PHYSICS REPORTS (Review Section of Physics Letters) 77, No. 3 (1981) 169–192. North-Holland Publishing Company

Topics in Quantum Probability

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0. Introduction

Quantum theory is so much a new probability as it is a new mechanics. More precisely, as Feynman says, the probabilities one meets in quantum theory are of the same type as those met in any other statistical theory; what radically changes is the way of computing them, i.e., the mathematical model. Is such a new, "non-Kolmogorovian" mathematical model necessary? or can everything be done within the framework of the classical theory of probability and of stochastic processes? Are there some features, qualitatively new with respect to the classical model, which arise from the inner development of the quantum probabilistic model (just as non-Euclidean geometry is not simply a translation of classical geometry in a more general context)? Can some concepts or results of quantum probability be of any use for physicists?

In what follows we deal with some of these questions. For reasons of space the discussion will be very sketchy and prevalence will be given to motivations and results rather than general definitions and proofs.

In section 1 we discuss the necessity of a mathematical model for the stochastic processes arising in quantum theory and extend to arbitrary (discrete) observables Wigner's proof [23] of Bell's inequality [10] for spin observables. (A much more thorough discussion of these arguments is contained in [8].)

In section 2 we introduce the concept of *conditional density matrix* which plays, for transition probabilities, the role played for probabilities by von Neumann density matrix.

In section 3 we use the concept of conditional density matrix to produce many examples of quantum Markov chains, and in section 4 we show in what sense all 1-dimensional nearest neighbours quantum lattice systems can be described by quantum Markov chains. The heuristic considerations of section 5 motivate the introduction of continuous time quantum processes, and in particular, quantum Markov processes (sections 6 and 7). In this context we prove a general quantum Feynman–Kac formula. For further informations and examples cf. [2, 3, 4, 5, 7].

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1. Insufficiency of the classical stochastic processes for quantum theory

By observable, in this section, we mean "observable which assumes a discrete set of values". Let A, B, C, ... be observables whose values we denote $(a_\alpha), (b_\beta), (c_\gamma), \ldots$ respectively. According to classical probability theory the mathematical model for description of these observables is given by a stochastic process, i.e. a set of random variables $\xi_A, \xi_B, \xi_C, \ldots$ taking values $(a_\alpha), (b_\beta), (c_\gamma), \ldots$ and defined on a probability space (Ω, ϑ, μ). The quantum mechanical description of these observables is given by a complex Hilbert space $\mathcal{H}$ and orthonormal basis $(\varphi_\alpha), (\psi_\beta), (\chi_\gamma), \ldots$ whose statistical meaning is specified by the well known relations

$$\text{Prob}\{A = a_\alpha | B = b_\beta\} = |\langle \varphi_\alpha, \psi_\beta \rangle|^2; \qquad \text{etc.} \tag{1}$$

where $\text{Prob}\{\cdot | \cdot\}$ means conditional probability. As shown by J. von Neumann [22] all the statistical assertions of quantum theory can be reduced to the computation of the conditional probabilities (1). We will say that a quantum mechanical description of the observables A, B, C, ... is equivalent to a classical one if there exist a probability space (Ω, ϑ, μ) and random variables $\xi_A, \xi_B, \xi_C, \ldots$ defined on (Ω, ϑ, μ) and taking values $(a_\alpha), (b_\beta), (c_\gamma), \ldots$ such that for each $\alpha, \beta, \gamma, \ldots$

$$|\langle \varphi_\alpha, \psi_\beta \rangle|^2 = E^\mu\{\xi_A = a_\alpha | \xi_B = b_\beta\} = \frac{\mu(A_\alpha \cap B_\beta)}{\mu(B_\beta)} \tag{2}$$

and similarly for the other indices. Here

$$A_\alpha = \{\omega \in \Omega : \xi_A(\omega) = a_\alpha\}; \qquad B_\beta = \cdots. \tag{3}$$

In other words, a quantum mechanical description is equivalent to a classical one if the quantum mechanical transition probabilities can be computed through a classical stochastic process.
In the following we will prove that usually quantum mechanical descriptions do not allow any classical equivalent in the sense specified above.
Each kind of description imposes some constraints (inequalities) on the transition probabilities which are universal for the models of that description, but in general are not satisfied by the models of the other one (cf. [8] for more precise results).

Proposition 1. In the above notations let be given a quantum mechanical description of two observables A, B such that all the transition probabilities (1) are strictly positive. Then a necessary condition for it to be equivalent to a classical description is that both A and B take only a *finite* number of values. If this is the case, then a classical description equivalent to the quantum mechanical one exists if and only if A and B take the same number of distinct values.
Proof. The quantum mechanical transition probabilities are symmetric, i.e.

$$\text{Prob}\{A = a_\alpha | B = b_\beta\} = \text{Prob}\{B = b_\beta | A = a_\alpha\} \tag{4}$$

hence if they admit a classical model it must satisfy, for any α, β:

$$\frac{\mu(A_\alpha \cap B_\beta)}{\mu(A_\alpha)} = \frac{\mu(A_\alpha \cap B_\beta)}{\mu(B_\beta)}. \tag{5}$$

Because of the strict positivity assumption this is equivalent to

$$\mu(A_\alpha) = \mu(B_\beta)\,; \qquad \forall \alpha, \beta$$

i.e. $\mu(A_\alpha) = \mu(B_\beta) = c$ – independent of α, β. Therefore

$$\mu(\Omega) = c \cdot (\text{number of distinct } a_\alpha) = c \cdot (\text{number of distinct } b_\beta)\,. \tag{6}$$

Thus, if $\mu(\Omega) = 1$, the number of distinct values of A must be finite and equal to the number of distinct values of B.
If this condition is satisfied let $n < +\infty$ be this number. Then $c = 1/n$ and a classical model for this process always exists. In fact we can take for Ω the interval $[0, 1]$ for μ the Lebesgue measure on $[0, 1]$, for A_α the interval $[(\alpha - 1)/n,\ \alpha/n[$, $\alpha = 1, \ldots, n$, and then define B_β as $\cup_{\alpha=1}^{n} A_{\alpha,\beta}$ where for each α, $A_{\alpha,1}, A_{\alpha,2}, \ldots, A_{\alpha,n}$ is a partition of A_α satisfying

$$\mu(A_{\alpha,\beta}) = \frac{1}{n}\,\mathrm{Prob}\{A = a_\alpha | B = b_\beta\} = |\langle \varphi_\alpha, \psi_\beta \rangle|^2 \cdot \frac{1}{n} \tag{7}$$

Remark 1. In case of existence the equivalent classical model is unique up to stochastic equivalence if we impose the (minimality) condition that the σ-algebra ϑ is generated by the random variables ξ_A, ξ_B.
Remark 2. If we renounce to the requirement that (Ω, ϑ, μ) be a probability space and allow $\mu(\Omega) = +\infty$, then for *couples* of observables we can always build a kind of classical model. However for *triples* the situation is worse even in the case of finitely many values. In fact one has:

Proposition 2. A necessary condition for a quantum description of three observables A, B, C, with transition probabilities $P(\bar{A}_\alpha|\bar{B}_\beta)$, $P(\bar{B}_\beta|\bar{C}_\gamma)$, $P(\bar{C}_\gamma|\bar{A}_\alpha)$ (we write $\bar{A}_\alpha$, $\bar{B}_\beta$, $\bar{C}_\gamma$ for $A = a_\alpha$, $B = b_\beta$, $C = c_\gamma$) to be equivalent to a classical one is that for every subset F of the index set, and for each α, γ:

$$\left| \sum_{\beta \in F} [P(\bar{A}_\alpha|\bar{B}_\beta) - P(\bar{B}_\beta|\bar{C}_\gamma)] \right| \leq 1 - P(\bar{A}_\alpha|\bar{C}_\gamma) \tag{8}$$

(and the other inequalities obtained by circular permutation of A, B, C keeping the same indices α, β, γ).
Proof. A classical model for the triple A, B, C must be a model for each couple. Therefore, according to Proposition 1 we must have, for any such model: $\mu(A_\alpha) = \mu(B_\beta) = \mu(C_\gamma) = c$; and we can choose $c = 1$ (to include also the case $\mu(\Omega) = +\infty$). Thus, in the notations of Proposition 1 we must have, for each subset F of the index set and for each α, γ:

$$\begin{aligned} P(\bar{A}_\alpha|\bar{C}_\gamma) &= \mu(A_\alpha \cap C_\gamma) = \sum_\beta (A_\alpha \cap B_\beta \cap C_\gamma) \\ &\leq \sum_{\beta \in F} \mu(A_\alpha \cap B_\beta) + \sum_{\beta \notin F} \mu(B_\beta \cap C_\gamma) \\ &= \sum_{\beta \in F} P(\bar{A}_\alpha|\bar{B}_\beta) + \sum_{\beta \notin F} P(\bar{B}_\beta|\bar{C}_\gamma) \\ &= \sum_{\beta \in F} P(\bar{A}_\alpha|\bar{B}_\beta) + 1 - \sum_{\beta \in F} P(\bar{B}_\beta|\bar{C}_\gamma) \end{aligned} \tag{9}$$

and the inequality (9) for an arbitrary subset F is equivalent to the inequality (8).
The limitation imposed by condition (8) on the transition probabilities is nontrivial. For example if F is a set of a single element, say β, and $\mathcal{H} = \mathbb{R}^3$, the three vectors

$$\varphi_\alpha = (1,0,0)\,; \qquad \psi_\beta = \left(\tfrac{1}{2}, -\tfrac{1}{2}, \left(\tfrac{1}{2}\right)^{1/2}\right)\,; \qquad \chi_\gamma = (1-\varepsilon, [2\varepsilon - \varepsilon^2]^{1/2}, 0)$$

are such that (8) is not satisfied if $\varepsilon < 1/34$. In the particular case in which the observables A, B, C take only the values ± 1, it is not difficult to see that as a consequence of inequality (8), the correlation functions of the random variables ξ_A, ξ_B, ξ_C, must satisfy

$$|\mu(\xi_A \cdot \xi_B) - \mu(\xi_B \cdot \xi_C)| \leq 1 - \mu(\xi_A \cdot \xi_C) \tag{10}$$

which is Bell's inequality (cf. [21]).

