Jean Tavernier¹

Received May 16, 1975

The Kac ring model is studied rigorously. Considered as an isolated system, its description is given in classical and quantum mechanics; the definition of the quantum states is made precise. The most interesting results are: (1) In the classical model, except for pathological cases, equilibrium is obtained independently of the initial state in the thermodynamic limit of a probabilistic theory; (2) as long as the number of sites and polarizations is finite, the master equation does not apply; (3) the explicit form of the non-Markovian terms in the evolution equation is obtained; (4) the memory of the initial state disappears from the evolution equation of the diagonal part of the density operator for a large class of nontrivial scattering operators. Finally, several unsolved problems are mentioned.

KEY WORDS: Quantum and classical models; equilibrium attainment; thermodynamic limit; density operator; master equation; non-Markovian terms; memory of initial state.

1. INTRODUCTION

In 1956 Kac⁽¹⁾ suggested a simple model for studying the problem of a physical system relaxing toward equilibrium.

The structure and classical and quantum descriptions of this model were

¹ Université Paris VI, Groupe de Physique des Solides E.N.S., Paris, France.

^{© 1976} Plenum Publishing Corporation, 227 West 17th Street, New York, N.Y. 10011. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, microfilming, recording, or otherwise, without written permission of the publisher.

studied and completed by Dresden⁽²⁾ in 1962 and have been recently analyzed in detail by him.⁽³⁾

The main features of Ref. 3 that have motivated the writing of this paper are the following:

- 1. In classical mechanics, the probabilistic description is obtained by averaging the distribution function.
- 2. In the quantum description, the master equation is used in an unusual form; it is given in terms of the occupation probability of the eigenstates of the one-particle position operator; usually the eigenstates considered are those of the unperturbed evolution operator.
- 3. The transition probability involved in the master equation is not symmetric with respect to the connected states.
- 4. The master equation is tentatively used to describe the Kac ring model and it is recognized that it does not apply to the magnetic depolarization process.

In order to get a better insight into the problems arising from Dresden's paper, we intend to deal with the following points:

- (a) We study the classical description of a generalized Kac model in the framework of a probabilistic theory; on the one hand, we prove that equilibrium is, in general, not obtained when the number of sites allowed to the particles is given; on the other hand, the relaxation toward equilibrium is obtained in the thermodynamic limit, independently of the initial state.
- (b) We specify and extend the quantum description of the Kac model, with particular emphasis on the definition of the evolution operators and the eigenstates.
- (c) We show that, for a given number of sites, the master equation cannot be deduced from the evolution equation of the density operator; the non-Markovian terms always remain and the offdiagonal part of the density operator at the initial time appears in the evolution equation of the diagonal part.
- (d) We look at what happens when the number of sites increases to infinity.

In addition, we prove that:

- 1. The time average of the observable "polarization" or "color" in Dresden's language commutes with the ensemble average in the classical description; it is worth noting that this observable specifies the macroscopic state of the system.
- 2. The system is not ergodic in the classical version.

3. In the limit of the number of sites increasing to infinity, the transition probability connecting two eigenstates of the unperturbed evolution operator depends only on the polarization states.

To conclude, the intention of this paper is to study the Kac model in more detail than has been done until now and to prove that the master equation does not apply.

The results we have obtained are complementary to those of Dresden. In fact, his main concern was with the Liouville and master equations as basic laws of evolution; the process of equilibrium attainment is investigated by an averaging method with respect to the scatterer distribution.

The reader interested in physical realizations of the model is referred to the very interesting examples and comments given by Dresden.

In Section 2, classical and quantum descriptions are specified. The Sections 3 and 4 are concerned with the above-mentioned points (a)-(d).

2. DESCRIPTION OF THE MODEL

The model suggested by Kac consists of N particles located respectively at N sites (numbered 1, 2,..., N) arranged into a circle. The evolution of the system is achieved in a discrete manner; the particle located at site j at time tjumps to the adjoining site j + 1 at time t + 1. Furthermore, these particles can take on one of two different intrinsic states (white or black) and the evolution of one particle from site j to site j + 1 occurs with or without a change of state according to whether or not there is scattering between sites jand j + 1.

Taking into account this model and its extended form given by Dresden, in which the particles remain independent, we propose the following generalization: The independent particles can take on one of S intrinsic states and the scattering effect is described in terms of probability theory.

We specify the mathematical structure of the model and point out its general properties and limits of validity.

2.1. Classical Description

We shall use the following notation: E is the set of intrinsic states for one particle; G_N is the set of sites allowed to a particle (the group of integers modulo N); D is the set of states for one scatterer (a subset of the set of mappings from E to E; this last set will be denoted F); $\mathscr{E} = E^N$ is the set of intrinsic states for the N-particle system; and $\mathscr{D} = D^N$ is the set of states for the N scatterers or configurations.

The state of a particle at time $t \in \mathbb{N}$ is

$$e_t = (j_t, \sigma_t) \in G_N \times E \tag{1}$$

The evolution operator for one particle $U = VU_0$ is the composite of the following mappings: (a) the unperturbed evolution operator:

$$U_0: \quad (j,\sigma) \to (j+1,\sigma) \tag{2}$$

and (b) the scattering operator:

$$V: (j, \sigma) \to (j, v_j \sigma) \tag{3}$$

where $v_i \in D$.

Therefore, we have by definition

$$e_{t+1} = (j_{t+1}, \sigma_{t+1}) = Ue_t = (j_t + 1, v_{j_t}\sigma_t)$$
(4)

The unperturbed evolution being trivial, we introduce an "intermediate representation" by defining

$$\xi_t = U_0^{-t}(e_t) = (j_0, \sigma_t)$$
(5)

and consequently

$$\xi_{t+1} = (j_0, v_{j_0+t}\sigma_t) \tag{6}$$

The evolution of the particle located at site j at time zero is then given by the relation

$$\sigma_{t+1} = v_{j+t}\sigma_t \tag{7}$$

The intermediate description of the N-particle system is defined by the mapping

$$\mathbf{\sigma}_t \in \mathscr{E} \to \mathbf{\sigma}_{t+1} = {}^t \mathbf{V}(\mathbf{\sigma}_t) \in \mathscr{E}$$
(8)

where ${}^t V \in \mathscr{D}$ is deduced from the configuration $V \in \mathscr{D}$ of the scatterers through the mapping

$$\mathbf{V} = (v_1, v_2, ..., v_N) \to {}^t \mathbf{V} = (v_{t+1}, ..., v_{t+N}), \qquad t \in \mathbb{Z}$$
(9)

We write as V^{-1} the mapping of $[\mathscr{P}(E)]^{\mathbb{N}}$ into itself, where $\mathscr{P}(E)$ is the set of all subsets of E, defined by

$$\mathbf{V}^{-1} = (v_1^{-1}, v_2^{-1}, ..., v_N^{-1})$$
(10)

It is an easy matter to verify that

$$({}^{t}\mathbf{V})^{-1} = {}^{t}(\mathbf{V}^{-1}) \tag{11}$$

In the same way it can be shown that

$${}^{t}(\mathbf{V}\mathbf{W}) = {}^{t}\mathbf{V}{}^{t}\mathbf{W}, \qquad t \in \mathbb{Z}, \quad \mathbf{V} \text{ and } \mathbf{W} \in F^{N}$$
(12)

$$t'(t\mathbf{V}) = t' + t\mathbf{V}, \qquad t \text{ and } t' \in \mathbb{Z}, \quad \mathbf{V} \in F^N$$
 (13)

$${}^{N}\mathbf{V} = \mathbf{V}, \qquad \mathbf{V} \in F^{N} \tag{14}$$

104

Thus we have proved that F^N is a group with operators whose domain of operators is G_N and \mathcal{D} has G_N as a group of operators.

Finally, a probabilistic description of the evolution will be defined by a given law of probability on the set $\mathscr{D} \times \mathscr{E}$ at the initial time; the law of probability at time t + 1 will be obtained from that at time t through the use of the evolution mapping

$$f_t: \quad (\mathbf{V}, \, \mathbf{\sigma}) \in \mathscr{D} \, \times \, \mathscr{E} \to (\mathbf{V}', \, {}^t \mathbf{V} \mathbf{\sigma}) \in \mathscr{D} \, \times \, \mathscr{E} \tag{15}$$

where V' would be different from V if the interaction between the particles and the scatterers modified the state of the latter.

In the following, we shall suppose the stability of the scatterers by writing

$$\mathbf{V} = \mathbf{V}'$$

As far as the law of initial probability is concerned, we shall formulate a hypothesis of independence:

$$P_0(\mathbf{V}, \boldsymbol{\sigma}) = P(\mathbf{V})p_0(\boldsymbol{\sigma}) \tag{16}$$

We shall write $p_t(\sigma)$ for the probability of the state σ at time t.

2.2. Quantum Description

We take the space of intrinsic states as \mathbb{C}^{s} . The set of sites is still the group G_{N} of the integers modulo N.

