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Models in Nonequilibrium Quantum Statistical Mechanics

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In this paper, quantum versions of statistical models are constructed. All aspects of the systems can be explicitly solved. It is possible to give magnetic realizations of these models. The most interesting conclusions are: (1) the state for time going to infinity is approached in an oscillatory manner in the quantum case; (2) in both classical and quantum cases, the exact description gives limiting states which remember the initial specifications; and (3) in these models, the time evolution generally cannot be described, even approximately, by a master equation.

KEY WORDS: Master equation; Liouville equation; reversibility and irreversibility; quantum statistical mechanics; relationship between master and Liouville equations; quantum and classical models; persistent initial conditions; persistent states.

1. BACKGROUND AND MOTIVATION

A few years ago, a study was published⁽¹⁾ in which several models devised by Kac⁽²⁾ were investigated. The purpose of this study was to clarify and discuss some old and fundamental questions in nonequilibrium *classical* statistical mechanics, using the Kac models as examples. The precise point at issue was the relation between the Liouville equation and the master equation. In the Liouville-type description, the system is described by a phase-

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space density function $\rho(\mathbf{p}_1\mathbf{q}_1,..., \mathbf{p}_N\mathbf{q}_N, t)$ which satisfies the Liouville equation. Macroscopic quantities of physical interest are obtained by some appropriate averaging. The time evolution is treated according to the precise dynamics without invoking any probability or statistical notions.

The master equation method describes the system by the master probability function $W(\mathbf{p}_1\mathbf{q}_1,..., \mathbf{p}_N\mathbf{q}_N, t)$. The time evolution of the master function is given in terms of a basic transition probability. This transition probability *simulates* the exact dynamics of the system. Thus the time evolution in the master equation approach *does* contain stochastic elements, in contrast to the Liouville method. The general relation between the Liouville equation and the master equation has been extensively discussed.(3-6) The special feature of the models discussed(1) previously is that *both* the master equation and the Liouville equation could be solved *exactly*, so that a direct comparison between the two treatments could be made. The somewhat surprising result obtained was that these two methods in general do *not* give the same results. To be sure, for special initial states, for limited time intervals, or for descriptions of limited accuracy, the results do coincide, but this is not the general situation. These models therefore demonstrate explicitly that there exist models (and presumably physical situations) whose time evolution can *not* be described by the usual, convenient master equation, but instead must be described by the Liouville formalism. Although this result is not altogether unexpected, there are very few explicit examples illustrating this behavior.

In this paper, a similar discussion of a quantum mechanical modification of these models will be presented. Since it is not at all obvious that the results obtained from a study of such contrived models (either classical or quantum mechanical) are particularly pertinent to or relevant for the description of realistic physical systems, it may be of interest to enumerate some of the reasons for undertaking such an investigation.

(a) It was already noted that the Kac models are some of the very few systems for which both the Liouville and master equations can be exactly and explicitly solved. There does not appear to be any quantum mechanical system allowing a similar detailed treatment.[3] The models constructed here are desigened to provide examples of such systems. Thus it is possible to test whether the introduction of quantum notions alters the relationship between the master equation and the Liouville equation, or whether that classical relationship is effectively unchanged. The relation *is* altered.

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[3] It should be noted that there are a number of interesting exactly soluble quantum statistical models (compare Lieb(7) and Yang(8)); but all these models deal with equilibrium phenomena, while the present study is concerned with-nonequilibrium properties. In a recent study,(9) the Liouville equation for the XY model was exactly solved, but no comparison with the master equation was undertaken.

(b) There are many investigations[4,10–13] which study the circumstances under which the quantum mechanical master equation (usually called the Pauli equation) can be obtained from the quantum mechanical Liouville equation (which is just the equation of motion of the density matrix). In this reduction, many approximations have to be made. Having exactly soluble models available allows a concrete discussion of the validity of these procedures. Thus in these models, it is possible to assess the error made when the exact description is replaced by a quantum mechanical master or Pauli equation. In addition, having explicit expressions for the exact solutions of both the Liouville and master equations enables one to study the relationships between the *solutions* as well as those between the equations. This, of course, is impossible in more realistic circumstances, where only approximate solutions of both equations are known.

(c) It is, of course, well known that the use of probability in classical physics is quite distinct from its use in quantum mechanics. In particular, a classical system in which interactions take place with a prescribed probability is intrinsically different from a quantum system. The models constructed in this paper demonstrate this difference in an almost dramatic manner. As such, they provide instructive and transparent examples of the different roles probability notions play in classical and quantum situations.

(d) The classical Kac models describe highly artificial and contrived physical situations. They deal with objects (called either balls or particles) which are capable of just two states, or two colors. The only dynamical element introduced is the possibility of a change of color at well-defined, fixed locations. The underlying physical picture suggesting this model is a beam of particles all moving in the same direction with the same speed, which can scatter elastically from a number of fixed obstacles. The obstacles are so arranged that the particles either continue or reverse their velocities. The two colors of the objects in the model correspond obviously to the two directions of the particle velocity. In a more realistic picture, the scattering (still elastic) could produce velocities in any direction (still with the same magnitude), which in the model language would correspond to balls capable of a continuum of colors. Thus the restriction to just two colors is oversimplified and artificial. However, in a quantum mechanical context, it is not at all unusual to deal with observables which are capable of just *two* quantum states. A system of particles of spin $\frac{1}{2}$ (or isotopic spin $\frac{1}{2}$) is an obvious example. In fact, any system composed of objects that are capable of two quantum states, provided with a suitable mechanism which can produce transitions between these quantum states at definite locations, is a perfectly good example of a quantum Kac model. The fact that all the physically interesting realizations of the Kac models involve quantum mechanics in an essential manner was one of the main reasons for investigating possible quantum modifications of these models. It is interesting that even though the original motivation for these models came from classical physics, the quantum mechanical extensions actually describe more realistic physical situations.

(e) Another, rather different reason for a restudy of the Kac models (and possible extensions) is the somewhat unsettled status of nonequilibrium statistical mechanics. It has been repeatedly emphasized(14) that the calculation of experimentally observable entities (such as transport coefficients) from the basic equations (such as the Liouville equation) is far from straightforward. It is now known through the work of Cohen and Dorfman(15) Kawasaki and Oppenheim,(16) Sengers,(17) and Ernst,(18) among others, that there occur divergences in the density expansion of the transport coefficients. These divergences and the related nonanalytic density dependence follow via a lengthy but well-defined procedure from the Liouville equation. The same results are obtained if the Kubo formula is used(15,17) for the calculation of the transport coefficients. Because of the unexpected and unintuitive character of these results, it would be extremely interesting if one could construct models which would elucidate some features of this surprising behavior. Unfortunately, the Kac models do not possess sufficient dynamic and geometric complexity to exhibit the divergence phenomenon. In fact, the models discussed previously were even too simple to define entities which could be considered as analogs of the transport parameters. In the process of constructing quantum models, it will be necessary to first construct classical models which possesses more structure than the previous ones. For these models, one *can* obtain a nontrivial response to an outside field. Thus in this case, an appropriate modification of the Kubo formula can be constructed. One has the possibility of obtaining transport-like parameters and it is possible to study density-like expansions. Even for these very simple models, the actual analysis is already involved; one of the main conclusions is that rather trivial and reasonable appearing assumptions about the initial state, and especially about the asymptotic time behavior, have an enormous effect on the existence and character of the expansions of the transport parameters. Interesting as this is, these aspects of the models are merely suggestive at this point; the main purpose of this paper is to study, using the models, the equivalence and relevance (or nonequivalence and lack of relevance) of the methods used in nonequilibrium quantum statistical mechanics. In a later study, the significance of models for the divergence problems will be treated in detail.

The paper is divided into seven sections. Section 2 contains a brief recapitulation of the notations and results of the classical discussion.(1) The succeeding section contains a modification of the classical models which consists in the introduction of a *classical stochastic* element in the dynamics.

This modification is useful both as a preliminary to the quantum extension and as a means to introduce an additional parameter in the problem. It is this new parameter which later allows the construction of transport quantities. The appropriate modifications of the model rules, which would yield a genuine quantum system are developed in a heuristic fashion in section 4. The main point is the recognition that in terms of the highly schematized dynamics of the model, the only remaining quantum mechanical feature is the superposition principle. Section 4 also contains the calculation of the one-particle (quantum) distribution function. The general formalism is set up in Section 5. The Liouville and master equations are obtained; contracted distribution functions and reduced density matrices are defined. It is possible —in principle, in any case—to obtain exact expression for *all* the reduced matrices. An explicit expression will be derived for the two-particle density matrix. Section 6 contains a discussion for the results obtained in particular comparisons of the answers obtained by the different methods. The main qualitative result is that the differences between the master equation and the Liouville equation are *more* pronounced in the quantum discussion than in the classical model. Using these exact results, it is also possible to investigate which of the assumption needed$^{(14)}$ in the general reduction of the Liouville equation to the master equation are applicable in this case.

It is demonstrated in Section 7 that a more or less realistic physical model provides an interesting realization of this quantum model. A polarized beam of particles with spin $\frac{1}{2}$ which are scattered by random ferromagnetic impurities (so they can flip the spin) located in a plane perpendicular to the plane of polarization is an example of a physical system which is exactly described by the model rules. Actually, the precise system consists of a number of independent beams all polarized in the same way. The "magnetic" example also allows the introduction of "outside" magnetic fields in a natural way. Thus the stage is set for a study of the "response" of this magnetic system to arbitrary outside fields, and with it, the calculation of the magnetic transport parameters. The dependence of these parameters on the density can now be investigated.

The final section contains a number of disconnected comments and remarks. Applications of the general formalism to other physical systems, such as the $K\overline{K}$ meson system, are briefly indicated. The possibility and utility of the extension of the formalism to systems capable of more than two quantum states are discussed. Further generalizations and especially the possibility of using these models to investigate density and other (μ) expansions are noted. Finally, there is a summary of the main results and a collection and assessment of the unsolved and partially solved problems.

2. CLASSICAL MODELS; BACKGROUND AND COMMENTS

The primitive dynamics embodied in the simple systems studied here can most conveniently be expressed in the language of a model. Consider a set of n equidistant points on a circle. A set of n objects (balls, for example) is placed on the n points. These balls can have *two* colors, black or white. A set of m fixed points ($m \ll n$) on the circle are marked. The fraction of the marked points is $\mu = m/n \ll 1$. During each elementary time interval, all the balls move *one* step counterclockwise with the rule that when a ball *leaves* a marker, it will change its color. If the initial color distribution and something about the marker distribution are given, the problem is the description of the time evolution of the color scheme. This is the classical problem discussed by Dresden.(1) Actually, the problem treated there in greatest detail was a slight modification of the situation described here; instead of one Kac ring.[4] an *ensemble* of such rings was considered. Each ring contains a well-defined set (both in number and location) of markers. The *ensemble* average of the number of markers at a given place over the ensemble of rings is μ. If the initial color scheme of the ensemble is given, the problem is again the description of the various aspects of the time evolution of the color scheme.

This general type of problem can be discussed on a variety of levels, which may be described as the Newton, Liouville, master, and Boltzmann level, respectively.[5]

2.1. The "Newtonian" Level

On this level, one deals with well-defined mechanical equations, their analysis, and consequences, No statistics or probability is used anywhere.

The following notation is used:

$$\epsilon_p = \begin{cases} +1 & \text{if the point } p \text{ is unmarked } (p = 1,\ldots, n) \\ -1 & \text{if the point } p \text{ is marked} \end{cases} \tag{1}$$

$$\eta_p(t) = \begin{cases} +1 & \text{if the ball at } p \text{ at time } t \text{ is white} \\ -1 & \text{if the ball at } p \text{ at time } t \text{ is black} \end{cases} \tag{2}$$

The variables $\eta_p(t)$ change in time; they are the dynamical variables of the system; the set of $\{\epsilon_p\}$ characterizes the location and number of interactions, and it, in a certain sense, represents the Hamiltonian of the system [of

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[4] The model described here is often referred to as "Kac ring," after its originator.

[5] This is a convenient and suggestive nomenclature which will be used throughout this paper.

Eqs. (21) and (23)]. The model rules may be summarized as an equation of motion for a single object,

$$\eta_{p+1}(t+1) = \epsilon_p \eta_p(t) \tag{3}$$

Equation (3) ("Newton's equation of motion") yields the expression for any $\eta_p(t)$ for all p and t in terms of the initial state as

$$\eta_p(t) = \epsilon_{p-1}\epsilon_{p-2} \cdots \epsilon_{p-t}\eta_{p-t}(0) \tag{4}$$

From Eq. (4), all quantities referring to a single ring can be calculated; for example, the number of white balls at any time is

$$N_W(t) = \tfrac{1}{2}n + \tfrac{1}{2}\sum_{p=1}^{n} \eta_p(t) \tag{5}$$

with $\eta_p(t)$ determined by Eq. (4).

It is clear from these formulas that all results depend explicitly on the set $\{\epsilon\}$, as could be anticipated from Eq. (3). Thus these formulas [Eq. (4) in particular] provide the solution to the *mechanical* problem: no statistical or probability notions or averaging processes are needed or used. If, however, the set of $\{\epsilon\}$ is not or only partially given, or if the initial state itself is only given in a probability sense, statistical methods are needed to obtain results of physical interest. This is accomplished by representing the actual system by an appropriate ensemble, and this leads to the Liouville level.

2.2. The Liouville Level of Description

The *state* of a single Kac ring at a given time is completely specified by the set of n numbers

$$\boldsymbol{\eta}(t) = \begin{pmatrix} \eta_1(t) \\ \eta_2(t) \\ \vdots \\ \eta_n(t) \end{pmatrix} \tag{6}$$

The $\eta_i(t)$ values are either $+1$ or -1. The phase space Γ of this dynamical system is thus the space of 2^n sequences, each sequence consisting of $(+1)$ and (-1), n in all. Consider now an ensemble of Kac rings; then the state of the ensemble is described by a density function $\rho(\eta_1 \cdots \eta_n, t)$; ρ is a nonnegative function defined on the space of sequences Γ; ρ is normalized to unity:

$$\sum_{\eta_1} \cdots \sum_{\eta_n} \rho(\eta_1 \cdots \eta_n, t) = 1 \tag{7}$$

Each member of the ensemble is a Kac ring with a definite number and a definite location of the markers; however, both may vary from ring to ring.

The ensemble is specified by the requirement that the probability that there is a marker at a given point j shall be μ, which is independent of j and n. This expresses in a more precise manner that for an individual ring, the fraction of the marked points is μ. In terms of the ϵ variables, the specification of the ensemble is

$$\text{Prob}(\epsilon_j = -1) = \mu \tag{8a}$$

$$\text{Prob}(\epsilon_j = +1) = 1 - \mu \tag{8b}$$

Equations (8a) and (8b) can be combined as

$$\text{Prob}(\epsilon) = \tfrac{1}{2} + \tfrac{1}{2}(1 - 2\mu)\,\epsilon \tag{8c}$$

From Eqs. (8a–c), it follows immediately that

$$\text{Prob}(\epsilon_j \epsilon_k) = (\text{Prob}\ \epsilon_j)(\text{Prob}\ \epsilon_k) \tag{8d}$$

The ensemble average (or ϵ average) of a quantity Q which depends on the ϵ variables is defined as

$$\langle Q\rangle_\epsilon = \sum_{\epsilon_1} \cdots \sum_{\epsilon_n} \text{Prob}(\epsilon_1 \cdots \epsilon_n)\, Q(\epsilon_1 \cdots \epsilon_n) \tag{8e}$$

This represents the result of averaging a physical quantity Q over all marker positions. The set of markers itself is specified by the formulas (8a) and (8b). The average of ϵ is given by Eq. (8e) as

$$\langle \epsilon \rangle = \sum_{\epsilon} \epsilon\, \text{Prob}(\epsilon) = 1 - 2\mu \tag{8f}$$

The average of products is obtained by combining Eqs. (8f) and (8d).

$$\langle \epsilon_1\,, \epsilon_2\,, \ldots, \epsilon_s\rangle_\epsilon = (1 - 2\mu)^s \tag{8g}$$

The motion of the balls on a given ring is still described by Eq. (3); this yields for the time evolution of the ensemble density function

$$\rho(\eta_1\,, \ldots, \eta_n\,, t + 1) = \rho(\epsilon_1\eta_2\,, \epsilon_2\eta_3\,, \ldots, \epsilon_n\eta_1\,, t) \tag{9}$$

Equation (9) is the Liouville equation for the model. As in ordinary statistical mechanics, it is useful to introduce *contracted* distribution functions defined by[6]

$$f^j(\alpha, t) = \sum_{\eta_1} \cdots \sum_{\eta_n} \rho(\eta_1 \ldots \eta_j = \alpha, \ldots, \eta_n\,, t) \tag{10a}$$

$$f^{jk}(\alpha, \beta, t) = \sum_{\eta_1} \cdots \sum_{\eta_n} \rho(\ldots \eta_j = \alpha, \ldots, \eta_k = \beta, \ldots, t) \tag{10b}$$

$$\vdots$$

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[6] Strictly speaking, one should write $f_1^j(\alpha, t)$, $f_2^{jk}(\alpha, \beta, t)$, indicating the one-, two-,..., particle character of these functions. The notation used should hopefully be clear enough.

Note that $f^j(\alpha, t)$ and $f^{jk}(\alpha, \beta, t)$ are normalized by Eq. (7).

$$\sum_{\alpha} f^j(\alpha, t) = 1, \qquad \sum_{\alpha,\beta} f^{jk}(\alpha, \beta, t) = 1 \tag{10c}$$

[In (10a), one does *not* sum over η_j ; it has a specified value α; in (10b), one does not sum over η_j and η_k , etc.]

These contracted distribution functions satisfy equations[7] which can be obtained by combining (9) and (10):

$$f^j(\alpha, t) = f^{j-1}(\epsilon_{j-1}\alpha, t-1) \tag{11a}$$

$$f^{jk}(\alpha, \beta, t) = f^{j-1,k-1}(\epsilon_{j-1}\alpha, \epsilon_{k-1}\beta, t-1) \tag{11b}$$

Equations (9) and (11) show explicitly that the time evolution of the system is determined by the set $\{\epsilon\}$; *no* stochastic elements are involved in the dynamical description of the system. This can also be seen from the solutions of Eqs. (9) and (11). Suppose that $\rho(\eta, 0)$, the initial density function, is given in terms of a set of coefficients b as

$$\rho(\eta, 0) \equiv g(\eta) = (1/2^n) + \sum_k b_k\eta_k + \sum_{k<l} b_{kl}\eta_k\eta_l + \cdots \tag{12}$$

Then the solution becomes

$$\begin{aligned}\rho(\eta, t) = (1/2^n) &+ \sum_k b_k\epsilon_k\epsilon_{k+1} \cdots \epsilon_{k+t-1}\eta_{k+t} \\ &+ \sum_{k<l} b_{kl}\epsilon_k \cdots \epsilon_{k+t-1}\epsilon_l \cdots \epsilon_{l+t-1}\eta_{k+t}\eta_{l+t} + \cdots\end{aligned} \tag{13}$$

$$f^j(\alpha, t) = \tfrac{1}{2} + 2^{n-1}\alpha b_{j-t}\epsilon_{j-t} \cdots \epsilon_{j-1} \tag{14}$$

$$\begin{aligned}f^{jk}(\alpha, \beta, t) = \tfrac{1}{4} + 2^{n-2}(&b_{j-t}\epsilon_{j-t} \cdots \epsilon_{j-1}\alpha + b_{k-t}\epsilon_{k-t} \cdots \beta \\ &+ b_{j-t,k-t}\alpha\beta\epsilon_{j-1} \cdots \epsilon_{j-t}\epsilon_{k-1} \cdots \epsilon_{k-t})\end{aligned} \tag{15}$$

These formulas exhibit the dependence of the various distribution functions on the initial configuration (the b's) and the dynamics (the ϵ's). If these are given, there just remains the analysis of the expressions (13)–(15). In many actual situations, however, the ϵ's (or the b's) are *not* known as such, but instead, a probability distribution of these variables is given. For example, the probability distribution (8) of the ϵ variables corresponds to the physical situation where markers are distributed over a Kac ring with *all* marker configurations equally likely, so that the average number of markers is μn.

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[7] The functions ρ, f^j, f^{jk}, etc. will be referred to as the "Liouville hierarchy."