2. The density matrix and the conditional density matrix

In this section we shall deal only with observables taking a finite number of values.

Let (S_a), where a belongs to an index set T, be a family of physical observables each of which takes values in a finite set S of real numbers independent of a (say, T = the unit sphere in $\mathbb{R}^3$ and S_α = the spin of a particle in the a-direction), the classical model for a probabilistic description of this family, i.e. a classical stochastic process, is defined by a probability space (Ω, ϑ, μ) and a one to one correspondence among the observables (S_a) and a set of random variables on (Ω, ϑ, μ). In this way we identify the observables (S_a) with real functions belonging to the algebra $L_C^\infty(\Omega, \vartheta, \mu)$.

In the quantum model for the statistical description of the family (S_a) one identifies the observables S_a with Hermitian operators in a matrix algebra M and assigns a density matrix or, equivalently a state φ (normalized, positive, linear functional) on this matrix algebra. In the classical case the algebra is infinite dimensional (if T is an infinite set) and commutative, in the quantum case it is finite dimensional and non commutative. The infinite dimensionality arises from the fact that in the classical case the measure μ contains information not only on the distributions of the single observables S_a, but also on their joint distributions, and in the quantum case these ones have no physical meaning if the observables are not compatible. Thus the quantum model can be thought as a way of synthetizing the information contained in infinitely many classical stochastic models (one for each maximal set of compatible observables) in a single mathematical structure (the couple $\{M, \varphi\}$ of the matrix algebra M and the state φ) without introducing quantities devoid of direct physical meaning (the joint distributions of sets of incompatible observables). The distribution of each random variable S_a has a density with respect to the uniform measure (the one which assigns measure 1 to each point of S), and the quantum counterpart of this fact was discovered by Von Neumann who realized that the quantum analogue of the uniform measure on S, and of the densities of probability measures with respect to the uniform one are given respectively by the (non-normalized) trace τ_o on M and the *density matrices* in M, i.e. those operators $W_o \in M$ satisfying

$$W_o \geq 0 \qquad \tau_o(W_o) = 1\,.$$

In classical probability theory besides the probabilities a fundamental role is played, by the conditional

probabilities. They concern a compound system, say the "union" of two systems 1 and 2, and theoretically one can look at them in two different ways:

(i) As providing a statistical description of the system 1 after that an actual measurement has led to a complete information concerning the system 2.

(ii) As a way of reducing the theoretical description (i.e. the mathematical model) of the compound system 1+2 to a mathematical model concerning only system 2 (as, for example, in the Ford–Kac–Mazur model, one reduces the description of the system heat bath + mechanical system, to a description concerning only the mechanical system. In the model this reduction is accomplished by taking a conditional expectation (cf. [14, 18]).

In the classical case these two interpretations correspond to the same mathematical situation. In the quantum case the situation (i) corresponds to a conditioning on a *commutative* algebra because the measurements performed on system 2 must be compatible; while in case (ii) the conditioning can take place on an arbitrary algebra (as, for example, when we reduce, by taking a partial trace, observables concerning the space $\mathcal{H}_1 \otimes \mathcal{H}_2$ to observables concerning only $\mathcal{H}_2$ (cf. section 5 for a further discussion of this point)). The formalism of density matrices is sufficient (up to inessential modifications) to deal with case (i), while both for physical and mathematical reasons it is desirable to dispose of a technical tool which allows to handle the general situation. This is the motivation for the introduction of the concept of *conditional density matrix.*

The following heuristic considerations show in what sense the conditional density matrix plays in quantum theory the role played by the transition probability density in classical probability theory. Let $S = \{1, \ldots, n\} \subseteq \mathbb{R}$ and let μ: $(i,j) \in S \times S \to p(i,j) \in [0,1]$ be a probability measure on $S \times S$. The marginal probability μ_o: $j \in S \to p_j^o$ is defined by

$$p_i^o = \sum_{j \in S} p(i,j) .$$

The conditional probability of the couple (i,j), given its first component, is (we assume that $p(i,j) > 0$ for each i and j)

$$p(j|i) = p(i,j)/p_i^o$$

and the μ-conditional expectation of a random variable a: $(i,j) \in S \times S \to a(i,j) \in \mathbb{C}$ is defined by

$$E(a)(i) = \sum_{j \in S} a(i,j)\, p(j|i) .$$

The μ-conditional expectation E can be considered as an operator E: $L^\infty(S \times S, \mu) \to L^\infty(S, \mu_o)$ and, since in our simple example $L^\infty(S, \mu_o)$ can be identified with the algebra D of all diagonal $n \times n$ matrices, we can consider E as a linear operator E: $D \otimes D \to D$. Now, fixing a set of matrix units (e_{ij}) in M ($\Sigma_j e_{jj} = 1$ and $e_{ij} e_{hk} = \delta_{jh} e_{ik}$), we can explicitly give the identifications

$$b \in L^\infty(S, \mu_o) \mapsto \sum_{j \in S} b(j) e_{jj} ,$$

$$a \in L^\infty(S \times S, \mu) \mapsto \sum_{i,j \in S} a(i,j) e_{ii} \otimes e_{jj}$$

and with these identifications we have, for $a \in L^\infty(S \times S, \mu)$

$$\mu(a) = \int a \, d\mu = \tau(Wa)$$

where τ is the trace on $M \otimes M$ and the density matrix W is given by

$$W = \sum_{ij} p(i,j) e_{ii} \otimes e_{jj} \; ; \qquad W_o = \sum_j p_j^o e_{jj} \, . \tag{1}$$

In these notations it is not difficult to see (cf. [1]) that the μ-conditional expectation can be written as

$$E(a) = E^o(W_o^{-1} W a) \tag{2}$$

where E^o: $M \otimes M \to M$ is the partial trace uniquely defined by the property $E^o(a \otimes b) = a \cdot \tau_o(b)$ or, more explicitly:

$$E_o: \sum_{i,j,h,k} a_{ij,hk} e_{ij} \otimes e_{hk} \in M \otimes M \to \sum_{ij} \left[\sum_h a_{ij,hh} \right] e_{ij} \in M \tag{2a}$$

and

$$W_o = \sum_j p_j^o e_{jj} \tag{3}$$

is the marginal (reduced) density matrix (we identify M with $M \otimes 1 \subseteq M \otimes M$).
Symmetrizing the right hand side of (2) we obtain

$$E(a) = E^o(W_o^{-1/2} W^{1/2} a W^{1/2} W_o^{-1/2}) \, . \tag{4}$$

The right hand side of (4) defines a map E: $M \otimes M \to M$ such that

$$E \text{ is a (completely) positive map} \tag{5}$$

$$E(1) = 1 \tag{6}$$

$$\mu(a) = \mu_o(E(a)) \; ; \qquad a \in M \otimes M \, . \tag{7}$$

Remark now that the right hand side of (4) is well defined for arbitrary density matrices W, W_o (we will always assume that the operators we are dealing with are invertible), and also in this case the properties (5), (6), (7) are satisfied.
In the classical case, i.e. when the density matrices W, W_o can be both diagonalized in the same system of matrix units and, in that system have the form (1) the matrix

$$K = W^{1/2} W_o^{-1/2} \tag{8}$$

has the form

$$K = \sum_{ij} [p(j|i)]^{1/2} e_{ii} \otimes e_{jj} \, . \tag{9}$$

In the quantum case the expression (8) is still well defined and satisfies

$$E^{\circ}(K^{*}K) = 1 \tag{10}$$

which is the quantum formulation of the usual classical condition

$$\sum_{j} p(j|i) = 1 .$$

Definition 1. Any operator $K \in \mathrm{M} \otimes \mathrm{M}$ satisfying (10) will be called a *conditional density matrix.*

Remark 1. As shown by equality (9), K is the analogue of the *square root* of the transition probability matrix, rather than of the transition probability matrix itself. Moreover the square root has been introduced, in the symmetrization (4), in an apparently artificial and not intrinsically motivated way. As a matter of fact there are some mathematical considerations, connected with non-commutative Radon–Nikodym theorems and Tomita's theory, which show that the square root in (4) appears in an absolutely necessary and canonical way (cf. [9] for the proof of this assertion).