In the Schrödinger representation, the instantaneous state of a particle is a mapping ψ from G_N into \mathbb{C}^S ; all the mappings from G_N into \mathbb{C}^S are squareintegrable for the normalized Haar measure on G_N .

In the following we shall take the Hilbert space of the wave functions $\mathscr{L}^2(G_N, \mathbb{C}^S)$ to be the Hilbert space $\mathscr{H} = [\mathbb{C}^S]^N$ with the canonical Hermitian product

$$\langle \psi | \varphi
angle = (1/N) \sum_{j \in G_N} \langle \psi(j) | \varphi(j)
angle_{\mathbb{C}^S}$$

where $\psi(j) \in \mathbb{C}^s$ is the *j*th component of ψ .

As in the case of the classical description, the evolution operator is obtained as the product of the unperturbed evolution operator U_0 with the scattering operator V.

2.2.1. Unperturbed Evolution Operator. We shall start by defining the position operator X for one particle by

$$X\psi(k) = e^{2i\pi k/N}\psi(k) \tag{17}$$

It is clear that this operator is unitary and that the set of its eigenvalues is

nothing but the roots of order N of unity; the latter is canonically isomorphic to G_N .

In short, we shall say that the wave function ψ describes a particle located at site $j \in G_N$ if

$$X\psi(k) = \delta_{jk} e^{2i\pi j/N} \psi(k) \tag{18}$$

The eigenvectors $\chi_{j\sigma}$ ($\sigma \in \mathbb{C}^{S}$) associated with the position $j \in G_{N}$ are such that

$$x_{j\sigma}(k) = \sigma \,\delta_{jk} \tag{19}$$

(the multiplicity of each eigenvalue is S).

The evolution operator must therefore be such that

$$U_0\chi_{j\sigma} = \chi_{j+1,\sigma} \tag{20}$$

By analyzing a wave function $\psi \in \mathscr{H}$ with respect to the basis composed of the eigenvectors of X, we verify, as expected, that

$$U_0 \psi(k) = \psi(k - 1)$$
(21)

It is clear that U_0 is a unitary operator and that its eigenvalues are

$$e^{-2i\pi n/N}, \quad n = 1, 2, ..., N$$
 (22)

The eigenvectors $\nu_{n\sigma}$ ($\sigma \in \mathbb{C}^{S}$) associated with the eigenvalue $e^{-2i\pi n/N}$ are such that

$$\nu_{n\sigma}(k) = e^{2i\pi n/N} \nu_{n\sigma}(k-1)$$
(23)

We shall put

$$\nu_{n\sigma} = (e^{2i\pi n/N}\sigma, e^{4i\pi n/N}\sigma, ..., \sigma)$$
(24)

(the multiplicity of each eigenvalue is S).

If the S polarizations are chosen to be an orthonormalized basis of \mathbb{C}^s , the vectors $\nu_{n\sigma}$ make an orthonormalized basis of \mathscr{H} .

2.2.2. Scattering Operator V and Evolution Operator U. The quantum transposition of the model used in the classical description of the scattering system is obtained by putting

$$V\chi_{j\sigma} = \chi_{j,v_{j-1}(\sigma)} \tag{25}$$

where v_j is a linear operator of \mathbb{C}^s , for every $j \in G_N$.

Clearly, there must be at least one scatterer such that the associated scattering operator is different from a scalar operator of modulus one. Otherwise any eigenstate of the unperturbed system also would be an eigenstate of the perturbed system.

Moreover, since the evolution operator $U = VU_0$ is unitary, V is a unitary operator of \mathcal{H} and consequently v_j is a unitary operator of \mathbb{C}^s .

106

Finally, for any wave function $\psi \in \mathscr{H}$ the definition (25) leads to

$$V\psi(k) = v_{k-1}[\psi(k)]$$
(26)

and by introducing, for all $t \in \mathbb{Z}$, the mapping

$$V = (v_1, ..., v_N) \in [\mathscr{L}(\mathbb{C}^S)]^N \to {}^tV = (v_{1-t}, ..., v_{N-t})$$
(27)

(the subscripts are to be counted modulo N), we establish the relation:

$$U_0^{\ t} V = {}^t V U_0^{\ t} \tag{28}$$

which will be used in Section 4.

The operators v_j are to be defined in terms of the properties of the scatterers by noticing that the matrix element

 $\langle \sigma | v_j \sigma'
angle$

represents the probability amplitude for the transition from the state of polarization σ' to that of polarization σ when the particle state is affected by a scatterer located between sites j and j + 1; in fact, we have

$$U\chi_{j\sigma} = \chi_{j+1,\nu_j(\sigma)} \tag{29}$$

On the other hand, note that the intermediate description, eliminating the trivial evolution U_0 operator, is obtained from the Schrödinger wave functions by putting

$$\psi_t^{(I)} = U_0^{-t} \psi_t^{(S)} \tag{30}$$

The evolution operator between times t and t + 1 is then

$$U_t^{(\mathrm{I})} = U_0^{-(t+1)} V U_0^{(t+1)}$$
(31)

and we easily verify that

$$U_t^{(I)}\psi(k) = v_{k+t}[\psi(k)] \quad \text{for any} \quad \psi \in \mathscr{H}$$
(32)

In particular, we have

$$\psi_{t+1}^{(I)}(k) = U_t^{(I)}\psi_t^{(I)}(k) = v_{k+t}[\psi_t^{(I)}(k)]$$
(33)

This is the quantum translation of the relation (7).

The statistical description of the system will be based on the use of the density operator ρ_t , the evolution equation of which is, in the Schrödinger representation,

$$\rho_{t+1} = U\rho_t U^* \tag{34}$$

3. CLASSICAL DESCRIPTION OF THE EVOLUTION

3.1. Law of Probability

The probabilistic model introduced in Section 2.1 allows us to compute the probability $p_t(\sigma)$ of the *N*-particle system to be found in intrinsic state σ at time *t*.

This computation is given in Appendix A. The result is

$$p_t(\boldsymbol{\sigma}) = \sum_{\mathbf{V} \in \mathcal{D}} P(\mathbf{V}) p_0(\mathbf{V}^{-1} \mathbf{V}^{-1} \cdots \mathbf{v}^{(t-1)} \mathbf{V}^{-1}(\boldsymbol{\sigma}))$$
(35)

In particular for the mechanical evolution the laws of probability P and p_0 are

$$P(\mathbf{V}) = \delta_{\mathbf{V},\mathbf{V}'}, \qquad p_0(\mathbf{\sigma}) = \delta_{\mathbf{\sigma},\mathbf{\sigma}'}$$

where V' and σ' are, respectively, some fixed elements of \mathcal{D} and \mathscr{E} .

Then we have

$$p_t(\mathbf{\sigma}) = 1 \quad \text{if} \quad \mathbf{\sigma}' \in ({}^{t-1}\mathbf{V}' \cdots \mathbf{V}')^{-1}(\mathbf{\sigma})$$

= 0 otherwise (36)

This result agrees with the relation (8), according to which

$$\boldsymbol{\sigma}_t = {}^{t-1} \mathbf{V}' \cdots \mathbf{V}'(\boldsymbol{\sigma}') \tag{37}$$

In particular, if V is the unit mapping of \mathscr{E} , we have $\sigma_t = \sigma'$; the intrinsic state of the particles does not change.

3.2. Study of a Simple Model

The preceding results are used to analyze the following model: Let E be the group of the roots of order S of unity, and D be the translation group of E (isomorphic to E).

For any element $\epsilon \in E$ the associated translation v_{ϵ} will be assimilated to this element by the definition

$$v_{\epsilon}(\sigma) = \epsilon \sigma$$
 for any $\sigma \in E$

The model studied by Dresden is contained in the particular case S = 2. The law of probability (35) is then written

$$p_t(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\epsilon} \in \mathscr{E}} P(\boldsymbol{\epsilon}^{-1}) p_0(\boldsymbol{\epsilon}^{-1} \boldsymbol{\epsilon} \cdots \boldsymbol{t}^{-1} \boldsymbol{\epsilon} \boldsymbol{\sigma})$$
(38)

From ${}^{N} \boldsymbol{\epsilon} = \boldsymbol{\epsilon}$, it is clear that $p_{t}(\boldsymbol{\sigma})$ is a periodic function whose period is a submultiple of NS.

Consequently, and as expected, the irreversibility phenomenon does not occur in the preceding description for any finite N.

