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New quantum rules for dissipative systems.

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Abstract

It is difficult to incorporate the concept of interacting physical particles in the frame of conventional quantum mechanics. It comes from the fact the in this formalism the hamiltonian plays a dual role as the generator of motion and as the observable associated with the energy. As a result it is easy to define either a representation in which particles interact but are not well defined (a representation in which the hamiltonian is not diagonal) or a representation in which the units are well defined but do **not** interact. We expect that in the search for a representation in which we may speak of **both** well defined and still interacting particles, the distinction between reversible and irreversible processes should play a basic role. Certainly we do not want to eliminate irreversible processes such as scattering, production or decay which are basically related to the mechanisms through which we observe particles.

To distinguish between reversible and irreversible processes we have to work in a representation such that a Liapounov function (the "entropy") may be ascribed to the time evolution of the system. The introduction of such a representation through a specific class of non-unitary transforms is described. We then propose new quantum rules directly applicable to dissipative systems with a Liapounov function. For systems with a discrete spectrum these new quantum rules reduce trivially to the usual quantum rules as formulated by Born, Jordan and Heisenberg.

The theory is applied to a simple field theoretical model - the so-called Friedrichs model-for which all calculations can be performed exactly. The results are most encouraging. In this new perspective the problem of "elementary" particles comes only after the formulation of the second law of thermodynamics (through the introduction of a Liapounov function). Elementary particles express in a simple way the time evolution of the field in terms of the various irreversible processes in which they participate.

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1. Introduction - Quantum Rules for Dissipative Systems.

There is, at present, much interest in irreversible processes occuring at various levels of description[1].

On the macroscopic level, much work has been devoted to "dissipative structures" arising in non equilibrium conditions. The point here that is essential for us is that dissipative structures imply the validity of the Second Law - the law of increase of entropy through dissipation. From the microscopic point of view, it has been shown that one can construct non unitary transformations ("star unitary" transformations) leading to "Liapounov representations", i.e. representations of dynamics which display, on the microscopic level, the basic thermodynamic distinction between reversible and irreversible processes[2]. More precisely, such a representation is characterized by the existence, in the thermodynamic limit, of a Liapounov function Ω which behaves like the entropy : it varies monotonously in time as the result of microscopic irreversible processes such as scattering, production and decay of particles.

These results are of obvious interest for one of the basic questions of modern physics : the dynamical definition of "elementary particles". In the standard

approach, one starts with a hamiltonian involving "bare" particles (for instance, electrons and photons) and an interaction. Some part of this interaction is then used to define the "physical" particles through renormalization[3]. The rest must then be used to describe the "true" evolution. The difficulties associated with this program are well-known[4]. One is always faced with a fundamental dilemma : either one works in a representation in which units are interacting but have no well defined energies (the energy is "partly" between the particles and leads to virtual processes) or one transforms to an unitarily equivalent representation in which particles do not interact (i.e. a representation in which the total hamiltonian is diagonal).

Is there a way out ? The distinction between reversible and irreversible processes on the microscopic level opens new possibilities. Indeed , in sufficiently complex systems, the interaction must clearly not be completely transformed away. We certainly do not want to eliminate irreversible processes such as scattering, decay... as these are the very processes through which we observe particles. Whatever the transformation we perform, we should keep the particles embedded in the physical evolution as expressed by the increase of entropy. This is the reason why we believe that the progress achieved in the theory of irreversible processes is also of interest in this new context.

From the mathematical point of view we may present this dilemma in the following way. In the formulation of quantum mechanics in terms of state vectors, the hamiltonian plays a dual role as the generator of the evolution (Schrödinger equation) and the energy observable (the eigenvalues of H determine the energy spectrum). To get out of the dilemma mentioned above, one may try to dissociate these two roles of H. Indeed, if we think, for instance, of an unstable particle, it is characterized by two different quantities : its energy and its life time. If the two roles of H are separated , one may hope that, once the transition to continuous spectrum is performed, it may be possible to discuss these two aspects separately.

To achieve this, a superoperator formalism[5] is required in which "superoperators" act on operators, such as the density operator ρ . Indeed the time evolution of the density matrix ρ is given by the Liouville-von Neumann equation :

$$i \frac{\partial \rho}{\partial t} = L \rho \tag{1.1}$$

where L is the superoperator corresponding to the commutator with H :

$$L = [H, \ ]_- \tag{1.2}$$

or, more explicitly :

$$L = H \times 1 - 1 \times H \tag{1.3}$$

Thus, the generator of the motion is the Liouvillian superoperator L while the energy H, as an observable operator, is an object of a different nature. An interesting additional feature is that this distinction may be introduced at the very same superoperator level. Indeed, we may define a superoperator $\mathcal{H}$ corresponding to the anticommutator with the hamiltonian :

$$\mathcal{H} = \frac{1}{2} [H, \ ]_+ = \frac{1}{2} (H \times 1 + 1 \times H) \tag{1.4}$$

The average value of the energy is then given by :

$$\langle H \rangle = Tr (\mathcal{H} \rho) = Tr\, H \rho \tag{1.5}$$

Of course, each of the two superoperators L and $\mathcal{H}$ is related in a simple way to H and their common origin shows up in the fact that L & $\mathcal{H}$ always commute

$$[L, \mathcal{H}]_- = 0 \tag{1.5'}$$

However, as we shall see, when, for systems with a continuous spectrum, we go through a non unitary transformation to a Liapounov representation, the relation between the transformed L and $\mathcal{H}$ is no longer so simple, through they will keep commuting.

Indeed these non-unitary transformations are also in general "non factorizable" and do not conserve the structure (1.3) and (1.4) of superoperators L and $\mathcal{H}$.

Let Λ be an invertible non unitary transformation leading to a new representation where the state is given by

$$ {}^{\flat}\rho = \Lambda^{-1} \rho \qquad (1.6) $$

The above considerations lead us to propose the following quantization rules :

a) go to a Liapounov representation ${}^{\alpha}\rho$ in which the distinction between reversible and irreversible processes is explicitly displayed. More precisely, look for transformations such that the quadratic functional

$$ \Omega = \mathrm{Tr}\ {}^{\alpha}\rho^{\dagger}\,{}^{\alpha}\rho \qquad (1.7) $$

decreases monotonously in time :

$$ \frac{d\Omega}{dt} \leq 0 \qquad (1.8) $$

b) among these representations ${}^{\alpha}\rho$, choose those ${}^{\flat}\rho$ which lead to states without dispersion for arbitrary functions of H, i.e. such that

$$ \langle H^n \rangle = \sum_i E_i^n \, {}^{\flat}\rho_{ii} \qquad (1.9) $$

where ${}^{\flat}\rho_{ii}$ is the diagonal element of ${}^{\flat}\rho$ in a representation where H_o is diagonal. (In (1.9) and later on the notation used obviously includes discrete as well as continuous cases).

Representations such that conditions a) and b) are satisfied will be called "physical". In such representations, we may speak of units with well defined energies E_L (see 1.9), evolving in time (see 1.8)*). These two rules, which we shall describe in more details in sections 2 and 3, replace the Born-Heisenberg-Jordan quantization rules (see e.g. Jammer[6]) :

a) consider canonical representations of motion
b) among them, choose those which diagonalize H .

The aim of this paper is to show that such transformations exist in the case of the simplest field theoretical model, the so-called Friedrichs' model which we have already studied in previous publications[7)8)]. The simplicity of this model stems from the fact that we may limit ourselves to the one particle sector. (It is, in a sense, a "one dimensional" model). The results are most encouraging : in particular the energy and the inverse life time of the decaying state appear as diagonal matrix elements of two different superoperators : one of the (transformed) $\mathcal{H}$ and the other of the (transformed) L. Although the above rules do not

*) Physical representations are of course particular Liapounov representations. So that, as, like in previous work, we are looking for special classes of Liapounov representations, we shall use ${}^{\flat}\rho$ as a unifying notation.

lead to an unique Λ-transformation (neither do the Born-Heisenberg-Jordan rules), they are however sufficient to determine completely these matrix elements ; as far as such partial results are concerned, they are identical with those obtained using the Green's function approach[9]. Some further conditions (weak coupling limit, symmetry considerations) lead to the choice of a well-defined Λ-transformation. As we shall see in the corresponding representation, the equations of motion for the density matrix involve only observable quantities such as life-times, emission, absorption and scattering cross sections.