Remark 2. The non uniqueness of the square root of a positive operator introduces a certain amount of non uniqueness also in the conditional density matrix associated to a state. We will see that this non uniqueness lies at the root of the invariance under gauge transformations of the quantum Markov chains. In order to make clear the origin of this non uniqueness, let us prove a structure theorem which connects the general Definition 1 of conditional density matrix, with the particular form (8) which we arrived to through the previous heuristic considerations.

Theorem 2. For any conditional density matrix $K \in \mathrm{M} \otimes \mathrm{M}$, there exist density matrices $W \in \mathrm{M} \otimes \mathrm{M}$ and $W_{\circ} \in \mathrm{M}$ ($\cong \mathrm{M} \otimes 1$), and a unitary operator $U \in \mathrm{M} \otimes \mathrm{M}$ such that:

$$K = W^{1/2} U W_{\circ}^{-1/2} ; \qquad E^{\circ}(W) = W_{\circ} . \tag{11}$$

Proof. For any density matrix $W_{\circ} \in \mathrm{M}$, $KW_{\circ}K^{*}$ is a density matrix in fact it is positive and

$$\tau(KW_{\circ}K^{*}) = \tau(K^{*}KW_{\circ}) = \tau_{\circ}(E^{\circ}(K^{*}K)W_{\circ}) = \tau_{\circ}(W_{\circ}) = 1 . \tag{12}$$

Thus the map $W_{\circ} \mapsto E^{\circ}(KW_{\circ}K^{*})$ maps into itself the set of density matrices in M, hence it has a fixed point $W_{\circ}$

$$E^{\circ}(KW_{\circ}K^{*}) = W_{\circ} . \tag{13}$$

Denote W the density matrix $KW_{\circ}K^{*}$. Then W satisfies the second equality of (11) because of (13) and $W^{1/2}$ and $W_{\circ}^{1/2}K^{*}$ have the same modulus. Hence if $UW_{\circ}^{1/2}K^{*}$ is the polar decomposition of $W_{\circ}^{1/2}K^{*}$, U is unitary (as already asserted, in this section, all the density and conditional density matrices are supposed to be invertible) and one has

$$KW_{\circ}^{1/2} = |W_{\circ}^{1/2}K^{*}|U^{*} = W^{1/2}U^{*}$$

which is equivalent to the first equality in (11) with U^{*} instead of U.

Remark 1. If $W \in \mathrm{M} \otimes \mathrm{M}$ and $W_o \in \mathrm{M} \otimes 1$ are compatible (i.e. $E^o(W) = W_o$) density matrices, then $K = W^{1/2} W_o^{-1/2}$ is always a conditional density matrix, but in general it is not true that, given an arbitrary unitary operator $U \in \mathrm{M} \otimes \mathrm{M}$ the operator $W^{1/2} U W_o^{-1/2}$ is a conditional density matrix. For this to be the case it is necessary and sufficient that

$$E^o(U^* W U) = W_o \tag{14}$$

or, equivalently, that

$$\tau_o(W_o b) = \tau(WUbU^*); \qquad \forall b \in \mathrm{M} (\cong \mathrm{M} \otimes 1). \tag{15}$$

From (14) and (15) it follows that if U belongs to any of the following three sets then $W^{1/2} U W_o^{-1/2}$ is a conditional density matrix

$$\mathrm{I}(W) = \text{unitaries in } \mathrm{M} \otimes \mathrm{M} \text{ commuting with } W \tag{16}$$

$$\mathrm{I}(W_o) = \text{unitaries in M commuting with } W_o \tag{17}$$

$$\mathrm{I}(\mathrm{M}') = \text{unitaries in } 1 \otimes \mathrm{M} \tag{18}$$

and the same is true if $U = U_1 U_2 U_3$ with $U_1 \in \mathrm{I}(W)$, $U_2 \in \mathrm{I}(W_o)$, $U_3 \in \mathrm{I}(\mathrm{M}')$. In particular all the unitaries in the multiplicative group generated by $\mathrm{I}(W_o)$ and $\mathrm{I}(\mathrm{M}')$ enjoy this property. (The structure of the unitaries which enjoy this property is described in [9].)

Remark 2. We can use any transition probability matrix p_{ij} on the space $\mathrm{S} \times \mathrm{S}$ $(i, j \in \mathrm{S})$, to lift any probability measure (p_i^o) on S into a probability measure $p(i, j)$ on $\mathrm{S} \times \mathrm{S}$, defined by $p(i, j) = p_i^o p_{ij}$. The construction of classical Markov chains is based on the iteration of this lifting procedure. The next theorem provides the quantum analogue of this lifting procedure, on which the construction of quantum Markov chains will be based.

Theorem 3. $K \in \mathrm{M} \otimes \mathrm{M}$ is a conditional density matrix if and only if, for each density matrix $W_o \in \mathrm{M}$, $K W_o K^*$ is a density matrix $\in \mathrm{M} \otimes \mathrm{M}$.

Proof. The necessity has been proved in the proof of Theorem 2. Conversely, if $K W_o K^*$ is a density matrix for any density matrix $W_o \in \mathrm{M}$, then if

$$E^o(K^* K) = \sum_j \lambda_j P_j; \qquad P_j \in \mathrm{M}; \qquad P_j^2 = P_j; \qquad \lambda_j \in \mathbb{R}$$

is the spectral decomposition of $E^o(K^* K)$, one has

$$1 = \tau_o\left(E^o(K^* K) \frac{1}{\tau_o(P_j)} P_j\right) = \frac{\lambda_j}{\tau_o(P_j)}$$

hence $\lambda_j = \tau_o(P_j)$ for each j. But if P_j is not atomic, then there exists a projection $Q_j \in \mathrm{M}$ such that $0 < Q_j < P_j$. For this we should have

$$1 = \tau_o\left(E^o(K^* K) \frac{1}{\tau_o(Q_j)} Q_j\right) = \frac{\lambda_j}{\tau_o(Q_j)}$$

which is impossible since it would imply that $\tau_o(Q_j) = \lambda_j = \tau_o(P_j)$, against the assumption that $Q_j < P_j$. Hence all the P_j must be atomic and therefore all the λ_j must be equal to 1. Thus $E^o(K^*K) = \Sigma_j P_j = 1$, i.e. K is a conditional density matrix.

3. Examples of quantum Markov chains

We shall not discuss here the general structure theory of quantum Markov chains (cf. [1] and [6] for this) but shall limit ourselves to give some simple prescriptions for the construction of quantum Markov chains.

Let us begin with the classical case. Let $S = \{1, 2, \ldots, n_0\}$ $(n_0 \in \mathbb{N})$. A classical (homogeneous) Markov chain with state space S is completely determined by a couple $\{W_o, P\}$ where $W_o = (P_j^o)$ is a probability measure on S and $P = (P_{ij})$ $(i, j \in S)$ is a transition probability matrix.

The classical Markov chain associated to such a couple is the stochastic process (ξ_n) $n \in N$ uniquely defined (up to stochastic isomorphism) by the joint distributions

$$\mu([\xi_0 = j_0] \cap [\xi_1 = j_1] \cap \cdots \cap [\xi_n = j_n]) = P_{j_0} P_{j_0 j_1} \cdot \ldots \cdot P_{j_{n-1} j_n}. \tag{1}$$

An equivalent way of assigning the process is to give the finite dimensional correlations of functions of the random variables ξ_n

$$\mu(a_0(\xi_0) \cdot a_1(\xi_1) \cdot \ldots \cdot a_n(\xi_n)) = \int a_0(\xi_0) \cdot \ldots \cdot a_n(\xi_n)\, d\mu \tag{2}$$

where $a_1, \ldots, a_n \in L^\infty(S) \cong D$ (cf. section 2). Using the notations introduced in section 2, the explicit form of the correlation functions (2) for the Markov chain $\{W_o, P\}$ can be written as

$$\mu(a_0(\xi_0) \cdot \ldots \cdot a_n(\xi_n)) = \varphi_o(\mathscr{E}(a_0 \otimes \mathscr{E}(a_1 \otimes \cdots \otimes \mathscr{E}(a_n \otimes 1)) \cdots)) \tag{3}$$

where the linear operator $\mathscr{E}$: $D \otimes D \to D$ is characterized by

$$\mathscr{E}(a \otimes b) = a \cdot P(b) \tag{4}$$

$$P: a \in D \cong L^\infty(S) \to Pa \in D; \qquad (Pa)(j) = \sum_k P_{jk} a(k). \tag{5}$$