In order to understand where the irreversible evolution comes from, let us study the mean value of the observable

$$A(\boldsymbol{\sigma}) = \sum_{i \in G_N} \sigma_i \tag{39}$$

We have

$$\langle A \rangle_t = \sum_{\boldsymbol{\sigma} \in \mathscr{E}} A(\boldsymbol{\sigma}) p_t(\boldsymbol{\sigma}) = \sum_{i \in G_N} \langle \epsilon_i \epsilon_{i+1} \cdots \epsilon_{i+t-1} \rangle \langle \sigma_i \rangle_0$$
(40)

where

$$\begin{split} \langle \sigma_i \rangle_0 &= \sum_{\boldsymbol{\sigma} \in \mathscr{E}} \sigma_i p_0(\boldsymbol{\sigma}) \\ \langle \epsilon_i \epsilon_{i+1} \cdots \epsilon_{i+t} \rangle &= \sum_{\boldsymbol{\varepsilon} \in \mathscr{E}} (\epsilon_i \cdots \epsilon_{i+t}) P(\boldsymbol{\varepsilon}) \end{split}$$

Finally, suppose the random variables ϵ_i to be independent with the same law of probability; then we get

$$\langle A \rangle_t = \langle \epsilon^k \rangle^{t - (k-1)N} \langle \epsilon^{k-1} \rangle^{kN-t} \langle A \rangle_0 \tag{41}$$

for $(k - 1)N + 1 \le t \le kN$, k = 1, 2, ..., S; and

$$\langle A \rangle_{t+NS} = \langle A \rangle_t$$

where

$$\langle \epsilon^k \rangle = \sum_{l=1}^{S} e^{(2i\pi/S)kl} p(l)$$

p(l) being the probability of the scattering state $e^{2i\pi l/s}$.

It is clear that

$$|\langle \epsilon^k \rangle| \leq 1, \qquad k = 1, 2, \dots, S \tag{42}$$

Furthermore, we observe that $\langle A \rangle_t = 0$ for every t as soon as $\langle A \rangle_0 = 0$; then the system is in statistical equilibrium. When $\langle A \rangle_0 \neq 0$ the system does not return to its equilibrium state for all finite N.

Now, what happens as far as the evolution is concerned when N goes to infinity with $\langle A \rangle_0 \neq 0$?

For any fixed t, as soon as N is greater than t, (41) leads to

$$\langle A_N
angle_t = \langle \epsilon
angle^t \langle A_N
angle_0$$

where the subscript N on A reminds us that A_N describes an N-site system.

If we suppose that the thermodynamic limit exists at the initial time, that is,

$$\lim_{N\to\infty}\frac{1}{N}\langle A_N\rangle_0=a$$

then the thermodynamic limit exists for any time and we have

$$a_t = \lim_{N \to \infty} \frac{1}{N} \langle A_N \rangle_t = \langle \epsilon \rangle^t a$$

Finally, in the thermodynamic limit, as soon as $|\langle \epsilon \rangle| < 1$ the observable a_t decreases exponentially to zero when t goes to infinity; the preceding condition means that the scatterers are efficient.

A detailed study of this problem has been given recently by Coopersmith and Mandeville,⁽⁴⁾ using Dresden's formalism. These papers give an analysis of the subsystem relaxation and a description of the fluctuations.

On the other hand, a simple computation given in Appendix B shows that taking the time average and taking the mean value with respect to the initial state are two commuting operations when applied to the observable A defined by (39).

The studied system displays all the main features of a good physical system but in spite of this it is not ergodic, as shown in Appendix C, for $N \ge 3$ and for every S.

4. QUANTUM DESCRIPTION OF THE EVOLUTION

4.1. Notations

The evolution is defined through the density operator ρ , whose evolution equation is now analyzed.

Let \mathscr{A} be the Hilbert algebra of the operators on $\mathscr{H} = (\mathbb{C}^{S})^{N}$ with the Hermitian product

$$\langle A|B\rangle = \operatorname{Tr} A^*B, \quad A \text{ and } B \in \mathscr{A}$$
 (43)

Let us introduce the complementary orthogonal projectors \mathscr{D} and $\mathscr{D}' = \mathscr{I} - \mathscr{D}$ defined by

$$\langle n\sigma | \mathscr{D}(A)n'\sigma' \rangle = \langle n\sigma | An\sigma \rangle \,\delta_{nn'} \,\delta_{\sigma\sigma'}, \qquad A \in \mathscr{A} \tag{44}$$

where $n\sigma$ stands for the eigenstate $\nu_{n\sigma}$ of the unperturbed evolution operator U_0 . [I is such that $\mathcal{I}(A) = A$ for every $A \in \mathcal{A}$.]

Let \mathscr{U}_0 , \mathscr{U} , and \mathscr{V} be the unperturbed and perturbed evolution operators and the scattering operator associated, respectively, to the operators U_0 , U, and V through definitions similar to

$$\mathscr{U}_0(A) = U_0 A U_0^* \quad \text{for all} \quad A \in \mathscr{A}$$
 (45)

It is clear that the following properties are true:

$$\mathcal{U}_0, \mathcal{U}, \text{ and } \mathscr{V} \text{ are unitary operators}$$

 $\mathcal{D}\mathcal{U}_0 = \mathcal{U}_0 \mathcal{D} = \mathcal{D}$ (46)
 $[\mathcal{D}(A)]^* = \mathcal{D}(A^*)$

4.2. Decomposition of the Evolution Equation

Let us consider \mathscr{A} as the direct sum of the Hilbert subspaces $\mathscr{D}(\mathscr{A})$ and $\mathscr{D}'(\mathscr{A})$.

The density operator is decomposed in the form

$$\rho_t = R_t + S_t, \quad \text{where} \quad R_t = \mathscr{D}(\rho_t), \quad S_t = \mathscr{D}'(\rho_t)$$
(47)

In the matrix notation, the evolution equation (34) can be written

$$R_{t+1} = \mathscr{U}_{00}(R_t) + \mathscr{U}_{01}(S_t), \qquad S_{t+1} = \mathscr{U}_{10}(R_t) + \mathscr{U}_{11}(S_t)$$
(48)

where:

$$\begin{aligned}
\mathcal{U}_{00} &= \mathcal{D}\mathcal{U}\mathcal{D} = \mathcal{D}\mathcal{V}\mathcal{D}, & \mathcal{U}_{01} = \mathcal{D}\mathcal{U}\mathcal{D}' = \mathcal{D}^{1}\mathcal{V}\mathcal{D}' \\
\mathcal{U}_{10} &= \mathcal{D}'\mathcal{U}\mathcal{D} = \mathcal{D}'\mathcal{V}\mathcal{U}, & \mathcal{U}_{11} = \mathcal{D}'\mathcal{U}\mathcal{D}'
\end{aligned} \tag{49}$$

Let us remark that $\mathscr{U}_{01}^* = (\mathscr{U}^*)_{10}$.

Then, it is an easy matter to verify that, for all $t \ge 0$,

$$R_{t+1} - \mathscr{U}_{00}(R_t) = \mathscr{U}_{01}\mathscr{U}_{11}^t(S_0) + \sum_{\tau=1}^t \mathscr{U}_{01}\mathscr{U}_{11}^{\tau-1}\mathscr{U}_{10}(R_{t-\tau})$$
(50)

and

$$S_{t+1} - \mathscr{U}_{11}(S_t) = \mathscr{U}_{10}\mathscr{U}_{00}^t(R_0) + \sum_{\tau=1}^t \mathscr{U}_{10}\mathscr{U}_{00}^{\tau-1}\mathscr{U}_{01}(S_{t-\tau})$$
(51)

It follows that the diagonal matrix elements of the density operator are given by the equation

$$\rho_{n\sigma}(t+1) = \sum_{n'\sigma'} |\langle n\sigma | Un'\sigma' \rangle|^2 \rho_{n'\sigma'}(t) + \langle n\sigma | \mathscr{U}_{01} \mathscr{U}_{11}^t(S_0) n\sigma \rangle + \sum_{\tau=1}^t \langle n\sigma | \mathscr{U}_{01} \mathscr{U}_{11}^{\tau-1} \mathscr{U}_{10}(R_{t-\tau}) n\sigma \rangle$$
(52)

where we have put

$$\rho_{n\sigma}(t) = \langle n\sigma | \rho_t n\sigma \rangle \tag{53}$$

This equation contains non-Markovian terms, which we are going to study in detail.

A tedious calculation, given in Appendix D, shows that

$$\langle \alpha | \mathscr{U}_{01} \mathscr{U}_{11}^{\tau-1} \mathscr{U}_{10}(R) \alpha \rangle = \sum_{\alpha'} P(\alpha \alpha'; \tau) \rho_{\alpha'}$$
(54)

where α stands for $n\sigma$.

The transition probabilities are defined as follows:

$$P(\alpha\alpha'; \tau) = \sum_{k=1}^{\tau+1} (-1)^{k+1} \sum_{i_1+\ldots+i_k=\tau+1} P_{i_1\ldots i_k}(\alpha, \alpha')$$
(55)

(the i_l are positive integers different from zero), with

$$P_{i_1\dots i_k}(\alpha, \alpha') = \sum_{\alpha_1\dots\alpha_{k-1}} P_{i_1}(\alpha, \alpha_1) P_{i_2}(\alpha_1, \alpha_2) \cdots P_{i_k}(\alpha_{k-1}, \alpha') \quad \text{for } k \ge 2$$
$$= P_{i_1}(\alpha, \alpha') \quad \text{for } k = 1$$
(56)

$$P_{l}(\alpha, \alpha') = |\langle \alpha | U^{l} \alpha' \rangle|^{2} = |\langle \alpha | V^{-1} V \cdots (l-1) V \alpha' \rangle|^{2}$$
(57)

The last form is obtained by using (28).