To obtain physical results for that case, one must average the expressions for $\rho, f^j, f^{jk}, \ldots$ over all marker configurations. Defining as before

$$\langle Q\rangle_\epsilon = \sum_{\epsilon_1} \cdots \sum_{\epsilon_n} \operatorname{Prob}(\epsilon_1 \cdots \epsilon_n)\, Q(\epsilon_1 \cdots \epsilon_n) \tag{16}$$

one finds[8]

$$\begin{aligned}\langle\rho(\boldsymbol{\eta}, t)\rangle_\epsilon = {} & (1/2^n) + \sum_k b_k(1-2\mu)^t\, \eta_{k+t} \\ & \sum_{k<l} b_{kl}(1-2\mu)^{\Delta(l,k,t)}\, \eta_{k+t}\eta_{l+t} + \cdots\end{aligned} \tag{17}$$

$$\langle f^j(\alpha, t)\rangle_\epsilon = \tfrac{1}{2} + 2^{n-1}\, b_{j-t}\alpha(1-2\mu)^t \tag{18}$$

$$\begin{aligned}\langle f^{jk}(\alpha, \beta, t)\rangle_\epsilon = {} & \tfrac{1}{4} + 2^{n-2}[(1-2\mu)^t\,(\alpha b_{j-t} + \beta b_{k-t}) \\ & + (1-2\mu)^{\Delta(j,k,t)}\, b_{j-t,k-t}\alpha\beta]\end{aligned} \tag{19}$$

$$\Delta(j, k, t) = \begin{cases} 2t, & j-k \geqslant t \\ 2(j-k), & j-k < t \end{cases} \tag{20}$$

These results no longer depend on the ϵ variables; they represent *averages* over all the marker configurations of the exact dynamics of the system. It is through the ϵ-averaging process that nonmechanical or stochastic elements enter the description. For many physical situations, (for example, in impurity scattering, where the location of the impurites is not known) such averaged quantities are just the ones needed for the physical description.

To emphasize further the mechanical nature of the Liouville equation, it is instructive to introduce the Hamiltonian matrix H which governs the dynamics. Define the matrix H by

$$H = \begin{pmatrix} & \epsilon_1 & & & \\ & & \epsilon_2 & & \\ & & & \ddots & \\ & & & & \epsilon_{n-1} \\ \epsilon_n & & & & \end{pmatrix} \tag{21}$$

It is easy to check that H has the property

$$H\begin{pmatrix}\eta_1 \\ \vdots \\ \eta_n\end{pmatrix} = \begin{pmatrix}\epsilon_1\eta_2 \\ \epsilon_2\eta_3 \\ \vdots \\ \epsilon_n\eta_1\end{pmatrix}, H^t\begin{pmatrix}\eta_1 \\ \vdots \\ \eta_n\end{pmatrix} = \begin{pmatrix}\epsilon_1\epsilon_2 \cdots \epsilon_t\eta_{t+1} \\ \epsilon_2\epsilon_3 \cdots \epsilon_{t+1}\eta_{t+2} \\ \vdots \\ \epsilon_n\epsilon_1 \cdots \epsilon_{n-1}\eta_t\end{pmatrix} \tag{22}$$

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[8] See especially Dresden[(1)] for more details.

Thus H, acting on a state η, yields, by Eqs. (22) and (9), the state from which that state came an elementary time earlier. As written, H propagates the system *back* in time. The (anti) time-evolution operator H depends exclusively on the ϵ variables, it is independent of the time and the initial conditions. Both these features are typical of mechanical time-evolution operators. In terms of H, the solution of the Liouville equation can be written in the compact form

$$\rho(\eta, t) = \rho((H^t\eta), 0) \tag{23}$$

This gives the form (13) immediately.

H has the further properties that

$$HH^T = H^T H = 1 \tag{24a}$$

$$H^{2n} = 1 \tag{24b}$$

Here, H^T is the transpose of H; since the ϵ's are real, (24a) expresses the unitarity of H. Equation (24b) expresses the essential periodicity of the system, which can be observed directly from (22) and the fact that

$$\epsilon_1\epsilon_2 \cdots \epsilon_t\epsilon_{t+1} \cdots \epsilon_{t+2n} = \epsilon_1 \cdots \epsilon_t .$$

Since H is unitary, its eigenvalues have absolute value 1: from (24b), it follows further that the eigenvalues of H are $e^{\pi ij/n}$, $j = 0, \ldots, n - 1$. Since H is unitary, it can be diagonalized by a unitary matrix U so that

$$UHU^{-1} = D \tag{25}$$

with D diagonal, with diagonal elements $(e^{\pi ij/n})$. U depends only on $\{\epsilon\}$ and n. It follows from (25) that the matrix H^t which occurs in the Liouville equation satisfies

$$H^t = U^{-1}D^tU \tag{26a}$$

Consequently, acting on a state, it yields

$$(H^t\eta) = \begin{pmatrix} \sum\limits_j \gamma_{1j}e^{\pi ijt/n} \\ \vdots \\ \sum \gamma_{nj}e^{\pi ijt/n} \end{pmatrix} \tag{26b}$$

Here, the γ_{kj} depend on the initial condition and the set $\{\epsilon\}$, but *not* on the time. The complete time dependence of $(H^t\eta)$ is explicitly exhibited in (26b). The time dependence of ρ of proceeds via an analysis of (23), while the time dependence of $\langle\rho\rangle_\epsilon$ requires the ensemble average.

2.3. The Master Level

Since the quantities of physical interest are usually ensemble averages, there is a considerable interest in setting up time-evolution equations which incorporate the probability aspects of the problem directly in the dynamics. The hope is that such equations will be simpler to solve and yet provide a reasonably accurate (if not exact) description of the averaged quantities of physical interest, thus avoiding the necessity of solving the exact equations and averaging their solutions. Such kinetic or master equations play a significant role in all of statistical mechanics; the Boltzmann equation is perhaps the best-known example.

In this model, the master equation requires the construction of a transition probability $P(\boldsymbol{\delta} \mid \boldsymbol{\eta})$, which gives the probability that, given that the system is in state $\boldsymbol{\delta}$, it will be in state $\boldsymbol{\eta}$ one elementary time interval later. With $\boldsymbol{\eta}$ and $\boldsymbol{\delta}$ fixed and given vectors, such a transition requires that $\eta_{j-1} = \epsilon_j\delta_j$ or $\epsilon_j = \delta_j\eta_{j-1}$. For a given ring, i.e., a given set of ϵ variables, this relation is either true or false. If, however, the $\{\epsilon\}$ are considered as random variables, the probability that $\epsilon_j = \delta_j\eta_{j+1}$ is given by [see Eq. (8c)]

$$\mathrm{Prob}(\epsilon_j = \delta_j\eta_{j+1}) = \tfrac{1}{2} + \tfrac{1}{2}(1 - 2\mu)\, \delta_j\eta_{j-1} \tag{27}$$

Therefore the transition probability $P(\boldsymbol{\delta} \mid \boldsymbol{\eta})$ is

$$P(\boldsymbol{\delta} \mid \boldsymbol{\eta}) = \prod_{j=1}^{n} \tfrac{1}{2}[1 + (1 - 2\mu)\, \delta_j\eta_{j-1}] \tag{28}$$

The master equation is defined by

$$\varphi(\boldsymbol{\eta}, t + 1) = \sum_{\boldsymbol{\delta}} P(\boldsymbol{\delta} \mid \boldsymbol{\eta})\, \varphi(\boldsymbol{\delta}, t) \tag{29}$$

It does not describe the time evolution of a single system, but it gives a stochastic representation of a time evolution in which the model rules ($\epsilon_j = \delta_j\eta_{j-1}$) are satisfied in some average sense. It is *this* feature which gives rise to the expectation that as long as one is interested in ensemble averages (such as an average over the markers), the master equation will give an adequate description. It is an important aspect of the present studies to investigate to what extent these expectations are valid.

Contracted distributions obtained from φ are defined as before

$$F^j(\alpha, t) = \sum_{\eta_1} \cdots \sum_{\eta_n} \varphi(\eta_1, \eta_j = \alpha, \dots, \eta_n, t) \tag{30a}$$

$$F^{jk}(\alpha, \beta, t) = \sum_{\eta_1} \cdots \sum_{\eta_n} \varphi(\eta_1, \dots, \eta_j = \alpha, \dots, \eta_k = \beta, \dots, \eta_n, t) \tag{30b}$$

Equations (29) and (30) yield equations for F, which are the counterpart of (11a),

$$F^j(\alpha, t) = \tfrac{1}{2} + \tfrac{1}{2}(1 - 2\mu)\, \alpha \sum_{\eta} \eta F^{j-1}(\eta, t - 1) \tag{31a}$$

$$\begin{aligned} F^{jk}(\alpha, \beta, t) = \tfrac{1}{4} + \tfrac{1}{4}(1 - 2\mu)\Big\{\alpha \sum_{\gamma} \gamma F^{j-1}(\gamma, t - 1) \\ + \beta \sum_{\gamma} \gamma F^{k-1}(\gamma, t - 1)\Big\} \\ + \tfrac{1}{4}(1 - 2\mu)^2\, \alpha\beta \sum_{\gamma\gamma'} \gamma\gamma' F^{j-1,k-1}(\gamma, \gamma', t - 1) \end{aligned} \tag{31b}$$

The Liouville hierarchy (9) and (10) could be rigorously solved with the initial condition $\rho(\boldsymbol{\eta}, 0) = g(\boldsymbol{\eta})$; the master equation hierarchy can also be exactly solved. Using the same initial condition $\varphi(\boldsymbol{\eta}, 0) = g(\boldsymbol{\eta})$ with g given by (12) yields

$$\varphi(\boldsymbol{\eta}, t) = 2^n + (1 - 2\mu)^t \sum_{k} b_k \eta_{k+t} + (1 - 2\mu)^{2t} \sum_{k,l} b_{kl} \eta_{k-t} \eta_{l-t} \tag{32a}$$

$$F^j(\alpha, t) = \tfrac{1}{2} + 2^{n-1} b_{j-t} \alpha (1 - 2\mu)^t \tag{32b}$$

$$\begin{aligned} F^{jk}(\alpha, \beta, t) = \tfrac{1}{4} + \tfrac{1}{4}(1 - 2\mu)^t\, 2^n (\alpha b_{j-t} + \beta b_{k-t}) \\ + \tfrac{1}{4}(1 - 2\mu)^{2t}\, b_{j-t,k-t}\, \alpha\beta 2^n \end{aligned} \tag{32c}$$

As was to be expected, the solutions of the master hierarchy do not depend on the ϵ variables. The parameter μ and the initial data $\{b\}$ determine the solutions uniquely.

It is again possible to give a matrix transcription of the master equation, analogous to the matrix transcription (23) of the Liouville equation. For this purpose, consider the set of values φ_p which $\varphi(\boldsymbol{\delta}, t)$ assumes when $\boldsymbol{\delta} = \delta_1, \delta_2, \ldots, \delta_n$ runs through its allowed values. Thus $\varphi_p(t)$ is one of 2^n components, p corresponding to a specific set of values of $\delta_1 \cdots \delta_n$. Then $P(\boldsymbol{\delta} \mid \boldsymbol{\eta})$ becomes a $2^n \times 2^n$ matrix and (29) can be written as

$$\varphi_p(t) = \sum_{q} \varphi_q(t - 1)\, P_{qp} \tag{33a}$$

or using an obvious matrix product notation,

$$\varphi_p(t) = (P^t)_{qp}\, \varphi_q(0) \tag{33b}$$

The matrix P is Hermitian. It is possible to find the eigenvalues and the matrix that diagonalizes P. This information combined with (33b) yields an alternate derivation of (32a).

The master hierarchy, in particular Eq. (31a) for F_1, can be given a direct kinetic interpretation. Using the fact that $F^j(\eta, t) + F^j(-\eta, t) = 1$ and $\eta^2 = 1$, Eq. (31a) can be put in the form

$$F^j(\alpha, t) = \mu + (1 - 2\mu)\, F^{j-1}(\alpha, t - 1) \tag{34}$$

This is the form which can immediately be understood as a gain–loss equation. The F^1 level of description in the master hierarchy will be called the Boltzmann level. On this level, the dynamics is described in probability terms; thus the probability for a color change at a point is the same as the probability of finding a marker at that point. This probability is μ, the fraction of the marked points. Hence one can write immdediately

$$F^j(\alpha, t) = (1 - \mu)\, F^{j-1}(\alpha, t - 1) + \mu(1 - F^{j-1}(\alpha, t - 1)) \tag{35}$$

Equation (35) states that the color state α at j at t can originate from a color state α at $j - 1$ at $t - 1$, if there is *no* marker at $j - 1$, *or* from a color state $-\alpha$ at $j - 1$ at $t - 1$ coupled with the presence of a marker at $j - 1$. This is just the usual kinetic argument for a gain–loss equation. It is clear that (35) is the same as (34).

A similar kinetic interpretation can be given for (31b).

2.4. Comparison

The formulas given allow a direct comparison of the results of the two methods. For example, (18) and (32b) show that

$$\langle f^j(\alpha, t)\rangle_\epsilon = F^j(\alpha, t) \tag{36a}$$

$$\langle f^{jk}(\alpha, \beta, t)\rangle_\epsilon \neq F^{jk}(\alpha, \beta, t) \tag{36b}$$

On the f^1 level, the time dependence of the ensemble average of the exact dynamics is the same as the time dependence produced by the average dynamics. However, this equality no longer holds rigorously for the more detailed descriptions of the system as given by f^2 and F^2, respectively. However, even on the f^2 level, there are time intervals and special initial configurations for which the two descriptions are approximately the same.[9] Thus one can state precisely that for this model, the ϵ or ensemble average of f^1 is exactly the same as the stochastic dynamics of the master equation for F^1; for higher distributions, the exact identity no longer holds, but there is a well-defined approximate relationship.

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[9] See Reference 1 for a more detailed comparison. The most important feature is that, because of the Δ occurring in $\langle f_1{}^2\rangle_\epsilon$ [compare Eqs. (19) and (20)], $\langle f^{jk}\rangle_\epsilon$ and F^{jk} remain unequal even if $t \to \infty$.

In this model (as in statistical mechanics generally), it is possible to define other averages which satisfy different equations. For example, the *local* color average at a point at time t is

$$\bar{\eta}_j(t) = \sum_{\eta} \eta f^{j}(\eta, t) \tag{37}$$

This quantity is analogous to the local velocity in kinetic theory:

$$\mathbf{u}(\mathbf{x}, t) = \int d^3v \, \mathbf{v} f(\mathbf{x}, \mathbf{v}, t)$$

It is easy to show from (37) and (11a) that $\bar{\eta}_j$ satisfies the *mechanical* equations of motion (3). Take the local average of (11a),

$$\bar{\eta}_j(t) = \sum_{\eta} \eta f^{j-1}(\epsilon_{j-1}\eta, t-1) = \epsilon_{j-1}\bar{\eta}_{j-1}(t-1) \tag{38a}$$

This is the Newton equation (3). Equation (38a) can be solved directly [or alternately, (37) can be used in conjunction with (14)] to give the solution

$$\bar{\eta}_j(t) = 2^n b_{j-t}\epsilon_{j-t} \cdots \epsilon_{j-1} \tag{38b}$$

It is interesting to note that the local average (37) still possesses the strict periodicity $\bar{\eta}_j(t+2n) = \bar{\eta}_j(t)$, as can be seen from (38b). This, of course, must be true since the local averages are described by the same equations as the original reversible dynamics. Only after taking the ensemble average (ϵ average) does the usual thermodynamic approach to equilibrium appear; from (38b) and (8g), there follows

$$\langle \bar{\eta}_j(t) \rangle_\epsilon = 2^n b_{j-t}(1-2\mu)^t \tag{39}$$

It is also possible to define color correlation functions using higher distribution functions: for example,

$$\overline{\alpha_j \beta_k}(t) = \sum_{\alpha} \sum_{\beta} \alpha\beta f^{jk}(\alpha, \beta, t) \tag{40a}$$

From the known solutions, these can be analyzed; it is easy to check that in general they do *not* factor:

$$\overline{\alpha_j \beta_k} \neq \bar{\alpha}_j \bar{\beta}_k \tag{40b}$$

Although it is not essential for the following, it is interesting to observe that it is also possible to define a *mechanical* time average

$$\langle \eta_j(t) \rangle_t \equiv (1/t) \sum_{\tau=0}^{t} \eta_j(\tau) \tag{41a}$$

It is easy to show [using Eq. (3)] that this time average satisfies

$$\langle \eta_{j+1} \rangle_{t+1} = [t/(t+1)]\, \epsilon_j \langle \eta_j \rangle_t + [1/(t+1)]\, \eta_{j+1}(0) \tag{41b}$$

This is not identical with the mechanical equation; if, however, $t \gg 1$ (but still $n \gg t$), one sees that the time average satisfies the mechanical equation approximately; hence in the limit that $n \to \infty$, $t \to \infty$ afterwards, the time average satisfies the equation

$$\langle \eta_{j+1} \rangle_{t+1} \sim \epsilon_j \langle \eta_j \rangle_t \tag{41c}$$

which is the *same* as the equation the color average satisfies. Hence in an approximate (well-defined!) sense, $\langle \eta_j \rangle_t = \bar{\eta}_j(t)$.

3. A CLASSICAL MODEL WITH EXPLICIT PROBABILITIES[10]

The model described in Section 2 was a strictly mechanical, deterministic model; probability elements were introduced only as a convenient means to describe the model. It is possible, and for the later discussion of quantum models necessary, to study classical models which explicitly contain probability notions. In the context of the models discussed in Section 2, the model rules are changed to the effect that if a ball leaves a marker (j), it will change color with *probability* λ_j. If a ball leaves an unmarked place, it will *certainly not* change color. (It will remain unchanged with probability one.) Thus the model now has a mixed character; it possesses a well-defined mechanics, described by the set $\{\epsilon\}$, and it contains stochastic elements through the stipulation that the change in the dynamical variables is described in a probability sense only. There are now two levels of description possible: the Liouville level, in which the $\{\epsilon\}$ variables are rigorously described, with the outcome of a color change described by the probabilities λ_j, and the master level, which treats both the collision process and the marker configurations on a probability basis. Since the underlying dynamics is only specified in a probability sense, no Newtonian level description is possible. The main result of this section is that even in this model, the $\{\epsilon\}$-averaged Liouville hierarchy is *not* identical with the master function, although there is less difference than in the previous case. Specifically, the two solutions do approach each other for long times.

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[10] Anyone interested solely in the quantum models could in principle skip this section. However, its content is essential for the comparisons to be carried out in Sections 6 and 7, and is probably generally instructive. In this section, locations are denoted by $p = 1, \ldots, n$, (as before), but also by j, k (Latin letters), and color variables are η or α, β (Greek letters).

A separate reason for studying this model is that through the introduction of the position-dependent (j-dependent) probabilities λ_j, the possibility of a stochastic model for a spatially inhomogeneous Boltzmann equation is opened up.. There are at the present time no stochastic models known which reproduce a Boltzmann-type equation with outside forces and streaming terms. Writing $\lambda_j = \lambda_0 + \rho v_j$, where λ_0 is independent of j, ρ is a small paremeter, and v_j depends on j, it can be shown that the introduction of an outside field (represented by ρ) can produce a spatial inhomogeneity in the system. In this manner, one may hope to simulate the effect of external fields.