The operator $\mathscr{E}$: $D \otimes D \to D$ is positive and satisfies

$$\mathscr{E}(1 \otimes 1) = 1. \tag{6}$$

The expression (3) for the correlation functions of a classical Markov chain can be generalized to a quantum theoretical context in the following way: Let $\mathscr{E}$: $M \otimes M \to M$ be a completely positive linear map satisfying (6), and let $\varphi_o(\cdot) = \tau_o(W_o \cdot)$ be any state on M. Define, for any natural integer n and any $a_0, \ldots, a_n \in M$

$$\varphi_{[0,n]}(a_0 \otimes a_1 \otimes \cdots \otimes a_n) = \varphi_o(\mathscr{E}(a_0 \otimes \mathscr{E}(a_1 \otimes \cdots \otimes \mathscr{E}(a_n \otimes 1)) \cdots)), \tag{7}$$

then one can prove (cf. [1]) that there exist a unique state (on the algebra $\otimes_{\mathbb{N}} \mathrm{M}$) whose finite dimensional correlation functions are given by the right hand side of (3).
Any state constructed in this way will be called a (homogeneous) *quantum Markov chain.*
Remark 1. Complete positivity is an important technical requirement. It guarantees not only that the map $\mathscr{E}$: $\mathrm{M}\otimes\mathrm{M}\to\mathrm{M}$ is positive but also that for any other matrix algebra N, the linear map characterized by

$$b\otimes x\in \mathrm{N}\otimes(\mathrm{M}\otimes\mathrm{M})\to b\otimes\mathscr{E}(x)\in\mathrm{N}\otimes\mathrm{M}$$

is positive (this is in general false for arbitrary positive maps, cf. [17]). Without this requirement we could not guarantee that the right hand side of (3) is positive whenever all the observables $a_0, a_1, \ldots, a_n$ are positive. Here we have required the complete positivity of the operator $\mathscr{E}$ from the beginning, but it is a satisfactory feature of the theory that this technical requirement follows from the quantum formulation of the Markov property (cf. [2, 3]). In the commutative case positivity and complete positivity are the same thing.
Remark 2. In the classical case a (homogeneous) Markov chain is determined by a couple $\{W_0, P\}$ where W_0 is a probability density in D and P: $\mathrm{D}\to\mathrm{D}$ is a positive, identity preserving map (cf. formula (4)). While a (homogeneous) quantum Markov chain is determined by the couple $\{W_0, \mathscr{E}\}$ where W_0 is a density matrix in M and $\mathscr{E}$: $\mathrm{M}\otimes\mathrm{M}\to\mathrm{M}$ is a completely positive identity preserving map. We see here a non trivial difference between the classical and the quantum case: if we think in terms of matrices, since D has dimension n, W_0 is determined (prescinding from the constraints) by n numbers and P by n^2. Since M has dimenison n^2 by a direct analogy one would expect, in the quantum case, W_0 to be determined by n^2 numbers, as it is, and $\mathscr{E}$ by n^4, as it is not since, being a linear map $\mathrm{M}\otimes\mathrm{M}\to\mathrm{M}$ it is determined by n^6 numbers. The point is that in the quantum case the operator $\mathscr{E}$ cannot have the structure given by equality (4) since, because of non-commutativity, the right hand side of (4) in general will not be positive, even if both a and b are positive. This is the reason why many attempts of a direct transplantation of the structure of classical Markov chains to a quantum context lead to pathological features such as complex probabilities or complex expectation values of positive observables.
Any completely positive identity preserving operator $\mathscr{E}$: $\mathrm{M}\otimes\mathrm{M}\to\mathrm{M}$ will be called a *transition expectation.* The following proposition clarifies the structure of transition expectations and provides a link between transition expectations and conditional density matrices.

Proposition 1. A linear map $\mathscr{E}$: $\mathrm{M}\otimes\mathrm{M}\to\mathrm{M}$ is completely positive if and only if it has the form

$$\mathscr{E}(x)=\sum_j E^{\circ}(K_j^* x K_j)\,; \qquad x\in\mathrm{M}\otimes\mathrm{M} \tag{8}$$

where $K_j\in\mathrm{M}\otimes\mathrm{M}$ and E°: $\mathrm{M}\otimes\mathrm{M}\to\mathrm{M}$ is the partial trace (cf. section 2, formula (2a)).
Proof. It is known that any map of the form (8) is completely positive [17, 20]. Conversely, let $\mathscr{E}$: $\mathrm{M}\otimes\mathrm{M}\to\mathrm{M}$ be a completely positive map. Identifying M with $\mathrm{M}\otimes 1$ we can consider $\mathscr{E}$ as a particular completely positive map $\mathrm{M}\otimes\mathrm{M}\to\mathrm{M}\otimes\mathrm{M}$ (will range $\mathrm{M}\otimes 1$). A lemma of Kraus [20] implies that all such maps have the form

$$\mathscr{E}(x)=\sum_j K_j^* x K_j \tag{9}$$

where $K_j \in \mathrm{M} \otimes \mathrm{M}$. Since the range of $\mathscr{E}$ is $\mathrm{M} \otimes 1$ we have

$$\mathscr{E}(x) = E^{\circ}(\mathscr{E}(x)) = \sum_j E^{\circ}(K_j^* x K_j)$$

and this proves the assertion.
In particular, if $K \in \mathrm{M} \otimes \mathrm{M}$ is any conditional density, then

$$\mathscr{E}(x) = E^{\circ}(K^* x K); \qquad x \in \mathrm{M} \otimes \mathrm{M} \tag{10}$$

is a transition expectation.
This provides a simple prescription to build up quantum Markov chains, namely:
(i) take any matrix $K \in \mathrm{M} \otimes \mathrm{M}$ such that $E^{\circ}(K^* K) = 1$ (i.e. a conditional density matrix) and any density matrix $W_{\circ} \in \mathrm{M}$;
(ii) form the transition expectation $\mathscr{E}$ according to (10);
(iii) define, for each $n \in \mathbb{N}$, the correlation functions according to (3).
Then by the general result mentioned before, these will be the correlation functions of a unique quantum Markov chain. Such a quantum Markov chain can be easily described in terms of density matrices, in fact one has:

$$\varphi_{\circ}(\mathscr{E}(a_0 \otimes \mathscr{E}(a_1 \otimes \cdots \otimes \mathscr{E}(a_n \otimes 1)) \cdots)) = \tau_{[0,n+1]}(W_{[0,n+1]}(a_0 \otimes a_1 \otimes \cdots \otimes a_n)) \tag{11}$$

where $\tau_{[0,n+1]}$ denotes the trace on $\mathrm{M}_{[0,n+1]} = \mathrm{M} \otimes \mathrm{M} \otimes \cdots \otimes \mathrm{M}$ ($(n+1)$ times) and $W_{[0,n+1]}$ is the density matrix in $\mathrm{M}_{[0,n+1]}$ defined by

$$W_{[0,n+1]} = K_n K_{n-1} \cdots K_0 W_0 K_0^* K_1^* \cdots K_n^* \tag{12}$$

where K_m is the matrix K considered as an element of

$$\underbrace{1 \otimes \cdots \otimes 1}_{m-1} \otimes \underbrace{\mathrm{M} \otimes \mathrm{M}}_{m,\, m+1} \otimes \underbrace{1 \otimes \cdots \otimes 1}_{n-m-1} = \mathrm{M}_{[m,m+1]}.$$

(Remark that in (11) we compute an n-correlation using a density matrix in $\mathrm{M}_{[0,n+1]}$, this is a "tail effect".)
Finally let us consider the operator

$$Z: a \in \mathrm{M} \to Z(a) = \mathscr{E}(1 \otimes a) \in \mathrm{M} \tag{13}$$

naturally associated to the transition expectation $\mathscr{E}$. It is a completely positive identity preserving map (in particular the adjoint of Z maps density matrices into density matrices) and, as already remarked, contrarily to the classical situation, it *does not* contain sufficient information to recover the quantum Markov chain (this is the key difference between the classical and the quantum case). However it contains enough information to determine both the ergodic behaviour and the stationarity of the chain. In fact one easily sees that for given $\{W_{\circ}, \mathscr{E}\}$ the corresponding quantum Markov chain is stationary if

(and only if)

$$\tau_o(W_o Z(a)) = \tau_o(W_o a)\,; \qquad \forall a \in \mathrm{M} \tag{14}$$

and, because of the equality

$$\varphi(a_0 \otimes a_1 \otimes \cdots \otimes a_m \otimes 1 \otimes \cdots \otimes 1 \otimes a_{n+1} \otimes \cdots \otimes a_{n+k}) = \varphi(a_0 \otimes a_1 \otimes \cdots \otimes \cdots a_m \otimes Z^{n-m}[\mathscr{E}(a_{n+1} \otimes \mathscr{E}(\cdots \otimes \mathscr{E}(a_n \otimes 1))])$$

a stationary quantum Markov chain will be strong mixing with exponential decay of correlations if 1 is the only eigenvalue of Z of absolute value 1 and is simple (cf. [3]).