Taking into account the definitions (24) and (27), we obtain the explicit form of P_l as

$$P_{l}(\alpha, \alpha') = \left| \frac{1}{N} \sum_{k=1}^{N} \left\{ \exp\left[\frac{2i\pi}{N} \left(n' - n\right)k\right] \right\} \langle \sigma | v_{k} v_{k-1} \cdots v_{k-l+1} \sigma' \rangle \right|^{2}$$
(58)

In the particular case where v_k is independent of k, we find

$$P_{l}(\alpha, \alpha') = \delta_{nn'} |\langle \sigma | v^{l} \sigma' \rangle|^{2}$$
⁽⁵⁹⁾

where again α stands for $n\sigma$.

Finally, Eq. (52) becomes, for all $t \ge 0$,

$$\rho_{\alpha}(t+1) = \sum_{\tau=0}^{t} \sum_{\alpha'} P(\alpha\alpha'; \tau) \rho_{\alpha'}(t-\tau) + \sum_{\alpha'\alpha''} P(\alpha; \alpha'\alpha''; t) S_{\alpha'\alpha''}(0) \quad (60)$$

where the transition probability $P(\alpha \alpha'; \tau)$ is defined by (55) and (56); $P(\alpha; \alpha' \alpha''; t)$ is given explicitly in Appendix D.

For the unperturbed system $(U = U_0)$ it is easily verified that

$$\rho_{\alpha}(t+1) = \rho_{\alpha}(t)$$

Remarks. The evolution equation (34) written in the form

$$\rho_{t-1} = U^* \rho_t U$$

allows us to show that the diagonal part of the density operator is given, for all $t \leq 0$, by the equation

$$R_{t-1} = \tilde{\mathscr{U}}_{00}(R_t) + \sum_{\tau=1}^{|t|} \tilde{\mathscr{U}}_{01} \tilde{\mathscr{U}}_{11}^{\tau-1} \tilde{\mathscr{U}}_{10}(R_{t+\tau}) + \tilde{\mathscr{U}}_{01} \mathscr{U}_{11}^{|t|}(S_0)$$
(61)

where the $\tilde{\mathcal{U}}_{ij}$ are defined by (49) for the operation $U^{-1} = U^*$ instead of U.

Then we can deduce that the diagonal matrix elements of the density operator satisfy

$$\rho_{\alpha}(t-1) = \sum_{\tau=0}^{|t|} \sum_{\alpha'} \widetilde{P}(\alpha\alpha';\tau) \rho_{\alpha'}(t+\tau) + \sum_{\alpha'\alpha''} \widetilde{P}(\alpha;\alpha'\alpha'';|t|) S_{\alpha'\alpha''}(0)$$
(62)

where it is easy to verify that

$$\tilde{P}(\alpha\alpha';\tau) = P(\alpha'\alpha;\tau)$$

$$\tilde{P}(\alpha;\alpha'\alpha'';|t|) = \sum_{k=1}^{|t|+1} (-1)^{k+1} \sum_{i_1+\ldots+i_k=|t|+1} P_{i_1}(\alpha''\alpha';\alpha'''\alpha''') P_{i_2\ldots i_k}(\alpha''',\alpha)$$
(63)

If we put, for all $t \leq 0$,

$$P(\alpha\alpha';t) = P(\alpha'\alpha;|t|), \qquad P(\alpha;\alpha'\alpha'';t) = \tilde{P}(\alpha;\alpha'\alpha'';|t|)$$
(64)

we obtain

$$\rho_{\alpha}(t-1) = \sum_{\tau=0}^{t} \sum_{\alpha'} P(\alpha\alpha'; \tau) \rho_{\alpha'}(t-\tau) + \sum_{\alpha'\alpha''} P(\alpha; \alpha'\alpha''; t) S_{\alpha'\alpha''}(0) \quad (65)$$

In the term $P(\alpha; \alpha'\alpha''; t)$, α stands for (α, α) .

We can then observe that the transition from the evolution equation for $t \ge 0$ to that corresponding to $t \le 0$ is obtained through the rule

$$P(\alpha, \alpha'; \tau) \to P(\alpha'\alpha; -\tau)$$
$$P(\alpha_1\alpha_2; \alpha_3\alpha_4; t) \to P(\alpha_4\alpha_3; \alpha_2\alpha_1; -t)$$

4.3. Properties of the Transition Probabilities

First of all, let us remark that the transition probability $P_1(\alpha, \alpha')$ which would occur in a hypothetical master equation is symmetric with respect to the connected states if the perturbation theory is taken up to the second order. In fact, if we write

$$V = I + W$$

where W is to be considered as a perturbation, the unitarity of V implying

$$W + W^* = -WW^*$$

we have, with evident notation

$$|U_{\alpha\alpha'}|^2 = |V_{\alpha\alpha'}|^2 = |W_{\alpha\alpha'}|^2 = |W_{\alpha'\alpha}|^2$$
 for $\alpha \neq \alpha'$

by neglecting the terms of order greater than two.

Now, the definition (55) of the transition probability can be rewritten in a

Jean Tavernier

more compact form by denoting P_l the real positive-definite matrix onto the set of the eigenstates of U_0 , defined by (57).

For any set $(i_1, ..., i_k)$ of positive integers different from zero, we put

$$P_{i_1...i_k} = P_{i_1} P_{i_2} \cdots P_{i_k} \tag{66}$$

and (52) becomes

$$P(\tau) = \sum_{k=1}^{\tau+1} (-1)^{k+1} \sum_{i_1 + \dots + i_k = \tau+1} P_{i_1 \dots i_k}$$
(67)

In Appendix E it is shown that the generating function of the transition matrices $P(\tau)$,

$$F(z) = \sum_{\tau=0}^{\infty} P(\tau) z^{\tau}$$
(68)

is related to the generating function of the matrices P_l ,

. . .

$$f(z) = \sum_{l=1}^{\infty} P_l z^l \tag{69}$$

through the relation

$$zF(z) = f(z)[I + f(z)]^{-1}$$
(70)

The transition matrix $P(\tau)$ appears as the coefficient of $z^{\tau+1}$ in $f(z)[I + f(z)]^{-1}$; so the process will be Markovian iff

$$f(z)[I + f(z)]^{-1} = \lambda z$$
 (71)

where λ , which is nothing but $P(0) = P_1$, is a matrix with a norm less than one.

This condition, equivalent to

$$f(z) = \lambda (I - \lambda z)^{-1} z \tag{72}$$

leads to the very restrictive relation

$$P_l = \lambda^l = P_1^l$$
 for any $l = 1, 2,...$ (73)

Then the lemma proved in Appendix F shows that the process is a Markovian one if and only if the evolution operation U commutes with the unperturbed evolution operator U_0 or, in other words, the scattering operator V commutes with U_0 .

This property is in disagreement with the hypothesis following (25), so we must conclude that the evolution process cannot be Markovian; it is therefore incorrect to apply the master equation to describe the Kac ring model.

On the other hand, it is shown in Appendix G that the condition eliminating the memory of the off-diagonal part of the density operator at time zero in (60) is much less restrictive than the preceding one; there exist some evolution operators U that do not commute with U_0 and such that $P(\alpha; \alpha'\alpha''; t) = 0$ For instance, if the number of polarizations S equals two, the scattering operator V defined by (25) with

$$v_k = \begin{pmatrix} 0 & \xi_k \\ \eta_k & 0 \end{pmatrix}$$
 where $|\xi_k \eta_k| = 1$ (74)

in the basis comprised of the eigenstates of polarization in \mathbb{C}^2 , leads to $\tilde{P}_i = 0$ [see definition (G.1)].

Finally, Theorem 1 proved in Appendix H shows that the limit, when N goes to infinity, of the transition probability $P_l(\alpha, \alpha')$ defined by (58) depends only on the polarizations σ and σ' of the states α and α' insofar as the sequence

$$\frac{1}{N}\sum_{k=1}^{N} \langle \sigma | v_k v_{k-1} \cdots v_{k-l+1} \sigma' \rangle$$

has a limit when N goes to infinity.

Theorem 2 of Appendix H improves the preceding result by showing that it is valid for the case where the limit of the site configuration is taken as follows: The abscissas (in increasing order) $(y_k(N))_{k=1,...,N}$ of the sites allowed to the N particles are such that the family of sequences indexed by $N: [x_k(N) = y_k(N)/y_N(N)]_{k=1,...,N}$, tends asymptotically, when N goes to infinity, toward a sequence equally distributed on the interval [0, 1].

