscr{B}\}$ and $\{\mathscr{R}\}$ constitute convex sets which are generated by their extremal elements. The pure density matrices, $\mathscr{R}^2 = \mathscr{R}$ are the extremal elements. We can go from any pure denisty matrix to any other pure density matrix by a transformation in $SU(N)$.

The combined density matrix is said to be separable [7] if it can be expressed in the form

$$\mathscr{R}_{aj,bk} = \sum_r \lambda_r \rho^I_{ab}(r) \times \rho^{II}_{jk}(r); \quad \lambda_r > 0, \ \sum_r \lambda_r = 1.$$

It is of some interest to find the extremal separable density matrices. We do this for a bipartite qubit system.

The most general bipartite qubit system density matrix may be written

$$\mathscr{R} = \tfrac{1}{4}\{1 \times 1 + \vec{a}.\vec{\sigma} \times 1 + 1 \times \vec{b}.\vec{\tau} + \sigma_j \times \tau_k C_{jk}\},$$

where a_j, b_j, c_{jk} are real parameters. They must satisfy

$$\mathscr{R} \geqslant 0.$$

Such density matrices form a convex set. We could make $SU(2) \times SU(2)$ "local" transformations to put $\mathscr{R}$ in a canonical form:

$$\mathscr{R} = \tfrac{1}{4}\{1 + a_j\sigma_j + b_j\tau_j + \gamma_j\sigma_j\tau_j\}.$$

We may use the standard representations

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \tau_1; \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \tau_2; \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

to write $\mathscr{R}$ as a 4×4 matrix. When $\mathscr{R}$ is pure

$$\mathscr{R}^2 = \mathscr{R}.$$

All 2×2 and 3×3 minors as well as $\mathscr{R}$ itself have zero determinants. In terms of the parameters these imply

$$(1 \pm a_3)^2 = (b_3 + \gamma_3)^2 + a_1^2 + a_2^2,$$

$$(1 \pm b_3)^2 = (a_3 \pm \gamma_3)^2 + b_1^2 + b_2^2,$$

$$(1 \pm \gamma_3)^3 = (a_3 \pm b_3)^2 + (\gamma_1 \mp \gamma_2)^2,$$

$$1 + (a_1 - \mathrm{i}a_2)(b_1 + \mathrm{i}b_2) + (a_1 + \mathrm{i}a_2)(b_1 - \mathrm{i}b_2) = (a_1^2 + a_2^2) + b_1^2 + b_2^2 + (\gamma_1 + \gamma_2)^2.$$

These equations imply

$$a_3 = \gamma_3 b_3, \quad b_3 = \gamma_3 a_3, \quad \gamma_3 = a_3 b_3 - \gamma_1 \gamma_2.$$

If $a_3 \neq 0$, it follows that

$$\gamma_3 = \pm 1, \quad b_3 = \gamma_3 a_3.$$

Therefore $1 \mp \gamma_3 = 0$ and so $\gamma_1 \pm \gamma_2 = 0$ and $a_3 \mp b_3 = 0$. So for $a_3 \neq 0$, we have the additional restrictions

$$(1 \pm a_3)^2 = \gamma_3^2 (1 \pm a_3)^2 + a_1^2 + a_2^2,$$

$$(1 \pm b_3)^2 = \gamma_3^2 (1 \pm b_3)^2 + b_1^2 + b_2^2.$$

So

$$a_1 = a_2 = b_1 = b_2 = 0, \quad a_3 = \pm b_3, \quad b_3 = \pm 1$$

and

$$(1 \pm \gamma_3)^2 = a_3^2 (1 \pm \gamma_3)^2 + (\gamma_1 \mp \gamma_2)^2,$$

$$\gamma_1 = \mp \gamma_2, \quad a_3^2 = 1.$$

The possible solutions are

$$\gamma_3 = +1; \quad a_3 = +b_3 = \pm 1; \quad \gamma_1 = \gamma_2 = b_1 = b_2 = a_1 = a_2 = 0,$$

$$\gamma_3 = -1; \quad a_3 = -b_3 = \pm 1; \quad \gamma_1 = \gamma_2 = b_1 = b_2 = a_1 = a_2 = 0.$$

These relations are equivalent since the local transformations

$$\mathrm{e}^{\mathrm{i}\sigma_2 \pi/2} \quad \text{and} \quad \mathrm{e}^{\mathrm{i}(\sigma_2 + \tau_2)\pi/2}$$

transform them into each other.