4. The 1-dimensional, nearest-neighbour quantum lattice systems as quantum Markov chains

Consider $\mathbb{Z}$ as a 1-dimensional lattice. To each point of $\mathbb{Z}$ we associate a quantum system, say a spin system, with Hilbert space H and denote $M = B(\mathrm{H})$ the bounded operators on H (for simplicity we assume that $\dim \mathrm{H} < +\infty$, but with simple assumptions on the free and the interacting Hamiltonians this restriction can be avoided).
Let $h = h^* \in \mathrm{M}$ be the Hamiltonian of the single spin system, and $V = V^* \in \mathrm{M} \otimes \mathrm{M}$ the (nearest neighbour) interaction Hamiltonian. Our aim is to give a meaning to a Hamiltonian for the infinite system whose formal, heuristic expression is

$$H = H_0 + H_1 = \sum_{n=-\infty}^{+\infty} h_n + \sum_{n=-\infty}^{+\infty} V_{n,n+1} \tag{1}$$

where h_n (resp. $V_{n,n+1}$) denotes h (resp. V) as acting on the space of the nth (resp. of the nth and $(n+1)$th) spin system. More precisely, we will give a meaning to the formal (equilibrium) density matrix

$$W(\mathrm{H}) = \frac{1}{Z}\exp\{-\beta(H_0 + H_1)\}\,; \qquad \beta > 0 \tag{1a}$$

where, formally $Z = \mathrm{Tr}(\exp\{-\beta(H_0 + H_1)\})$.
The usual way of achieving this is by means of a cut-off-and-take-limits procedure (i.e. the formal sum in (1) is substituted by a finite sum, say from $-N$ to N; the corresponding density matrix W_N defined by (1a) makes sense; and one considers limits as $N \to \infty$ of expectation values of (local) observables computed with W_N. However with this approach even for the simplest interactions of the form (1) one has little more than qualitative results (existence of the limit, regularity properties, ...) obtained, moreover, with a rather heavy technical machinery. What is worse with this approach is that the limits obtained in this way do not agree with the intuition coming from classical statistical mechanics according to which the finite range of the interaction corresponds to a locality property of the statistical correlations (i.e. a generalized Markov property, cf. [11, 12]).
In particular, in the 1-dimensional case, nearest neighbour interactions give rise to Markov chains. Adopting the point of view that one of the reasons of being of simple models is that they allow *simple* and *explicit* computations, and exploiting the analogy with the construction of quantum Markov chains, outlined in section 3, we suggest a different approach to this problem, which is based on the following:

Ansatz. The interaction potential defines a perturbation not directly of the equilibrium density matrix, but of the conditioned density matrix (i.e., not directly of the expectations, but of the conditional expectations of the (local) observables).

Remark. The point of view expressed in the ansatz above is the one generally adopted in the construction of mathematical models for classical statistical mechanics [11, 12]. In these cases one uses the interaction potential to perturb the conditional expectations associated to the free equilibrium state and to define a compatible system of conditional expectations. Then one looks for the existence and possible uniqueness of a probability measure compatible with this new set of conditional expectations (Dobruscin's theory); and such a probability measure is, by definition, an equilibrium state of the infinite system.
The construction is the following: define

$$W_o = e^{-h}/\tau_o(e^{-h}) \in M\,; \qquad \varphi_o^o(a) = \tau_o(W_o a)\,; \qquad a \in M \tag{2}$$

(where τ_o is the trace on M); $\varphi^o = \otimes_Z \varphi_o^o$. Then, formally

$$\varphi^o(\cdot) = \tau_Z\left(\exp\left\{-\sum_{n=-\infty}^{+\infty} h_n^{(x)}\right\}(\cdot)\right); \qquad h^{(x)} \equiv h - \log \tau_o(h) \tag{3}$$

where the right hand side is a purely symbolic notation which, however, becomes rigorous whenever we consider expectations of observables localized on a finite number of points. The state φ^o (free state) is a product state hence, trivially, a Markov state with transition expectations $\mathscr{E}^o$: $M \otimes M \to M$ characterized by

$$\mathscr{E}^o(a \otimes b) = a \cdot \varphi_o^o(b)\,; \qquad a, b \in M\,. \tag{4}$$

Let us define the perturbing conditional density matrix by:

$$K = e^{-V/2} \cdot \mathscr{E}^o(e^{-V})^{-1/2} \tag{5}$$

and use it to define the perturbed transition expectation:

$$\mathscr{E}(x) = \mathscr{E}^o(K^* x K) \qquad x \in M \otimes M \tag{6}$$

(it is easy to verify that $\mathscr{E}$: $M \otimes M \to M$ is effectively a transition expectation in the sense of section 3). Then we look for an $\mathscr{E}$-stationary distribution, i.e. a density matrix $V_o = e^{-R_o} \in M$ such that

$$\tau_o(V_o \mathscr{E}(1 \otimes a)) = \tau_o(V_o a)\,; \qquad a \in M \tag{7}$$

whose existence, if $\dim M < +\infty$, poses no problem (fixed point arguments) and whose uniqueness is often guaranteed by a variant (to include the non Hermitian case) of Gross's non commutative Perron theorem [15]. In terms of $\mathscr{E}$ and of $\psi_o(\cdot) = \tau_o(V_o \cdot)$, one can define a stationary quantum Markov chain φ on $\otimes_Z M$ which is characterized by

$$\varphi(a_{-m} \otimes a_{-(m-1)} \otimes \cdots \otimes a_0 \otimes a_1 \otimes \cdots \otimes a_n) = \psi_o(\mathscr{E}(a_{-m} \otimes \mathscr{E}(a_{-(m-1)} \otimes \cdots \otimes \mathscr{E}(a_n \otimes 1)) \cdots)) \tag{8}$$

keeping into account that

$$\mathscr{E}(x) = E^{\circ}(W_{\circ}^{1/2} K^* x K W_{\circ}^{1/2}) \tag{9}$$

(where $E^{\circ}(a \otimes b) = a \cdot \tau_{\circ}(b)$) we can compute the partial density matrices of the quantum Markov chain (8) using formula (12) of section 3, and obtain

$$W_{[-(n+1),n+1]} = H_n H_{n-1} \cdots H_{-n} V_{-n} H_{-n}^* H_{-(n-1)}^* \cdots H_n^* \tag{10}$$

where $H = K W_{\circ}^{1/2}$. If all the operators involved commute we can define the renormalized potential $V^{(r)} = V - \log \mathscr{E}^{\circ}(\mathrm{e}^{-V})^{-1/2}$ in terms of which we can express the formal density of the quantum Markov chain:

$$\varphi(\cdot) = \tau_{\mathbb{Z}}\left(\exp\left\{-\sum_{-\infty}^{+\infty} h_n^{(r)} - \sum_{-\infty}^{+\infty} V_{n,n+1}^{(r)} - R_{\circ}\right\}\right). \tag{11}$$

In this sense we claim that the quantum Markov chain (8) provides a rigorous expression for the formal Hamiltonian (1). Remark that with this construction *all the correlation functions are explicitly given* in terms of the initial data (i.e. h and V) by formula (8).

Let us mention a different way of associating a quantum Markov chain to the single-system Hamiltonian h and the nearest neighbour potential V: let $K_1 = \exp\{-\frac{1}{2}V\}$; define the (un-normalized) transition expectation $\mathscr{L}$: $\mathrm{M} \otimes \mathrm{M} \to \mathrm{M}$ by:

$$\mathscr{L}(x) = \mathscr{E}^{\circ}(K_1^* x K_1); \qquad x \in \mathrm{M} \otimes \mathrm{M}. \tag{12}$$

Consider the operator S: $a \in \mathrm{M} \to \mathscr{L}(1 \otimes a) \in \mathrm{M}$ and look for a $b \geq 0$ ($\neq 0$), such that

$$Sb = \lambda b; \qquad b \in \mathrm{M} \tag{13}$$

for some $\lambda > 0$. Define $\mathscr{E} = \mathscr{L}/\lambda$, and let $v_{\circ} = \lambda v / \tau_{\circ}(S^*(v))$ be any solution of

$$S^* v / \tau_{\circ}(S^* v) = v; \qquad \tau_{\circ}(v) = 1; \qquad \tau_{\circ}(S^*(v)a) = \tau_{\circ}(vS(a)) \tag{14}$$

(by fixed point arguments the solutions of both equations (13) and (14) always exist in the finite dimensional case). Define now $\varphi_{\circ}(a) = \tau_{\circ}(v_{\circ} a)/\tau_{\circ}(v_{\circ} b)$, where b is the operator defined by (13). Then the correlations

$$\varphi(a_{-m} \otimes \cdots \otimes a_n) = \varphi_{\circ}(\mathscr{E}(a_{-m} \otimes \mathscr{E}(a_{-(m-1)} \otimes \cdots \mathscr{E}(a_n \otimes b)) \cdots)) \tag{15}$$

define a unique stationary state on $\otimes_{\mathbb{Z}} \mathrm{M}$. If everything commute this state has the formal density

$$\varphi(\cdot) = \tau_{\mathbb{Z}}\left(\exp - \left\{\sum_{-\infty}^{+\infty} h_n^{(r)} + \sum_{-\infty}^{+\infty} V_{n,n+1} + \log b + R_1\right\}\right). \tag{16}$$

Comparing (16) with (11), we see that the two procedures differ in the fact that in the first case one