Of course, the Friedrich's model is a highly idealized model. Still, some very general and, we believe interesting features emerge which may have a wider range of applications :

a) in the conventional view, particles come first, the second law of thermodynamics (the Liapounov function) comes later. Here, the order is inverted - the second law (on the microscopic scale) is used to define the particles.

b) in the conventional view, quantization is performed on the level of operators ; here, it appears in conjunction with superoperators.*)

Let us now present more details about our method.

*) The distinction is somewhat similar to that between vector and tensor calculus. From this point of view "ordinary" quantum mechanics corresponds to the level of vector calculus.

2. Liapounov representations.

What we mean by Liapounov representations has been discussed in recent papers (see e.g. 2) and we shall only recall it briefly. Basically, they are obtained through non unitary transformations such that the distinction between reversible and irreversible processes is explicitly displayed in the equations of motion.

First of all, we restrict ourselves to non unitary transformations $\Lambda(L)$ such that :

a) the average value of observables is preserved

b) the theory admits equivalent formulations in Schrödinger and Heisenberg pictures

c) the hermitian character of supervectors is preserved. Indeed observable and density operators must remain hermitian operators in all representations.

The first condition means :

$$\langle A \rangle = \mathrm{Tr}\, A^+ \rho = \mathrm{Tr}\, ({}^{\flat}A)^+ {}^{\flat}\rho \qquad (2.1)$$

where ${}^{\flat}\rho$ is the transformed density operator given by (1.6) and ${}^{\flat}A$ the transformed observable (see appendix I)

$${}^{\flat}A = (A^+ \Lambda)^+ = \Lambda^+ A \qquad (2.2)$$

As, using the hermiticity of the superoperator L (see appendix 1), the equation of evolution for (hermitian) observables in the Heisenberg picture is

$$i\frac{dA}{dt} = AL = -LA \tag{2.3}$$

The second condition b) is satisfied when (2.2) is related to (1.6) by L-inversion, i.e.

$$^{\flat}A = \Lambda^{-1}(-L)\,A \tag{2.4}$$

Combining these two requirements, we obtain the star-unitarity condition :

$$\Lambda^{*}(L) \equiv \Lambda^{+}(-L) = \Lambda^{-1}(L) \tag{2.5}$$

(As in our previous work we use the star notation for hermitian conjugation combined with L-inversion). The third property of Λ has been called adjoint symmetry and noted (see Appendix I)

$$\Lambda = \Lambda^{a} \tag{2.6}$$

It is interesting to notice that the three conditions we imposed on $\Lambda(L)$ may be satisfied by two types of transformations

$$^{\flat}A = \Lambda^{-1}(\pm L)\,A \tag{2.4a}$$

with

$$\Lambda^{+}(L) = \Lambda^{-1}(\pm L) \tag{2.5a}$$

The sign + corresponds to the usual, unitary transformations, the sign - to the starunitary ones. Unitary transformations are of no interest in the construction of the Liapounov functional. That is the reason why we turn to the second class which satisfy the starunitary condition (2.5).

In the new, starunitarily equivalent, representation, the Liouville equation (1.1) becomes :

$$i\frac{\partial\,^{\flat}\rho}{\partial t} = \phi\,^{\flat}\rho \tag{2.7}$$

where the generator of motion, ϕ, is related to L by a similitude :

$$\phi = \Lambda^{-1} L \Lambda \tag{2.8}$$

and is star hermitian :

$$(i\phi)^{*} = i\phi \tag{2.9}$$

Again the two possibilities corresponding to (2.5a) lead to the two classes

$$i\phi^{+}(L) = i\phi(\pm L) \tag{2.9a}$$

The choice of the - sign leads to new possibilities of direct relevance for the microscopic theory of irreversible processes. Indeed ϕ may then be split into two parts,

respectively even and odd with respect to L-inversion :

$$\phi = {}^{e}\phi + {}^{o}\phi \tag{2.10}$$

$${}^{e}\phi(L) = {}^{e}\phi(-L) \tag{2.11}$$

$${}^{o}\phi(L) = -\,{}^{o}\phi(-L) \tag{2.12}$$

In order that the new representation be a Liapounov representation, condition (1.8) must be satisfied. This implies the well-known "dissipativity condition" :

$$-i\,{}^{e}\phi \leq 0 \tag{2.13}$$

The decomposition (2.10) of ϕ transposes, into the microscopic description, the distinction between reversible and irreversible processes. Our first quantum rule means that we have to look for particles in a Liapounov representation in which (2.13) is satisfied. Particles have, in this sense, to be embedded in "becoming" as expressed by the change in time of the Liapounov functional Ω.

The remarkable properties of starunitary transformations should be clear at this point.*) Whenever they may be constructed we transform the description of the time evolution in terms of a hermitian operator (L) into a description displaying explicitly the dissipativity due to irreversible processes. Once (2.13) is satisfied we may define the Liapounov function as in (1.7) and verify the inequality (1.8).

*) The relation between starunitary transformations and Liouville's theorem will be studied in a separate paper[10].

3. Physical representations.

We now turn to our second quantum rule, which can be expressed as a condition on the transformed superoperator :

$${}^{\Lambda}\mathcal{H} = \Lambda^{-1}\,\mathcal{H}\,\Lambda \tag{3.1}$$

Indeed, from (1.4), we easily obtain

$$H^{n} = 1.\,\mathcal{H}^{n} \tag{3.2}$$

hence

$$\langle H^{n}\rangle = \mathrm{Tr}\, H^{n}\rho = \mathrm{Tr}\, 1.\mathcal{H}^{n}\rho = \mathrm{Tr}\, {}^{\Lambda}1.({}^{\Lambda}\mathcal{H})^{n}\,{}^{\Lambda}\rho \tag{3.3}$$

where

$${}^{\Lambda}1 = 1.\Lambda = \Lambda^{+}.1 \tag{3.4}$$

In order that (3.3) reduces to (1.9), we first impose that the unity supervector is conserved by the Λ-transformation :

$$1.\Lambda = \Lambda^{+}.1 = 1 \tag{3.5}$$

This property insures the form invariance of the trace under the transformation :

$$\mathrm{Tr}\,\rho = \mathrm{Tr}\, 1.\rho = \mathrm{Tr}\,{}^{\Lambda}1.{}^{\Lambda}\rho = \mathrm{Tr}\,{}^{\Lambda}\rho \tag{3.6}$$

To go further, let us use for operators and superoperators a matrix representation in which H_o is diagonal (see appendix 1) ; (3.3) becomes :

$$\langle H^n \rangle = \sum_{ikl} \left[({}^{\flat}\mathcal{H})^n \right]_{ii,kl} {}^{\flat}\rho_{kl} \tag{3.7}$$

To obtain the equivalence between (3.7) and (1.9), it is sufficient to require that Λ puts ${}^{\flat}\mathcal{H}$ into a canonical form, i.e. is such that :

$${}^{\flat}\mathcal{H}_{ii,ii} = E_i \tag{3.8}$$

$${}^{\flat}\mathcal{H}_{ii,kl} = 0 \quad \text{for} \quad k \neq l \;\; \& \;\; k = l \neq i \tag{3.9}$$

When Λ satisfies all these conditions, we notice the following features :

a) the "state" ${}^{\flat}\rho_{ii} = 1$, ${}^{\flat}\rho_{kk} = 0$ for $i \neq k$, corresponds to a state with no dispersion in the energy,

b) the "energy levels" correspond to fully diagonal elements of the superoperator ${}^{\flat}\mathcal{H}$.