5. CONCLUSION

We shall not enumerate the main results obtained in this work; this has been done in the introduction. Here we emphasize the most important limitations of the considered models and point out what points it would be interesting to study.

First of all, the classical and quantum models are only concerned with independent-particle systems. It would be certainly fruitful to remove this hypothesis as long as the new models would admit rigorous treatment without appealing to perturbation theory, which is, in general, hardly justified.

In the classical description, we have only considered a cyclic model of polarization and to study the return toward equilibrium in the thermodynamic limit we have supposed that the scatterers were independent and described by the same probability law. Nevertheless, we do not think these restrictions to be essential in proving the general properties of the studied system.

What we have done in terms of a quantum description is clearly incomplete. In particular, it would be essential to describe what happens in the limit where the number of sites goes to infinity; but, according to the discussion at the end of Section 4.3 and the relation (73), it seems reasonable to think that the system will not become Markovian in this limit. Nevertheless, this very important problem remains open.

Finally, we have proved that the memory of the off-diagonal part contained in the density operator at the initial time is eliminated from the evolution equation of the diagonal part even for some nontrivial scattering operators; it would be very interesting to define the class of scattering operators that ensure the elimination of the memory effect; moreover, a physical understanding of their properties would be certainly fruitful.

To conclude, we remark that the Kac ring model, although very fascinating in its simplicity and its mathematical tractability, is not the best one to be studied in the framework of the master equation. In fact, we are tempted to conjecture that the master equation applies, in the case of an isolated system, only when a continuous spectrum of eigenstates is obtained for the unperturbed evolution operator, in the thermodynamic limit. Thus, we expect the master equation to be valid for describing the Kac ring model in the limit of a continuous spectrum of polarizations and not only in the case where Sgoes to infinity.

This model was already suggested by Dresden as a "more realistic picture which corresponds to balls capable of a continuum color." But its study remains open.

APPENDIX A. THE PROBABILITY $p_t(\sigma)$

According to the probabilistic model given at the end of Section 2.1, we are able to determine $p_i(\sigma)$ as follows.

From the definition, the probability $P_1(\mathbf{V}, \boldsymbol{\sigma})$ induced onto the set $\mathcal{D} \times \mathcal{E}$, at time one, by the mapping f_0 is

$$P_1(\mathbf{V}, \mathbf{\sigma}) = P_0(\mathbf{V}, \mathbf{V}^{-1}\mathbf{\sigma}) = P(\mathbf{V})p_0(\mathbf{V}^{-1}\mathbf{\sigma})$$
(A.1)

and the probability of state σ at time one is

$$p_1(\boldsymbol{\sigma}) = \sum_{\mathbf{V} \in \mathscr{D}} P(\mathbf{V}) p_0(\mathbf{V}^{-1}\boldsymbol{\sigma})$$
(A.2)

Now, through the mapping f_1 , we have successively

$$P_2(\mathbf{V}, \boldsymbol{\sigma}) = P_1(\mathbf{V}, {}^{1}\mathbf{V}^{-1}\boldsymbol{\sigma}) = P_0(\mathbf{V}, \mathbf{V}^{-1}{}^{1}\mathbf{V}^{-1}\boldsymbol{\sigma})$$
(A.3)

and

$$p_2(\boldsymbol{\sigma}) = \sum_{\mathbf{V} \in \mathscr{D}} P(\mathbf{V}) p_0(\mathbf{V}^{-1} \mathbf{V}^{-1} \boldsymbol{\sigma})$$
(A.4)

We thus see that (35) is true at times one and two; an easy recursion procedure proves (35).

APPENDIX B. MEAN VALUES OF OBSERVABLE A DEFINED BY (39)

In the framework of the model used in Section 3.2, the *i*th component of the state at time t ($1 \le t \le NS$) can be written

$$\sigma_{i}(t) = \epsilon_{i+t-1} \cdots \epsilon_{i+1} \epsilon_{i} \sigma_{i}, \qquad 1 + (k-1)N \leq t \leq kN, \quad k = 1, \dots, S$$
(B.1)

where σ_i is the *i*th component of the initial state.

Remembering the counting modulo N of indices, (B.1) becomes

$$\sigma_{i}(t) = \mu^{k-1} \epsilon_{i} \epsilon_{i+1} \cdots \epsilon_{i+t-1-(k-1)N} \sigma_{i}$$
(B.2)

with $\mu = \prod_{i=1}^{N} \epsilon_i$.

The time average of $\sigma_i(t)$ is

$$\bar{\sigma}_{i} = \frac{1}{NS} \sum_{t=1}^{NS} \sigma_{i}(t) = 0 \quad \text{if} \quad \mu \neq 1$$

$$= \frac{\sigma_{i}}{N} \sum_{t=1}^{N} \epsilon_{i} \cdots \epsilon_{i+t-1} \quad \text{if} \quad \mu = 1$$
 (B.3)

On the other hand, since the ensemble average of $\sigma_i(t)$ is

 $\langle \sigma_i(t) \rangle = \mu^{k-1} \epsilon_i \cdots \epsilon_{i+t-1-(k-1)N} \langle \sigma_i \rangle, \quad 1 + (k-1)N \leq t \leq k_N$ (B.4) its time average is

$$\overline{\langle \sigma_i \rangle} = 0 \qquad \text{if } \mu \neq 1$$
$$= \frac{\langle \sigma_i \rangle}{N} \sum_{t=1}^N \epsilon_i \cdots \epsilon_{i+t-1} \qquad \text{if } \mu = 1 \qquad (B.5)$$

Thus we verify that (B.5) is the ensemble average of (B.3):

$$\overline{\langle \sigma_i \rangle} = \langle \overline{\sigma}_i \rangle \tag{B.6}$$

The preceding result is extended by linearity to prove that it stands for observable A.

APPENDIX C. NONERGODICITY OF THE SYSTEM WHEN $N \ge 3$

A definition⁽⁵⁾ of ergodicity is that the entity

$$(1/NS)\sum_{i=1}^{NS} f(\boldsymbol{\sigma}_i) \tag{C.1}$$

where $\sigma_t = {}^{t-1} \epsilon \cdots {}^1 \epsilon \epsilon \sigma$, must be independent of $\sigma \in \mathscr{E}$ for all complex-valued functions f.

Since a basis of functions over \mathscr{E} is given by the set $\{\delta_{\xi}\}_{\xi \in \mathscr{E}}$ with

$$\begin{split} \delta_{\boldsymbol{\xi}} \colon & \boldsymbol{\sigma} \in \mathscr{E} \mapsto \delta_{\boldsymbol{\xi}}(\boldsymbol{\sigma}) = 1 & \text{if } \boldsymbol{\xi} = \boldsymbol{\sigma} \\ &= 0 & \text{if } \boldsymbol{\xi} \neq \boldsymbol{\sigma} \end{split} \tag{C.2}$$

the statement (C.1) is equivalent to requiring that

$$(1/NS)\sum_{t=1}^{NS} \delta_{\xi}(\sigma_t)$$
(C.3)

is independent of σ for all $\xi \in \mathscr{E}$.

From the definition,

$$\frac{1}{NS}\sum_{t=1}^{NS} \delta_{\xi}(\boldsymbol{\sigma}_t) = \frac{1}{NS} |\{t: \boldsymbol{\sigma}_t = \boldsymbol{\xi}, 1 \leq t \leq NS\}|$$
(C.4)

where $|\{\cdots\}|$ stands for the number of elements of the set $\{\cdots\}$.

For a fixed $\xi \in \mathscr{E}$ let us define

 $A(\mathbf{\sigma}) = \{t: \ \mathbf{\sigma}_t = \mathbf{\xi}, \ 1 \leqslant t \leqslant NS\}$ (C.5)

When $\sigma \neq \sigma'$, it is not hard to show that

$$A(\mathbf{\sigma}) \cap A(\mathbf{\sigma}') = \emptyset \tag{C.6}$$

Suppose $|A(\sigma)|$ independent of σ ; then

$$\left|\bigcup_{\boldsymbol{\sigma}\in\mathscr{E}}A(\boldsymbol{\sigma})\right| = N^{S}|A(\boldsymbol{\sigma})| \leq NS$$
 (C.7)

since

$$\bigcup_{\boldsymbol{\sigma}\in\mathscr{E}}A(\boldsymbol{\sigma})\subseteq\{1,2,...,NS\}$$

Therefore, if the system is to be ergodic, we must have

$$|A(\mathbf{\sigma})| \leqslant SN^{1-s} \tag{C.8}$$

But, for all S and as soon as $N \ge 3$, it is easy to verify that

$$|A(\sigma)| < 1$$

The conclusion is obtained by remarking that for all ξ there exists at least one element σ such that $A(\sigma) = \emptyset$.