"renormalizes" also the interaction Hamiltonian, while in the second case only the "free" Hamiltonian is renormalized and a "boundary term at ∞" (i.e. $\log b$ appears).
In order to understand better the difference between these two procedures let us briefly discuss to what it amounts in the case of classical spin systems (1-dimensional Ising model). Assume that the interaction between spin i at the nth site and spin j at the $(n+1)$th site of the lattice is given by a number $V_{ji} = V_{ij} \in \mathbb{R}$. To this interaction we can associate an un-normalized transition matrix

$$A = (A_{ij}); \qquad A_{ij} = \exp(-V_{ij}). \tag{17}$$

Assuming, for simplicity that $h_0 = 0$ (no free part in the Hamiltonian) we have two ways of normalizing this transition matrix. One consists in forming the *conditioned partition function*

$$Z(i) = \sum_j \exp(-V_{ij})$$

and then define the transition (transfer) matrix $P = (P_{ij})$

$$P_{ij} = \mathrm{e}^{-V_{ij}}/Z(i). \tag{18}$$

The equilibrium state of the system is then defined to be the (unique) stationary Markov chain with transfer matrix given by (18). In this approach the conditioned partition function $i \mapsto Z(i)$ corresponds to the term $\mathscr{E}^0(\mathrm{e}^{-V})$ in (5) and the transfer matrix (18) to the perturbing conditional density matrix (5). The second approach is suggested by the cut-off-and-take-limits procedure, according to which for each $N \in \mathbb{N}$ one defines a probability density on the $[0, N]$ spin space $S \times S \times \cdots \times S$ $(N+1)$ times (let us restrict for simplicity to the one-sided lattice) spin configuration $(j_0, j_1, \ldots, j_N)$ $(j_k \in S)$ assigns the probability

$$\exp\Big\{-\sum_{k=1}^{N} V_{j_{k-1}j_k}\Big\} \Big/ \sum_{j_0, \ldots, j_n} \exp\Big\{-\sum_{k=1}^{N} V_{j_{k-1}j_k}\Big\} \tag{19}$$

the correlation functions for this probability measure are given by

$$\varphi_{[0,N]}(a_0(\sigma_0) \cdot a_1(\sigma_1) \cdot \ldots \cdot a_n(\sigma_n)) = \tau_0(a_0 \cdot (Aa_1 \cdot (Aa_2 \cdot (\cdots Aa_N)) \cdots))/\tau_0(A^{N+1} \cdot 1) \tag{20}$$

where $a: j \in S \to a(j) \in \mathbb{R}$ is any function: $1: S \to \mathbb{R}$ is the constant function $1(j) = 1$, $j \in S$: $\tau_0(a) = \Sigma_{j \in S} a(j)$, and σ_k denotes the spin variable at site k. The infinite volume limit procedure requires to look for limits, as $k \to +\infty$ of expectation values of the form:

$$\varphi_{[0,N+k]}(a_0(\sigma_0) \cdot \cdots \cdot a_N(\sigma_N)) = \tau_0(a_0 \cdot (Aa_1 \cdot (\cdots A(a_N \cdot (A^k 1)) \cdots))/\tau(A^{N+k+1}). \tag{21}$$

Now it is well known (Perron theorem) that there exists a real $\lambda > 0$ and a vector $b = (b_j)_{j \in S}$ with strictly positive components such that

$$Ab = \lambda b; \qquad \tau_0(b) = 1 \tag{22}$$

$$\lim_k \lambda^{-k} A^k(a) = b \cdot \tau_0(ba) \tag{23}$$

uniformly in a: $S \to \mathbb{R}$, with $\sup |a_{(i)}| \leq 1$. Therefore the limit of (21), for $k \to +\infty$, exists for every $N \in \mathbb{N}$, and every $a_0, \ldots, a_N$: $S \to R$, and is equal to

$$\tau_o\left(a_0 \cdot \left(\frac{A}{\lambda} a_1 \cdot \left(\frac{A}{\lambda} a_2 \cdot \left(\cdots \frac{A}{\lambda}(a_N b) \cdots\right)\right)\right)\right). \tag{24}$$

The equilibrium state is then defined to be the (unique) stationary Markov chain with transfer matrix given by

$$Q = (q_{ij}); \qquad q_{ij} = \frac{1}{\lambda} b_i^{-1} e^{-V_{ij}} b_j. \tag{25}$$

This is the classical analogue of the state defined by (15). In general the stationary Markov chains associated to these two transition probabilities (i.e. (18) and (24)) will be different.

Remark 1. The formal density (11) has been obtained in the assumption that all the operators involved mutually commute. If this is not the case then substituting λV for V (λ-small) and using (10) we find that the equality

$$\overline{W}_{[-n,n]} = \exp\left\{-\frac{1}{2}\left[\sum_{l=-n}^{n} h_l^{(\omega)} + \lambda \sum_{l=-(n-1)}^{n-1} V(l, l+1)\right]\right\} \cdot e^{-R_\omega}$$
$$\cdot \exp\left\{-\frac{1}{2}\left[\sum_{l=-n}^{n} h_l^{(\sigma)} + \lambda \sum_{l=-(n-1)}^{n-1} V(l, l+1)\right]\right\}$$

holds at first order in λ for every n.

Remark 2. The construction (8) can be dualized; i.e. one can define a quantum Markov chain by substituting in (8)

$$\rho_o(\mathscr{E}(\cdots \mathscr{E}(\mathscr{E}(a_{-m} \otimes 1) \otimes a_{-(m-1)}) \otimes \cdots) \otimes a_n) \tag{26}$$

where ρ_o, instead of (7), satisfies

$$\rho_o(\mathscr{E}(a \otimes 1)) = \rho_o(a); \qquad a \in \mathrm{M}. \tag{27}$$

In the case of one-sided lattices, the choice of the right hand side (8) corresponds to the inside (past) conditioning the outside (future); the choice of (26) to the outside (exterior) conditioning the inside (interior).

Summing up: the perturbation theory described above can in principle be applied to all nearest neighbour (or, with minor modifications, finite range) potentials and leads to a new class of quantum mechanical states (quantum Markov chains) with a simple structure which can be explicitly expressed in terms of the interaction potentials and which essentially agree, at first order, with the states suggested by perturbation theory. In particular one could apply this technique to the Ising or Heisenberg chain (cf. [19]) or to the Kondo Hamiltonian (cf. [24]).

Whether or not the resulting states have a physical interest is a question that cannot be solved on a purely mathematical ground.

5. The Feynman formula: heuristic motivation

The importance of the Feynman integral in quantum theory is essentially linked to two main features: (i) it provides a new, although heuristic, technique of quantization applicable to a wide class of classical dynamical systems; (ii) it provides a new perturbation technique for a Schrödinger evolution, based on a formal functional integral.

Many attempts have been made to give a rigorous mathematical foundation to this functional integral.

In this section we shall discuss the heuristic motivations of a new approach to this problem, which is mainly concerned with the second of the two features of the Feynman integral quoted above. In position representation, the Feynman formula for the kernel of a Schrödinger semi-group is

$$\psi(x, t; x_o, t_o) = \int_{[x_o t_o \to x t]} \exp\{iS_{[t_o,t]}(\omega)\}\mathcal{D}(d\omega) \tag{1}$$

where $[x_o t_o \to x t]$ denotes the space of all the "trajectories" of the system from the space-time point (x_o, t_o) to the space-time point (x, t), $\hbar = 1$, and $S_{[t_o,t]}(\omega)$ denotes the classical action in the time interval $[t_o, t]$ along the trajectory ω.

$\psi(x, t; x_o, t_o)$ is the transition amplitude for the system to be at x at time t if it was at x_o at time t_o.

Let us rewrite the expression (1) in the symbolic notation

$$\psi_t = \exp\{iS_{[t_o,t]}\}\psi_o \tag{2}$$

where we consider $\exp\{iS_{[t_o,t]}\}$ as a unitary operator but, for the moment, we do not specify neither the explicit form of this operator, nor the Hilbert space where it acts.

Since ψ_t is an amplitude, it is not a physically measurable quantity. The interesting, and measurable, objects in quantum theory are not the transition *amplitudes* by themselves, but the transition *probabilities* which are given by:

$$|\langle \varphi_t, \psi_{t_o}\rangle|^2 = \text{Prob}\{\varphi; t|\psi_o; t_o\} \tag{3}$$

where φ is any state. Denoting τ the trace on the Hilbert space where $\exp\{iS_{[t_o,t]}\}$ acts, one has

$$\text{Prob}\{\varphi; t|\psi_o; t_o\} = \tau(P_{[\varphi_{t_o}]}P_{[\psi_t]}) = \tau(\exp\{-iS_{[t_o,t]}\}P_{[\varphi]}\exp\{iS_{[t_o,t]}\}P_{[\psi_o]}) \tag{4}$$

where, for any state χ, $P_{[\chi]} = |\chi\rangle\langle\chi|$ is the orthogonal projection in the χ-direction. If, instead of a single projection $P_{[\varphi]}$, we consider a general observable of the form

$$A = \sum_j \lambda_j P_{[\varphi_j]} \tag{5}$$

(or limits thereof), the corresponding formula will be:

$$E\{A; t|\psi_o; t_o\} = \tau(\exp\{-iS_{[t_o,t]}\}A_t \exp\{iS_{[t_o,t]}\}P_{[\psi_o]}) \tag{6}$$

where the label t (in A_t) does not denote the Heisenberg evolute of A, but the fact that the measurement of A takes place at time t. This gives the conditional expectation of the observable A at time t given that the state of the system at time t_o is ψ_o.