3.1. The Liouville Level[11] ($f^{(1)}$)

The system will be described by the probability functions $f^j(\alpha, t)$. $f^{jk}(\alpha, \beta, t)$; no higher distribution functions need be considered here. The normalizations are

$$\sum_{\alpha} f^j(\alpha, t) = 1 \tag{42a}$$

$$\sum_{\alpha} f^{jk}(\alpha, \beta, t) = f^k(\beta, t) \tag{42b}$$

Equation (42b) emphasizes that f^{jk} is the *joint* probability of finding the object at j of color α *and* the object at k of color β at time t. The model rules are summarized in the equation

$$f^{j+1}(\alpha, t+1) = \tfrac{1}{2}(1+\epsilon_j) f^j(\alpha, t) + \tfrac{1}{2}(1-\epsilon_j)[(1-\lambda_j) f^j(\alpha, t) + \lambda_j f^j(-\alpha, t)] \tag{43a}$$

Since the color variables have only the values -1 and 1, Eq. (43a) indicates the ways in which a color state α at $k+1$ and $t+1$ can be obtained from a state α at j at t (meaning *no* color change), or from a state $-\alpha$ at j at t (showing that a change has taken place). Using $f^j(\alpha, t) - f^j(-\alpha, t) = 1$. Eq. (43a) assumes the form

$$f^{j+1}(\alpha, t+1) = f^j(\alpha, t)[1 - \lambda_j(1-\epsilon_j)] + \tfrac{1}{2}\lambda_j(1-\epsilon_j) \tag{43b}$$

One should expect that in the special case that $\lambda_j = \lambda = 1$ for all j, (43b) should reduce to the equation of motion for the f_1 function of the previous section Eq. (11a). One obtains for $\lambda = 1$,

$$f^{j+1}(\alpha, t+1) = \epsilon_j f^j(\alpha, t) + \tfrac{1}{2}(1-\epsilon_j) \tag{43c}$$

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[11] All the results in this and the next section can be straightforwardly verified by elementary means just by showing that the equations written express the model rules correctly. On occasion, this verification becomes quite involved; even so, the proofs have merely been indicated; the omitted parts just take patience.

and [from Eq. (11a)]

$$f^{j-1}(\alpha, t + 1) = f^{j}(\epsilon_j x, t)$$

These two equations do have the same content, since one can establish the *identity*

$$f^{j}(\epsilon_j \alpha, t) = \epsilon_j f^{j}(\alpha, t) + \tfrac{1}{2}(1 - \epsilon_j) \tag{44}$$

[Equation (44) depends *only* on the fact that α and ϵ_j assume just the values ± 1 and the normalization of f. Thus in contrast to the equation of motion (43c) and (11a), which only hold for $\lambda = 1$, Eq. (44) is a valid identity for any (one-particle) distribution function.] Returning to the basic equation (43b), it is very suggestive to introduce

$$\epsilon_j' \equiv 1 - \lambda_j(1 - \epsilon_j) \tag{45}$$

In terms of ϵ_j' the distribution function $f^{j}(\alpha, t + 1)$ for the stochastic model satisfies[12]

$$f^{j-1}(\alpha, t + 1) = \epsilon_j' f^{j}(\alpha, t) + \tfrac{1}{2}(1 - \epsilon_j') \tag{46a}$$

This equation can be iterated immediately to yield for all real ϵ_j'

$$f^{j}(\alpha, t) = \tfrac{1}{2} - \tfrac{1}{2}\epsilon'_{j-1} \cdots \epsilon'_{j-t} + \epsilon'_{j-1} \cdots \epsilon'_{j-t} f^{j-t}(\alpha, 0) \tag{46b}$$

The initial condition $\rho(\alpha, 0)$ as given by Eq. (12) yields the initial condition for f^{j}:

$$f^{j}(\alpha, 0) = \tfrac{1}{2} + 2^{n-1}\alpha b_j \tag{46c}$$

This, used in (46a), gives the explicit solution for f as

$$f^{j}(\alpha, t) = \tfrac{1}{2} + 2^{n-1}\epsilon'_{j-1} \cdots \epsilon'_{j-t} b_{j-t}\alpha \tag{46d}$$

It is important to observe that although this solution contains the $\{\epsilon\}$ variables explicitly, the distribution function is no longer periodic, in contrast to the previous model [see Eqs. (14) and (24b)]. *Formally*, this lack of periodicity comes from the fact that this solution contains ϵ with $(\epsilon_j')^2 \neq 1$, while the previous solutions contained ϵ with $\epsilon_j^2 = 1$. *Physically*, the continued operation of a random element in the dynamics precludes an exact periodicity of the system.

It is again appropriate to average over all the marker positions. Using

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[12] This equation for f^j (with $\lambda \neq 1$) has the same structure as the equation for f^j with $\lambda = 1$ [Eq. (43b)]. Just ϵ_j is replaced by ϵ_j'.

the definition (45) for ϵ_j' and the properties of the $\{\epsilon\}$ ensemble given by Eqs. (8a)–(8g), it is straightforward to establish that

$$\langle \epsilon_j' \rangle = 1 - 2\lambda_j \mu \tag{47a}$$

$$\langle \epsilon_j' \epsilon_k' \rangle = \langle \epsilon_j' \rangle \langle \epsilon_k' \rangle, \qquad j \neq k \tag{47b}$$

$$\langle (\epsilon_j')^2 \rangle = 1 - 4\lambda_j \mu (1 - \lambda_j) \tag{47c}$$

Equation (47c) represents the main difference with the previous case, where $\epsilon_j^2 = 1$; hence $\langle \epsilon_j^2 \rangle = 1$. With these formulas, the ϵ averaging can easily be carried out. The result is

$$\langle f^j(\alpha, t) \rangle_\epsilon = \tfrac{1}{2} + 2^{n-1} b_{j-t} \alpha \prod_{\tau=1}^{t} (1 - 2\mu\lambda_{j-\tau}) \tag{48a}$$

$$\langle f^j(\alpha, t) \rangle_\epsilon = \tfrac{1}{2} + 2^{n-1} b_{j-t} \alpha (1 - 2\lambda\mu)^t, \qquad \lambda_j = \lambda \tag{48b}$$

The second form (48b) refers to a model where all the probabilities λ_j are the same. The ϵ-averaged distribution function for the stochastic model has exactly the same structure as the ϵ-averaged mechanical model [see Eq. (18)]. It just appears as if the marker density μ has been decreased by a factor λ (the probability of a change) to yield an effective marker density $\mu\lambda$. This is intuitively reasonable (in fact, pretty obvious).

It is, however, amusing to see how the j dependence of the probability can simulate a location- (j-) dependent color. Suppose $\lambda_j = 1 - \rho v_j$, where ρ is small; assume further that initially all balls have the same color, thus $f_j(\alpha = 1, 0) = 1$; this gives $b_j = (\tfrac{1}{2})^n$ [from Eq. (46d)]. Expanding the product in (48a) and keeping just terms linear in ρ gives

$$\langle f^j(\alpha, t) \rangle_\epsilon \approx \tfrac{1}{2} + \tfrac{1}{2}\alpha \left[(1 - 2\mu)^t + (1 - 2\mu)^{t-1}\, 2\rho\mu \sum_{\tau=1}^{t} v_{j-\tau} \cdots \right] \tag{49a}$$

For long times $\langle f \rangle_\epsilon$ approaches $\tfrac{1}{2}$, independent of j. The "average" color[13] at j computed from (49a) and (37) is

$$\bar{\alpha}_j(t) = \left[(1 - 2\mu)^t + (1 - 2\mu)^{t-1}\, 2\rho\mu \sum_{\tau=1}^{t} v_{j-\tau} \right] \tag{49b}$$

This relation shows that for long times, the average color approaches 0. (If $\alpha = +1$ is white and $\alpha = -1$ is black, the value $\alpha = 0$ would be the

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[13] Strictly speaking, the variable used in (49a) is the local average of the ensemble average, $\overline{\langle \alpha_j \rangle}_\epsilon = \sum_\epsilon \alpha \langle f^j(\alpha, t) \rangle_\epsilon$. The simplified notation should not cause too much confusion.

average, presumably grey!) However, (49b) also shows that for *finite* times, the average color varies from place to place; for example.

$$\bar{\alpha}_j(t) - \bar{\alpha}_{j-1}(t) = 2\rho\mu(1 - 2\mu)^{t-1}(v_{j-1} - v_{j-t-1}) \tag{49c}$$

This difference clearly goes to zero for *large* t; however, in the model where $\mu = 0$, this difference vanishes for all t. Thus the introduction of a j-dependent probability λ_j causes the average local color to become dependent on position.

3.2. The Liouville Level (f^2)

It is again fairly straightforward to derive an equation for the time variation of $f^{jk}(\alpha, \beta, t)$. It is just necessary to enumerate the circumstances which can give rise to a particular color configuration at particular locations. The result is[14]

$$f^{j+1,k+1}(\alpha, \beta, t + 1) = A_{jk} f^{jk}(\alpha, \beta, t) + B_{jk} f^j(\alpha, t) + B_{kj} f^j(\alpha, t) \times C_{jk} \tag{50}$$

$$\begin{aligned} A_{jk} &= \lambda_j\lambda_k\epsilon_j\epsilon_k + \epsilon_j\lambda_j(1 - \lambda_k) \\ &\quad + \epsilon_k\lambda_k(1 - \lambda_j) + (1 - \lambda_j)(1 - \lambda_k) \end{aligned} \tag{51a}$$

$$B_{jk} = \tfrac{1}{2}[-\lambda_j\lambda_k\epsilon_j\epsilon_k + \epsilon_j\lambda_j\lambda_k + \epsilon_k(\lambda_j\lambda_k - \lambda_k) + (\lambda_k - \lambda_j\lambda_k)] \tag{51b}$$

$$C_{jk} = \tfrac{1}{4}\lambda_j\lambda_k(1 - \epsilon_j)(1 - \epsilon_k) \tag{51c}$$

It can indeed be checked that (50)–(51c) incorporate all the model rules. If $\lambda_j = \lambda = 1$, the $f^{(2)}$ equation for the previous case (without stochastic elements) should be recovered. One finds from (50) that it reduces to

$$\begin{aligned} f^{j-1,k+1}(\alpha, \beta. t + 1) &= \epsilon_j\epsilon_k f^{jk}(\alpha, \beta, t) + \tfrac{1}{2}(\epsilon_j - \epsilon_j\epsilon_k) f^j(d, t) \\ &\quad + \tfrac{1}{2}(\epsilon_k - \epsilon_j\epsilon_k) f^k(\beta, t) + \tfrac{1}{4}(1 - \epsilon_j)(1 - \epsilon_k), \quad (\lambda = 1) \end{aligned} \tag{52a}$$

This should be compared with Eq. (11b), which describes this same situation:

$$f^{j+1,k+1}(\alpha, \beta, t + 1) = f^{jk}(\epsilon_j\alpha, \epsilon_k\beta. t), \qquad \lambda = 1$$

That these equations have the same content follows from the *identity*

$$\begin{aligned} f^{jk}(\epsilon_j\alpha, \epsilon_k\beta, t) &= \epsilon_j\epsilon_k f^{jk}(\alpha, \beta, t) + \tfrac{1}{2}\epsilon_j(1 - \epsilon_k) f^j(\alpha, t) \\ &\quad + \tfrac{1}{2}(1 - \epsilon_j)\, \epsilon_k f^k(\beta, t) + \tfrac{1}{4}(1 - \epsilon_j)(1 - \epsilon_k) \end{aligned} \tag{52b}$$

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[14] No summation of any kind is implied by indices occurring twice.

Equation (52b) again follows, as did (44), for all normalized probability functions, from the assumed properties of α, β, ϵ. It is both interesting and important to observe that the introduction of the ϵ_j' variables allows the two-particle equation (50) to be written in the form

$$\begin{aligned} f^{j+1,k+1}(\alpha, \beta, t+1) &= \epsilon_j'\epsilon_k' f^{jk}(\alpha, \beta, t) + \tfrac{1}{2}\epsilon_j'(1-\epsilon_k')f^j(\alpha, t) \\ &\quad + \tfrac{1}{2}(1-\epsilon_j')\,\epsilon_k' f^k(\beta, t) + \tfrac{1}{4}(1-\epsilon_j')(1-\epsilon_k') \end{aligned} \tag{53}$$

The structure of (53), the equation for the two-particle distribution function *with general* λ_j, is identical with that of Eq. (52a) for the two-particle distribution function with $\lambda_j = \lambda = 1$: just the ϵ_j in the ($\lambda = 1$) equation must be replaced by ϵ_j' in λ_j equation.

This procedure can be generalized to all distribution functions $f^1, f^2, \ldots, \rho$. First, generalizations of the identities (44) and (52b) are needed for $\rho(\epsilon_1\eta_2, \epsilon_2\eta_3, \ldots, \epsilon_n\eta_1, t)$. These identities have the character that the ϵ's act not on the independent variables, but on the functions ρ, f^1, etc., as in (44) and (52b). In this way, one obtains an expansion of $\rho(\eta_1 \cdots \eta_n, t)$, $f^j(\eta, t)$. The Liouville equation is obtained by equating $\rho(\eta_1 \cdots \eta_n, t+1)$ to the expansion with all the ϵ_j variables replaced by ϵ_j' as in (45).

Since the solution of the Liouville hierarchy (9) and (11) was obtained by iteration in which no use was made of the special properties of the ϵ variables, it follows that the present hierarchy (46a) and (53) can be solved in the identical manner. In fact, the Liouville hierarchy for arbitrary λ_j can be immediately and exactly solved by replacing ϵ_j in the former solutions by ϵ_j'. Thus the solution of (53) with initial condition (46c) derived from (12),

$$f^j(\alpha, 0) = \tfrac{1}{2} + 2^{n-1}\alpha b_j$$

and

$$f^{jk}(\alpha, \beta, 0) = \tfrac{1}{4} + 2^{n-2}(b_j\alpha + b_k\beta + b_{j,k}\alpha\beta)$$

is just given by

$$\begin{aligned} f^{jk}(\alpha, \beta, t) &= \tfrac{1}{4} + 2^{n-2}(b_{j-t}\epsilon'_{j-t} \cdots \epsilon'_{j-1}\alpha + b_{k-t}\epsilon'_{k-t} \cdots \epsilon'_{k-1}\beta) \\ &\quad + 2^{n-2}b_{j-t,k-t}\epsilon'_{j-t} \cdots \epsilon'_{j-1}\epsilon'_{k-t} \cdots \epsilon'_{k-1}\alpha\beta \end{aligned} \tag{54}$$

It is again straightforward to obtain the ϵ average of $f^{jk}(\alpha, \beta, t)$. The terms linear in α and β, will involve an average of t factors ϵ', and will contribute, by (47b), $(1-2\lambda\mu)^t$ (if all $\lambda_j = \lambda$). The term in $\alpha\beta$ will give a result that is dependent on the *overlap* of the chains of ϵ's. One finds, using (47a–c),

$$\langle \epsilon'_{j-t} \cdots \epsilon'_{j-1}\epsilon'_{k-t} \cdots \epsilon'_{k-1} \rangle = (1-2\mu\lambda)^{2t} \qquad \text{if} \quad t \leqslant j-k \tag{55a}$$

$$\langle \epsilon'_{j-t} \cdots \epsilon'_{j-1}\epsilon'_{k-t} \cdots \epsilon'_{k-1} \rangle = (1-2\mu\lambda)^{2(j-k)}\,[1-4\mu\lambda(1-\lambda)]^{k-j+t} \qquad \text{if} \quad t > j-k \tag{55b}$$

Thus for times $t > j - k$, one obtains

$$\langle f^{jk}(\alpha, \beta, t)\rangle_\epsilon = \tfrac{1}{4} + 2^{n-2}(1 - 2\lambda\mu)^t(\alpha b_{j-t} + \beta b_{k-t}) + 2^{n-2}(1 - 2\lambda\mu)^{2(j-k)}\alpha\beta[1 - 4\mu\lambda(1 - \lambda)]^{k-j+t} \tag{56}$$

For times $t \leqslant j - k$, the last term is given by (55a). It is interesting to note if $\lambda = 1$, the case of *no* overlap, Eq. (55a) is only slightly altered; however, for $\lambda = 1$, the time dependence in the overlap terms disappears, they just become $(1 - 2\mu)^{2(j-k)}$. It is this persistence in the overlap terms which spoils the agreement between the master equation and the Liouville equation even for long times in the $\lambda = 1$ case. If, however, $\lambda \neq 1$, the overlap terms depend on time; since $[1 - 4\mu\lambda(1 - \lambda)]$ is less than one, they become less important as t increases.

The same features persist if the λ variables differ from point to point. Characteristically, an average such as (55a) becomes a product

$$\prod_{\tau=1}^{t} (1 - 2\mu\lambda_{j-\tau})(1 - 2\mu\lambda_{k-\tau})$$

The complete hierarchy is explicitly soluble and all the ϵ averages can be performed.

3.3. The Master Level, Comparison

To obtain the master equation, it is necessary to construct the transition operator $P(\boldsymbol{\delta} \mid \boldsymbol{\eta})$ similar to (28) which takes the altered model rules into account. A color δ_j at location j an elementary time later becomes a color η_{j+1} at $j + 1$. If *no* color change has taken place, $\delta_j\eta_{j+1} = +1$; while $\delta_j\eta_{j+1} = -1$ if a color change has occurred. The master description dynamics assigns a probability $\mu\lambda_j$ to a color change and a probability $1 - \mu\lambda_j$ to "no change." Therefore

$$\begin{aligned} P(\delta_j \to \eta_{j+1}) &= \tfrac{1}{2}(1 - \delta_j\eta_{j+1})\,\mu\lambda_j + \tfrac{1}{2}(1 + \delta_j\eta_{j+1})(1 - \mu\lambda_j) \\ &= \tfrac{1}{2}[1 + \delta_j\eta_{j+1}(1 - 2\mu\lambda_j)] \end{aligned} \tag{57a}$$

Consequently the transition operator becomes

$$P(\boldsymbol{\delta} \mid \boldsymbol{\eta}) = \prod_{j=1}^{n} \tfrac{1}{2}[1 + \delta_j\eta_{j+1}(1 - 2\mu\lambda_j)] \tag{57b}$$

It differs from (28) only through the replacement of μ by $\mu\lambda$. The master equation is [P is given by (57b)]

$$\varphi(\boldsymbol{\eta}, t + 1) = \sum_{\boldsymbol{\delta}} P(\boldsymbol{\delta} \mid \boldsymbol{\eta})\, \varphi(\boldsymbol{\delta}, t) \tag{57c}$$

It appears as if the decrease in effectiveness in producing transitions through the introduction of the probabilities λ_j is totally accounted for in P by a decrease in the effective marker density. Since the master level gives an overall "averaged" description of the dynamics, it is to be expected that the introduction of the λ_j could be so expressed. Formally, the master hierarchy is exactly the same as that obtained before; just μ should be replaced by $\lambda\mu$, and powers $(1 - 2\mu)^t$ by products of t factors. The results for F^j and F^{jk} are (as always, with the same initial conditions)

$$F^j(\alpha, t) = \tfrac{1}{2} + 2^{n-1} b_{j-t}\alpha \prod_{\tau=1}^{t} (1 - 2\lambda_{j-\tau}\mu) \tag{58a}$$

$$\begin{aligned} F^{jk}(\alpha, \beta, t) = \tfrac{1}{4} + 2^{n-2} \Big[& \alpha b_{j-t} \prod_{\tau=1}^{t} (1 - 2\lambda_{j-\tau}\mu) \\ & + \beta b_{k-t} \prod_{\tau=1}^{t} (1 - 2\lambda_{k-\tau}\mu) \\ & + \alpha\beta b_{k-t} \prod_{\tau=1}^{t} (1 - 2\lambda_{j-\tau}\mu)(1 - 2\lambda_{k-\tau}\mu) \Big] \end{aligned} \tag{58b}$$

The equation for $F^j(\alpha, t)$ again has a direct kinetic interpretation as a gain–loss equation. Using the familiar arguments, one writes

$$\begin{aligned} F^{j+1}(\alpha, t + 1) &= F^j(\alpha, t)(1 - \mu) + F^j(\alpha, t)\,\mu(1 - \lambda) \\ &\quad + [1 - F^j(\alpha, t)]\,\mu\lambda \\ &= \mu\lambda + (1 - 2\mu\lambda)\,F^j(\alpha, t) \end{aligned} \tag{58c}$$

Equation (58c) enumerates the ways in which the color α can be produced at location $j + 1$ at time $t + 1$, and assigns them their appropriate probabilities. Clearly, (58c) is the same as (34) with μ replaced by $\mu\lambda$. Equation (58c) can also be obtained by summing (57c) over all η, except η_j, which is equal to α.

The comparison between the master and Liouville hierarchies can just be read off from (58a), (58b), and (48a) and (55a) (55b), and (56). The results are

$$\langle f^j(\alpha, t)\rangle_\epsilon = F^j(\alpha, t) \tag{59a}$$

$$\langle f^{jk}(\alpha, \beta, t)\rangle_\epsilon = F^{jk}(\alpha, \beta, t), \qquad t \leqslant j - k \tag{59b}$$

$$\langle f^{jk}(\alpha, \beta, t)\rangle_\epsilon \neq F^{jk}(\alpha, \beta, t), \qquad t > j - k \tag{59c}$$

The difference noted in (59c) originates in the overlap terms. Although the two solutions are *not* equal for any finite time $t > j - k$, the terms which are different individually go to zero as t becomes large. This is in sharp contrast to the mechanistic model, where the corresponding terms are $(1-2\mu)^{2(t-k)}$ (in the Liouville equation) and $(1-2\mu)^{2t}$ (in the Master description). Here, one term becomes small as t becomes large, while the other remains constant. Thus the Master equation in the stochastic model gives for long times a better approximation to the Liouville equation than in the mechanistic model. Even so, it is a quantitative question (depending on t, b_k, λ, μ, and the accuracy needed) to decide whether the use of the Master solution is legitimate in any particular case, even in the stochastic model.