To conclude this section, let us mention that, for systems with discrete spectrum, this method leads to no new results ; it is just the transcription in the superoperator formalism of the usual quantization rules. This will be shown in more details in section 5, but, before, we shall briefly recall the main steps involved in the construction of Λ .

4. Quantization in the superoperator formalism.

The first step in the construction of Λ is the introduction of a complete set of hermitian eigenprojectors ${}^{(\nu)}Q$ of the unperturbed Liouvillian L_o . For the unperturbed evolution, each of these projectors defines a subdynamics :

$$\left[{}^{(\nu)}Q , L_o \right]_- = 0 \tag{4.1}$$

It has been shown[11] through the analysis of the resolvent $(z - L)^{-1}$ of the Liouvillian L, that similarly it is possible to decompose the evolution of the interacting system ($\lambda \neq o$) into various subdynamics by means of a complete set of mutually orthogonal superprojectors ${}^{(\nu)}\Pi$ such that

$$\left[{}^{(\nu)}\Pi , L \right]_- = 0 \tag{4.2}$$

These projectors are star hermitian :

$${}^{(\nu)}\Pi^* = {}^{(\nu)}\Pi \tag{4.3}$$

One then looks for a starunitary transformation $\Lambda(L)$ such that the ${}^{(\nu)}\Pi$'s are related to the ${}^{(\nu)}Q$'s through

$${}^{(\nu)}\Pi = \Lambda \, {}^{(\nu)}Q \, \Lambda^* = \Lambda \, {}^{(\nu)}Q \, \Lambda^{-1} \tag{4.4}$$

with the further requirement :

$$\Lambda(\lambda \to o) = 1 \tag{4.5}$$

which guarantees that, when $\lambda \to 0$ (and thus $L \to L_0$), ${}^{(\nu)}\Pi$ reduces to ${}^{(\nu)}Q$.

Combining (4.2), (4.4) and (2.8), one obtains

$$[{}^{(\nu)}Q, \Phi]_- = 0 \tag{4.6}$$

Thus, the existence of subdynamics makes it possible to require that the generator of evolution is block-diagonal The dissipativity condition (2.13) can also be discussed in each subspace separately.

Let us now turn our attention to the further restrictions introduced by our second quantum rule. The interesting point is that, to define E_i, we need not the complete knowledge of Λ, but only a "part" which can be determined separately.

It is quite remarkable that we can also require that the transformed energy superoperator be block-diagonal. This is a direct consequence of the fact that, in the original representation, the superoperators $\mathcal{H}$ and L commute. Then $\mathcal{H}$ commutes with the resolvent of L, thus with each of the super-projectors ${}^{(\nu)}\Pi$ constructed using this resolvent. Transforming the vanishing commutator using (3.1) and (4.4),

one gets

$$\Lambda^{-1}[{}^{(\nu)}\Pi, \mathcal{H}]\Lambda = [\Lambda^{-1}{}^{(\nu)}\Pi\Lambda, \Lambda^{-1}\mathcal{H}\Lambda]_- = [{}^{(\nu)}Q, {}^{\flat}\mathcal{H}] = 0 \tag{4.7}$$

In the special case $\nu = 0$ (${}^{(\nu)}Q$ is the projector on the null-space of L_0), (4.7) leads, in the tetradic notation, to :

$${}^{\flat}\mathcal{H}_{ii,k\ell} = {}^{\flat}\mathcal{H}_{k\ell,ii} = 0 \quad \text{for} \quad k \neq \ell \tag{4.8}$$

i.e. part of condition (3.9) is already fulfilled. Condition (3.8) and the remaining part of condition (3.9) are conditions on the superoperator ${}^{(0)}Q\,{}^{\flat}\mathcal{H}\,{}^{(0)}Q$: it must be diagonal. Taking into account (3.1), we thus see that our second rule does not involve the complete Λ but only the superoperator $\Lambda^{(0)}Q$.

To make contact with our previous work, it is useful, at this stage, to introduce some notations. Because of the special role of the ${}^{(0)}\Pi$ subspace (this subspace contains the invariants, in particular H), we shall denote it simply Π and use P instead of ${}^{(0)}Q$. Thus :

$$P \equiv {}^{(0)}Q \qquad , \Pi \equiv {}^{(0)}\Pi = \Lambda P \Lambda^{-1} \tag{4.9}$$

If σ is an arbitrary supervector, we denote by σ_0 and σ_c the set of non vanishing elements of $P\sigma$ (diagonal elements) and of $(1-P)\sigma$ (off diagonal elements). Similarly, if $\mathcal{A}$ is an arbitrary superoperator, we note $a_{00}, a_{c0}, a_{0c}, a_{cc}$ the sets of non vanishing elements of $P\mathcal{A}P, (1-P)\mathcal{A}P,$

$P\mathcal{A}(1-P)$, $(1-P)\mathcal{A}(1-P)$. The matrices associated with σ and $\mathcal{A}$ can then be written in terms of the sub-matrices associated with these quantities :

$$\sigma = \begin{pmatrix} \sigma_o \\ \sigma_c \end{pmatrix} \qquad \mathcal{A} = \begin{pmatrix} a_{oo} & a_{oc} \\ a_{co} & a_{cc} \end{pmatrix} \tag{4.10}$$

It has been shown that the superoperator Π takes the form :

$$\Pi = \begin{pmatrix} A & AD \\ CA & CAD \end{pmatrix} \tag{4.11}$$

where $A \left(\equiv \Pi_{oo}\right)$ is a starhermitian superoperator

$$A = A^* \tag{4.12}$$

and C and D are star hermitian conjugates :

$$C = D^* \tag{4.13}$$

The important point is that the non vanishing elements of $(1-P)\Pi$ (second line in 4.11) can be obtained by the action of the superoperator C on the non vanishing elements of $P\Pi$ (first line in 4.11). In other words, the off-diagonal elements of a Π -projection are linear functionals of the diagonal elements

$$(\Pi\rho)_c = C(\Pi\rho)_o \tag{4.14}$$

As already mentioned, to discuss our second quantum rule, we need only the ΛP part of Λ , i.e. the submatrices Λ_{oo} and Λ_{co} . As in our previous work, we shall use the notation :

$$\Lambda_{oo} \equiv \chi \qquad \text{i.e.} \quad \Lambda_{aa,bb} \equiv \chi_{aa,bb} \tag{4.15}$$

As a consequence of our above definitions and of (4.9), we obtain

$$\Pi_{oo} \equiv A = \chi\chi^* \tag{4.16}$$

$$\Pi_{co} \equiv CA = \Lambda_{co}\Lambda_{oo}^* \tag{4.17}$$

Using (4.15) and (4.16), (4.17) becomes :

$$\Lambda_{co} = C\chi \tag{4.18}$$

C is determined as soon as the problem of the construction of Π is solved (this involves analytic continuation and has been discussed elsewhere[1]). As far as χ is concerned, the choice is restricted by (4.16) and also by conditions (2.6), (3.5) and (4.5) which, in the tetradic notation imply (see appendix I) :

$$\chi_{aa,bb} = \chi^{cc}_{aa,bb} \tag{4.19}$$

i.e. χ must be real

$$1 = \sum_{\alpha} \chi_{aa,\beta\beta} \tag{4.20}$$

$$\chi_{aa,\beta\beta}(\lambda \to 0) = \delta_{a\beta} \tag{4.21}$$

The diagonalization of $P\,{}^{t}\mathcal{H}\,P$ will bring further conditions on χ.