If we split the "action operator" $S_{[t_o t]}$ into two terms, corresponding, respectively to "free" and "interaction" action:

$$S_{[t_o,t]} = S^{\circ}_{[t_o,t]} + S^{\mathrm{I}}_{[t_o,t]} \tag{7}$$

and, with a little violence to mathematics to be justified a posteriori, write

$$\exp\{-\mathrm{i}S_{[t_o,t]}\} = \exp\{-\mathrm{i}S^{\circ}_{[t_o,t]}\}\exp\{-\mathrm{i}S^{\mathrm{I}}_{[t_o,t]}\} \tag{8}$$

then the expectation value of A at time t given ψ_o at time t_o becomes

$$\tau(\exp\{\mathrm{i}S^{\circ}_{[t_o,t]}\}P_{[\psi_o]}\exp\{-\mathrm{i}S^{\circ}_{[t_o,t]}\}\cdot\exp\{-\mathrm{i}S^{\mathrm{I}}_{[t_o,t]}\}A_t\exp\{\mathrm{i}S^{\mathrm{I}}_{[t_o,t]}\}). \tag{9}$$

Keeping in mind that in the quantum case ψ_o defines a pure state, we remark that in the classical Feynman–Kac formula for the heat equation we meet an expression which is the analogue of (9), namely:

$$\int \exp\{-\tfrac{1}{2}S^{\circ}_{[t_o,t]}\}P_{[x_o]}\exp\{-\tfrac{1}{2}S^{\mathrm{I}}_{[t_o,t]}\}A_t\mathscr{D}(\mathrm{d}\omega) \tag{10}$$

where $P_{[x_o]}$ is the characteristic function of the set of all trajectories starting at x_o at time t_o; A_t is a functional of the process at time t; i.e. $A_t = A(x_t)$;

$$S^{\circ}_{[t_o,t]} = \int_0^t \left(\frac{\mathrm{d}x_s}{\mathrm{d}s}\right)^2 \mathrm{d}s \qquad \text{(formally)} \tag{11}$$

$$S^{\mathrm{I}}_{[t_o,t]} = \int_0^t V(x_s)\,\mathrm{d}s \qquad (V\text{-potential}) \tag{12}$$

and $\int(\cdots)\mathscr{D}(\mathrm{d}\omega)$ denotes the formal infinite-dimensional Lebesgue measure. Now, the rigorous notation for the formal expression (10) is

$$E^{\circ}_{[t_o]}(\exp\{-\tfrac{1}{2}S^{\mathrm{I}}_{[t_o,t]}\}A_t)(x_o) \tag{13}$$

where $E^{\circ}_{[t_o]}(\cdots)(x_o)$ denotes the conditional expectation at time t_o of the Wiener process evaluated at x_o. In order to exploit this analogy in the quantum case, let us remark that if the initial state ψ_o, corresponding to the preparation of the system at time t_o, is an eigenstate of a (discrete) observable B whose full set of eigenstates is (ψ_j), then according to the quantum theory of measurement we can define the observable:

$$E(A;t|\mathrm{B};t_o) = \sum_j \tau(\exp\{\mathrm{i}S^{\circ}_{[t_o,t]}\}P_{[\psi_j]}\exp\{-\mathrm{i}S^{\circ}_{[t_o,t]}\}\cdot\exp\{-\mathrm{i}S^{\mathrm{I}}_{[t_o,t]}\}A_t\exp\{\mathrm{i}S^{\mathrm{I}}_{[t_o,t]}\})\cdot P_{[\psi_j]} \tag{14}$$

which is the conditional expectation of A at time t given B at time t_o.

Remark 1. The *original* von Neumann formulation of the quantum measurement process ([22] chap. VI) is in terms of states and density matrices; however it is more appropriate both from the mathematical (cf. [4]) and the physical point of view to consider (14) as the conditional expectation of A given B. In particular, if an a priori probability distribution, say (P_j), for the states (ψ_j) is known and one forms the density matrix $W = \Sigma_j p_j P_{[\Psi_j]}$, the corresponding expectation value of A agrees with the usual rules of probability theory.

Remark 2. If the act of conditioning is going to have a physical meaning it must be on an *Abelian* algebra. In fact conditioning at time t_o means to measure a certain set of observables at time t_o, hence these observables must be compatible.

However, the example of quantum Markov chains (cf. section 3) shows that conditioning (or "quasi-conditioning") on a non-commutative algebra might be a useful mathematical tool and, even if not of direct physical significance, it might reflect in the mathematical model some physical properties of the system. For example, the finite range of the interaction potential will be reflected by a generalized quantum Markov property of the conditional (or quasi-conditional) expectations even if these operators take values on a non-commutative algebras. For these reasons, in the following (cf. section 7) we shall omit the restriction that the range of the conditional expectation be an Abelian algebra. In particular, we will drop the symbol B from the expression (14) and use the notation:

$$E^{\circ}_{\{t_o\}}(\exp\{-iS^{I}_{[t_o,t]}\}A_t \exp\{iS^{I}_{[t_o,t]}\}) = \sum_j \tau(\exp\{iS^{\circ}_{[t_o,t]}\}P_{[\psi_i]} \exp\{-iS^{\circ}_{[t_o,t]}\} \cdot \exp\{-iS^{I}_{[t_o,t]}\}A_t \exp\{iS^{I}_{[t_o,t]}\})P_{[\psi_j]} . \tag{15}$$

Now, in the Feynman–Kac formula for the Wiener process we have that:

$$E^{\circ}_{\{0\}}(\exp\{-\tfrac{1}{2}S^{I}_{[0t]}\}A_t) = \exp\{-t(H_0 + V)\}A \tag{16}$$

where H_0 is the generator of the process, V the "potential function", and we have put $t_o = 0$.

Thus analogy with the classical Feynman–Kac formula leads us to the following problem: can we give a meaning, in an appropriate mathematical context, to expressions such as

$$E^{\circ}_{\{t_o\}}(\exp\{-iS^{I}_{[t_o t]}\}A_t \exp\{iS^{I}_{[t_o t]}\}) \tag{17}$$

in such a way that:

(i) $E^{\circ}_{\{t_o\}}$ are conditional expectations

(ii) $\exp\{iS^{I}_{[t_o,t]}\}$ are unitary operators

(iii) the maps A (quantum observable) $\mapsto A_t$ are isomorphisms and, moreover

$$E^{\circ}_{\{0\}}(\exp\{-iS^{I}_{[0t]}\}A_t \exp\{iS^{I}_{[0t]}\}) = \exp\{it(H_0 + V)\}A \exp\{-it(H_0 + V)\} \tag{18}$$

for some H_0 (free Hamiltonian) and V (potential)?

In the following we will show that the answer to this problem is, in general, affirmative. Moreover our technique will be applicable not only to evolutions of Heisenberg type, but also to some dissipative quantum evolutions.

6. Quantum stochastic processes

A solution of the problem formulated in the preceding sections can be given in the framework of quantum stochastic processes. For a detailed discussion of this topic, we refer to [5] and to the papers of J.T. Lewis and A. Frigerio in this issue; here we will limit ourselves to make a few comments on the heuristic content of the general definitions.

A classical stochastic process is usually determined by the assignment of a family $(X_t)_{t\in T}$ of random variables defined on a probability space (Ω, ϑ, μ) and with values on a state space (S, B); for us the index set T will be $\mathbb{R}$ or $\mathbb{R}^+$ and we interpret it as "time". To be precise, this is a realization of a stochastic process, and different realization are stochastically equivalent. There are many different concepts of "stochastic equivalence" but we shall not discuss them here in detail. What is important for us is that all these concepts of stochastic equivalence recognize as essential features of a process (i.e. as those invariants which characterize the equivalence) the expectation values of particular classes of localized functionals of the process (the differences among the various concepts of stochastic equivalence are due to the different choices of these classes of functionals).

A *localized functional* of the process (X_t) is a function $F(\{X_s\}_{s\in I})$ of a sub-set of the random variables $(I \subseteq T)$, i.e. a function which does not depend on the whole trajectory, but only on a part of it. Some stochastic processes are characterized up to equivalence by the expectation values of functionals localized on finite sets (time correlations), for some others (e.g. random fields) we need more general localized functionals. Usually bounded functionals are sufficient and, since the arithmetical operations, complex conjugation and limits in the sup-norm preserve localizations, one can associate to each sub-set I of the index set T (= $\mathbb{R}$ or $\mathbb{R}^+$) the algebra (C*-algebra) of all bounded functional of the process localized in I (or, more generally, the C*-algebra generated by a particular class of bounded functionals localized in I). Let us denote by A_I this algebra. If the index set I is properly chosen A_I will not depend on the realization of the process, but only on its equivalence class. Clearly

$$I \subseteq J \Rightarrow A_I \subseteq A_J\,. \tag{1}$$

Therefore, choosing a family $\mathcal{F}$ of sub-sets of the index set such that for any $I_1, I_2 \in \mathcal{F}$ there is a $J \in \mathcal{F}$ containing both I_1 and I_2, the C*-algebra A-closure in sup-norm of $\bigcup\{A_I: I \in \mathcal{F}\}$ will still depend only on the process, and not on a particular realization of it. The probability measure defines an expectation function (state) on A which we will denote μ. The triple $\{A, (A_I)_{I\in\mathcal{F}}, \mu\}$ is thus an invariant of the process. For some relations of stochastic equivalence it is a complete set of invariants, in the sense that it characterizes the process up to equivalence for some other we still need to specify a set of generators inside each local algebra A_I and require that the isomorphism maps generators into generators.