APPENDIX D. NON-MARKOVIAN TERMS

We want to get an explicit expression for the terms of the form

$$N_{\mathfrak{r}} = \langle \alpha | \mathscr{U}_{01} \mathscr{U}_{11}^{\mathfrak{r}-1} \mathscr{U}_{10}(R) \alpha \rangle = \langle \alpha | (\mathscr{U} \mathscr{D}')^{\mathfrak{r}} \mathscr{U}(R) \alpha \rangle$$
(D.1)

where the right-hand expression is obtained from definitions (49) and $\mathscr{D}(R) = R$.

Let A be an operator on the Hilbert space \mathscr{H} ; the operator \mathscr{A} associated with the operator A on \mathscr{H} and defined by $\mathscr{A}(T) = ATA^*$ for all $T \in \mathscr{L}(\mathscr{H})$ admits, with respect to the basis $\{|\alpha\rangle\langle\alpha'|\}$ generated by the basis of the eigenvectors of U_0 in \mathscr{H} , the matrix elements

$$A(lphaeta;\gamma\delta)=\langlelpha|A\gamma
angle\overline{\langleeta|A\delta
angle}$$

Then we have

$$\langle \alpha | \mathscr{A}(T) \alpha' \rangle = \sum_{\alpha'' \alpha'''} A(\alpha \alpha'; \alpha'' \alpha''') \langle \alpha'' | T \alpha''' \rangle$$
 (D.2)

and by iteration

$$\langle \alpha | \mathscr{A}_{1} \mathscr{D}' \mathscr{A}_{2} \mathscr{D}' \cdots \mathscr{A}_{m-1} \mathscr{D}' \mathscr{A}_{m}(T) \alpha' \rangle$$

$$= \prod_{k=1}^{m} A_{k}(\alpha_{i_{k-1}} \alpha_{j_{k-1}}; \alpha_{i_{k}} \alpha_{j_{k}}) \prod_{k=1}^{m-1} (1 - \delta_{\alpha_{i_{k}} \alpha_{j_{k}}}) \langle \alpha_{i_{m}} | T \alpha_{j_{m}} \rangle$$
(D.3)

with $\alpha_{i_0} = \alpha$ and $\alpha_{j_0} = \alpha'$.

In particular, we get

$$N_{\tau} = \prod_{k=1}^{\tau+1} U(\alpha_{i_{k-1}}\alpha_{j_{k-1}}; \alpha_{i_{k}}\alpha_{j_{k}}) \prod_{k=1}^{\tau} (1 - \delta_{\alpha_{i_{k}}\alpha_{j_{k}}}) \delta_{\alpha_{i_{\tau+1}}\alpha_{j_{\tau+1}}}\rho_{\alpha_{i_{\tau+1}}}$$
(D.4)

where $\alpha_{i_0} = \alpha_{j_0} = \alpha$.

In the preceding formulas, the sum over the repeated indices is implied. The last result takes the form

$$N_{\tau} = \sum_{\alpha'} P(\alpha \alpha'; \tau) \rho_{\alpha'}$$
(D.5)

with

$$P(\alpha\alpha'; \tau) = \prod_{k=1}^{\tau+1} U(\alpha_{i_{k-1}}\alpha_{j_{k-1}}; \alpha_{i_k}\alpha_{j_k}) \prod_{k=1}^{\tau} (1 - \delta_{\alpha_{j_k}}\alpha_{j_k})$$

and $\alpha_{i_{\tau+1}} = \alpha_{j_{\tau+1}} = \alpha'$.

Let us introduce (i) the sets $\mathscr{S} = \mathscr{T} \times \mathscr{T}$ where \mathscr{T} is the eigenvector set of U_0 , $\Delta = \{(\alpha, \alpha) : \alpha \in \mathscr{T}\}$ is the diagonal of \mathscr{S} , and $T = \{1, 2, ..., \tau\}$; and (ii) the mappings

$$\chi: \quad \gamma = (\gamma_1 \cdots \gamma_\tau) \in \mathscr{S}^T \mapsto \chi(\gamma) = \prod_{k \in T} [1 - \chi_\Delta(\gamma_k)]$$

which is the characteristic function of the subset $\overline{\Delta}^T$ of \mathscr{S}^T , where $\overline{\Delta}$ is the

Jean Tavernier

complement of Δ in \mathscr{S} ; χ_{Δ} is the characteristic function of Δ ; and

$$\widetilde{U}$$
: $\gamma \in \mathscr{S}^T \mapsto \widetilde{U}(\gamma) = \prod_{k=1}^{i+1} U(\gamma_{k-1}; \gamma_k)$

with $\gamma_0 = (\alpha, \alpha)$ and $\gamma_{\tau+1} = (\alpha', \alpha')$.

Thus we get the following expression for $P(\alpha \alpha'; \tau)$:

$$P(\alpha\alpha'; \tau) = \sum_{\gamma \in \mathscr{S}^T} \tilde{U}(\gamma)\chi(\gamma)$$
(D.6)

in which it is clear that

$$\chi(\gamma) = \sum_{k=0}^{\tau} (-1)^k \sum_{\substack{S \subset T \\ |S|=k}} \prod_{j \in S} \chi_{\Delta}(\gamma_j) = \sum_{k=0}^{\tau} (-1)^k \sum_{\substack{S \subset T \\ |S|=k}} \chi_{\Delta}s(\gamma_S) \quad (D.7)$$

where γ_s is the restriction of γ to the subset S of T and χ_{Δ^s} is the characteristic function of Δ^s , with $\chi_{\Delta^s}(\gamma_s) = 1$ when $S = \emptyset$.

Now, putting

$$S = \{m_1, ..., m_k\}$$
 with $1 \leq m_1 < m_2 \cdots < m_k \leq \tau$

we have

$$\tilde{U}(\gamma) = \prod_{j=1}^{k+1} \prod_{l=m_{j-1}}^{m_j-1} U(\gamma_l; \gamma_{l+1})$$
(D.8)

with $m_0 = 0$ and $m_{k+1} = \tau + 1$.

Inserting (D.7) into formula (D.6), we get

$$P(\alpha\alpha';\tau) = \sum_{k=0}^{\tau} (-1)^k \sum_{\substack{S \subset T \\ |S| = k}} \sum_{\gamma_S \in \mathscr{S}^S} \chi_{\Delta S}(\gamma_S) \sum_{\overline{\gamma} \in \mathscr{S}^{\overline{S}}} \widetilde{U}(\gamma)$$
(D.9)

where γ is defined through its restrictions γ_s and $\overline{\gamma}$.

Taking account of (D.8), we obtain

$$\chi_{\Delta s}(\gamma_{s}) \sum_{\bar{\gamma} \in \mathscr{S}^{s}} \tilde{U}(\gamma) = \prod_{j=1}^{k+1} P_{m_{j}-m_{j-1}}(\alpha_{m_{j-1}}, \alpha_{m_{j}})$$

where

$$P_{m_j-m_{j-1}}(\alpha_{m_{j-1}}, \alpha_{m_j}) = \sum_{\gamma \in \mathscr{S}^{S_j}} \prod_{l=m_{j-1}}^{m_j-1} U(\gamma_l, \gamma_{l+1})$$

with $\gamma_{m_j} = (\alpha_{m_j}, \alpha_{m_j})$ for all $m_j \in S$ and

$$S_j =]m_{j-1}, m_j[, \qquad \tilde{S} = \bigcup_{j=1}^{k+1} S_j$$

Then, the expression (D.9) for $P(\alpha \alpha'; \tau)$ becomes

$$P(\alpha \alpha'; \tau) = \sum_{k=0}^{1} (-1)^{k} \sum_{(m_{1} \cdots m_{k}) \in T^{k}} P_{m_{1} \cdots m_{k}}(\alpha, \alpha')$$
(D.10)

where

$$P_{m_1...m_k}(\alpha, \alpha') = \sum_{(\alpha_{m_1}\cdots\alpha_{m_k})\in \mathcal{F}^k} \prod_{j=1}^{k+1} P_{m_j-m_{j-1}}(\alpha_{m_{j-1}}, \alpha_{m_j})$$

Finally, the mapping

$$(m_1,...,m_k) \in T^k \to (i_1,...,i_{k+1})$$

where $i_l = m_l - m_{l-1}$ is a nonzero positive integer and $\sum_{l=1}^{k+1} i_l = \tau + 1$ according to (D.8), allows us to write:

$$P(\alpha\alpha'; \tau) = \sum_{k=1}^{\tau+1} (-1)^{k+1} \sum_{\substack{i_1 \cdots i_k \\ \sum i_l = \tau+1}} P_{i_1 \cdots i_k}(\alpha, \alpha')$$
(D.11)

with

$$P_{i_1\dots i_k}(\alpha, \alpha') = \sum_{(\alpha_1 \cdots \alpha_{k-1}) \in \mathcal{F}^{k-1}} \prod_{l=1}^k P_{i_l}(\alpha_{l-1}, \alpha_l) \quad \text{if } k \ge 2$$

= $P_{i_1}(\alpha, \alpha') \quad \text{if } k = 1$ (D.12)

where $\alpha_0 = \alpha$, $\alpha_k = \alpha'$, and

$$P_{l}(\alpha, \alpha') = |\langle \alpha | U^{l} \alpha' \rangle|^{2}$$
 (D.13)

Let us remark that the $P_i(\alpha, \alpha')$ are just the diagonal matrix elements of the operator \mathscr{U}^i with respect to the basis $\{|\alpha\rangle\langle\alpha'|\}$.