As already mentioned, the knowledge of ΛP is sufficient to determine $P\,{}^{t}\mathcal{H}\,P$. It also allows to determine the $P\phi P$ part of the collision operator. Before we conclude this section, let us notice that, if we combine (2.8), (3.1) and the block-diagonality conditions (4.6), (4.7), we obtain the relations

$$\phi_{oo} = \chi^{-1}\,\tilde{L}\,\chi \tag{4.22}$$

$${}^{t}\mathcal{H}_{oo} = \chi^{-1}\,\tilde{\mathcal{H}}\,\chi \tag{4.23}$$

where

$$\tilde{L} = L_{oc}\,C$$

$$\tilde{\mathcal{H}} = \mathcal{H}_{oo} + \mathcal{H}_{oc}\,C \tag{4.24}$$

(4.25)

(note that $L_{oo} = 0$).

The operator $\tilde{L}$ is the evolution operator for the diagonal elements of the Π projection of ρ. Indeed, combining (1.1), (4.2) for $\nu = o$ and (4.14), we have :

$$i\,\frac{\partial(\Pi\rho)_o}{\partial t} = (\Pi L\rho)_o = (L\Pi\rho)_o = L_{oc}(\Pi\rho)_c = \tilde{L}\,(\Pi\rho)_o \tag{4.26}$$

Also, if we take into account the fact that regular invariants are in the Π-subspace, i.e. that one can show that :

$$H\Pi = H \tag{4.27}$$

we have :

$$\langle H\rangle = \mathrm{Tr}\,H\rho = \mathrm{Tr}\,H\Pi\rho = \mathrm{Tr}\,\mathcal{H}\,\Pi\rho$$
$$= \mathrm{Tr}\,\{\mathcal{H}_{oo}(\Pi\rho)_o + \mathcal{H}_{oc}(\Pi\rho)_c\} = \mathrm{Tr}\,\tilde{\mathcal{H}}\,(\Pi\rho)_o \tag{4.28}$$

i.e. provided H is replaced by $\tilde{\mathcal{H}}$, the average value of the energy may be expressed in terms of the diagonal elements of $\Pi\rho$.

Another way to express the average energy is

$$\langle H\rangle = \mathrm{Tr}\,{}^{t}H\,{}^{t}\rho \tag{4.29}$$

where ${}^{t}H$ is the transformed observable :

$${}^{t}H = H\Lambda = \Lambda^{+}H \tag{4.30}$$

This operator is diagonal ; indeed, using (4.27) and (4.28), the hermiticity of ${}^{\flat}H$ and P, we have :

$$ {}^{\flat}H = H\pi\Lambda = H\Lambda P = {}^{\flat}H P = P\,{}^{\flat}H \tag{4.31} $$

The sole knowledge of χ allows us to determine this operator. Indeed, using (4.30), we have :

$$ H_o = (PH)_o = (P\Lambda' {}^{\flat}H)_o = (P\Lambda' P\,{}^{\flat}H)_o = \chi'({}^{\flat}H)_o \tag{4.32} $$

or equivalently :

$$ ({}^{\flat}H)_o = \chi'^{-1} H_o \tag{4.33} $$

(As in our previous work, the dash sign designates the L inversion).

5. Systems with discrete spectrum.

Before applying these rules to the Friedrichs' model, let us consider the case of discrete systems and discuss the link between the above method and the usual technique.

Starting with the Liouville equation (1.1), we may proceed in two different ways. The usual way consists in looking for <u>particular</u> solutions of (1.1) corresponding to a <u>factorized</u> density operator :

$$ \rho = |\Psi\rangle\langle\Psi| \tag{5.1} $$

$|\Psi\rangle$ obeys the Schrödinger equation and the standard eigenvalue problem leads to quantization with, as eigenvectors, probability amplitudes. This procedure corresponds therefore to a factorization of the space $\mathcal{H}^{(2)}$ of density operators into an exterior <u>product</u> of two Hilbert spaces $\mathcal{H}$ for <u>probability amplitudes</u>

$$ \mathcal{H}^{(2)} = \mathcal{H} \otimes \mathcal{H} \tag{5.2} $$

In the second method, $\mathcal{H}^{(2)}$ is written as a sum of two subspaces, symbolically :

$$ \mathcal{H}^{(2)} = \pi + (1-\pi) \tag{5.3} $$

(For discrete systems, the projector Π introduced in section 4, is the projector on the zero-eigenvalue of L). The eigenvalue problem is then formulated in the Π-space alone. This leads to an eigenvalue problem for "probability eigenfunctions" (and not amplitudes). Conditions (3.8), (3.9), allowing the determination of energy levels, extend to dissipative systems part of this method (the determination of eigenvalues). For this reason, we shall summarize it briefly here (for more details, see the original papers[12)13)].

We consider the hamiltonians H_o and H with

$$H = H_o + \lambda V \tag{5.4}$$

with eigenvectors $|n\rangle$ and $|\tilde{n}\rangle$ and eigenvalues E^o_n, E_n
We introduce the unitary transformation :

$$U = \sum_n |\tilde{n}\rangle\langle n| \tag{5.5}$$

which transforms H into ${}^UH$:

$${}^UH = U^{-1} H U \tag{5.6}$$

corresponding to eigenvectors $|n\rangle$ and energies E_n . The determination of E_n (and V) corresponds to the usual eigenvalue problem in Hilbert space. Equivalently, we may work in the space of density operators and look for a Λ-transformation which diagonalizes both $\mathcal{H}$ and L

given in (1.3), (1.4). Such a transformation is given by the factorizable unitary superoperator :

$$\Lambda = U \times U^+ \qquad (\Lambda_{ij,kl} = U_{ik}\, U^{cc}_{jl}) \tag{5.7}$$

This transformation has all the properties mentionned above. First of all, its unitarity is a consequence of the general requirement of star unitarity plus the additional property of invariance under L-inversion :

$$\Lambda = \Lambda' \tag{5.8}$$

Furthermore, we have

$$\phi_{ij,kl} = \delta_{ik}\,\delta_{jl}\,(E_i - E_j) \tag{5.9}$$

$${}^{\flat}\mathcal{H}_{ij,kl} = \delta_{ik}\,\delta_{jl}\,\tfrac{1}{2}(E_i + E_j) \tag{5.10}$$

For $i = j$, (5.10) is just (3.8), (3.9). Also, combining (5.7) and (4.15), we have :

$$\chi_{ii,jj} = |U_{ij}|^2 \tag{5.11}$$

Hence, using also (5.8), (4.33) becomes :

$$({}^{\flat}H)_{ij} = \delta_{ij} \sum_k |U_{ik}|^2 E^o_k = \delta_{ij} E_i \tag{5.12}$$

and ${}^{\flat}H$ is identical with ${}^UH$.

The link (4.9) between the projectors on the zero eigenvalue of L and L_0 is just the transcription in superoperator language of the relation between $|\tilde{n}\rangle$ and $|n\rangle$.

The interesting point is that we may determine χ (hence E_i) directly, without using (5.11). For this, we start from (4.28) and consider the eigenvalue problem in the Π -subspace :

$$\tilde{\mathcal{H}}\, \varphi_n = E_n\, \varphi_n \qquad (5.13)$$

where φ_n is an eigenprobability (not an eigen amplitude) corresponding to E_n. (This was first done in two papers by Prigogine, George and Rae[12)13)]). Equivalently, we may look for a similitude such that the operator

$$U\tilde{\mathcal{H}} = \chi^{-1}\, \tilde{\mathcal{H}}\, \chi \qquad (5.14)$$

is diagonal (This operator, defined in Π -subspace, is identical to ${}^{\flat}\mathcal{H}_{oo}$) :

$$U\tilde{\mathcal{H}}_{ii,kk} = E_i\, \delta_{ik} \qquad (5.15)$$

This is nothing else than condition(3.8) and part of (3.9).

In the case of a discrete spectrum, nothing new - at least from the "practical" point of view - has been achieved. Both methods of quantization are equivalent.

One may even state that our approach appears here as unnecessarily cumbersome. Still, we believe that, even in this case, it has some conceptual value.* It is indeed unexpected that the classical eigenvalue problem can still be viewed in a new way !