The other possibility is $a_3 = b_3 = 0$ and $\gamma_3 \neq 0_2$. Consequently

$$\gamma_3 = -\gamma_1 \gamma_2$$

$$1 + \gamma_3^2 = \gamma_1^2 + \gamma_2^2$$

so that

$$\gamma_1^2 \gamma_2^2 - \gamma_1^2 - \gamma_2^2 + 1 \equiv (\gamma_1^2 - 1)(\gamma_2^2 - 1) = 0.$$

So the solutions are

$$\gamma_1 = \pm 1 \quad \gamma_2 = +1 \quad \gamma_3 = \mp 1,$$

$$\gamma_1 = \pm 1 \quad \gamma_2 = -1 \quad \gamma_3 = \pm 1,$$

which are equivalent by the local unitary transformation $\mathrm{e}^{\mathrm{i}\tau_2 \pi/2}$.

A third possibility is $a_3 = b_3 = b_3 = 0$. Then

$$a_1^2 + a_2^2 = b_1^2 + b_2^2 = 1.$$

Using the determinant of the 3×3 minor we get

$$1 + \{(a_1 - \mathrm{i}a_2)(b_1 + \mathrm{i}b_2) + (a_1 + \mathrm{i}a_2)(b_i - \mathrm{i}b_2)\}(\gamma_1 + \gamma_2) = a_1^2 + a_2^2 + b_1^2 + b_2^2 + (\gamma_1 + \gamma_2)^2. \tag{1}$$

Reality of $(\gamma_1 + \gamma_2)$ requires the restriction

$$\frac{a_1 - \mathrm{i}a_2}{a_1 + \mathrm{i}a_2} = \frac{b_1 - \mathrm{i}b_2}{b_1 + \mathrm{i}b_2} = \mathrm{e}^{2\mathrm{i}\theta}.$$

A unitary transformation

$$\mathrm{e}^{\mathrm{i}(\sigma_3+\tau_3)\pi/2}.$$

Could make $a_2 = b_2 = 0$, and then $a_1 = \pm b_1 = \gamma_1 b_1$. This is equivalent to the case $a_3 = b_3\gamma_3$; $a_3^2 = b_3^2 = 1$ by the local unitary transformation

$$\mathrm{e}^{\mathrm{i}(\sigma_2+\tau_2)\pi/4}.$$

Thus the extremal elements are of the form

(A) $\mathscr{R} = \frac{1}{4}(1 + \sigma_3)(1 + \tau_3)$,

(B) $\mathscr{R} = \frac{1}{4}(1 - \sigma_1\tau_1 - \sigma_2\tau_2 - \sigma_3\tau_3)$.

The extremal elements of the class (A) are given by

$$\vec{a}^2 = \vec{b}^2 = 1.$$

They form an invariant class under a partial time reversal transformation

$$\vec{\sigma} \to \vec{\sigma}, \quad \vec{\tau} \to -\vec{\tau}, \quad \vec{\sigma}.\vec{\tau} \to -\vec{\sigma}\vec{\tau}$$

and are simply reducible.

$$R = \rho^I \times \rho^{II}.$$

The class (B) is not an invariant class under the partial time reversal. The extremal elements of the set of separable matrices are the six vertices of the octahedron which is obtained by the intersection of the original tetrahedron by its reflection $\gamma_1 \to -\gamma_1$, $\gamma_2 \to -\gamma_2$, $\gamma_3 \to -\gamma_3$.