4. THE QUANTUM MODEL; A HEURISTIC DISCUSSION

4.1. The Model

In ordinary quantum theory, the state of the system at time t is described by the state vector $|\psi(t)\rangle$. It is related to the state vector at time 0 by a unitary time-evolution operator

$$|\psi(t)\rangle = e^{-iHt}\,|\psi(0)\rangle \tag{60a}$$

The Hamiltonian H, contains the dynamics of the system. The probability W that at time t the quantum system is in a state χ (say an eigenstate of some operator) is the square of an amplitude $a(t)$,

$$W(t) = |\langle\chi\,|\,\psi(t)\rangle|^2 \equiv |a(t)|^2 \tag{60b}$$

These well-known notions will now be applied to the present model. To construct such a quantum mechanical version of the models, it is first necessary to describe the state of a single object.[15] A state is described by a vector $|p, \eta, t\rangle$ which gives information about the location (p) and color (η) at time t. Since the model rigidly prescribes the motion of the balls along the ring, it is only necessary to stipulate the manner in which the color changes can occur. The color scheme and the position can be described independently of each other. Formally, $|p, \eta\rangle = |p\rangle \otimes |\eta\rangle$, a state of a single object can be written as a direct product of a state $|p\rangle$ in R_n, giving the position, and a state $|\eta\rangle$, giving information about the color in C_2, where R_n is a real n-dimensional space, C_2 is a two-dimensional complex vector space, and $\otimes$ denotes the direct (tensor) product. The "color" space C_2 is spanned by the color eigenvectors $|\eta^+\rangle$, $|\eta^-\rangle$, corresponding to color eigenstates. An obvious representation of these states is given by

$$|\eta^+\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \qquad |\eta^-\rangle = \begin{pmatrix}0\\1\end{pmatrix} \tag{61a}$$

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[15] The genuine generalization to the many-particle system will be given in Section 5.

One could introduce a color operator Q which has as only two eigenstates, $|\eta^+\rangle$ with eigenvalue $+1$, and $|\eta^-\rangle$ with eigenvalue -1. It clearly would have the matrix representation

$$Q = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

A general state in C_2, i.e., a general superposition of color eigenstates, is

$$|p, \eta\rangle = C_1 \,|p, \eta^+\rangle + C_2 \,|p, \eta^-\rangle \tag{61b}$$

$$|C_1|^2 + |C_2|^2 = 1 \tag{61c}$$

In such a state, the probability that a color measurement at p would give white is $|C_1|^2 = |\langle\eta^+ \,|\, p, \eta\rangle|^2$ [compare (60b)]; it would give black with probability $|C_2|^2 = |\langle\eta^- \,|\, p, \eta\rangle|^2$.

The distinguishing quantum feature is precisely that an object can be in a mixed color state such as (61b). In a *classical* description, a ball is either white or black; one can describe the *changes* from one to another in a probability manner as was done in Section 3, but the state itself refers to a definite color. In quantum theory, by contrast, the state *itself* contains both color possibilities.

The time-evolution operator for the model must be so chosen that when a ball leaves an unmarked point, its color state is not changed. However, when a ball leaves a marked point, its color state must undergo a change described by an operator which does not have the color states as eigenstates or which is *not* diagonal in the color representation. In that case, even a pure color state becomes a superposition of color states, which is the essential (in fact only) quantum theoretical ingredient in the model. Thus the quantum modification of the model described in Section 3 must have the property that if a ball in a *color eigenstate* leaves a marked point p, it will change color with probability λ_p and will not change with probability $(1 - \lambda_p)$.[16] (It should be pointed out that if a ball leaving a marker would *certainly* change color, a pure color state would necessarily evolve into a different, but again pure state. The only characteristic quantum mechanical superposition of states would then result from the initial mixture and not from the dynamics. For that reason, it was felt preferable to construct the model so that the mixing was an intrinsic feature; this demands the introduction of λ. This, of course, has the consequence that the quantum model should properly be compared with a classical model of the same character, thus containing the same λ. This was the main reason for the Discussion of section 3.)

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[16] Most of the formulas will be written for λ independent of p. The modifications introduced by the p dependence are usually straightforward, and only occasionally noted.

4.2. The Schrödinger Equation[17]

To construct the operator which describes this time evolution, it is best to start from E_p :

$$E_p = \tfrac{1}{2}(1 + \epsilon_p)\, 1 + \tfrac{1}{2}(1 - \epsilon_p)\, S_p \tag{62}$$

E_p must be thought of as a 2 × 2 matrix, acting in the color subspace. If p is not marked, E_p clearly is the unit matrix. The model rules just described require that S_p have the properties

$$S_p\, |\eta_p{}^{+}\rangle = e^{i\alpha}(1 - \lambda)^{1/2}\, |\eta^{+}_{p+1}\rangle + e^{i\beta}\lambda^{1/2}\, |\eta^{-}_{p+1}\rangle \tag{63a}$$

$$S_p\, |\eta_p{}^{-}\rangle = e^{i\gamma}\lambda^{1/2}\, |\eta^{+}_{p+1}\rangle + e^{i\delta}(1 - \lambda)^{1/2}\, |\eta^{-}_{p+1}\rangle \tag{63b}$$

Equation (61b), combined with (63a), shows that S_p acting on a color state (say; white) at p yields a state at $p + 1$ having a probability $1 - \lambda$ of being white and a probability λ of being black, which is just what the model requires. In the color representation, the matrix S_p assumes the form

$$S_p = \begin{pmatrix} e^{i\alpha}(1 - \lambda)^{1/2} & e^{i\gamma}\lambda^{1/2} \\ e^{i\beta}\lambda^{1/2} & e^{i\delta}(1 - \lambda)^{1/2} \end{pmatrix} \tag{63c}$$

The phases α, β, γ, and δ are *real* constants, independent of the color. If one requires that the time-evolution operator is unitary (as is customary in quantum mechanics), and further, that the matrix S_p becomes the *unit* matrix as $\lambda \to 0$, just one of the phases remains free:

$$S_p = \begin{pmatrix} (1 - \lambda)^{1/2} & e^{i\gamma}\lambda^{1/2} \\ -e^{-i\gamma}\lambda^{1/2} & (1 - \lambda)^{1/2} \end{pmatrix} \tag{63d}$$

The phase γ will be taken zero.[18] The evolution of the system is now summarized by the equation for the state vectors:

$$|\eta_{p+1}(t + 1)\rangle = E_p\, |\eta_p(t)\rangle \tag{64a}$$

This is the analog of the Schrödinger equation; it can easily be checked that the requirements of the model are all satisfied. Equation (64a) is a typical quantum mechanical equation, if the set $\{\epsilon\}$ and λ are given (i.e., the Hamiltonian is given); it contains probability notions precisely to the extent that quantum mechanics always does; but there are no other stochastic or statistical elements contained in the description.

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[17] Compare Section 2.1.

[18] In Section 7, the physical significance of the phase γ will be further discussed. For the present, it is sufficient to note that S as given by (63d) with $\gamma = 0$ gives a dynamics in harmony with the required model rules, although these rules do not determine S uniquely.

It is simple to solve the Schrödinger equation by interation; Eq. (64a) gives immediately

$$| \eta_p(t)\rangle = E_{p-1} \cdots E_{p-t} \, | \eta_{p-t}(0)\rangle \tag{64b}$$

The product of the E operators plays the role of the exponential operator in (60a).

4.3. An Example

To illustrate the characteristic differences encountered in this quantum model, it is interesting to discuss a specific physical situation. Assume that at time $t = 0$, all objects are in the same pure color state,

$$| \eta_p(0)\rangle = | \eta^+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad p = 1, \ldots, n \tag{65}$$

What is wanted is the probability that at time t, ball p is white (i.e., is in the same color state). The answer to this problem on the classical Liouville level is for the boundary conditions obtained from (46b) and (48b) as

$$f^{p}(1, t) = \tfrac{1}{2} + \tfrac{1}{2}\epsilon'_{p-1} \cdots \epsilon'_{p-t} \tag{66a}$$

$$\langle f^{p}(1, t)\rangle_\epsilon = \tfrac{1}{2} + \tfrac{1}{2}(1 - 2\lambda\mu)^t \tag{66b}$$

The method to be followed in the quantum case is clear enough in principle. One clearly can compute $\eta_p(t)$ from (64b) with the boundary condition (65). Then the desired probability is, by (60b),

$$W_p(t) = | a_p(t)|^2 = |\langle \eta^+ | \eta_p(t)\rangle|^2 \tag{67}$$

It is also clear that the expression for the probability will explicity depend on ϵ variables, which will enter W_p through $\eta_p(t)$. Substituting the expression (62) for E_p in (64*b*), one obtains for $| \eta_p(t)\rangle$ a *sum* of terms of the type

$$\begin{aligned} &(\tfrac{1}{2})^t \, (1 + \epsilon_{p-1})(1 + \epsilon_{p-2}) \cdots (1 + \epsilon_{p-r})(1 - \epsilon_{p-r-1}) \\ &\qquad \cdots (1 - \epsilon_{p-t}) \, S_{p-r-1} \cdots S_{p-t} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{aligned} \tag{68}$$

These sums tend to get somewhat complicated; however, there are two simplifying features. One is that the ϵ variables occur in products with no ϵ variable occurring twice, multiplying the S matrices. The other is that the matrices

$$S_p = \begin{pmatrix} (1 - \lambda_p)^{1/2} & \lambda_p^{1/2} \\ -\lambda_p^{1/2} & (1 - \lambda_p)^{1/2} \end{pmatrix} \tag{69a}$$

can all be diagonalized by the same unitary matrix[19]:

$$U = (1/\sqrt{2})\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \tag{69b}$$

$$S_p = UD_pU^{-1}, \qquad D_p = \begin{pmatrix} \Lambda_p & \\ & \Lambda_p{}^* \end{pmatrix} \tag{69c}$$

$$\Lambda_p = (1 - \lambda_p)^{1/2} + i\lambda_p^{1/2} \tag{69d}$$

The fact that all the S matrices can be diagonalized by the same U allows a very simple reduction of the products of the S matrices and the vector

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

occurring in (68) to a simple vector. To obtain W_p, it is first necessary to take the scalar product of that vector with (1, 0). It is here that the fact that that the ϵ variables factor becomes very important. One finds, for example, for $t = 2$,

$$\begin{aligned} a_p(2) &= \langle \eta^+ \mid \eta_p(2) \rangle \\ &= \tfrac{1}{4}\{(1 + \epsilon_{p-2})(1 + \epsilon_{p-1}) + \tfrac{1}{2}(1 - \epsilon_{p-2})(1 + \epsilon_{p-1})(\Lambda + \Lambda^*) \\ &\quad + \tfrac{1}{2}(1 + \epsilon_{p-2})(1 - \epsilon_{p-1})(\Lambda + \Lambda^*) \\ &\quad + \tfrac{1}{2}(1 - \epsilon_{p-2})(1 - \epsilon_{p-1})[\Lambda^2 + (\Lambda^*)^2]\} \end{aligned} \tag{70a}$$

Finally, this expression has to be squared to obtain $W_p(2)$. Some simplifications occur in this process. Since $\epsilon^2 = 1$, all mixed products in this square disappear; they always contain terms such as $(1 - \epsilon_{p-2})(1 + \epsilon_{p-2})$, which vanish. For $W_p(t)$, one obtains polynomials of degree $2t$ in Λ and Λ^*, with coefficients which depend on ϵ. This is in general as far as the analysis can be carried out. The result is the answer to the quantum mechanical problem posed.

As an example of the type of expression obtained, the specific result for $W_p(2)$ is:

$$\begin{aligned} W_p(2) = \tfrac{1}{4}\{&(1 + \epsilon_{p-2})(1 + \epsilon_{p-1}) + (1 - \epsilon_{p-2})(1 + \epsilon_{p-1})(1 - \lambda) \\ &+ (1 + \epsilon_{p-2})(1 - \epsilon_{p-1})(1 - \lambda) + (1 - \epsilon_{p-2})(1 - \epsilon_{p-1}(1 - 2\lambda)^2)\} \end{aligned} \tag{70b}$$

The structure of $W_p(t)$ is an obvious generalization of (70b). This formula is the quantum counterpart of (66a) evalutated for $t = 2$:

$$f_p(1, t = 2) = \tfrac{1}{2} + \tfrac{1}{2}[1 - \lambda(1 - \epsilon_{p-1})][1 - \lambda(1 - \epsilon_{p-2})] \tag{70c}$$

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[19] The formulas as written hold in the general case where λ depends on p. The p is omitted again after formula (69d).

It can be seen immediately that these results have a similar structure both are quadratic functions of λ with ϵ-dependent coefficients. The coefficients, however, are different. These differences persist for all t.

4.4. The ϵ-Averaging Process

To obtain results of physical interest in the classical case, one had to average over $\{\epsilon\}$. In the quantum mechanical context, a similar average has to be carried out. This, properly speaking, is an analysis on the Liouville level; the dynamics is solved in terms of the ϵ variables. to the bitter end, and the final answer is averaged over ϵ. Thus

$$\langle W_p(t)\rangle_\epsilon = \langle | a_p(t)|^2\rangle_\epsilon = \langle |\langle\eta^+ | \eta_p(t)\rangle|^2\rangle_\epsilon \tag{71a}$$

The reason for the repetition of this formula is to stress that the squaring of the amplitude has to take place *before* the averaging over ϵ is carried out. The dynamics gives as quantity of physical interest $|a_p|^2 = W_p$; only after the dynamical calculation is completed should the ϵ average be taken. With the explicit form of $a_p(t)$, of which (71a) gives a sample, $|a_p(t)|^2$ can be calculated in terms of Λ and ϵ variables. The ϵ averaging can then be obtained in the usual straightforward, but tedious fashion.

It is more instructive to proceed in a slightly different fashion (the answer is of course the same). Start again by considering (64b); however, assume that of the t points, exactly r ($<t$) are marked. Since the state only changes at such marked points and S is independent of p,

$$|\eta_p(t)\rangle = S^r | \eta_{p-t}(0)\rangle = S^r \begin{pmatrix}1\\0\end{pmatrix} \tag{71b}$$

Using the fact that S can be diagonalized by U [Eq. (69c)] gives

$$|\eta_p(t)\rangle = UD^rU^{-1} \begin{pmatrix}1\\0\end{pmatrix} \tag{71c}$$

With the explicit form of U and D, this is easy to evaluate and

$$\langle\eta^- | \eta_p(t)\rangle = \tfrac{1}{2}[\Lambda^r + (\Lambda^*)^r] \tag{72}$$

$$W_p(r, t) = \tfrac{1}{4} | \Lambda^r + (\Lambda^*)^r |^2 \tag{73}$$

This is the probability that the ball at t at p shall be white *provided* that there are r markers in the interval $p - 1, \ldots, p - t$. The latter probability itself is

$$\mathscr{G}(r) = [t!/r!(t - r)!]\, \mu^r(1 - \mu)^{t-r} \tag{74}$$

This is a consequence of the assumed marker distribution. Averaging $W_p(r, t)$ over all marker distributions gives the needed ϵ average of W_p,

$$\langle W_p(t) \rangle_\epsilon = \sum_{r=0}^{t} W_p(r, t)\, \mathscr{G}(r)$$

$$= \tfrac{1}{4} \sum_{r=0}^{t} |\Lambda^r + (\Lambda^*)^r|^2\, [t!/s!(t-r)!]\, \mu^r (1-\mu)^{t-r} \qquad (75a)$$

This sum can be carried out using (69d); the answer is

$$\langle W_p(t) \rangle_\epsilon = \tfrac{1}{2} + \tfrac{1}{2}\, \mathrm{Re}\{1 - 2\lambda\mu + 2i\mu[\lambda(1-\lambda)]^{1/2}\}^t \qquad (75b)$$

The detailed analysis of this expression will be postponed till later, but it is perhaps useful to mention that this expression is strikingly different from the classical result (66b). As $t \to \infty$, $\langle W_p(t) \rangle_\epsilon$ does approach $\frac{1}{2}$, but not at all monotonically. Instead, it oscillates with a decreasing amplitude and a frequency ν

$$\nu = (1/2\pi) \tan^{-1}[2\mu(\lambda - \lambda^2)^{1/2}/(1 - 2\lambda\mu)] \qquad (75c)$$

Hence the classical and quantum mechanical results are distinct before the $\{\epsilon\}$ averaging is carried out [as illustrated by (70b) and (70c)]; but more surprisingly, they also are quite different *after* this averaging has been performed.

5. THE QUANTUM MODEL; EXACT DISCUSSION

5.1. The State Space and the Density Matrix

To give a description of the dynamics of the system as a whole, rather then just of its individual constituents (as was done in Section 4), it is necessary to construct the space of states of the system. Since the balls move independently of each other; the state of the system at *any* time t is a tensor product[20] of the states of the individual objects:

$$|j, t\rangle = \prod_{p=1}^{n} \otimes\, |\alpha_p, p, t\rangle \qquad (76a)$$

Here, $|x_p, p, t\rangle$ is the color state at location p at time t; it is, as was noted in Section (4), a vector in the two-dimensional complex color subspace $C_\mu^{(2)}$. The state $|j, t\rangle$ is a vector in 2^n-dimensional tensor product space C.

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[20] A tensor product will always be denoted by $\prod_p \otimes$. Ordinary products will be written in the usual way, $\prod_p$.

The time evolution of the system as described by the Liouville equation is therefore an equation of motion for vector $|j, t\rangle$ in C. Equation (76a) holds for *all* times; in particular for $t = 0$:

$$|j, 0\rangle = \prod_{p=1}^{n} \otimes \, |\alpha_p, p, 0\rangle \tag{76b}$$

The state $|j, 0\rangle$ depends explicitly on the values α_p ($p = 1, 2,..., n$); it describes the initial color configuration. As written, the states $|\alpha, p, 0\rangle$ could be color eigenstates (eigenstates of Q_p) or not.

To construct the density matrix of the system, it is simplest to recall that for *any* system, the density matrix $\rho(t)$ can be obtained in the following fashion. Let $|j\rangle$ be a complete orthonormal set of states which spans the phase space of the system, but which is otherwise arbitrary. Assume that the initial density operator is given:

$$\rho(0) = \sum_j b_j \, |j\rangle\langle j| \tag{77}$$

Then the density matrix at time t is

$$\rho(t) = \sum_j b_j \, |j, t\rangle\langle j, t| \tag{78}$$

In (78), $|j, t\rangle$ is the state which evolves via the dynamics of the system from the state $|j\rangle$ at time $t = 0$. (For a Hamiltonian system, $|j, t\rangle = e^{-iHt}|j\rangle$.) The coefficients b_j determine the ensemble. To apply (77) and (78) to the model, assume that the initial state is a tensor product of color eigenstates[21,22]

$$|j, 0\rangle = \sum_{p=1}^{n} \otimes \, |\eta, p, 0\rangle \tag{79}$$

Thus $\rho(0)$ can be written (exhibiting all indices) as

$$\rho(0) = \sum_{\eta_1} \cdots \sum_{\eta_n} b_{\eta_1 \cdots \eta_n} \prod_{p=1}^{n} \otimes \, |\eta_p, p, 0\rangle\langle \eta_p, p, 0| \tag{80}$$

The initial color configuration is given by the $b_{\eta_1 \cdots \eta_n}$. If these coefficients have the special property that

$$b_{\eta_1 \cdots \eta_n} = \prod_{p=1}^{n} b_{\eta_p} \tag{81}$$

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[21] An effort has been made to denote color eigenstates by $|\eta, p, 0\rangle$, while general states are written as $|\alpha, p, 0\rangle$.

[22] It is straightforward to check that these eigenstates are complete and orthonormal.

the initial distribution is *factored*. (This is sometimes called an *uncorrelated* initial distribution.) It will be seen later that factored initial distributions lead to substantial simplifications in the formalism, although their special *physical* properties are not quite so obvious.

The specification (80) of the initial density matrix is one where the initial density matrix is diagonal in the color representation. For, taking the matrix elements of $\rho(0)$ between color eigenstates $\eta_1' \cdots \eta_n'$, $\eta_1'' \cdots \eta_n''$ yields

$$\langle \eta_1' \cdots \eta_n' \mid \rho(0) \mid \eta_1'' \cdots \eta_n'' \rangle = \delta_{\eta_1'\eta_1''} \cdots \delta_{\eta_n'\eta_n''} b_{\eta_1' \cdots \eta_n'} \tag{82}$$

Equation (82) also shows that $\rho(0)$ determines and is determined by b.

To use the expression (78) for the density matrix at time t, it is only necessary to find the state $\mid j, t \rangle$ into which $\mid j, 0 \rangle$ evolves after a time t under the time evolution as specified by the model rules.

5.2. The Time Evolution

The state of the system at time t is the tensor product

$$\mid j, t \rangle = \prod_{p=1}^{n} \otimes \mid \alpha, p, t \rangle \tag{83a}$$

Similarly, at time $t - 1$,

$$\mid j, t+1 \rangle = \prod_{p=1}^{n} \otimes \mid \alpha, p, t+1 \rangle \tag{83b}$$

Both $\mid j, t \rangle$ and $\mid j, t+1 \rangle$ are vectors in C. $\mid \alpha, p, t \rangle$ is a vector in the color subspace C_p. This subspace is associated with the *location* p, *not* with the particular ball. For this reason, the notation $\mid \alpha_p, p, t \rangle$ is really redundant.[23] This is a color state at location p at time t, and it is specified completely by writing $\mid \alpha, p, t \rangle$. The model rules relate $\mid \alpha, p+1, t+1 \rangle$ in subspace C_{p-1} to $\mid \alpha, p, t \rangle$ in subspace C_p, by E_p:

$$\mid \alpha, p+1, t+1 \rangle = E_p \mid \alpha, p, t \rangle \tag{84}$$

[E_p is given by Eqs. (62) and (63d)].