We can sum up the main conclusion of the above qualitative analysis in the assertion: up to stochastic equivalence the theory of classical stochastic processes is the theory of local algebras (i.e. families (A_I) satisfying (1)) with a state on them. Because of this equivalence, and of the fact that local algebras have been introduced in quantum theory with motivations completely independent on the theory of stochastic processes [16], it is natural to define a quantum stochastic process just as a triple $\{A, (A_I)_{I\in F}, \mu\}$ with all the properties listed above and without the restriction that the algebra A be Abelian.

Remark. In this definition of quantum stochastic processes we adopt an intrinsic point of view in the sense that the random variables themselves play no role, but only the bounded functionals of them. From this point of view, the choice of a specific set of random variables is similar to the choice of a basis in a vector space.

If, in analogy with the classical situation, we want to single out a set of random variables which define the process we can do this, in the present context, by using $*$-homomorphisms (cf. [7]).

7. The quantum Feynman–Kac formula

Let $\{A, (A_I)_{I\in\mathscr{F}}, \mu\}$ be a quantum stochastic process in the sense of the preceding sections.
To fix the ideas $\mathscr{F}$ will now be the family of all (closed, open, half-closed, bounded or not) intervals of $\mathbb{R}$ and the parameter $t\in\mathbb{R}$ will be interpreted as *time*. Let $I\in\mathscr{F}$; a linear map E_I: $A\to A_I$ will be called a *conditional expectation* if

$$E_I \text{ is positivity preserving} \tag{1}$$

$$E_I(1) = 1 \tag{2}$$

$$E_I(a\cdot b) = E_I(a)\cdot b\,; \qquad a\in A\,; \qquad b\in A_I\,. \tag{3}$$

In the classical case these properties, together with the μ-invariance

$$\mu(E_I(a)) = \mu(a)\,; \qquad a\in A \tag{4}$$

uniquely characterize the conditional expectation associated to μ and relative to the σ-algebra generated by the functions in A_I.
Let $(E_I)_{I\in\mathscr{F}}$ be a family of conditional expectations, E_I: $A\to A_I$, satisfying the compatibility condition

$$I\subseteq J \Rightarrow E_I\cdot E_J = E_I\,. \tag{5}$$

Let U_t: $A\to A$ be a 1-parameter group of $*$-automorphisms of A (time-shift) such that for each $I\in\mathscr{F}$ and $t\in\mathbb{R}$, the covariance conditions:

$$U_t(A_I) = A_{I+t} \tag{6}$$

$$U_t^{-1}\cdot E_{I+t}\cdot U_t = E_I \tag{7}$$

are satisfied.
Finally we assume that the system (E_I) of conditional expectations satisfies the following *Markov Property*:

$$E_{]-\infty,t]}(A_{[t,+\infty[}) \subseteq A_t\,; \qquad t\in\mathbb{R}\,. \tag{8}$$

Systems $\{A, (A_I), (E_I), U_t\}$ with the above properties are often naturally associated to models of free or quasi-free systems (cf. [7]). To such a system one can associate a "free" evolution on the "time-zero algebra" A_0 (we have $\{0\} = [0, 0]\in\mathscr{F}$ and we denote $A_0 = A_{(0)}$):

$$P_0^t = E_{]-\infty,0]}U_t \restriction A_0\,: \quad A_0\to A_0 \tag{9}$$

the evolution (semi-group) property follows from

$$P_0^t P_0^s = E_{]-\infty,0]} U_t E_{]-\infty,0]} U_s$$
$$= E_{]-\infty,0]} E_{]-\infty,t]} U_{t+s} = E_{]-\infty,0]} U_{t+s} = P_0^{t+s} . \tag{10}$$

The fact that P_0^t maps A_0 into itself is a consequence of the Markov property (8).
In order to perturb the free evolution P_0^t, let us consider a family of operators $(M_t)_{t>0}$ satisfying

$$M_t \in A_{[0,t]} \tag{11}$$

$$M_{t+s} = M_t \cdot U_t(M_s) \quad \text{(1-cocycle identity)} . \tag{12}$$

Any such a family will be called a *Markovian cocycle* (Markovian because of the localization property (11)). Typical examples of Markovian cocycles are

$$M_t = \exp\left\{-\tfrac{1}{2}\int_0^t V_s \, ds\right\} \qquad \text{(Hermitian Markovian cocycle)} \tag{13}$$

$$M_t = T\left(\exp\left\{i\int_0^t V_s \, ds\right\}\right) \qquad \text{(unitary Markovian cocycle)} \tag{14}$$

where T denotes the time-ordered exponential and $V_s = U_s V_0$; V_0 being any Hermitian operator in A_0 (potential). In terms of the free evolution P_0^t and of the Markovian cocycle $(M_t)_{t>0}$, we can define the perturbed evolution P^t by:

$$P^t(a_0) = E_{]-\infty,0]}(M_t U_t(a_0) M_t^*) ; \qquad a_0 \in A_0 . \tag{15}$$

Again the fact that P^t maps A_0 into itself follows from the Markov property and from (11). Moreover

$$P^t P^s(a_0) = E_{]-\infty,0]}(M_t U_t\{E_{]-\infty,0]}(M_s U_s(a_0) M_s^*)\} \cdot M_t^*)$$
$$= E_{]-\infty,0]}(M_t \cdot E_{]-\infty,t]}\{U_t(M_s)\, U_{t+s}(a_0)\, U_t(M_s)^*\} \cdot M_t^*)$$
$$= E_{]-\infty,0]} E_{]-\infty,t]}(M_t\, U_t(M_s)\, U_{t+s}(a_0)\, U_t(M_s)^* \cdot M_t^*)$$
$$= E_{]-\infty,0]}(M_{t+s} U_{t+s}(a_0) M_{t+s}) = P^{t+s}(a_0) . \tag{16}$$

Therefore P^t is effectively an evolution. In order to relate the two evolutions above, let

$$\delta_0 = \lim_{t \downarrow 0} \frac{1}{t}(P_0^t - 1) \tag{17}$$

be the infinitesimal generator of the free evolution. To compute the infinitesimal generator of the perturbed evolution remark that for any $a_0 \in A_0$

$$\frac{1}{t}\cdot(P^t-1)a_0=\frac{1}{t}\{E_{]-\infty,0]}(M_t\,U_t(a_0)\,M_t^*)-a_0\}$$

$$=\frac{1}{t}\{E_{]-\infty,0]}U_t(a_0)-a_0\}+E_{]-\infty,0]}\left\{\frac{1}{t}[M_t\cdot U_t(a_0)\cdot M_t^*-a_0]\right\}$$

$$=\frac{1}{t}\{P_0^t-1\}(a_0)+E_{]-\infty,0]}\left\{\frac{1}{t}[M_t\,U_t(a_0)\,M_t^*-a_0]\right\}$$

therefore

$$\delta(a_0)=\lim_{t\downarrow 0}\frac{1}{t}(P^t-1)(a_0)=\delta_0(a_0)+\{A_0\cdot a_0+a_0A_0^*\} \tag{18}$$

where

$$A_0=\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0}M_t=\lim_{t\downarrow 0}\frac{1}{t}[M_t-1]\,. \tag{19}$$

In particular, if M_t has the form (13)

$$\delta=\delta_0+\tfrac{1}{2}\{V_0,\cdot\}$$

where $\{\cdot,\cdot\}$ denotes the anti-commutator, and if M_t has the form (14)

$$\delta=\delta_0+\mathrm{i}[V_0,\cdot]$$

where $[\cdot,\cdot]$ denotes the commutator.
Moreover, if the free evolution P_0^t, was of Heisenberg type, i.e. $\delta_0=\mathrm{i}[H_0,\cdot]$ then using the Markov property to substitute $E_{\{0\}}$ for $E_{]-\infty,0]}$, we have

$$P^ta_0=\exp\{\mathrm{i}t(H_0+V)\}\cdot a_0\cdot\exp\{-\mathrm{i}t(H_0+V)\}$$

$$=E_{\{0\}}\left(T\left[\exp\left\{\mathrm{i}\int_0^t V_s\,\mathrm{d}s\right\}\right]\cdot U_t(a_0)\cdot T\left[\exp\left\{\mathrm{i}\int_0^t V_s\,\mathrm{d}s\right\}\right]^*\right)$$

which, up to notations is equality (18) of section 5.
In this sense we claim that the formalism outlined above provides a possible framework in which the heuristic considerations of section 5 acquire a rigorous meaning (cf. [5] for a more detailed discussion and [7] for an application to a concrete model).

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