When we go to more general systems, involving a continuous spectrum the quantities $\tilde{\mathcal{H}}, \Pi, \ldots$ can be obtained by analytical continuation. It is thus very natural to try to apply this new approach to quantization of dissipative systems. This is what we have done for the Friedrichs' model, which we consider as a kind of test case. (For this reason we have discussed this model at various stages of the development of our microscopic theory of irreversible processes[7)8)].

*) One may even argue that it is natural to consider the Liouville operator L (and not the Hamiltonian H) as the operator for time displacement. Indeed contrary to H which is a positive operator, the spectrum of L covers in general the real line from $-\infty$ to $+\infty$. As the result Pauli's well-known argument (Jammer[6)] p. 141) which leads to reject the existence of a conjugate time operator associated with time displacement does not apply.
It is interesting that von Neumann has called this limitation of the hamiltonian formulation of quantum mechanics "an essential,... in fact, the chief weakness of quantum mechanics" (Jammer[6)] p. 150).

6. The Friedrichs' model.

Even for this simple model, the calculations are often lengthy. To keep this paper to a reasonable length, we are bound to refer to earlier papers and specially to the paper by De Haan and Henin[8]. Only calculations going beyond those given in that paper will be presented here ; they essentially deal with the consequences of our second quantum rule. To discuss this, we only need the ΛP part of Λ , i.e. (see (4.14) and (4.16)) the operators C and χ .

The construction of a Liapounov representation according to the technique summarized in section 4 completely determines C and gives some conditions on χ . Moreover, in the Friedrichs' model, the collision operator ϕ_{oo} is even in L in the weak coupling limit. As $\tilde{L}$ and A are also even in L, it is possible to require (see (4.14), (4.20)) that χ shares this property

$$\chi = \chi' \tag{6.1}$$

This is a sufficient condition for $\phi_{..}$ to be even in L in all orders in the coupling constant λ . With this additional condition, only a single group of matrix elements of χ are not yet determined. They can be further

specified with the help of our second quantum rule. This still leaves some slight indetermination ; symmetry considerations, however, can be used to choose a uniquely defined transformation.

As well-known, in the Friedrichs' model, a state $|1\rangle$ interacts with a set of states $\{|k\rangle\}$ through

$$H = \omega_1 |1\rangle\langle 1| + \sum_k \omega_k |k\rangle\langle k| + \lambda \sum_k \{ v_k |1\rangle\langle k| + v_k^{cc} |k\rangle\langle 1| \} \tag{6.2}$$

where $v_k \left(= \langle 1|V|k\rangle \right)$ is assumed of order $L^{-3/2}$, L^3 being the volume of the quantization box. It is very important to specify the volume dependence as we shall need it to obtain asymptotic expansions valid for large volumes. It is only at the end, in the evaluation of average values of observables, that we can go to the limit of infinite volumes.

As long as the spectrum is discrete, the eigenvalues of H are solutions of the dispersion equation

$$\eta(z) = 0 \tag{6.3}$$

where

$$\eta(z) = z - \omega_1 - \sum_k \frac{|v_k|^2}{z - \omega_k} \tag{6.3'}$$

In the continuous spectrum limit, the sum over k becomes an integral

$$\eta(\zeta) = \zeta - \omega_1 - \int d\omega_k \frac{|v(\omega_k)|^2}{\zeta - \omega_k} \tag{6.4}$$

where $v(\omega_k)$ is defined by the relation

$$\lim_{L^3 \to \infty} \sum_k |v_k|^2 = \int d\omega_k \, |v(\omega_k)|^2 \tag{6.5}$$

The equation

$$\eta^+(\zeta) = 0 \tag{6.6}$$

with $\eta^+(\zeta)$ the analytic continuation of $\eta(\zeta)$ from above admits a complex root $(\omega_1 + \zeta)$ in the lower half plane

$$\eta^+(\omega_1 + \zeta) = 0 \quad , \quad \lim_{\lambda \to 0} \zeta = 0 \tag{6.7}$$

In the Green's function approach, the inverse life time $(+i\theta)$ of the unstable state is given by the imaginary part of this root :

$$\theta = \zeta - \zeta^{cc} \tag{6.8}$$

while the energy is associated with the real part :

$$\Omega_1 = \omega_1 + \frac{\zeta + \zeta^{cc}}{2} \tag{6.9}$$

The sets of non vanishing elements of $P\phi P$, $P^+ \mathcal{H} P$ are given by (4.22) and (4.23), together with (4.24) and

(4.25). All operators needed for the expression of π have been calculated explicitly in the paper by De Haan and Henin.[8] Let us quote here the expressions obtained for the matrix elements of $\tilde{L}$ when only dominant terms with respect to L^3 are kept* :

$$\tilde{L}_{11,11} = \theta \tag{6.10}$$

$$\tilde{L}_{11,kk} = -\theta a_k \tag{6.11}$$

$$\tilde{L}_{kk,11} = \theta b_k \tag{6.12}$$

$$\tilde{L}_{kk,kk} = \lambda^2 |v_k|^2 \left(\frac{1}{\eta^+(\omega_k)} - \frac{1}{\eta^-(\omega_k)} \right) \equiv i w_k \tag{6.13}$$

$$\tilde{L}_{kk,k'k'} = \frac{1}{\theta} \tilde{L}_{kk,11} \tilde{L}_{11,kk} + i w_{kk'} \tag{6.14}$$

where

$$a_k = \lambda^2 \frac{|v_k|^2}{|\eta^+(\omega_k)|^2} \tag{6.15}$$

$$b_k = \lambda^2 |v_k|^2 \frac{1}{(s + \omega_1 - \omega_k)\zeta (s' + \omega_1 - \omega_k)\zeta^{cc}} \tag{6.16}$$

---

*In reference [8], $\tilde{L}$ is noted Ⓗ.

$$w_{kk'} = 2\pi \lambda^4 |v_k|^2 |v_{k'}|^2 \frac{1}{|\eta^+(\omega_k)|^2} \delta(\omega_k - \omega_{k'}) \tag{6.17}$$

In the expression of b_k appear the symbols of "deferred" analytic continuation $\frac{1}{(s+\omega_1-\omega_k)_\zeta}$, $\frac{1}{(s'+\omega_1-\omega_k)_{\zeta^{cc}}}$.

They mean that, in integrations over ω_k , the integration has to be performed with s in S^+ (s' in S^-), then the expression is to be analytically continued to ζ in S^- (ζ^{cc} in S^+).

The corresponding elements of $\tilde{\mathcal{H}}$ can be obtained in a similar way (see appendix II) :

$$\tilde{\mathcal{H}}_{11,11} = \Omega_1 \tag{6.18}$$

$$\tilde{\mathcal{H}}_{11,kk} = (\omega_k - \Omega_1)\, a_k \tag{6.19}$$

$$\tilde{\mathcal{H}}_{kk,11} = (\Omega_1 - \omega_k)\, b_k \tag{6.20}$$

$$\tilde{\mathcal{H}}_{kk,kk} = \omega_k \tag{6.21}$$

$$\tilde{\mathcal{H}}_{kk,k'k'} = \frac{\lambda^4 |v_k|^2 |v_{k'}|^2}{|\eta^+(\omega_{k'})|^2} \mathcal{P}\left(\frac{1}{\omega_{k'} - \omega_k}\right) - (\Omega_1 - \omega_k)\, b_k\, a_{k'} \tag{6.22}$$

where $\mathcal{P}$ denotes the Cauchy principal part. It is interesting that the inverse life time $i\theta$ appears in the $11-11$ matrix element of $\tilde{L}$ (see (6.10)) . This is a direct result of analytic continuation and does not involve transformation theory. We note also that $\tilde{\mathcal{H}}$ is off-diagonal. We cannot ascribe well defined energies to the particles. Finally, the time evolution as described by $\tilde{L}$ is difficult to understand in physical terms. For instance there appears a dissymmetry between emission and absorption as described by $\tilde{L}_{11,kk}$ and $\tilde{L}_{kk,11}$. Can a physically acceptable description be reached through the χ transformation in (4.22), (4.23) ? This is what we have to study now.