There are also two continuous parameter extremal density matrices for which

$$\gamma_3 = +1; \quad a_3 = +b_3 = \cos\theta; \quad \gamma_1 = \gamma_2 = \sin\theta; \quad b_1 = b_2 = a_1 = a_2 = 0$$

$$\gamma_3 = -1; \quad a_3 = -b_3 = \cos\phi; \quad \gamma_1 = \gamma_2 = \sin\phi; \quad b_1 = b_2 = a_1 = a_2 = 0$$

and the ones obtained by permutation of the indices 1, 2, 3. These correspond to pure entangled states.

7. Concluding remarks

In this paper, which is really a sequel to the author's basic paper of 1961 on stochastic dynamics of quantum mechanical systems, we have introduced the notion of a stochastic map of the density matrices generalizing their conventional unitary evolution [1]. A probability weighted average of such unitary evolutions is a type of stochastic map in which both decoherence and dephasing arise. Interference between the various component unitary evolutions will contribute to (partial) suppression of the off diagonal elements: this is decoherence. Yet this is not the most general stochastic map. In any such map phase relations are lost which provide dephasing. These two are intimately related.

It is shown that any stochastic map may be viewed as the contraction of a unitary evolution of an extended system. This extension is by coupling a reservoir system with density matrix τ to the primary system with density matrix ρ by a generic Hamiltonian. To produce decoherence and dephasing it is not sufficient that the reservoir affects the primary system with (possibly time dependant) interactions: to produce a stochastic map, the reservoir must react to the primary system. In the second order this reaction produces "propogator modifications" in the primary system. It is this two-step self-interaction that leads to decoherence [6].

Not only is such a mechanism capable of producing stochastic evolution of the primary system, but we also show that it is the only mechanism by "unfolding" the stochastic evolution to a type of unitary evolution of the combined system of the system of interest and the reservoir. This extension is not unique, not even as to the size of the reservoir. It is however remarkable that the combined system need only a modest $N^2 \times N^2$ reservoir at most.

Since density matrices form a (compact) convex set the stochastic maps also form a convex set. Those elements which are not a convex combination of two mappings are called extremal maps. They are the building blocks for any

stochastic map. It is shown that the reservoir need have only $R \leqslant N$ dimensions to get an extremal map [3,4]. All the extremal maps can be computed by a simple algebraic process [4] which is illustrated for qubits and qutrits with obvious generalization to any dimension.

For bipartite systems we have the case of quantum entanglement and quantum separability. The simplest separable state has its density matrix as the direct product of the reduced density matrices. A convex combination of such simply separable states is the generic separable state. In contrast, like the singlet state of two qubits, there are states which cannot be expressed as probabilistic sum of simply reducible density matrics. The generic two qubit system can be easily expressed in a simple canonical form by local $SU(2) \otimes SU(2)$ transformations:

$$\rho = \tfrac{1}{4}(1 + \vec{a}.\vec{\sigma} + \vec{b}.\vec{\tau} + \mathscr{C}_n \sigma_n \tau_n).$$

Any other bipartite density matrix may be obtained by a suitable $SU(2) \otimes SU(2)$ transformation. The extreme elements can be determined in terms of the nine parameters separated into two classes each, in turn, labelled by three nonzero parameters. The parameters that determine the extreme elements form the vertices of a regular tetrahedron. Not all of the extreme elements are separable. Using the Peres criterion [7] we could show that the nonnegative separable matrices are bounded by a regular octahedron in appropriate parameters.

From each stochastic map we can construct a semigroup of evolutions. If the stochastic map is completely positive, the resulting semigroup is also completely positive. Some examples of such a construction [8] is given explicitly. The generators of the semigroup form a convex cone, with extremal elements being the generators of the cone. The relaxation parameters of a finite level system obeying a completely positive semigroup obey certain inequalities. For relaxation of a qubit we recover the familiar results which imply in particular that in axially symmetric relaxtion the axial relaxation rate cannot be greater than twice the transverse relaxation rate; a restriction obeyed by all experimental results.

This paper is an attempt to tie together the work of the last four decades on quantum stochastic processes done under different notations and different contexts. Many of the "new" results in this field are reproductions of old results and which appear "new" since the old results are not cited.

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