Combining (83b) and (84), one has

$$\mid j, t+1 \rangle = \prod_{p=1}^{n} \otimes E_{p-1} \mid \alpha, p-1, t \rangle \tag{85}$$

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[23] Even so, this notation is often convenient as a bookkeeping device; it is used as such in what follows.

Since the products in (85) and (83a) are over all $p = 1,\dots, n$, both $|j, t\rangle$ and $|j, t + 1\rangle$ are vectors in the tensor product space C. However, the operator E_p takes a vector from the subspace C_p and constructs from it a vector in C_{p+1} ; the dynamics can *not* be described in a single-color subspace; only by taking the tensor product (either with a cyclic boundary condition $p + n = p$, or an infinite tensor product) can the time evolution of the total system be described.

Iteration of (84) gives

$$| \eta, p, t\rangle = E_{p-1} \cdots E_{p-t} \, | \eta, p - t, 0\rangle \tag{86}$$

(Here, the color variable on the right-hand side is written as η, to indicate that the initial state is a color eigenstate.) The states of the complete system are, from (83a),

$$| j, t\rangle = \prod_{p=1}^{n} \otimes E_{p-1} \cdots E_{p-t} \, | \eta, p - t, 0\rangle \tag{87}$$

Using this expression in (78) and putting in all the indices gives

$$\begin{aligned} \rho(t) = \sum_{\eta_1} \cdots \sum_{\eta_n} b_{\eta_1 \cdots \eta_n} \prod_{p=1}^{n} \otimes \, & E_{p-1} \cdots E_{p-t} \, | \eta_{p-t} \, , p - t, 0\rangle \\ & \times \langle \eta_{p-t} \, , p - t, 0 \, | \, E^{+}_{p-t} \cdots E^{+}_{p-1} \end{aligned} \tag{88}$$

This is the explicit expression for the density matrix. It contains the coefficients b, which describe the ensemble; the dynamics is contained in the products of the E operators, and the many-body character is expressed by the tensor products. The quantities of greatest physical interest are the matrix elements of $\rho(t)$ between states of the complete system. These states themselves are tensor products

$$| \alpha\rangle = \prod_{p} \otimes \, | \alpha_p\rangle$$

The matrix elements can be obtained directly from (88), or alternately (78) gives

$$\langle \alpha \, | \, \rho(t) | \, \beta\rangle = \sum_{j} b_j \, \langle \alpha \, | \, j, t\rangle\langle j, t \, | \, \beta\rangle \tag{89}$$

In (89), both $\langle \alpha \, |$ and $| \, j, t\rangle$ are tensor products; using the formula (generally valid for tensor products)

$$\langle a \otimes b \, | \, a' \otimes b'\rangle = \langle a \, | \, a'\rangle\langle b \, | \, b'\rangle \tag{90}$$

one obtains

$$\begin{aligned}\langle\alpha_1 \cdots \alpha_p \cdots | \rho(t) | \beta_1 \cdots \beta_p \cdots\rangle &= \sum_{\eta_1} \cdots \sum_{\eta_n} b_{\eta_1\cdots\eta_n} \prod_p \langle\alpha_p | E_{p-1} \cdots E_{p-t} | \eta_{p-t}, p-t, 0\rangle \\ &\quad \times \langle\eta_{p-t}, p-t, 0 | E^\dagger_{p-t} \cdots E^\dagger_{p-1} | \beta_p\rangle \end{aligned} \tag{91}$$

Equation (91) contains only *ordinary* products; the application of (90) has eliminated the tensor products.

With the formulas (88) and (91), the calculation of the density matrix has been completed. These formulas are not too transparent as they stand; before considering simplifications, a few comments concerning the derivation might clarify the nature of these results. Using (78) and (83a), $\rho(t)$ can be written as

$$\rho(t) = \sum_{\eta_1} \cdots \sum_{\eta_n} b_{\eta_1\cdots\eta_n} \prod_p \otimes | \eta_p, p, t\rangle\langle\eta_p, p, t | \tag{88'}$$

with $|\eta_p, p, t\rangle$ given by (86). The complexity of this expression stems from the fact that the *same* E_p operator occurs in many different vectors, which in turn occur in the tensor product. As an example, take $t = 4$ and consider

$$|\eta, p-1, 4\rangle = E_{p-2}E_{p-3}E_{p-4}E_{p-5} | \eta, p-5, 0\rangle \tag{92a}$$

$$|\eta, p, 4\rangle = E_{p-1}E_{p-2}E_{p-3}E_{p-4} | \eta, p-4, 0\rangle \tag{92b}$$

$$|\eta, p+1, 4\rangle = E_{p}E_{p-1}E_{p-2}E_{p-3} | \eta, p-3, 0\rangle \tag{92c}$$

The tensor product constructed from these vectors to obtain $\rho(4)$ from (88′) will contain, as can be seen, a number of factors $E_{p-2} \cdot E_{p-3}$. This can be written down easily enough, but the formulas become a little involved. The ϵ averaging which eventually has to be carried out becomes particularly complicated, precisely because of the occurrence of the ϵ terms in each factor E.

It might appear that the dynamics as given by (85) is very trivial. That is in fact not the case. To see precisely what is involved, consider a case where $n = 3$. Then, (83a) reads

$$|j, t\rangle = |\alpha, 1, t\rangle \otimes |\alpha, 2, t\rangle \otimes |\alpha, 3, t\rangle \tag{93}$$

Here,

$$|\alpha, p, t\rangle = a_p \begin{pmatrix}1\\0\end{pmatrix} + b_p \begin{pmatrix}0\\1\end{pmatrix}, \qquad p = 1, 2, 3 \tag{94}$$

$|\alpha, p, t\rangle$ is a vector in the two-dimensional subspace C_p with components a_p and b_p; however, $|j, t\rangle$ is a vector in the $2^3 = 8$-dimensional space C. Its components are (using the standard realization of the tensor product)[24]

$$|j, t\rangle = \begin{pmatrix} a_1a_2a_3 \\ a_1a_2b_3 \\ a_1b_2a_3 \\ a_1b_2b_3 \\ b_1a_2a_3 \\ b_1a_2b_3 \\ b_1b_2a_3 \\ b_1b_2b_3 \end{pmatrix} \tag{95}$$

The state vector $|j, t + 1\rangle$ is given by (95) as

$$|j, t + 1\rangle = (E_1 |\alpha, 1, t\rangle) \otimes (E_2 |\alpha, 2, t\rangle) \otimes (E_3 |\alpha, 3, t\rangle) \tag{96}$$

The known expression for E_p gives components of the vectors: $E_p |\alpha, p, t\rangle$. Write for convenience

$$(E_p |\alpha, p, t\rangle) = \begin{pmatrix} l_pa_p + m_pb_p \\ n_pa_p + o_pb_p \end{pmatrix}, \qquad p = 1, 2, 3 \tag{97a}$$

Here l, m, n, and o are known coefficients determined by E_p: for example,

$$l_p = \tfrac{1}{2}(1 + \epsilon_p) + \tfrac{1}{2}(1 - \epsilon_p)(1 - \lambda)^{1/2} \tag{97b}$$

It should be noted particularly that the vector $E_p |\alpha, 1, t\rangle$ is contained in the subspace C_{p+1}; thus in this example, $E_1 |\alpha, 1, t\rangle \in C_2$. With the explicit forms (97a) and (96), and using the same realization of the tensor product in C, the components of $|j, t + 1\rangle$ can be obtained as

$$|j, t + 1\rangle = \begin{pmatrix} (l_3a_3 + m_3b_3)(l_1a_1 + m_1b_1)(l_2a_2 + m_2b_2) \\ \vdots \\ (n_3a_3 + o_3b_3)(n_1a_1 + o_1b_1)(n_2a_2 + o_2b_2) \end{pmatrix} \tag{98}$$

The effect of the time-evolution operator (for one step) is to produce $|j, t + 1\rangle$, Eq. (98), from $|j, t\rangle$, Eq. (95). Clearly, $|j, t + 1\rangle$ is much more complicated than $|j, t\rangle$ and no immediately obvious operator exists in C which produces $|j, t + 1\rangle$ directly from $|j, t\rangle$. In fact, it is only through the use of the tensor product (96) that one can establish a simple formal relation between $|j, t + 1\rangle$ and $|j, t\rangle$. However, as can be seen, the resulting dynamics is far from trivial.

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[24] See, for example, Jauch.(25)

It was mentioned, pretty much in passing, that the subspace $C_p^{(2)}$ is the two-dimensional color subspace associated with location p; the operator E_p, acts on vectors in this subspace and construct vectors in $C_{p+1}^{(2)}$ from them. Also, E_p refers to a location, not a particular object. Classically, one *could* follow a particular ball [for example, by following an object that initially ($t = 0$) is in a particular place]. Furthermore, the color change classically comes about because of the prescribed motion of the balls. Quantum mechanically, by contrast, the state is totally determined by the color configuration; it makes no sense to ask which ball is where; the specification of the color state vector $\prod_p \otimes |\eta, p, t\rangle$ gives all possible physical information. The change in the color configuration quantum mechanically is described by (84); this asserts that the state at $p + 1$ at $t + 1$ is determined in a prescribed manner by that at p at t. However, it is not at all necessary (although presumably legitimate) to associate this change of state with the actual motion of a physical object. This shows that indeed quantum mechanically E_p must be associated with a *location*, not with an object. It is in fact impossible to associate E_p with a particular ball. For, if this were done, the state of ball p at time t would be $E_{p+t-1} \cdots E_{p-1}E_p |\eta, p, 0\rangle$; here all operators $E_p, E_{p+1}, E_{p+2}, \ldots, E_{p+t-1}$ in this sequence would have to act in the subspace of ball p. However, another ball, say ball $p + 1$, is at time t in the state $E_{p+1}E_{p+t-1} \cdots E_{p+1} |\eta, p + 1, 0\rangle$. This would require $E_{p+1}, E_{p+2} \ldots$ to act in the subspace of ball $p + 1$. Thus E_{p+1} would have to act in two independent subspaces and this is impossible.

5.3. The Reduced Density Matrices

It will be assumed throughout that the trace of the density matrix is normalized to one. Thus

$$\sum_{\eta_1'} \cdots \sum_{\eta_n'} \langle \eta_1' \cdots \eta_n' | \rho(t) | \eta_1' \cdots \eta_n' \rangle = 1 \qquad (99a)$$

Equation (99a) in conjunction with (91) yields the condition on the coefficients b

$$\sum_{\eta_1} \cdots \sum_{\eta_n} b_{\eta_1 \cdots \eta_n} \equiv \left(\sum_{\eta}\right) b_{\eta_1 \cdots \eta_n} = 1 \qquad (99b)$$

(The essential element in the step from (99a) to (99b) is the completeness relation

$$\sum_{\eta_p} \langle \alpha, p, t | \eta_p, p \rangle \langle \eta_p, p | \alpha, p, t \rangle = 1 \qquad (100)$$

In Eq. (100), $|\eta_p, p\rangle$ are color eigenstates; they are summed; $\langle \alpha, p, t|$ is a general state in C_p; it is not summed.)

The density matrix assumes a particularly simple form in the case that the initial distribution factors. In that case, using Eq. (86),

$$\begin{aligned}\rho(t) &= \sum_{\eta_1} \cdots \sum_{\eta_n} (b_{\eta_1} \cdots b_{\eta_n}) \prod_{p} \otimes \, |\, \eta, p, t \rangle \langle \eta, p, t \,| \\ &= \prod_{p} \otimes \sum_{\eta_{p-t}} b_{\eta_{p-t}} E_{p-1} \cdots E_{p-t} \,|\, \eta_{p-t}\,, p - t, 0 \rangle \\ &\quad \times \langle \eta_{p-t}\,; p - t, 0 \,|\, E^{\dagger}_{p-t} \cdots E^{\dagger}_{p-1} \end{aligned} \tag{101}$$

The writing of this expression as a product of sums was possible only because b factored. It is further possible to exchange the summation over η_{p-t} in (101): with the E operators, define r_{p-t} by

$$r_{p-t}(0) = \sum_{\eta} b_{\eta} \,|\, \eta, p - t, 0 \rangle \langle \eta, p - t, 0 \,| \tag{102}$$

$r_{p-t}(0)$ is clearly an operator in the $(p - t)$th color subspace. $\rho(t)$ can be written as

$$\rho(t) = \prod_{p} \otimes E_{p-1} \cdots E_{p-t} r_{p-t}(0) \, E^{t}_{p-t} \cdots E^{t}_{p-1} \tag{103a}$$

Thus in the case of a *factored* initial distribution, the density matrix is an *n-fold tensor* product of $r_p(t)$.

$$\rho(t) = \prod_{p} \otimes \, r_{p-t}(t) \tag{103b}$$

$$r_{p-t}(t) = E_{p-1} \cdots E_{p-t} r_{p-t}(0) \, E^{\dagger}_{p-t} \cdots E^{\dagger}_{p-1} \tag{103c}$$

The normalization condition (99b) also becomes very simple for a factored initial state:

$$\sum_{\eta_1} \cdots \sum_{\eta_n} b_{\eta_1} b_{\eta_2} \cdots b_{\eta_n} = 1 \Rightarrow \sum_{\eta_p} b_{\eta_p} = 1 \tag{104}$$

It is interesting to observe that the operators r_p satisfy typical operator equations of motion. From (103c), it follows easily that

$$r_{p-t}(t + 1) = E_p r_{p-t}(t) \, E_p{}^{\dagger}$$

The physical discussion is facilitated by the introduction of the *reduced* density matrices, which correspond to contracted distribution functions in the classical case.

Various general formulas for the traces of tensor products are useful in this connection. If a_i and a_i' are vectors in a vector space V_i, and if A_i and A_i' are operators in the same space, then the following relations are satisfied:

$$\mathrm{Tr}(A_i \otimes A_j) = (\mathrm{Tr}_i\, A_i)(\mathrm{Tr}_j\, A_j) \tag{105a}$$

$$\mathrm{Tr}(A_i \otimes A_j) \cdot (A_i' \otimes A_j') = (\mathrm{Tr}_i\, A_iA_i')(\mathrm{Tr}_j\, A_jA_j') \tag{105b}$$

Here, $\mathrm{Tr}_i\, A_i$, means that the trace is to be taken in the vector space V_i. Further,

$$\begin{aligned}\sum_{a_2} \cdots \sum_{a_n} \langle a_1' \otimes a_2 \cdots \otimes a_n \,|\, A_1 \otimes A_2 \otimes \cdots A_n \,|\, a_1'' \otimes a_2 \cdots \otimes a_n\rangle \\ = \langle a_1' \,|\, A_1 \,|\, a_1''\rangle\, \mathrm{Tr}_2 A_2 \cdots \mathrm{Tr}_n\, A_n \end{aligned} \tag{105c}$$

The reduced density matrices are obtained by taking matrix elements of $\rho(t)$ [Eq. (88)] between color eigenstates of the system (these states, of course, are tensor products) and taking the trace over all but a certain number of color variables. Equation (88) can be used in conjunction with Eq. (105), or (91) can be applied directly. Using Eqs. (86), (88′), and (91), one obtains the expressions

$$\begin{aligned}\langle \eta_p' \,|\, \rho_1(p, t) \,|\, \eta_p''\rangle &\equiv \sum_{\eta_1'} \cdots \sum_{\eta_n'}{}' \langle \eta_1' \cdots \eta_p' \cdots \eta_n' \,|\, \rho(t) \,|\, \eta_1' \cdots \eta_p'' \cdots \eta_n'\rangle \\ &= \Big(\sum_{\eta'}\Big)' \Big(\sum_{\eta}\Big)\, b_{\eta_1\cdots\eta_n} \langle \eta_p' \,|\, \eta, p, t\rangle\langle \eta, p, t \,|\, \eta_p''\rangle \\ &\quad \times \prod_{s\neq p}{}' \langle \eta_s' \,|\, \eta, s, t\rangle\langle \eta, s, t \,|\, \eta_s'\rangle \end{aligned} \tag{106a}$$

$$\begin{aligned}&\langle \eta_p'\eta_q' \,|\, \rho_2(p, q, t) \,|\, \eta_p'', \eta_q''\rangle \\ &\quad\equiv \sum_{\eta_1'} \cdots \sum_{\eta_n'}{}'' \langle \eta_1' \cdots \eta_p' \cdots \eta_q' \cdots \eta_n' \,|\, \rho(t) \,|\, \eta_1' \cdots \eta_p'' \cdots \eta_q'' \cdots \eta_n'\rangle \\ &\quad= \Big(\sum_{\eta'}\Big)'' \Big(\sum_{\eta}\Big)\, b_{\eta_1\cdots\eta_n} \langle \eta_p' \,|\, \eta, p, t\rangle\langle \eta, p, t \,|\, \eta_p''\rangle \\ &\quad\quad \times \langle \eta_q' \,|\, \eta, q, t\rangle\langle \eta, q, t \,|\, \eta_q''\rangle \prod_{s\neq p\neq q}{}'' \langle \eta_s' \,|\, \eta, s, t\rangle\langle \eta, s, t \,|\, \eta_s'\rangle \end{aligned} \tag{106b}$$

Equations (106a) and (106b) are the definitions of the one- and two-particle density matrices.[25] The sum over η_i' in (106a) specifically excludes the pth color variable η_p'; similarly, the summations over η_p' and η_q' are excluded

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[25] The construction of higher density matrices is the obvious generalization of the procedure given.

in (106b). The notation $(\sum_{\eta'})'$ and $(\sum_{\eta'})''$ indicates this once more; while the prime on the products indicates that the terms $s = p$ in (106a) and $s = p$ and $s = q$ in (106b) are excluded. From these definitions and the completeness relation (100) (applied to the sums over η') it follows that *generally*

$$\langle \eta_p' \mid \rho_1(p, t) \mid \eta_p'' \rangle = \sum_{\eta_1} \cdots \sum_{\eta_n} b_{\eta_1 \ldots \eta_n} \langle \eta_p' \mid \eta, p, t \rangle \langle \eta, p, t \mid \eta_p'' \rangle \tag{107a}$$

$$\begin{aligned} &\langle \eta_p' \eta_q' \mid \rho_2(p, q, t) \mid \eta_p'' \eta_q'' \rangle \\ &\quad = \sum_{\eta_1} \cdots \sum_{\eta_n} b_{\eta_1 \ldots \eta_n} \langle \eta_p' \mid \eta, p, t \rangle \langle \eta, p, t \mid \eta_p'' \rangle \langle \eta_q' \mid \eta, q, t \rangle \langle \eta, q, t \mid \eta_q'' \rangle \end{aligned} \tag{107b}$$

These relations simplify considerably for the case of factored initial distributions. For example, the one-particle density matrix becomes

$$\begin{aligned} \langle \eta_p' \mid \rho_1(p, t) \mid \eta_p'' \rangle = \sum_{\eta_1} \cdots \sum_{\eta_{p-t}} \cdots \sum_{\eta_n} & b_{\eta_1} \cdots b_{\eta_{p-t}} \cdots b_{\eta_n} \\ & \times \langle \eta_p' \mid E_{p-1} \cdots E_{p-t} \mid \eta_{p-t}, p - t, 0 \rangle \\ & \times \langle \eta_{p-t}, p - t, 0 \mid E_{p-t}^{\dagger} \cdots E_{p-1}^{\dagger} \mid \eta_p'' \rangle \end{aligned} \tag{108a}$$

The summations[26] over all η except η_{p-t} can now be performed and give unity [Eq. (104)]. The remaining sum over η_{p-t} can be exchanged with the E operators; it just yields $r_{p-t}(0)$ [see Eq. (102)]. This, combined with (103c), gives

$$\langle \eta_p' \mid \rho_1(p, t) \mid \eta_p'' \rangle = \langle \eta_p' \mid r_{p-t}(t) \mid \eta_p'' \rangle \tag{108b}$$

In other words, the operator $r_{p-t}(t)$ is the one-particle density matrix. The form (103b), together with (108b), shows that the density matrix is the tensor product of one-particle density matrices:

$$\rho(t) = \prod_{p=1}^{n} \otimes \rho_1(p, t) \tag{109}$$

The analysis of the two-particle density matrix for the case of the factored initial distribution follows the same pattern; one obtains from (107b) the result

$$\langle \eta_p', \eta_q' \mid \rho_2(p, q, t) \mid \eta_p'', \eta_q'' \rangle = \langle \eta_p' \mid r_{p-t}(t) \mid \eta_p'' \rangle \langle \eta_q' \mid r_{q-t}(t) \mid \eta_q'' \rangle \tag{110}$$

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[26] It is perhaps worth recalling that the summations over η_p are sums over the *initial* pure color states. It is for this reason that the summation over η_{p-t} in (108a) has been explicitly displayed.