On the other hand, the term proportional to S_0 in (52) is of the form

$$M_t = \langle \alpha | \mathscr{U}_{01} \mathscr{U}_{11}^t(S) \alpha \rangle = \langle \alpha | (\mathscr{U} \mathscr{D}')^{t+1}(S) \alpha \rangle$$
 (D.14)

with $\mathscr{D}'(S) = S$, or

$$M_{t} = \prod_{k=1}^{t+1} U(\alpha_{i_{k-1}}\alpha_{j_{k-1}}; \alpha_{i_{k}}\alpha_{j_{k}})(1 - \delta_{\alpha_{i_{k}}\alpha_{j_{k}}})S_{\alpha_{i_{k}}\alpha_{j_{k}}}$$
(D.15)

with $\alpha_{i_0} = \alpha_{j_0} = \alpha$ and $S_{\alpha\alpha'} = \langle \alpha | S\alpha' \rangle$ (the sum over the repeated indices is implied).

Therefore, M_t can be written

$$M_t = \sum_{\alpha'\alpha''} P(\alpha; \alpha'\alpha''; t) S_{\alpha'\alpha''}$$
(D.16)

Jean Tavernier

where we have put

$$P(\alpha; \alpha' \alpha''; t) = \prod_{k=1}^{t+1} U(\alpha_{i_{k-1}} \alpha_{j_{k-1}}; \alpha_{i_k} \alpha_{j_k}) \prod_{k=1}^{t} (1 - \delta_{\alpha_{i_k} \alpha_{j_k}})$$
(D.17)

with $\alpha_{i_0} = \alpha_{j_0} = \alpha$, $\alpha_{i_{t+1}} = \alpha'$, and $\alpha_{j_{t+1}} = \alpha''$.

It is not difficult to verify that the proof leading to (D.11) can be carried over to the problem at hand; we evaluate (D.17) to get

$$P(\alpha; \alpha' \alpha''; t) = \sum_{k=1}^{t+1} (-1)^{k+1} \sum_{\substack{i_1 \cdots i_k \\ \sum i_l = t+1}} P_{i_1 \cdots i_k}(\alpha; \alpha' \alpha'')$$
(D.18)

(the i_l are positive integers different from zero), with

$$P_{i_{1}\cdots i_{k}}(\alpha; \alpha'\alpha'') = \sum_{\substack{(\alpha_{1}\cdots\alpha_{k-1})\in\mathscr{F}^{k-1}\\\alpha'''\in\mathscr{F}}} \left[\prod_{l=1}^{k-1} P_{i_{l}}(\alpha_{l-1}, \alpha_{l}) \right] P_{i_{k}}(\alpha_{k-1}\alpha_{k-1}; \alpha'\alpha'')$$
$$= \sum_{\alpha'''\in\mathscr{F}} P_{i_{1}\cdots i_{k-1}}(\alpha, \alpha''') P_{i_{k}}(\alpha'''\alpha'''; \alpha'\alpha'')$$
(D.19)

where

$$P_{l}(\alpha_{1}\alpha_{2}; \alpha_{3}\alpha_{4}) = \langle \alpha_{1} | U^{l}\alpha_{2} \rangle \overline{\langle \alpha_{3} | U^{l}\alpha_{4}} \rangle$$
 (D.20)

and $\alpha_0 = \alpha$.

The definition (D.20) is just that of the matrix elements of the operator \mathscr{U}^{l} with respect to the basis $\{|\alpha\rangle\langle\alpha'|\}$.

APPENDIX E. GENERATING FUNCTION OF THE TRANSITION PROBABILITIES

Introducing the power series F(z) constructed from the $P(\tau)$'s as coefficients, the definition (67) of the transition matrices gives

$$zF(z) = \sum_{\tau=0}^{\infty} P(\tau)z^{\tau} = \sum_{\tau=0}^{\infty} \sum_{k=1}^{\tau+1} (-1)^{k+1} \sum_{i_1+\dots+i_k=\tau+1} P_{i_1}z^{i_1}\dots P_{i_k}z^{i_k}$$
$$= \sum_{k=1}^{\infty} \sum_{\tau=k-1}^{\infty} (-1)^{k+1} \sum_{i_1+\dots+i_k=\tau+1} P_{i_1}z^{i_1}\dots P_{i_k}z^{i_k}$$
$$= \sum_{k=1}^{\infty} (-1)^{k+1} \left[\sum_{l=1}^{\infty} P_l z^l\right]^k$$
(E.1)

Now, defining the generating function of the matrices P_t ,

$$f(z) = \sum_{l=1}^{\infty} P_l z^l$$
 (E.2)

we obtain the following relation:

$$zF(z) = f(z)[I + f(z)]^{-1}$$
 (E.3)

It is not hard to make sure that the series F(z) and f(z) have a nonzero radius of convergence, since

$$\|P(\tau)\| = \sup_{\alpha\alpha'} |P(\alpha\alpha'; \tau)| \leq \sum_{k=1}^{\tau+1} \sum_{i_1+\cdots+i_k=\tau+1} \prod_{l=1}^k \|P_{i_l}\| \leq 2^{\tau}$$

This last result is a consequence of

$$||P_{l}|| = \sup_{\alpha'\alpha} |\langle \alpha | U^{l} \alpha' \rangle|^{2} \leq 1$$

and

$$|\{(x_1 \cdots x_k) \in \mathbb{N}^{+k}: x_1 + \cdots + x_k = n\}| = \binom{n-1}{k-1}$$
 (E.4)

where \mathbb{N}^+ is the set of nonzero positive integers.

The formula (E.4) is proved by iteration with respect to n and application of the combinatory algebra formula⁽⁶⁾

$$\sum_{j=k}^{n} \binom{j}{k} = \binom{n+1}{k+1}, \quad k = 0, 1, ..., n$$
 (E.5)

APPENDIX F. A LEMMA

Let \mathscr{H} be a Hilbert space and $\{e_i\}_{i\in\mathbb{N}}$ an orthonormal basis of \mathscr{H} . Any unitary operator U such that

$$|\langle e_i | U^2 e_j \rangle| = |\langle e_i | U e_j \rangle|^2 \quad \text{for any} \quad i, j \in \mathbb{N}$$
 (F.1)

is diagonal in the basis $\{e_i\}$.

Proof. With some obvious notations, let us rewrite (F.1) in the form:

$$|U_{ij}^2| = |U_{ij}|^2 (F.2)$$

The unitarity of operators U and U^2 gives, for all $j \in \mathbb{N}$,

$$\sum_{i} |U_{ij}^2| = 1 \quad \text{and} \quad \sum_{i} |U_{ij}^2|^2 = 1 \quad (F.3)$$

For all $j \in \mathbb{N}$, these two relations imply that there exists an integer $\alpha(j) \in \mathbb{N}$ such that

$$|U_{ij}^2| = \delta_{i,\alpha(j)} \tag{F.4}$$

and, consequently, there exists, for all *j*, a complex number λ_j of modulus one such that

$$U^2 e_j = \lambda_j e_{\alpha(j)} \tag{F.5}$$

Since the operator U^2 is a one-to-one mapping, α is a permutation of \mathbb{N} . Finally (F.1) leads to

$$|\langle e_i | U e_j \rangle| = \delta_{i,\alpha(j)} \tag{F.6}$$

and, consequently there exists, for all j, a complex number μ_j of modulus one such that

$$Ue_j = \mu_j e_{\alpha(j)} \tag{F.7}$$

From (F.5) and (F.7) it follows that

$$Ue_{\alpha(j)} = \lambda_j \overline{\mu}_j e_{\alpha(j)} \tag{F.8}$$

and the lemma is proved.

APPENDIX G. COMMENTS ON THE MATRICES $P(\alpha; \alpha'\alpha''; t)$

Let us denote by P_i , the matrix defined by (57) with \mathcal{T} (eigenvectors set of U_0) as the set of indices for the rows and columns, and by \tilde{P}_i the matrix

$$\widetilde{P}_{l}(\alpha; \alpha' \alpha'') = \langle \alpha | U^{l} \alpha \rangle \overline{\langle \alpha' | U^{l} \alpha'' \rangle}$$
(G.1)

where the rows and columns are respectively indexed by \mathcal{T} and \mathcal{T}^2 .