7. Liapounov and physical representations for the Friedrichs model.

The starunitarity condition for Λ leads to condition (4.16) for χ. The matrix elements of A are given in ref. [8]. From their order of magnitude with respect to L^3, one may deduce those of the matrix elements of χ :

$$\chi_{11,11} \sim O(1) \tag{7.1}$$

$$\chi_{11,kk} \ , \ \chi_{kk,11} \sim O(L^{-3}) \tag{7.2}$$

$$\chi_{kk,kk} = 1 + O(L^{-3}) \tag{7.3}$$

$$\chi_{kk,k'k'} \sim O(L^{-6}) \tag{7.4}$$

Using the notation

$$\phi_{aa,bb} = i W_{ab} \tag{7.5}$$

and (6.10) to (6.14), (4.22) leads to

$$W_{11} = -i\theta \tag{7.6}$$

$$W_{1k} = \frac{W_{11}}{\chi_{11,11}} \left(\chi_{11,kk} - a_k \right) \tag{7.7}$$

$$W_{k1} = W_{11} \left(b_k \chi_{11,11} - \chi_{kk,11} \right) \tag{7.8}$$

$$W_{kk} = -i\lambda^2 |v_k|^2 \left(\frac{1}{\eta^+(\omega_k)} - \frac{1}{\eta^-(\omega_k)} \right) \tag{7.9}$$

$$W_{kk'} = \frac{W_{k1} W_{1k'}}{W_{11}} + 2\pi \lambda^4 \delta(\omega_k - \omega_{k'}) \frac{|v_k|^2 |v_{k'}|^2}{|\eta^+(\omega_k)|^2} \tag{7.10}$$

for the relevant elements of ϕ in the π-subdynamics. The equations of motion for the diagonal elements of the density matrix in an arbitrary Liapounov representation are then :

$$\frac{\partial \rho_{11}}{\partial t} = W_{11} \rho_{11} + \sum_k W_{1k} \rho_{kk} \tag{7.11}$$

$$\frac{\partial \rho_{kk}}{\partial t} = W_{kk} \rho_{kk} + W_{k1} \rho_{11} + \sum_{k'} W_{kk'} \rho_{k'k'} \tag{7.12}$$

The matrix elements of χ must satisfy condition (4.16), (4.19), (4.20), (4.21). This is however insufficient to determine them completely. We notice however that the life time $\tau = -W_{11}^{-1}$ and the forward scattering W_{kk} do not depend on the particular Liapounov representation. They only involve analytic continuation (in the computation of $\tilde{L}$).

The arbitrariness in the determination of χ can be reduced by the requirement (6.1). This leads to (see appendix 3) :

$$\chi_{11,11} = \left(\frac{1}{|\eta'^{+}(\omega_1 + \xi)|^2} \right)^{1/2} \tag{7.13}$$

and a relation between $\chi_{11,kk}$ and $\chi_{kk,11}$:

$$\chi_{11,kk} = a_k + \chi_{11,11} \left(\chi_{11,11}\, b_k - \chi_{kk,11} \right) \tag{7.14}$$

As a consequence of this last relation, we obtain :

$$W_{1k} = W_{k1} \quad , \quad W_{kk'} = W_{k'k} \tag{7.15}$$

Symmetry between emission and absorption is now correctly introduced. To determine completely the evolution, there remains only one type of coefficients $(\chi_{kk,11})$ to be further specified. Independently of the value of these coefficients, it is possible to verify that the Liapounov inequality (2.13) is satisfied (see ref.[2] [14]).

Decay and scattering drive the system to equilibrium (as far as the restricted dynamics of the Friedrichs model allows).

To further specify χ , we now appeal to our second quantum rule. (At this point, we depart from our earlier work on the Friedrichs model where we used a

different method which, however, did not lead to dispersion-free energies). In an arbitrary Liapounov representation, the matrix elements of $P' \mathcal{H} P$ can be derived from (4.23) and (6.18) to (6.22). This gives :

$$^{\flat}\mathcal{H}_{11,11} = \Omega_1 \tag{7.16}$$

$$^{\flat}\mathcal{H}_{11,kk} = (\Omega_1 - \omega_k) \frac{1}{\chi_{11,11}} (\chi_{11,kk} - a_k) \tag{7.17}$$

$$^{\flat}\mathcal{H}_{kk,11} = (\Omega_1 - \omega_k)(b_k \chi_{11,11} - \chi_{kk,11}) \tag{7.18}$$

$$^{\flat}\mathcal{H}_{kk,kk} = \omega_k \tag{7.19}$$

$$^{\flat}\mathcal{H}_{kk,k'k'} = \lambda^4 \frac{|v_k|^2 |v_{k'}|^2}{|\eta^+(\omega_{k'})|^2} \mathcal{P}\left(\frac{1}{\omega_{k'} - \omega_k}\right) + \chi_{kk,k'k'}(\omega_k - \omega_{k'})$$
$$-(\Omega_1 - \omega_k) b_k (a_{k'} - \chi_{11,k'k'}) - \chi_{kk,11}(\omega_k - \Omega_1) \frac{1}{\chi_{11,11}} (a_{k'} - \chi_{11,k'k'})$$
$$- \chi_{kk,11}\, \chi_{11,k'k'} \frac{1}{\chi_{11,11}} (\omega_k - \omega_{k'}) \tag{7.20}$$

The transformation to a Liapounov representation has <u>not</u> altered the meaning of the diagonal elements $^{\flat}\mathcal{H}_{11,11}$ $^{\flat}\mathcal{H}_{kk,kk}$. Therefore, the results obtained by analytic continuation in section 6 are not altered. But as the

matrix ${}^{\flat}\mathcal{H}_{ii,jj}$ is not diagonal, we cannot speak of states of well defined energies. To obtain a "physical" representation, we must add the requirement of diagonality of ${}^{\flat}\mathcal{H}_{ii,jj}$, i.e. the conditions :

$$ {}^{\flat}\mathcal{H}_{11,kk} = 0 \qquad (7.21) $$

$$ {}^{\flat}\mathcal{H}_{kk,11} = 0 \qquad (7.22) $$

$$ {}^{\flat}\mathcal{H}_{kk,k'k'} = 0 \qquad (7.23) $$

To satisfy these conditions, we have to take the following expressions for the off-diagonal elements of χ :

$$ \chi_{11,kk} = \alpha_k - \beta_k \, \delta(\Omega_1 - \omega_k) \qquad (7.24) $$

$$ \chi_{kk,11} = \delta_k \chi_{11,11} + \alpha_k \, \delta(\Omega_1 - \omega_k) \qquad (7.25) $$

and also impose a condition on $\chi_{kk,k'k'}$. The coefficients α_k, β_k are, to a large extent arbitrary ; they must be such that conditions (4.19), (4.20) and (4.21) are satisfied (see also appendix 3).

From the point of view of the energies, the choice of a physical representation out of all Liapounov representations leads to no new result. The "energies" associated with the particles are Ω_1 and ω_k in agreement

with Green's function approach as stated in the introduction. But as all off-diagonal elements of ${}^{\flat}\mathcal{H}$ vanish, we may now associate Ω_1 and ω_k to the excitations of the system ; indeed, we have :

$$ \langle H \rangle = \Omega_1 \, {}^{\flat}\rho_{11} + \sum_k \omega_k \, {}^{\flat}\rho_{kk} \qquad (7.26) $$

and consider ${}^{\flat}\rho_{11}$, ${}^{\flat}\rho_{kk}$ as the probabilities of finding the corresponding excitations*. The special state

$$ {}^{\flat}\rho_{11} = 1 \quad , \quad {}^{\flat}\rho_{kk} = 0 \qquad \forall k \qquad (7.27) $$

corresponds to a state where only the unstable particle is present. This is a state without fluctuations (an expression similar to (7.26) holds for all powers of H), in which the energy is exactly Ω_1 .