There exists a general fomula relating matrix elements of tensor products of operators to individual matrix elements:

$$\langle a_1' \otimes a_2' \mid A_1 \otimes A_2 \mid a_1'' \otimes a_2'' \rangle = \langle a_1' \mid A_1 \mid a_1'' \rangle \langle a_2' \mid A_2 \mid a_2'' \rangle \tag{111}$$

Applying (111) to (110) and recognizing that the states denoted by η_p' and η_q' are in fact tensor products yields the result

$$\rho_2(p, q, t) = r_{p-t}(t) \otimes r_{q-t}(t) = \rho_1(p, t) \otimes \rho_1(q, t) \tag{112}$$

Similarly, one can show in general (for factored initial conditions) that the *m*th reduced density matrix is the *m*-fold tensor product of the one-particle density matrix. Collecting (112), (108b), and (103c), the final results for the one- and two-particle density matrices are

$$\rho_1(p, t) = r_{p-t}(t) = E_{p-1} \cdots E_{p-t} r_{p-t}(0)\, E_{p-t}^{\dagger} \cdots E_{p-1}^{\dagger} \tag{113a}$$

$$r_{p-t}(0) = \sum_{\eta} b_\eta \mid \eta, p-t, 0 \rangle\langle \eta, p-t, 0 \mid \tag{113b}$$

$$\rho_2(p, q, t) = \rho_1(p, t) \otimes \rho_1(q, t) \tag{113c}$$

It should be stressed that these results depend explicitly on the assumption that the initial distribution is factored. For general initial configurations, the one-particle density matrix is similar in structure to (113a). The two-particle density matrix, however, no longer possesses a tensor product structure. Using appropriately modified arguments, one finds in the *general* case

$$\rho_1(p, t) = E_{p-1} \cdots E_{p-t} r_{p-t}^{(1)}(0)\, E_{p-t}^{\dagger} \cdots E_{p-1}^{\dagger} \tag{114a}$$

$$r_{p-t}^{(1)}(0) = \sum_{\eta} C_\eta^{(1)} \mid \eta, p-t, 0 \rangle\langle \eta, p-t, 0 \mid \tag{114b}$$

Here, $C_\eta^{(1)}$ is given by

$$\sum_{\eta_1} \cdots \sum_{\eta_n}{}' b_{\eta_1 \ldots \eta_{p-t} \ldots \eta_n} = C_{\eta_{p-t}}^{(1)} \tag{114c}$$

Note that η_{p-t} is not summed in (114c). This results are indeed similar in form to Eqs. (113a) and (113b). The matrix elements of ρ_2 are given by

$$\begin{aligned} &\langle \eta_p' \eta_q' \mid \rho_2(p, q, t) \mid \eta_p'' \eta_q'' \rangle \\ &\quad = \sum_{\eta_{p-t}} \sum_{\eta_{q-t}} C_{\eta_{p-t},\, \eta_{q-t}}^{(2)} \langle \eta_p' \mid \eta, p, t \rangle\langle \eta, p, t \mid \eta_p'' \rangle \\ &\qquad \times \langle \eta_q' \mid \eta, q, t \rangle\langle \eta, q, t \mid \eta_q'' \rangle \end{aligned} \tag{115}$$

Here, $C^{(2)}_{\eta_{p-t}, \eta_{q-t}}$ is the sum of $b_{\eta_1 \cdots \eta_n}$ over all η's except η_{p-t} and η_{q-t}. If $C^{(2)}$ does not factor, the two-particle density matrix is not a tensor product; it cannot be reduced further. It would be very worthwhile to study the general case; for the present, however, just the factored case, which yields (113a–c), will be investigated further.

5.4. The Master Equation

In the quantum mechanical as in the classical master equation approach, the system is described by a probability function $\varphi(\eta_1', \ldots, \eta_n'; t)$, which gives the probability that object p is in eigenstate η_p' of the color operator Q_p. Since Q_p and $Q_{p'}$ commute, one can simultaneously specify all η_p'. The master equation gives the change of this function in time. The *independent* variables in φ are the *eigenvalues* of the color operators. A superposition of color states does not occur in the master description. The model is characterized by $P(\eta \mid \eta') \equiv P(\eta_1, \ldots, \eta_n \mid \eta_1', \ldots, \eta_n')$, which gives the transition probability from state $\eta_1' \ldots \eta_n'$ to $\eta_1 \ldots \eta_n$ in a unit time. The independence of the balls shows that P has a product structure:

$$P(\eta_1, \ldots, \eta_n \mid \eta_1', \ldots, \eta_n') = \prod_p P_1(\eta_p \mid \eta'_{p-1}) \tag{116}$$

The model rules assert the following:

(a) If point $p - 1$ is not marked, η_p and η'_{p-1} are the same:

$$P_1(\eta_p \mid \eta'_{p-1}) = \delta_{\eta_p, \eta'_{p-1}} \tag{117a}$$

(b) If point p is marked, η_p and η_{p-1} are different with probability λ:

$$P_1(\eta_p \mid \eta'_{p-1}) = \lambda(1 - \delta_{\eta_p, \eta'_{p-1}}) + (1 - \lambda)\, \delta_{\eta_p, \eta'_{p-1}} \tag{117b}$$

Since points are marked with probability μ, all the rules are collected in the expression for P_1:

$$P_1(\eta_p \mid \eta'_{p-1}) = (1 - 2\lambda\mu)\, \delta_{\eta_p, \eta'_{p-1}} + \lambda\mu \tag{117c}$$

The quantum mechanical master equation is

$$\varphi(\eta_1, \ldots, \eta_n; t + 1) = \sum_{\eta_1'} \cdots \sum_{\eta_n'} P(\eta_1, \ldots, \eta_n \mid \eta_1', \ldots, \eta_n')\, \varphi(\eta_1', \ldots, \eta_n'; t) \tag{118}$$

with P given by (116) as a product of n factors, with P_1 given in turn by (117c). The form (117c) contains exactly the same information as the classical expression (57a). It is written slightly differently, but it can be directly checked that (117c) is identical in content with the form

$$P_1(\eta_p \mid \eta'_{p-1}) = \tfrac{1}{2}[1 + \eta'_{p-1}\eta_p(1 - 2\lambda\mu)] \tag{117d}$$

(117d) is exactly the classical expression. The basic transition probability is the same in the classical and quantum mechanical master equations; the structure of the equations (118) and (57c) is also identical; hence all classical results obtained in Section (3.3) can be carried over without further change. Because of this identity, it is not really necessary to discuss (118) further. However, a few observations might be useful.

It is straightforward to check[27] that (118) possesses a factorization property; that is, if

$$\varphi(\eta_1, \ldots, \eta_n ; 0) = \prod_p \varphi_1(\eta_p, 0) \tag{119a}$$

then

$$\varphi(\eta_1, \ldots, \eta_n ; t) = \prod_p \varphi_1(\eta_p, t) \tag{119b}$$

where $\varphi_1(\eta_p, t)$ is given by

$$\varphi_1(\eta_p, t) = \sum_{\eta_{p-1}} \sum_{\eta_{p-2}} \cdots \sum_{\eta_{p-t}} P_1(\eta_p \mid \eta_{p-1}) \cdots P_1(\eta_{p-t+1} \mid \eta_{p-t})\, \varphi(\eta_{p-t}, 0) \tag{119c}$$

Thus if φ is factored initially, it remains factored for all times. (This is in marked contrast to the Liouville equation, where correlations are set up in time, even if the initial configuration is uncorrelated.)

Since the master equation can be solved for *arbitrary* initial conditions [see either (32a), (32c), or (50b)], it is not necessary to impose the initial factorization as expressed by (119a). *If*, however, one assumes that

$$\varphi_1(\eta_p, 0) = \tfrac{1}{2} + 2^{n-1} b_p \eta_p, \qquad \varphi(\eta, 0) = \prod_p \varphi_1(\eta_p) \tag{120}$$

it can be shown easily [combining (119c) and (117c)] that $\varphi_1(\eta_p, t)$ is given by

$$\varphi_1(\eta_p, t) = \tfrac{1}{2} + 2^{n-1} b_{p-t} \eta_p (1 - 2\lambda\mu)^t \tag{121}$$

This expression can be used in (119b) to give

$$\varphi(\eta_1, \ldots, \eta_n ; t) = 2^{-n} + (1 - 2\lambda\mu)^t \sum_p b_p \eta_{p+t}$$
$$+ (1 - 2\lambda\mu)^{2t} \sum_{p<q} b_p b_q \eta_{p-t} \eta_{q+t} \tag{122}$$

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[27] This can be done most easily by iteration of (118), using the initial condition (119a).

This result is of course the same as that obtained before [Eq. (32a)]: however, it is instructive to see how the initial factorization simplifies the calculation. The formulas given [(122) for the Master equation and (113) for the Liouville equation)] solve the quantum mechanical model for factored initial conditions.

5.5. The ϵ Averaging of ρ_1 [28]

The results obtained for the one- and two-particle density matrices depend through the operators E explicitly on the ϵ variables. As in the classical case, the quantities of physical interest (also those to be compared with the master description) are the ϵ averages of the observables. Since the matrix elements of the density matrix represent probabilities, these are the entities to be averaged. This is to be contrasted with the procedure used for (4.3), where amplitudes were computed and squared, and then the ϵ average was taken. Although the procedure is different, the physical principle is the same: the ϵ average is to be taken after the observables are obtained. To carry out this averaging process in a convenient manner, it is best to present a reinterpretation of the matrix elements of the one-particle density matrix. Using the abbreviation

$$O_p(\epsilon) \equiv E_{p-1} \cdots E_{p-t} \tag{123}$$

these matrix elements can be written as

$$\langle\eta_p'|\rho_1(p,t)|\eta_p''\rangle = \sum_\eta b_\eta \langle\eta_p'|O_p(\epsilon)|\eta\rangle\langle\eta|O_p(\epsilon)|\eta_p''\rangle \tag{124}$$

Here, η_p' and η_p'' are color eigenstates: the summation over η is a sum over the states present in the initial ensemble [see (102) and (108a)]. The matrix element

$$\langle\eta_p'|O_p(\epsilon)|\eta\rangle = \langle\eta_p'|E_{p-1}\cdots E_{p-t}|\eta, p-t\rangle$$

is to be understood in the following sense: $|\eta, p-t\rangle$ is a state in the $(p-t)$th color subspace: E_{p-t} acting on it produces a vector in the $(p-t+1)$-dimensional subspace, and E_{p-t+1} acts on it, etc. Thus, O_p acting on $|\eta, p-t\rangle$ yields a vector in the pth subspace; its scalar product with η_p' is the entity occurring in (124). The matrix element (124) can be further simplified by introducing the initial density matrix in the $(p-t)$th subspace as was done in (102):

$$r_{p-t}(0) = \sum_\eta b_\eta |\eta, p-t, 0\rangle\langle\eta, p-t, 0| \tag{125}$$

---

[28] This section contains a rather detailed description of the ϵ averaging. Anyone primarily interested in the physical applications could skip the details and just note the general method and results.

Equation (125) combined with (124) yields

$$\langle \eta_p' \,|\, \rho_1(p, t) \,|\, \eta_p'' \rangle = \langle \eta_p' \,|\, O_p(\epsilon)\, r_{p-t}(0)\, O_p^{-1}(\epsilon) \,|\, \eta_p'' \rangle \tag{126}$$

This formal result was obtained before; it is no more than a recasting of the matrix elements of the one-particle density matrix. For the present purposes, it is important to note the following interpretation of (126). Consider $r_{p-t}(0)$ as a 2×2 matrix whose matrix elements are

$$\langle \eta_{p-t}' \,|\, r_{p-t}(0) \,|\, \eta_{p-t}'' \rangle = \sum_{\eta} b_{\eta} \langle \eta_{p-t}' \,|\, \eta, p - t, 0 \rangle \langle \eta, p - t, 0 \,|\, \eta_{p-t}'' \rangle \tag{127}$$

η_{p-t}' and η_{p-t}'' are color eigenstates in the $(p - t)$th subspace [given by

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

as always]. The sum over η *has* to be over a complete set, which again could be the eigenstates

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

but this is not necessary. One can now, by direct calculation, verify the identity[29]

$$\langle \eta' \,|\, OrO^{\dagger} \,|\, \eta'' \rangle = \sum_{\eta} b_{\eta} \langle \eta' \,|\, O \,|\, \eta \rangle \langle \eta \,|\, O^{\dagger} \,|\, \eta'' \rangle \tag{128a}$$

This is valid for an arbitrary operator O. The right-hand side is identical in form and interpretation with (124). The left-hand side contains $OrO^{\dagger}$, which to be understood as an ordinary matrix product of 2×2 matrices; the matrix r is given by (127). Further, calling $OrO^{\dagger} = M$, the left-hand side of (128a) is to be understood as:

$$\langle \eta' \,|\, M \,|\, \eta'' \rangle = (\eta_1', \eta_2')(M)\begin{pmatrix} \eta_1'' \\ \eta_2'' \end{pmatrix} \tag{128b}$$

Combining (123), (124), and (128a) leads to the result

$$\rho_1(p, t) = E_{p-1} \cdots E_{p-t} r_{p-t}(0)\, E_{p-t}^{\dagger} \cdots E_{p-1}^{\dagger} \tag{129}$$

where now ρ_1 is an *ordinary matrix*[30] product of $(2t + 1)$ two-dimensional matrices with $r_{p-t}(0)$ given by (127). It is easy to show from (127) that r has the form

$$r_p(0) = \begin{pmatrix} \frac{1}{2} + c_p & z \\ z^* & \frac{1}{2} - c_p \end{pmatrix} \tag{130a}$$

---

[29] For convenience in writing, the indices have been omitted in (128a).

[30] The matrix form of E_p is given by (62) and (63d), or (132a).

Here, z is an arbitrary complex number, and c_p is real, $-\frac{1}{2} \leqslant c_p \leqslant \frac{1}{2}$. If the states η which are summed over in (127) are themselves color eigenstates, r_p reduces to

$$r_p(0) = \begin{pmatrix} \frac{1}{2} + c_p & 0 \\ 0 & \frac{1}{2} - c_p \end{pmatrix} \tag{130b}$$

The sum over η in (127) is a sum over those states that occur in the initial ensemble. Since it was assumed that the initial density matrix was diagonal in the color representation [see Eq. (80)], the states occurring in the initial ensemble are indeed color eigenstates. Thus, the form (130b) of r_p is the appropriate one to use.

The great advantage of the explicit matrix form of $\rho_1(p, t)$ is that now the ϵ averaging can be carried directly out:

$$\langle\rho_1(p, t)\rangle_\epsilon = \sum_{\epsilon_1} \cdots \sum_{\epsilon_n} P(\epsilon_1, \ldots, \epsilon_n)\, E_{p-1} \cdots E_{p-t} r_{p-t}(0)\, E_{p-t}^\dagger \cdots E_{p-1}^\dagger \tag{131}$$

The ϵ variables are contained in the E matrices; $P(\epsilon_1, \ldots, \epsilon_n)$ is the probability for a particular marker configuration. Although it would be possible using the expression (8) for P to evaluate (131), it is simpler and clearer to follow the method used previously in Section (4.3). Recall that the matrix expression for E_p is given by[31]

$$E_p = \tfrac{1}{2}(1 + \epsilon_p)\, 1 + \tfrac{1}{2}(1 - \epsilon_p)\, S \tag{132a}$$

$$S = \begin{pmatrix} (1-\lambda)^{1/2} & \lambda^{1/2} \\ -\lambda^{1/2} & (1-\lambda)^{1/2} \end{pmatrix} \tag{132b}$$

Further, S can be diagonalized by a unitary matrix U:

$$U = (1/\sqrt{2})\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \tag{132c}$$

$$S = UDU^{-1} \tag{132d}$$

$$D = \begin{pmatrix} \Lambda & \\ & \Lambda^* \end{pmatrix} \tag{132e}$$

$$\Lambda = (1-\lambda)^{1/2} + i\lambda^{1/2} \tag{132f}$$

To carry out the ϵ averaging of the product of matrices in (129), assume first that of the t points, $p - 1$ to $p - t$, exactly s are marked. The unmarked points yield E factors of unity [see (132a)]; each marked point contributes an S. Hence for s marked points, ρ_1 becomes

$$\rho_1(p, t, s) = S^s r_{p-t}(0)\, S^{-s} \tag{133}$$

---

[31] This is the identical nomenclature used in Section 4.3. It is repeated here to facilitate reading.

The average of ρ_1 is obtained by multiplying $\rho_1(p, t, s)$ by the probability that of the t points, s are marked, and summing over $s = 1, \ldots, t$. Therefore

$$\langle \rho_1(p, t) \rangle_\epsilon = \sum_{s=0}^{t} [t!/s!\,(t-s)!]\, \mu^s (1-\mu)^{t-s}\, S^s r_{p-t}(0)\, S^{-s} \tag{134}$$

The remainder of the calculation consists in evaluating the matrix product and performing the sum over s. Since S can be diagonalized by U, the calculation of S^s is straightforward and yields

$$S^s = \operatorname{Re} \left\{ \Lambda^s \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \right\} \tag{135a}$$

Using this result, matrix multiplication gives

$$S^s r_{p-t}(0)\, S^{-s} = \tfrac{1}{2}1 + \operatorname{Re}(c_{p-t} \Lambda^{2s} \sigma_0) \tag{135b}$$

Here, the form (130b) was used for the matrix r. The σ_0 is a 2×2 matrix (which will occur frequently)

$$\sigma_0 = \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix} \tag{136}$$

The matrix occurring in (134) has the simple form (135b). Of special importance is the simple s dependence of the matrix. Its occurrence as a power Λ^{2s} allows the application of the binomial theorem to obtain the sum in (134), with the result

$$\langle \rho_1(p, t) \rangle_\epsilon = \tfrac{1}{2}1 + c_{p-t} \operatorname{Re}\{[1 - 2\lambda\mu + 2i\mu(\lambda - \lambda^2)^{1/2}]^t \sigma_0\} \tag{137}$$

This is the final result for the one-particle density matrix; it is given here as a 2×2 matrix. All questions dealing with the one-particle distribution can be answered by (137).

5.6. The ϵ Averaging of ρ_2 [32]

Before calculating the ϵ average of ρ_2, it is useful to collect two results. Note first that (134) and (137) can be combined to give the sum formula

$$\langle \rho_1(p, t) \rangle_\epsilon = \sum_{s=0}^{t} [t!/s!\,(t-s)!]\, \mu^s (1-\mu)^{t-s}\, S^s r_{p-t}(0)\, S^{-s}$$

$$= \tfrac{1}{2}1 + c_{p-t} \operatorname{Re}\{R^t \sigma_0\} \tag{138a}$$

$$R \equiv 1 - 2\lambda\mu + 2i\mu(\lambda - \lambda^2)^{1/2} \tag{138b}$$

---

[32] See footnote 28 as the start of Section 5.5. The calculations in this section are somewhat long, a little tricky, and quite tedious. Some details are omitted.

This sum formula is valid for all values of t and all p. The second observation deals with the evaluation of the matrix product $S^s r_{p-t}(0)\,S^{-s}$. The same procedure [use of (132d)] can be employed to obtain another matrix product:

$$S^s\langle\rho_1(p,t)\rangle_\epsilon S^{-s} = \tfrac{1}{2}1 + c_{p-t}\,\mathrm{Re}(R^t\Lambda^{2s}\sigma_0) \tag{139}$$

Both these results will be needed; Λ is given by (132f).

The discussion leading to (129) for the one-particle density matrix can be repeated for the two-particle density matrix, so that ρ_2 can be written as

$$\begin{aligned}\rho_2(q,p,t) = {} & E_{q-1}\cdots E_{q-t}r_{q-t}(0)\,E_{q-t}^\dagger\cdots E_{q-1}^\dagger\\ & \otimes E_{p-1}\cdots E_{p-t}r_{p-t}(0)\,E_{p-t}^\dagger\cdots E_{p-1}^\dagger\end{aligned} \tag{140}$$

ρ_2 appears as a tensor product; each factor is an ordinary product of matrices. In (140), p is assumed larger than q; p, q, and t are given and fixed. The locations occurring in (140) are the points labeled $p-1,\ldots,q-t$. Divide this set of points into three nonintersecting sets:

(I) Points $p-1, p-2,\ldots,$ up to and including q.