Then, (D.18) defines a matrix P(t) by

$$P(t) = \sum_{k=1}^{t+1} (-1)^{k+1} \sum_{i_1 + \dots + i_k = t+1} P_{i_1 \dots P_{i_{k-1}}} \tilde{P}_{i_k}$$
(G.2)

The power series F(z) with the P(t)'s as coefficients is determined by

$$zF(z) = [I + f(z)]^{-1}\tilde{f}(z)$$
 (G.3)

where f(z) is defined in (E.2) and

$$\tilde{f}(z) = \sum_{l=1}^{\infty} \tilde{P}_l z^l \tag{G.4}$$

The matrix P(t) is the coefficient of z^{t+1} in (G.3).

The relation (60) will be independent of the off-diagonal elements of the density operator at time zero if and only if this series equals zero.

This statement is equivalent to

$$\tilde{f}(z) = 0 \tag{G.5}$$

that is to say,

$$\tilde{P}_l = 0$$
 for $l = 1, 2, ...$

We can verify that this last relation is satisfied by some operators that do not commute with U_0 .

In fact, if $\langle \alpha | U^l \alpha \rangle = 0$ for all *l* and all α , the Hamilton-Cayley theorem shows that the determinant of *U* equals zero; consequently, there does not exist any unitary operator satisfying (G.5).

The unitary operators compatible with (G.5) are, therefore, such that there exist l_0 and α_0 such that $\langle \alpha_0 | U^{l_0} \alpha_0 \rangle \neq 0$; in that case U^{l_0} is diagonal with respect to the basis of the eigenvectors of U_0 and $|\langle \alpha | U^{l_0} \alpha \rangle| = 1$ for all α .

The operators commuting with U_0 fulfill this condition, but there are also some others.

APPENDIX H. TWO THEOREMS

Theorem 1. Let (a_k) be a bounded sequence of complex numbers such that

$$\lim_{N\to\infty}\frac{1}{N}\sum_{k=1}^N a_k$$

exists and equals \bar{a} ; then

$$\lim_{N\to\infty}\frac{1}{N}\sum_{k=1}^N a_k e^{2i\pi kx/N}$$

exists for all real x, and equals $\bar{a}e^{i\pi x}(\sin \pi x)/\pi x$ (\bar{a} for x = 0).

For x = 0 the theorem is trivial. When $x \neq 0$ it is sufficient to show that

$$\lim_{N \to \infty} \frac{1}{N} \sum_{k=1}^{N} (a_k - \bar{a}) e^{2i\pi k x/N} = 0$$
(H.1)

since

$$\lim_{N \to \infty} \frac{1}{N} \sum_{k=1}^{N} e^{2i\pi k x/N} = e^{i\pi x} \frac{\sin \pi x}{\pi x}$$
(H.2)

Therefore the theorem will be proved at the same time as the following lemma.

Lemma. Let (b_k) be a bounded sequence of complex numbers such that

$$\lim_{N\to\infty}\frac{1}{N}\sum_{k=1}^N b_k = 0$$

Then, for all real x

$$\lim_{N\to\infty}\frac{1}{N}\sum_{k=1}^N b_k e^{2i\pi kx/N} = 0$$

Proof. We may clearly suppose that $|b_k| \leq 1$. By defining

$$S_k = (1/k) \sum_{l=1}^{k} b_l$$
 (H.3)

we have $|S_k| \leq 1$ and $\lim_{k \to \infty} S_k = 0$ (by hypothesis).

Jean Tavernier

Now, let us put

$$\sigma_N(x) = \frac{1}{N} \sum_{k=1}^N b_k e^{2i\pi k x/N} = \frac{1}{N} \sum_{k=1}^{N-1} k S_k e^{2i\pi k x/N} (1 - e^{2i\pi x/N}) + S_N e^{2i\pi x}$$

Taking the absolute value, we obtain

$$|\sigma_N(x)| \leq |S_N| + \frac{2\pi}{N^2} |x| \sum_{k=1}^{N-1} k|S_k|$$

which gives

$$|\sigma_N(x)| \leq |S_N| + 2\pi \frac{|x|}{N} \sum_{k=1}^N |S_k|$$

With the sequence (S_k) converging to zero, the preceding bound shows that the function sequence (σ_N) converges to zero, uniformly onto any compact set.

Theorem 2. Let (a_k) be a bounded sequence of complex numbers, x a positive real number, and (x_k) an increasing (strictly) sequence of real numbers, equally distributed onto the interval [0, x].

If

$$\lim_{N\to\infty}\frac{1}{N}\sum_{k=1}^N a_k$$

exists and equals \bar{a} , then

$$\lim_{N\to\infty}\frac{1}{N}\sum_{k=1}^N a_k e^{2i\pi x_k}$$

exists and equals $\bar{a}e^{i\pi x}(\sin \pi x)/\pi x$.

Let us recall that⁽⁷⁾ a sequence (x_k) is equally distributed onto the interval [0, x] if, and only if, for any Riemann-integrable function f, the following relation is satisfied:

$$\lim_{N \to \infty} \frac{1}{N} \sum_{k=1}^{N} f(x_k) = \int_0^x f(y) \frac{dy}{x}$$
(H.4)

In particular, we have

$$\lim_{N\to\infty}\frac{1}{N}\sum_{k=1}^{N}e^{2i\pi x_k}=e^{i\pi x}\frac{\sin\pi x}{\pi x}$$

To prove the theorem, it is sufficient to show that the following lemma is true.

Lemma. Let (b_k) be a bounded sequence of complex numbers such that

$$\lim_{N\to\infty}\frac{1}{N}\sum_{k=1}^N b_k = 0$$

Then we have

$$\lim_{N\to\infty}\frac{1}{N}\sum_{k=1}^N b_k e^{2i\pi x_k} = 0$$

where (x_k) stands for the equally distributed sequence introduced in the theorem.

Proof. We take $|b_k| \leq 1$. Introduce the sequence S_k defined by (H.3) and put

$$\sigma_N = \frac{1}{N} \sum_{k=1}^N b_k e^{2i\pi x_k}$$

which can be written

$$\sigma_N = S_N e^{2i\pi x_N} + \frac{1}{N} \sum_{k=1}^{N-1} k S_k (e^{2i\pi x_k} - e^{2i\pi x_{k+1}})$$

The modulus of σ_N is bounded by

$$|\sigma_N| \leq |S_N| + \frac{2\pi}{N} \sum_{k=1}^{N-1} k |S_k| (x_{k+1} - x_k)$$

But, for all $\epsilon > 0$, there exists an integer N_0 such that $|S_k| \leq \epsilon$ for all $k \geq N_0$. Consequently, for any $N \geq N_0$, we have the following bound:

$$|\sigma_N| \leq \epsilon + \frac{\pi x}{N} N_0(N_0 + 1) + \frac{2\pi \epsilon}{N} \sum_{k=1}^{N-1} k(x_{k+1} - x_k)$$

Moreover, it is clear that

$$\frac{1}{N}\sum_{k=1}^{N}k(x_{k+1}-x_{k})=x_{N}-\frac{1}{N}\sum_{k=1}^{N}x_{k}\leqslant x-\frac{1}{N}\sum_{k=1}^{N}x_{k}$$

and, from the basic property (H.4) of the equally distributed sequences

$$\limsup_{N\to\infty}\frac{1}{N}\sum_{k=1}^N k(x_{k+1}-x_k) \leqslant \frac{x}{2}$$

Thus, N can be chosen large enough to ensure that $|\sigma_N|$ will be as small as we wish; this completes the proof.

Remark. Theorem 2 remains valid if the sequence (x_k) is replaced by a family of sequences, indexed by N, strictly increasing, contained in [0, x], and asymptotically equally distributed over [0, x] when N goes to infinity.

More precisely, if $(x_k(N))_{k=1\cdots N}$ is such a family of sequences, for all α and β such that $0 \leq \alpha < \beta \leq x$ we have

$$\lim_{N \to \infty} \frac{\nu_{\alpha\beta}(N)}{N} = \frac{\beta - \alpha}{x}$$

where

$$\nu_{\alpha\beta}(N) = |\{k: 1 \leq k \leq N, x_k(N) \in [\alpha, \beta]\}|$$

REFERENCES

- 1. M. Kac, Bull. Roy. Soc. Belgium 42:356 (1956).
- 2. M. Dresden, in *Studies in Statistical Mechanics I*, de Boer and Uhlenbeck, eds., p. 303 (1962).
- 3. M. Dresden and F. Feiock, J. Stat. Phys. 4:111 (1972).
- 4. M. Coopersmith and G. Mandeville, J. Stat. Phys. 10:391, 405 (1974).
- 5. V. Arnold and A. Avez, Problèmes ergodiques de la mécanique classique, Gauthier-Villars (1967).
- 6. L. Comtet, Analyse combinatoire, Presses Universitaires de France (1970).
- 7. J. Bass, Cours de Mathématiques, Tome III, Masson et Cie (1971).