The arbitrariness on the elements of χ can be further reduced by imposing (6.1), i.e. (7.14), i.e.

$$ \chi_{11,11} \alpha_k = \beta_k \qquad (7.28) $$

As we have seen, this leads to a symmetric collision operator, given by (7.6), (7.9) and

$$ W_{1k} = W_{k1} = - W_{11} \alpha_k \, \delta(\Omega_1 - \omega_k) \qquad (7.29) $$

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*The Λ transformation is based on analytical continuation procedures, i.e. it is only defined for a restricted set of states and observables. The above interpretation holds only if $0 \leq {}^{\flat}\rho_{aa} \leq 1$ which is not necessarily the case for given initial conditions in the bare representation. (see § 8)

$$W_{kk'} = - W_{11}\, \alpha_k \alpha_{k'}\, \delta(\Omega_1 - \omega_k)\, \delta(\Omega_1 - \omega_{k'}) + w_{kk'} \qquad (7.30)$$

for this class of representations. In these expressions, as a consequence of (4.19) and (4.20), α_k is real and must satisfy the condition

$$\sum_k \alpha_k\, \delta(\Omega_1 - \omega_k) = 1 \qquad (7.31)$$

Among these representations, it is quite natural to choose for this model, the one which leads to isotropy of the emission and absorption process. This requirement leads to the identification of α_k with a mere kinematic factor :

$$\alpha_k = \frac{|v_k|^2}{|v(\omega_k)|^2} \qquad (7.32)$$

In conclusion, these results are most satisfactory : the emission and absorption probabilities are positive definite ; moreover, Fermi's golden rule applies now to all orders in the coupling constant, energy is conserved in each process (see (7.29)). As shown in appendix IV, this is not in contradiction with the existence of a finite line width in agreement with conventional Green's function approach. Also, it is shown in that appendix that $W_{kk'}$ is an excess scattering cross section : it is the difference between the total scattering cross section ($w_{kk'}$) and "resonant" scattering, i.e. that part of scattering consisting in the absorption of boson with energy $\omega_k = \Omega_1$ and subsequent emission, after a time of the order of the lifetime of the excited state, of a boson with the same energy.

8. Concluding remarks.

We have seen that, in the case of the Friedrichs model, there exist star unitary Λ transformations which satisfy the various requirements that we have imposed in order to obtain a physical representation. Taking into account specific features of the model, we have been naturally led to a unique choice for this transformation.

As indicated earlier, the Friedrichs model is a somewhat idealized model and the importance of our ideas can only be evaluated once the present results will be extended to more realistic situations. Nevertheless, they already indicate that the question : "What is an excited state?" is likely to receive an answer. From this point of view our interpretation of the diagonal elements of the density matrix in the physical representation is a separate postulate : it is valid only if

$$0 \leq {}^{\flat}\rho_{aa} \leq 1 \qquad (8.1)$$

From chosen initial conditions in the bare representation this may be satisfied or not, depending on the interaction. For instance, with the initial condition $\rho_{11}(0) = 1$, one obtains (see appendix 4), ${}^{\flat}\rho_{11}(0) = \chi_{11,11}$ and ${}^{\flat}\rho_{11}(0)$ does not satisfy (8.1) if $\chi_{11,11} > 1$. Conversely, one might encounter situations such that (8.1) is satisfied, but

when one goes back to the bare representation, the corresponding ρ does not possess all the properties required from a density operator. In other words, it is in general not possible to give a consistent interpretation in <u>both</u> the bare and the physical representations. Our attitude, in the discussion of our results, has been to depart from the bare representation and to grant an intrinsic status to the physical representation. This is in line with our general arguments according to which the distinction between reversible and irreversible processes is a prerequisite element for the definition of interacting physical particles.

APPENDIX I. MATRIX REPRESENTATION OF OPERATORS AND SUPEROPERATORS.

Let the density operator ρ and observables A have matrix elements ρ_{ab} and A_{ab} such that the diagonal elements of H ($H_{aa} = \omega_a$) define the unperturbed hamiltonian H_0 while the off-diagonal elements define the perturbation λV .

Then superoperators admit a tetradic representation. For instance, the Liouvillian has matrix elements

$$L_{ab,cd} = H_{ac}\,\delta_{db} - H_{db}\,\delta_{ac} \tag{AI.1}$$

and the energy superoperator has elements :

$$\mathcal{H}_{ab,cd} = \tfrac{1}{2}\left(H_{ac}\,\delta_{db} + H_{db}\,\delta_{ac}\right) \tag{AI.2}$$

If $\mathcal{A}$ is an arbitrary superoperator and σ an arbitrary supervector, one can associate through the scalar product (2.1) various conjugate superoperators to $\mathcal{A}$:

a) transposed operator : $\mathcal{A}\sigma = \sigma\,\mathcal{A}^{T}$ (AI.3)

b) adjoint superoperator : $\mathcal{A}\sigma = (\sigma^{+}\mathcal{A}^{+})^{+}$ (AI.4)

c) associated superoperator : $\mathcal{A}\sigma = (\mathcal{A}^{a}\sigma^{+})^{+}$ (AI.5)

In the tetradic notation, these relations lead to :

$$\mathcal{Q}_{ij,kl} = (\mathcal{Q}^T)_{lk,ji} = (\mathcal{Q}^+)^{cc}_{kl,ij} = (\mathcal{Q}^a)^{cc}_{ji,lk}$$

(AI.6)

As an example, the property of adjoint symmetry (2.6) of Λ takes the form :

$$\Lambda_{ab,cd} = \Lambda^{cc}_{ba,dc}$$

(AI.7)

APPENDIX 2. MATRIX ELEMENTS OF $\tilde{\mathcal{H}}$ FOR THE FRIEDRICHS' MODEL.

We start from (4.25). Taking into account

$$C_{ab,dd} = C^{cc}_{ba,dd}$$

(A2.1)

(which results from $\Pi = \Pi^a$ and guarantees (2.6)), we have at dominant order in L^3 :

$$\tilde{\mathcal{H}}_{11,11} = \omega_1 + Re\left\{\sum_k v_k^{cc} C_{k1,11}\right\}$$

(A2.2)

$$\tilde{\mathcal{H}}_{kk,kk} = \omega_k$$

(A2.3)

$$\tilde{\mathcal{H}}_{11,kk} = Re\left\{v_k^{cc} C_{k1,kk} + \sum_{k'} v_{k'}^{cc} C_{k'1,kk}\right\}$$

(A2.4)

$$\tilde{\mathcal{H}}_{kk,11} = Re\left\{v_k C_{1k,11}\right\}$$

(A2.5)

$$\tilde{\mathcal{H}}_{kk,k'k'} = Re\left\{v_k C_{1k,k'k'}\right\}$$

(A2.6)

Using the expressions of matrix elements of C given in [8] and writing $\eta^+(z)$ in the form :

$$\eta^+(z) = z - \omega_1 - f^+(z)$$

(A2.7)

we have

$$\tilde{\mathcal{H}}_{11,11} = \omega_1 + Re\left\{\lambda^2 \int d\omega_k \frac{|v(\omega_k)|^2}{(s+\omega_1-\omega_k)z}\right\} = \Omega_1$$

(A2.8)

$$\tilde{\mathcal{H}}_{11,kk} = Re\left\{\lambda^2 |v_k|^2 \left(\frac{1}{\eta^-(\omega_k)} + \frac{f^+(\omega_k)}{|\eta^+(\omega_k)|^2} - \frac{f^-(\omega_k+\xi)}{|\eta^+(\omega_k)|^2}\right)\right\}$$

$$= (\omega_k - \Omega_1)\, a_k \qquad \text{(A2.9)}$$

$$\tilde{\mathcal{H}}_{kk,11} = \tfrac{1}{2}\lambda^2 |v_k|^2 \left(\frac{1}{(s'+\omega_1-\omega_k)\xi^{cc}} + \frac{1}{(s+\omega_1-\omega_k)\xi}\right)$$

$$= (\Omega_1 - \omega_k)\, b_k \qquad \text{(A2.10)}$$

$$\tilde{\mathcal{H}}_{kk,k'k'} = \lambda^4 \frac{|v_k|^2 |v_{k'}|^2}{|\eta^+(\omega_k)|^2} \mathcal{P}\left(\frac{1}{\omega_{k'}-\omega_k}\right) - (\Omega_1-\omega_k)\, b_k\, a_{k'} \qquad \text{(A2.11)}$$

where a_k and b_k are given by (6.15), (6.16).