(II) Points $q-1, q-2,\ldots,$ up to and including $p-t$.

(III) Points $p-t-1,\ldots,$ up to and including $q-t$.

It is clear that set I will contain just matrices of the p chain, set III will contain just matrices of the q chain, while set II may contain matrices of both chains. If set II is not empty, there will be overlap between the chains. Whether the chains overlap depends on p, q, and t:

$$p-t \geqslant q, \qquad t \leqslant p-q \qquad \text{no overlap} \tag{141}$$

$$p-t < q, \qquad t > p-q \qquad \text{overlap} \tag{142}$$

Consider now a marker arrangement with s_1 markers in region I, s_2 in II, and s_3 in III. Since the E matrix for a marked point is just S, ρ_2 for this particular configuration becomes

$$\begin{aligned}\rho_2(q,p,t,s_1,s_2,s_3) = {} & S^{s_3}S^{s_2}r_{q-t}(0)\,S^{-s_2}S^{-s_3}\\ & \otimes S^{s_2}S^{s_1}r_{p-t}(0)\,S^{-s_1}S^{-s_2}\end{aligned} \tag{143}$$

Writing the product of S operators as S^{s_3}, S^{s_2} is done only to indicate the origin of the factors; these factors commute, of course. To obtain the ϵ

average of ρ_2 . $\rho_2(p, q, t, s_1, s_2, s_3)$ must be multiplied by the probability of this marker distribution and summed over s_1 . s_2 . s_3 :

$$\begin{aligned}\langle\rho_2(q, p, t)\rangle_\epsilon = \sum_{s_1=0}^{p-q} \sum_{s_2=0}^{q-p+t} \sum_{s_3=0}^{p-q} & \frac{(p-q)!}{s_1!\,(p-q-s_1)!}\,\mu^{s_1}(1-\mu)^{p-q-s_1} \\ & \times \frac{(q-p+t)!}{(q-p+t-s_2)!\,s_2!}\,\mu^{s_2}(1-\mu)^{q-p+t-s_2} \\ & \times \frac{(p-q)!}{s_3!\,(p-q-s_3)!}\,\mu^{s_3}(1-\mu)^{p-q-s_3} \\ & \times S^{s_3}S^{s_2}r_{q-t}(0)\,S^{-s_2}S^{-s_3} \otimes S^{s_2}S^{s_1}r_{p-t}(0)\,S^{-s_1}S^{-s_2} \qquad (144)\end{aligned}$$

The complexity in this formula clearly stems from the s_2 summation. which contains contributions from both factors in the tensor product.

In the case of *no* overlap, region II is empty, $s_2 = 0$, and the summations over s_1 and s_3 can be performed separately (note that in this case. s_1 and s_3 both run from 1 to t); using (138a), the result is simply

$$\langle\rho_2(q, p, t)\rangle_\epsilon = \langle\rho_1(q, t)\rangle_\epsilon \otimes \langle\rho_1(p, t)\rangle_\epsilon, \qquad t \leqslant p - q \qquad (145)$$

If there is no overlap. the averaged two-particle density matrix factors into a product of averaged one-particle density matrices, as could be anticipated. In the case that there is overlap (which will be assumed from now on). the s_1 and s_3 summations in (144) can still be carried out using (138). It is necessary to observe that the s_1 summation runs from 1 to $p - q$ in (144) instead of 1 to t in (138). Thus $\langle\rho_2\rangle_\epsilon$ simplifies to

$$\begin{aligned}\langle\rho_2(q, p, t)\rangle_\epsilon = \sum_{s_2=0}^{q-p+t} & \frac{(q-p+t)!}{(q-p+t-s_2)!\,s_2!}\,\mu^{s_2}(1-\mu)^{q-p+t-s_2} \\ & \times S^{s_2}\langle\rho_1(q, p-q)\rangle_\epsilon S^{-s_2} \otimes S^{s_2}\langle\rho_1(p, p-q)\rangle_\epsilon S^{-s_2} \qquad (146)\end{aligned}$$

Apart from the combinatorial factor, (146) contains precisely the matrix combination noted in (139). The purpose of the further reduction is to cast (146) in such a form that the s_2 summation can be performed. It is somewhat simpler to study the *correlation* function $X(q, p, t)$ instead of $\langle\rho_2\rangle_\epsilon$. The function X is defined by

$$X(q, p, t) = \langle\rho_2(q, p, t)\rangle_\epsilon - \langle\rho_1(q, t)\rangle_\epsilon \otimes \langle\rho_1(p, t)\rangle_\epsilon \qquad (147)$$

Substituting (139) in (146), constructing X as in (147), and using (138). there results

$$\begin{aligned}X(q, p, t) = c_{q-t}c_{p-t} \sum_{s_2=0}^{q-p+t} & \frac{(q-p+t)!}{(q-p+t-s_2)!\,s_2!}\,\mu^{s_2}(1-\mu)^{q-p+t-s_2} \\ & \times \{\mathrm{Re}(R^{p-q}\Lambda^{2s}\sigma_0) \otimes \mathrm{Re}(R^{p-q}\Lambda^{2s}\sigma_0) - \mathrm{Re}\, R^t\sigma_0 \otimes \mathrm{Re}\, R^t\sigma_0\} \\ & \qquad (148)\end{aligned}$$

Most of the calculation leading to (148) is routine manipulation; one does need the tensor product rule

$$(A + A') \otimes (B + B') = A \otimes B + A \otimes B' + A' \otimes B + A' \otimes B' \qquad (149a)$$

The terms occurring in (148) have an obvious enough origin; perhaps the only surprising feature is the absence of terms linear in c_{p-t}, which come in through (139) and (138a). For such terms, the s_2 sum can be evaluated; this shows that they indeed cancel. Equation (148) can be simplified further using the identity

$$\operatorname{Re} A \otimes \operatorname{Re} B = \tfrac{1}{4}(A \otimes B + A \otimes B^* + A^* \otimes B + A^* \otimes B^*) \qquad (149b)$$

Applying (149b) to the bracket in (148) gives

$$\{\cdots\} = \tfrac{1}{2}\operatorname{Re}\{(R^{2(p-q)}\Lambda^{4s_2} - R^{2t})\,\sigma_0 \otimes \sigma_0 + (|R|^{2(p-q)} - |R|^{2t})\,\sigma_0 \otimes \sigma_0^*\} \qquad (150)$$

At first sight, it may appear strange that the coefficients of $\sigma_0 \otimes \sigma_0$ and $\sigma_0 \otimes \sigma_0^*$ in (150) are not the same. One might expect $|R|^{2(p-q)}\,|\Lambda|^{4s_2}$ instead of $|R|^{2(p-q)}$ in the second term. This is in fact the case, but $|\Lambda| = 1$, as a glance at (132f) will show. With (150), the s_2 dependence is again a simple power, so that the sum over s_2 can be performed. If one resubstitutes the expression for R as given by (138a) in terms of Λ, noting that

$$R \equiv 1 - 2\lambda\mu - 2i\mu(\lambda - \lambda^2)^{1/2} = 1 - \mu + \mu\Lambda^2 \qquad (151)$$

the result of the summation is

$$\begin{aligned} X(q, p, t) = c_{q-t}c_{p-t}\operatorname{Re}\{&[1 - \mu + \mu\Lambda^2)^{2(p-q)}(1 - \mu + \mu\Lambda^4)^{t-p+q} \\ &- (1 - \mu + \mu\Lambda^2)^{2t}]\,\sigma_0 \otimes \sigma_0 + [|1 - \mu + \mu\Lambda^2|^{2(p-q)} \\ &- |1 - \mu + \mu\Lambda^2|^{2t}]\,\sigma_0 \otimes \sigma_0^*\} \end{aligned} \qquad (152)$$

Equation (152) gives X for times $t > p - q$. With (152) and (147), the two-particle density matrix is explicitly known; all questions concerning the two-particle distributions can be answered from (152).

The formulas (152) and (137) are perhaps the most important results of this paper, giving the exact one- and two-particle ϵ-averaged density matrices. In the next sections, the physical results which follow from these rather complicated expressions will be analyzed. To provide the model with some measure of physical relevance, the next section contains a "magnetic realization" of the model.

6. A MAGNETIC REALIZATION

The model rules of Section 4 were quantum mechanical versions of the rules of the classical models. As already noted in the introduction, these rules were abstracted from actual physical situations; however, the simplifications introduced were so drastic that it is not at all clear that the final models have anything to do with physics. It is therefore interesting to show that it is possible to construct a more or less realistic physical system which obeys the model rules set down in Section 4. The rules given there referred to the single-particle problem—this case will be considered first; the many-particle problem will be treated later.

Consider a straight line in the xy plane having a direction $\mathbf{e}$ given by

$$\mathbf{e} = \mathbf{e}_1 \cos \alpha + \mathbf{e}_2 \sin \alpha \tag{153}$$

The unit vectors in the x, y, z directions are $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$; α is the angle the line makes with the x axis. Assume that somewhere an origin is picked on this line; the line is divided into segments of size d. The distance s from the origin can be written as

$$s = qd + yd \tag{154}$$

Here, q is an integer 0, 1, 2,..... while y lies between 0 and 1. Imagine that a particle of spin 1/2 moves uniformly along this line. It moves as a classical particle with momentum p_e (momentum along e) and speed d/τ. It is also possible to consider this motion as a succession of steps of size d, each step taking a time τ. The trajectory may be considered as generated by the "Hamiltonian"

$$H_0 = p_e(d/\tau) \tag{155a}$$

The time-evolution operator for a time interval τ is

$$S_0 = e^{iH_0\tau} = e^{idp_e} \tag{155b}$$

S_0 describes the uniform motion of the particle along the line e. The particle has a spin $\frac{1}{2}$; hence it possesses a magnetic moment

$$\boldsymbol{\mu} = g\boldsymbol{\sigma} \tag{156}$$

g is the usual gyromagnetic ratio, $\boldsymbol{\sigma}$ is the Pauli matrix spin vector[33]:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{157}$$

---

[33] Notice that these σ matrices have nothing to do with the σ_0 matrix of the previous chapter. Notice further that $\hbar$ has been put equal to one.

Now introduce a magnetic field in the xy plane perpendicular to the line e. The magnitude of the field is a function of s, the distance along the classical path. The field is assumed to be [using (154)]

$$\mathbf{B}_q(s) = \tfrac{1}{2}(1 - \epsilon_q)\, B[\mathbf{e}_3 \times \mathbf{e}] \tag{158}$$

The field is in the xy plane, perpendicular to the direction of motion of the particle. ϵ_q is $+1$ or -1, as before. If $\epsilon_q = +1$, there is no magnetic field in the domain from qd to $(q + 1)\, d$. If $\epsilon_q = -1$, there is a magnetic field. Its magnitude is B; the vector product defines its direction. The magnetic interaction energy of the particle with the field is then [using (150) and (156)]

$$\begin{aligned} H_1 &= \tfrac{1}{2}(1 - \epsilon_q)\, gB\boldsymbol{\sigma} \cdot [\mathbf{e}_3 \times \mathbf{e}] \\ &= \tfrac{1}{2}(1 - \epsilon_q)\, gB(\sigma_y \cos\alpha - \sigma_x \sin\alpha) \end{aligned} \tag{159}$$

Because of the occurrence of the Pauli matrices, H_1 is a 2×2 matrix. The total Hamiltonian of the system is $H_0 + H_1$. The time-evolution operator for a time interval τ for this total system is [see (159) and (155a)]

$$S(\tau) = \exp[ip_0 d + \tfrac{1}{2}\tau g B(1 - \epsilon_q)(\sigma_y \cos\alpha - \sigma_x \sin\alpha)] \tag{160a}$$

Equation (160a) shows that the time-evolution operator splits up as a product; one factor S_0 describes the uniform motion along e, the other S_1 describes the interaction:

$$S_1 \equiv \exp[\tfrac{1}{2} i g\tau(1 - \epsilon_q)\, B(\sigma_y \cos\alpha - \sigma_x \sin\alpha)] \tag{160b}$$

The remaining discussion will just deal with the interaction. The known properties of the Pauli spin matrices make it possible to write S_1 as a 2×2 matrix

$$S_1(q) = \cos x_q + (i \sin x_q)(\sigma_y \cos\alpha - \sigma_x \sin\alpha) \tag{161a}$$

$$x_q \equiv \tfrac{1}{2}(1 - \epsilon_q)\, g\tau B \tag{161b}$$

Using the representation of the Pauli matrices (157), S_1 assumes the explicit form

$$S_1(q) = \begin{pmatrix} \cos x & (\sin x)\, e^{-i\alpha} \\ -(\sin x)\, e^{i\alpha} & \cos x \end{pmatrix} \tag{162}$$

If a point q is not marked, $\epsilon_q = 1$, so $x_q = 0$. In that case, (162) shows that S_1 for an unmarked point is unity. For a marked puint, $\epsilon_q = -1$, $x_q = g\tau B$.

Defining

$$\lambda = \sin^2(g\tau B), \qquad \lambda^{1/2} = \sin(g\tau B) \tag{163}$$

It is seen that S for a marked point has the form

$$S = \begin{pmatrix} (1-\lambda)^{1/2} & \lambda^{1/2}e^{-i\alpha} \\ -\lambda^{1/2}e^{i\alpha} & (1-\lambda)^{1/2} \end{pmatrix} \tag{164}$$

A glance at (63d) shows that this is precisely the time-evolution operator which the model rules required. The phase γ is just the angle $-\alpha$ which the line of motion makes with the x axis. If the motion of the particle is along the x axis, the phase disappears and S assumes the form used throughout this paper.

The physical picture which emerges is one where a particle of spin $\frac{1}{2}$, with a given initial spin, moves through a medium. At certain locations, there are ferromagnetic impurities producing local magnetic fields. These fields (in the xy plane) will produce changes in the spin state of the particle. If the initial state was assumed to be an eigenstate of the z component of the spin, the new state will no longer be an eigenstate of the z component, since the time-evolution operator contains the x and y components. One can compute and discuss the average of the spin in the z direction. The precise correspondence between model and example identifies the color eigenstates of the balls with the spin eigenstates of the particles; the markers correspond to local magnetic fields producing transitions; averaging over the markers corresponds to an average over all impurity locations. The approach to the color equilibrium is replaced by the depolarization of an initial beam of polarized particles. The most concrete physical picture which realizes this model is the depolarization of an initially polarized beam of neutrons which travels through a medium containing ferromagnetic impurities. The neutrons can be magnetically scattered. The time dependence of the polarization corresponds to the average number of balls of one color and requires the one-particle density matrix $\langle \rho_1 \rangle_\epsilon$. Spin–spin correlation functions would require a knowledge of $\langle \rho_2 \rangle_\epsilon$. One of the advantages of the magnetic version of the model is that it now becomes possible to introduce external fields in a natural way. A simple way to do this is to consider, instead of the field (158), which represented the internal field, a new field

$$\mathbf{B}_q = \tfrac{1}{2}(1-\epsilon_q)\,B[\mathbf{e}_3 \times \mathbf{e}] + F_q\mathbf{e}_3 \tag{165}$$

This clearly presents an additional field in the z direction. The new interaction energy is obtained in the obvious way; the magnetic part of the time evolution operator can be written (for a time interval τ) as

$$S = \exp\{i[x(\sigma_y \cos\alpha - \sigma_x \sin\alpha) + y\sigma_z]\} \tag{166a}$$

Here, x is the same as before[34]

$$x = x_q = \tfrac{1}{2}(1 - \epsilon_q)\, g\tau B_q \tag{166b}$$

$$y = y_q = g\tau F_q \tag{166c}$$

It is again possible, using the properties of the Pauli matrices, to write S as a 2×2 matrix similar to (161a):

$$\begin{aligned} S &= \cos r + i(\sin r)[(x/r)(\sigma_y \cos \alpha - \sigma_x \sin \alpha) + (y/r)\, \sigma_z] \\ r^2 &\equiv g^2\tau^2[\tfrac{1}{4}(1 - \epsilon_q)^2\, B^2 + F^2] \end{aligned} \tag{167}$$

Since all the essential physical features are already contained in the special case that $\alpha = 0$, this will be assumed.

Consider S for the case that $\epsilon_q = 1$, i.e., there is no local field. In the previous case, $S = 1$ if $\epsilon_q = 1$. In the present case, use of the explicit form of the Pauli matrices gives $S_+ \equiv S_q(\epsilon_q = +1)$:

$$S_+ = \begin{pmatrix} e^{ig\tau F} & 0 \\ 0 & e^{-ig\tau F} \end{pmatrix} \tag{168}$$

Thus the time development from a location without internal field is described by (168). The states do not remain unchanged under the action of S_+, but eigenstates remain eigenstate states. If

$$|\eta\rangle = c_1\,|\eta^+\rangle + c_2\,|\eta^-\rangle \tag{169a}$$

$$S_+\,|\eta\rangle = c_1 e^{ig\tau F}\,|\eta^+\rangle + c_2 e^{-ig\tau F}\,|\eta^-\rangle \tag{169b}$$

the probability of finding the spin up is $|c_1|^2$ in state $|\eta\rangle$; it is the same in the state $S_+\,|\eta\rangle$. The relative phases are changed by S_+, the probabilities are not. Hence the original model rule which required that the relative probabilities, for spins up or down, shall remain unchanged when spins move through an unmarked point (a point where there is no interaction) is still satisfied. This same rule is still valid when there is an additional outside field $\mathbf{F}_q\mathbf{e}_3$. If point q does possess a local field,

$$x = gB\tau \tag{170a}$$

$$y = gF\tau \tag{170b}$$

$$r^2 = x^2 + y^2 = g^2\tau^2(B^2 + F^2) \tag{170c}$$

$$\sin \varphi \equiv \frac{y}{r} = \frac{F}{(B^2 + F^2)^{1/2}} = \frac{F}{B}\left(1 - \frac{F^2}{2B^2} \cdots\right) \tag{170d}$$

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[34] Although x, y, B, and F all could depend on q (x always depends on q), the q index is often suppressed.

(170d) defines φ (the expansion is appropriate if the external field F is small compared to the internal field; it is obviously an expansion in powers of F/B).

It is straightforward to obtain the transition matrix $S_- \equiv S(\epsilon_\eta = -1)$ from (167) and (170a–d). The result can be written as

$$S_- = \begin{pmatrix} \cos r + i \sin \varphi \sin r & \cos\varphi \sin r \\ -\cos \varphi \sin r & \cos r - i \sin \varphi \sin r \end{pmatrix} \tag{171}$$

This is the form for the transition matrix if an outside field F is present. It should be contrasted with (162), which, written for the case $\alpha = 0$, is

$$S_-(F = 0) = \begin{pmatrix} \cos x & \sin x \\ -\sin x & \cos x \end{pmatrix} \tag{172a}$$

In the case $F = 0$, $y = 0$, $\varphi = 0$, and $x = r$; thus S_- reduces correctly to $S_-(F = 0)$. The introduction of $\lambda^{1/2} = \sin x$ transforms $S_-(F = 0)$ into the time-evolution matrix used throughout. If one introduces $\nu = 1 - \lambda$, the form of S becomes

$$S_-(F = 0) = \begin{pmatrix} \nu^{1/2} & (1 - \nu)^{1/2} \\ -(1 - \nu)^{1/2} & \nu^{1/2} \end{pmatrix} \tag{172b}$$

The expression for S_- with $F \neq 0$, Eq. (171), can be written in a very similar form by introducing

$$u^{1/2} = \cos r + i \sin \varphi \sin r \tag{173}$$

In terms of u, which is obviously complex, (171) can be written as

$$S_-(F) = \begin{pmatrix} u^{1/2} & (1 - |u|)^{1/2} \\ -(1 - |u|)^{1/2} & (u^*)^{1/2} \end{pmatrix} \tag{174}$$

It is clear that this matrix describes the same kind of process; $S_-(F)$ acting on a spin eigenstate yields a state which will be a mixture. The probability that *no* change has taken place is given by $|u|$ (this corresponds to $\nu = 1 - \lambda$ in the case where $F = 0$). The total time evolution is the result of many such actions. The explicit solubility of the $F = 0$ models depended on the fact that the $S_-(F = 0)$ matrix could be diagonalized by a matrix U which was *independent* of λ (or ν). Hence the action of many $S_-(F = 0)$ operators led to a power of a single matrix. The diagonalization becomes a good deal more involved for the case where S is given by (174).[35]

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[35] The projection techniques developed in a different context(19) allow an explicit solution of this case as well. The results are contained in a forthcoming publication.

It is clear, however, that the formalism given immediately suggests an approximation procedure in terms of powers of B/F. The matrix S_- can be expanded as a sum of matrices, assuming φ is small. Ordinary perturbation calculus can then be employed to obtain the response of the system to outside fields. Thus apart from providing an interesting example of the models, the magnetic realization also points to natural and hopefully useful extensions and modifications

7. COMPARISON OF THE RESULTS; CONCLUSION

7.1. General Remarks

The study presented in this paper dealt with various different ways of describing a particular model. In these discussions, the relationship between the different treatments is always of considerable importance. All the appraoches are designed to calculate the same physical quantities; since all led to equations which could be explicitly and rigorously solved, a direct comparison becomes possible. It is instructive to consider a few simple cases in some detail. It should be recalled that the descriptions are on the classical master level, described by (normalized) functions $F_p^1(\alpha, t)$, $F_{q,p}^2(\alpha, \beta, t)$. Alternately, there is the classical Liouville level ϵ-averaged, whose functions are denoted by $\langle f_p^1(\alpha, t)\rangle_\epsilon$, $\langle f_{q,p}^2(\alpha, \beta, t)\rangle_\epsilon$. On either level, one can have a stochastic element λ in the description: this λ is usually written near the formula. In the quantum case, there are again the master level functions $\varphi_p(\eta', t)$ and the Liouville level characterized by $\langle \rho_1(p)\rangle_\epsilon$ and $\langle \rho_2(q, p, t)\rangle_\epsilon$. To make the discussion concrete, *two* special problems will be considered on *all* levels.

Assume that the initial state ($t = 0$) is a state where all the spins[36] are in $+z$ eigenstates. (In the color language, all objects are known with certainty to have the same color.) The questions to be considered are as follows:

1. What is the probability that at time t, the spin at p is in the $+z$ direction?
2. What is the probability that at time t, the spin at p and the spin at q are both in the $+z$ direction?

Since the classical functions are already normalized, these are probabilities; hence question 1 requires the knowledge of $F_p^1(1, t)$ on the master level and $\langle f_p^1(1, t)\rangle_\epsilon$ on the Liouville level. Recall that the values of the

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[36] In this section, the model language and the language of the magnetic example will be used interchangeably.

classical variables indicate the color. The fact that the initial color was with certainty 1 is expressed by

$$F_p{}^1(1, 0) = 1 \tag{175a}$$

$$\langle f_p{}^1(1, 0)\rangle_\epsilon = 1 \tag{175b}$$

In the quantum case, probabilities are the matrix elements of the density matrix. Denote the color eigenstate by $|1\rangle$; then the probability that at time t, the color at p is $|1\rangle$ is determined by

$$\langle 1 \mid \rho_1(p, t) \mid 1\rangle_\epsilon \tag{176a}$$

In the master formulation, this same probability is given by $\varphi_p(\eta_p{}' = 1, t)$. The determination of the joint probabilities needed in question 2 demands a knowledge of the two-particle functions. On the master level, for example, one needs $F^2_{q,p}(1, 1, t)$. The quantum discussion consists in the calculation of $\langle 1 \otimes 1 \mid \rho_2(q, p, t) \mid 1 \otimes 1\rangle$. Since the general form of these entities is known, the detailed computation consists in evaluating these quantities for the specified initial condition and giving the independent variables numerical values, or calculating certain matrix elements.

7.2. The One-Particle Problem

The quantity which is calculated throughout in this section is the probability that at time t, the ball at p is white ($\alpha = 1$), but this *same* physical quantity is written in different ways, indicating the level of its calculation. The relevant formulas are (18), (32b), (48b), (58a), (75b), (121), and (137). The initial condition imposed yields for the classical coefficients [see (12)].

$$b_p = 1/2^n, \qquad p = 1,\ldots, n \tag{176b}$$

The initial condition gives for the coefficients c in (130b) the result

$$c_p = \tfrac{1}{2}, \qquad p = 1,\ldots, n \tag{176c}$$

With these coefficients, one obtains

$$F_p{}^1(1, t) = \tfrac{1}{2} + \tfrac{1}{2}(1 - 2\mu)^t \tag{177}$$

$$\langle f_p{}^1(1, t)\rangle_\epsilon = \tfrac{1}{2} + \tfrac{1}{2}(1 - 2\mu)^t \tag{178}$$

$$F_p{}^1(1, t) = \tfrac{1}{2} + \tfrac{1}{2}(1 - 2\lambda\mu)^t, \qquad \lambda \neq 1 \tag{179}$$

$$\langle f_p{}^1(1, t)\rangle_\epsilon = \tfrac{1}{2} + \tfrac{1}{2}(1 - 2\lambda\mu)^t, \qquad \lambda \neq 1 \tag{180}$$

$$\varphi_1(\eta_p{}^1 = 1, t) = \tfrac{1}{2} + \tfrac{1}{2}(1 - 2\lambda\mu)^t \tag{181}$$

$$\langle 1 \mid \rho_1(p, t) \mid 1\rangle_\epsilon = \tfrac{1}{2} + \tfrac{1}{2}\,\mathrm{Re}[1 - 2\lambda\mu + 2i\mu(\lambda - \lambda^2)^{1/2}]^t \tag{182}$$

Thus the *one*-particle probability distribution is the *same* for the classical master and Liouville equations, as well as the quantum mechanical master equation. The introduction of a stochastic element (λ) does *not* change the general character of the distribution function. In fact, the classical master equation with a stochastic element is precisely the same as the quantum master equation. The distribution functions approach the equilibrium state monotonically. The equilibrium state is a state where there are as many spins up as down; the beam is depolarized.

Expression (182), which gives the same quantity derived from the quantum Liouville equation, shows a drastically different behavior. It is still true that as $t \to \infty$, the system approaches equilibrium. To see this explicitly, write

$$1 - 2\mu\lambda + 2i\mu(\lambda - \lambda^2)^{1/2} = R_0 e^{i\theta} \tag{183a}$$

$$R_0^2 \equiv 1 - 4\mu\lambda(1 - \mu) \tag{183b}$$

$$\tan\theta = 2\mu(\lambda - \lambda^2)^{1/2}/(1 - 2\mu\lambda) \tag{183c}$$

The probability (182) then becomes:

$$\langle 1 \mid \rho_1(p, t) \mid 1 \rangle_\epsilon = \tfrac{1}{2} + \tfrac{1}{2} R_0^t \cos t\theta \tag{184}$$

It is easy to check that if $0 < \mu < 1$ and $0 < \lambda < 1$, $|R_0| < 1$. Consequently as $t \to \infty$, $R_0^t \to 0$, hence the probability approaches $\frac{1}{2}$ as $t \to \infty$. However, the approach is oscillatory, the frequency of the equally spaced oscillations is [see (183a–c)]

$$\nu_0 = (1/2\pi) \tan^{-1}[2\mu(\lambda - \lambda^2)^{1/2}/(1 - 2\mu\lambda)] \tag{185}$$

The system exhibits an *oscillatory* approach to equilibrium. This is a rather unusual phenomenon; it would mean, for example, that in the process of the depolarization of a polarized beam of particles, the value of the polarization would change from positive to negative and oscillate with decreasing amplitude and frequency given by (185) around its equilibrium value. It is clear that if any real significance can be attributed to this behavior, the master equation description is totally inadequate. It does not contain any oscillations at all. Presumably, the stochastic dynamical elements contained in the master equation have averaged out the actual oscillatory character inherent in the system.

It is interesting to observe how essential is the fact that $\lambda = 1$. It is clear that if $\lambda = 1$, $\nu_0 = 0$; furthermore, if $\lambda = 1$, Eq. (182) reduces to the classical expressions. Physically, $\lambda \neq 1$ means that the action of an impurity (a marker) on the spin states causes a spin eigenstate to go over in a *superposition* of eigenstates, not a single one. If λ were equal to 1, the state of the system at any time would be a tensor product of pure spin eigenstates. The fact that $\lambda \neq 1$ is what causes the mixing of the states. Since it is known that magnetic fields acting on spins do produce mixtures of eigenstates, it follows that the model rules correctly describe the quantum situation. For example, such processes as magnetic depolarization should be described in this manner. It further follows that the time evolution of such a process *cannot* be described by a master equation.

Remark. There does not seem to exist a simple process which produces the master result from the Liouville equation. Simple averaging, for example, does not eliminate the oscillations. The model rules do *not* determine the transition matrix S uniquely, but instead have a phase undetermined (see (63)d]. Thus it might appear that if one uses for S the expression

$$S = \begin{pmatrix} (1-\lambda)^{1/2} & e^{i\gamma}\lambda^{1/2} \\ -e^{-i\gamma}\lambda^{1/2} & (1-\lambda)^{1/2} \end{pmatrix} \tag{186}$$

and averages the final observables over γ, the quantum mechanical oscillations would indeed disappear.[37] This is a straightforward calculation (patterned after Section 4.3); however, the oscillations do not disappear; the final answer is again (182). This is physically to be expected from the magnetic example. The phase in that example indicates the direction of the trajectory in the xy plane. The magnetic field $\mathbf{B}$ is perpendicular to that line. If the line changes its orientation, so does $\mathbf{B}$; but $\mathbf{B}$ lies always (for any γ) in the xy plane; hence it is *always* in a plane perpendicular to the direction of the spin. The probability of a spin flip produced by a field in a plane perpendicular to the spin depends on the magnitude of the field, but not on the orientation of the field vector in that plane. Hence, all angles γ in S produce the same admixture of spin eigenstates. Averaging over the angle γ can then not have any effect. This is also shown by the explicit calculation.

7.3. The Two-Particle Distribution Functions

The quantity calculated in this section is the probability that at time t, the spin at p is up and the spin at q is also up. This is a *joint* probability. The necessary formulas are (19), (32c), (56), (58b), (122), (137), (147), and (152).

As before, it is only necessary to evaluate the constants from the initial data and substitute the values of the variables (in the classical case), or take the matrix elements (in the quantum case), It should be mentioned that the

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[37] It is not uncommon that an averaging of quantum mechanical phases leads to a classical result.

coefficients b_{pq} occurring in (19) and (32c) are by virtue of the initial conditions given by

$$b_{qp} = 1/2^n, \qquad q, p = 1, \ldots, n \tag{187}$$

The results in the usual notation are

$$F^2_{q,p}(1, 1, t) = \tfrac{1}{4} + \tfrac{1}{2}(1 - 2\mu)^t + \tfrac{1}{4}(1 - 2\mu)^{2t} \tag{188}$$

$$\langle f^2_{q,p}(1, 1, t)\rangle_\epsilon = \tfrac{1}{4} + \tfrac{1}{2}(1 - 2\mu)^t + \tfrac{1}{4}(1 - 2\mu)^{2t}, \qquad t \leqslant p - q \tag{189}$$

$$\langle f^2_{q,p}(1, 1, t)\rangle_\epsilon = \tfrac{1}{4} + \tfrac{1}{2}(1 - 2\mu)^t + \tfrac{1}{4}(1 - 2\mu)^{2(p-q)}, \qquad t > p - q \tag{190}$$

$$F^2_{q,p}(1, 1, t) = \tfrac{1}{4} + \tfrac{1}{2}(1 - 2\lambda\mu)^t + \tfrac{1}{4}(1 - 2\lambda\mu)^{2t} \tag{191}$$

$$\langle f^2_{q,p}(1, 1, t)\rangle_\epsilon = \tfrac{1}{4} + \tfrac{1}{2}(1 - 2\lambda\mu)^t + \tfrac{1}{4}(1 - 2\lambda\mu)^{2t}, \qquad t \leqslant p - q \tag{192}$$

$$\begin{aligned}\langle f^2(1, 1, t)\rangle_\epsilon &= \tfrac{1}{4} + \tfrac{1}{2}(1 - 2\lambda\mu)^t \\ &\quad + \tfrac{1}{4}(1 - 2\lambda\mu)^{2(p-q)}\,[1 - 4\mu\lambda(1 - \lambda)]^{q-p+t}, \qquad t > p - q\end{aligned} \tag{193}$$

$$\begin{aligned}&\langle 1, 1 \mid X(q, p, t) \mid 1, 1\rangle \\ &\quad = \tfrac{1}{4}\mathrm{Re}[(1 - \mu + \mu\Lambda^2)^{2(p-q)}\,(1 - \mu + \mu\Lambda^4)^{t-p+q} \\ &\qquad - (1 - \mu + \mu\Lambda^2)^{2t} + |1 - \mu + \mu\Lambda^2|^{2(p-q)} - |1 - \mu + \mu\Lambda^2|^{2t}]\end{aligned} \tag{194}$$

$$\begin{aligned}&\langle 1, 1 \mid \rho_2(q, p, t) \mid 1, 1\rangle \\ &\quad = \langle 1, 1 \mid X \mid 1, 1\rangle + \langle 1 \mid \rho_1(q, t) \mid 1\rangle\langle 1 \mid \rho_1(p, t) \mid 1\rangle\end{aligned} \tag{195}$$

$$\varphi_2(\eta_q{}' = 1, \eta_p{}' = 1; t) = \tfrac{1}{4} + \tfrac{1}{2}(1 - 2\lambda\mu)^t + \tfrac{1}{4}(1 - 2\lambda\mu)^{2t} \tag{196}$$

These joint probabilities show a great deal more variety in behavior than the single probabilities. Perhaps more important is the fact that the joint probabilities give much more detailed information about the system than do the single distribution functions. The master equations, both classical (188) and quantum mechanical (196), give, as always, the ordinary monotonic approach to equilibrium. The agreement between the classical Liouville equation and the classical master equation holds only for limited times[38] $t \leqslant p - q$ [see (189) and (190)]. Particularly noteworthy and new is the existence of *persistent* correlations as $t \to \infty$:

$$\langle f^2_{qp}(1, 1, t)\rangle_\epsilon \to \tfrac{1}{4} + \tfrac{1}{4}(1 - 2\mu)^{2(p-q)}$$

One would expect naively that f^2 approaches $\tfrac{1}{4}$. It is interesting that the introduction of a classical stochastic element leads to Eq. (193) for f^2, which,

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[38] It is interesting to note that these times of agreement get longer as the spins involved are farther apart.

although distinct from F^2, has at least the good taste to go to equilibrium as $t \to \infty$. Apparently the continued operation of the stochastic dynamics destroys the correlations. The quantum expression shows oscillations, as before; however, there are persistent correlations as well. Because of the presence of two different terms, $(1 - \mu + \mu\Lambda^2)$ and $(1 - \mu + \mu\Lambda^4)$, the time development of $\langle 1, 1, | X | 1, 1\rangle$ contains two distinct frequencies. The detailed analysis of Eq. (194) shows that there are beat frequencies as well. Both terms mentioned are less than one; this allows the long-time limit to be obtained rather easily. One finds

$$\lim_{t \to \infty} \langle 1, 1 \mid \rho_2(q, p, t) \mid 1, 1\rangle = \tfrac{1}{4} + \tfrac{1}{4}[1 - 4\lambda\mu(1 - \mu)]^{p-q} \tag{197}$$

This is the remaining persistent correlation. In the case $\lambda = 1$. Eq. (197) reduces to the classical result given in (190). Even so, it is somewhat surprising that the introduction of a *classical* stochastic element such as λ eliminates the persistent correlation giving f^2 a reasonable asymptotic behavior, while the quantum mechanical problem with $\lambda \neq 1$ still has a persistent correlation. This may seem strange in view of the comments made in connection with the classical case: The persistent correlations are destroyed by the continued operation of a stochastic element, as (193) shows explicitly. The explanation, which contains the essence of the difference between the classical and quantum descriptions, lies in the fact that in the quantum model with $\lambda \neq 1$, the dynamics as such does not contain any stochastic elements. There is a well-defined Hamiltonian and λ is determined by the system. In the magnetic example, λ is determined by the field: $\lambda = \sin^2(g\tau B)$. The interaction is given and fixed. The problem is an ordinary quantum mechanical problem, where probability notions enter solely through the interpretation of the state vector; the dynamics does not contain probability aspects. This system described on the Liouville level leads to persistent correlations, as Eq. (197) shows. This is to be contrasted with the classical ($\lambda = 1$) case, where the *interaction* contains the stochastic features; the states do not have any probability aspects. It is understandable that such a system would not possess any persistent correlations. Summarizing, one can say that probabilistic elements in the dynamics lead to the destruction of persistent correlation: pure dynamics in either the quantum or classical domain can lead to situations in which correlations persist for all time.

8. FINAL REMARKS

(a) The most striking phenomena exhibited by these models are (1) the occurrence of persistence correlation, and (2) an oscillatory approach to equilibrium.

The first-mentioned behavior means in particular that these systems, in their time behavior, do not approach the "obvious" thermodynamic equilibrium state as $t \to \infty$. The time limit *does* exist, but the state reached in time has rather unexpected and unintuitive properties [Eq. (197)].

The second type of behavior is perhaps a little less strange, but even so, the monotonic approach to equilibrium is often taken for granted. In fact, any discussion in which a relaxation time is assumed to exist presupposes this monotonic approach. Thus any system which does not exhibit the monotonic approach is worth investigating in detail.

Both behaviors 1 and 2 are *incompatible* with a master equation description. The models therefore provide specific examples of systems whose time behavior cannot be described and not even approximated by a master equation.

As in any study of models, there is always the nagging concern that the unusual phenomena studied are features of the special and contrived model and have no validity or significance beyond the confines of this artificial model. Stated less generously, the model is bad. For this reason, it would be extremely interesting if neutron depolarization experiments (or related spin echo experiments) could actually show examples of the oscillatory approach to equilibrium. It is believed that this oscillatory approach can and does occur in a variety of circumstances, but a precise characterization of a system exhibiting this behavior is still lacking.

(b) Several modifications and extensions of the models are possible: some may be useful. One could introduce a location-dependent interaction (as was done in Section 3): $\lambda_p = \lambda_0 + g_p$. Considering g_p as a perturbing external field allows both an exact and an approximate calculation to be performed. In this manner, one can—for these models, in any case—obtain a check on the validity of the Kubo formula. It would also be very interesting to construct a model in which the dependence on the density is less trivial than the dependence on μ in the ones considered. There are several ways of doing this: one could consider a model where the probability of a spin change would depend on the spin state of the neighbors. This would at the same time introduce interactions, a more complicated density dependence, and would yield a nonlinear model. Some of these models are still soluble.

(c) A variety of other modifications are possible. Instead of dealing with particles of spin $\frac{1}{2}$, one could consider particles of spin s. The appropriate values of the ϵ variables then would be the $2S + 1$ roots of unity. One can also alter the model rules so that the resulting system simulates a hysteresis-type behavior. Many other possibilities are open.

(d) The final utility of models is of course determined by the insight and knowledge they provide about realistic systems. One interesting possibility which is under active study is to see whether one can set up inequalities or "comparison theorems" which relate real systems and models. An example[39] would be a result showing that the susceptibility of a real three-dimensional system (with interactions between the constituents specified by a potential V) is always larger then, say, the product of the susceptibilities of three one-dimensional chains, each with a constant interaction given by the maximum of V. Thus the purpose would be to *bound* the physical characteristics of realistic systems (which of course cannot be computed) by those of models (which can be computed). If this program can ever be carried out, the models constructed here might give useful insights into the nonequilibrium behavior of quantum systems.

(e) This model differs from other exactly soluble models in several respects: (1) The model possesses both classical and quantum mechanical versions. (2) The master and Liouville equations can both be exactly solved. (3) Comparisons can be explicitly carried out between classical models with explicit stochastic elements and quantum systems.

Models investigated by other authors demonstrate some, but generally not all, of these features.

For example, Barouch *et al.*(9) solve the Liouville equation for the XY model in a homogeneous, time-dependent magnetic field. It was found in the thermodynamic limit that the limit of the magnetization as $t \to \infty$ is finite; but the system does not approach a thermal equilibrium state. The master equation was not studied for this model. Abraham *et al.*(20) studied the XY model where for $t \leq 0$, the system is in thermal equilibrium with a magnetic field acting on just a single spin. The magnetic field is now removed and the time evolution of the system is determined via the Liouville equation. The magnetization of the system now relaxes to its new equilibrium.

The first demonstration of the oscillatory approach to equilibrium for this model was given by Dresden.(21) Oscillatory behavior in the time evolution of spin systems was found by Walgraef and Borchmans.(22) These authors used a weak coupling expansion of the Liouville equation, basing their considerations on the Prigogine formalism.(3)

The system described here is (as the magnetic example suggests) closely related to the behavior of a two-level atom in an external field. The Liouville equation for this case was discussed by Muriel.(23)

The relationship and validity of the master equation is of special interest in the study of spontaneous emission of N two-level atoms (which itself is useful for the description of lasers). A master-type equation was employed for this purpose by Agarwal.(24) Since the system described is a good deal more complex than that described here, the Liouville equation was not investigated. It would be interesting to see whether the techniques of this

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[39] This is a pretty crazy example.

paper could be used to handle a more realistic and therefore more interesting physical situation. The limits of the validity of the master equation description of lasers would be particularly useful.

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