APPENDIX 3. LIAPOUNOV REPRESENTATION FOR THE FRIEDRICHS' MODEL. DETERMINATION OF χ .

From (4.16), we obtain the conditions

$$\chi_{11,11}\, \chi^*_{11,11} = A_{11,11} \qquad \text{(A3.1)}$$

$$\chi_{11,kk} + \chi_{11,11}\, \chi^*_{11,kk} = A_{11,kk} \qquad \text{(A3.2)}$$

$$\chi_{kk,11}\, \chi^*_{11,11} + \chi^*_{kk,11} = A_{kk,11} \qquad \text{(A3.3)}$$

$$\chi_{kk,11}\, \chi^*_{11,k'k'} + \chi_{kk,k'k'} + \chi^*_{kk,k'k'} = A_{kk,k'k'} \qquad \text{(A3.4)}$$

For this model, A is real, starhermitian and even in L (hence hermitian), i.e.

$$A_{aa,bb} = A^{cc}_{aa,bb} = A_{bb,aa} \qquad \text{(A3.5)}$$

Also, combining (6.1) and (4.19), we have :

$$\chi^*_{aa,bb} = \chi^+_{aa,bb} = \chi_{bb,aa} \qquad \text{(A3.6)}$$

and (A3.1) to (A3.4) lead to :

$$\chi_{11,11} = (A_{11,11})^{1/2} = \left(\frac{1}{|\eta^+(\omega_1+\xi)|^2}\right)^{1/2} \qquad \text{(A3.7)}$$

$$\chi_{11,kk} = A_{11,kk} - \chi_{kk,11}\, \chi_{11,11} \qquad \text{(A3.8)}$$

$$\chi_{kk,k'k'} + \chi_{k'k',kk} = A_{kk,k'k'} - \chi_{kk,11}\, \chi_{k'k',11} \qquad \text{(A3.9)}$$

Further requirements on χ are given by (4.20), (4.21), i.e. :

$$\chi_{11,11} + \sum_k \chi_{kk,11} = 1 \tag{A3.10}$$

$$\chi_{11,kk} + \sum_{k' \neq k} \chi_{k'k',kk} = 0 \tag{A3.11}$$

$$\lim_{\lambda \to 0} \chi_{kk,11} = \lim_{\lambda \to 0} \chi_{11,kk} = \lim_{\lambda \to 0} \chi_{kk,k'k'} = 0 \tag{A3.12}$$

If one takes into account the explicit expression of $A_{11,kk}$ (see ref.[8]), (A3.8) becomes :

$$\chi_{11,kk} = a_k + \chi_{11,11} \left(\chi_{11,11}\, b_k - \chi_{kk,11} \right) \tag{A3.13}$$

In a physical representation, $\chi_{11,kk}$ and $\chi_{kk,11}$ for instance, are of the form (7.24), (7.25). From (A3.10), we then obtain the condition

$$\sum_k \alpha_k\, \delta(\Omega_1 - \omega_k) = 1 \tag{A3.14}$$

when one takes into account

$$\sum_k b_k = \frac{\lambda^2}{\theta} \left(\int d\omega_k \, \frac{|v(\omega_k)|^2}{(s' + \omega_1 - \omega_k)\, \zeta^{cc}} - c.c. \right)$$

$$= \frac{1}{\theta} \left[f^-(\omega_1 + \zeta^{cc}) - c.c. \right] = -1 \tag{A3.15}$$

APPENDIX 4. FINITE LINEWIDTH FOR SPONTANEOUS EMISSION AND INTERPRETATION OF SCATTERING CROSS SECTION.

Let us first consider the spontaneous emission process, i.e. start with an initial condition of the type :

$$\rho_{11}^{\alpha}(0) \sim O(1) \quad , \quad \rho_{kk}^{\alpha}(0) \sim O(L^{-3}) \quad \forall k \tag{A4.1}$$

Then, if we keep only dominant terms with respect to L^3, the evolution equations (7.11), (7.12) reduce to :

$$\frac{\partial \rho_{11}^{\alpha}}{\partial t} = W_{11}\, \rho_{11}^{\alpha} \tag{A4.2}$$

$$\frac{\partial \rho_{k1}^{\alpha}}{\partial t} = W_{k1}\, \rho_{11}^{\alpha} \tag{A4.3}$$

These equations are easily solved :

$$\rho_{11}^{\alpha}(t) = e^{W_{11} t}\, \rho_{11}^{\alpha}(0) \tag{A4.4}$$

$$\rho_{kk}^{\alpha}(t) = \rho_{kk}^{\alpha}(0) + \frac{W_{k1}}{W_{11}} \left(e^{W_{11} t} - 1 \right) \rho_{11}^{\alpha}(0) \tag{A4.5}$$

$(W_{11} < 0)$. For

$$|W_{11}|\, t \gg 1 \tag{A4.6}$$

this gives :

$$ {}^{\alpha}\rho_{11}(\infty) = 0 $$

$$ {}^{\alpha}\rho_{kk}(\infty) - {}^{\alpha}\rho_{kk}(0) = -\frac{W_{k1}}{W_{11}}\,{}^{\alpha}\rho_{11}(0) \qquad \text{(A4.7)} $$

i.e. in a physical representation (see 7.27) :

$$ {}^{\flat}\rho_{kk}(\infty) - {}^{\flat}\rho_{kk}(0) = \alpha_k\,\delta(\Omega_1-\omega_k)\,{}^{\flat}\rho_{11}(0) \qquad \text{(A4.8)} $$

In the physical representation, the emission line is infinitely narrow.

The discussion of spontaneous emission in the Green's function approach is formulated in the bare particle description. One starts with the initial condition

$$ \rho_{11}(0) = 1 \;,\quad \rho_{kk}(0) = 0 = \rho_{1k}(0) = \rho_{k1}(0) = \rho_{kk'}(0) \qquad \text{(A4.9)} $$

and looks at the asymptotic distribution of bare bosons, i.e. at $\rho_{kk}(\infty)$.

Let us restrict ourselves to physical representations in which (6.1) (i.e. (A3.6) and (7.26)) is satisfied. Then using (1.6), (A4.9) gives an initial condition of the type (A4.1). More precisely, we have :

$$ {}^{\flat}\rho_{11}(0) = \chi^{*}_{11,11} = \chi_{11,11} \qquad \text{(A4.10)} $$

$$ {}^{\flat}\rho_{kk}(0) = \chi^{*}_{kk,11} = \chi_{11,kk} = \alpha_k - \alpha_k\,\delta(\Omega_1-\omega_k)\,\chi_{11,11} \qquad \text{(A4.11)} $$

We also have, taking into account (A4.7), (A4.8) :

$$ \rho_{kk}(\infty) = {}^{\flat}\rho_{kk}(\infty) \qquad \text{(A4.12)} $$

i.e. using (A4.8), (A4.10) and (A4.11) :

$$ \rho_{kk}(\infty) = \alpha_k = \frac{\lambda^2\,|v_k|^2}{|\eta^{+}(\omega_k)|^2} \qquad \text{(A4.13)} $$

which shows that there is a line shape in this description. (As well known, further approximations lead to the Lorentzian shape : in $\eta^{+}(\omega_k)$, one replaces $f^{+}(\omega_k)$ by $f^{+}(\omega_1) \simeq \Omega_1 + \frac{i\Theta}{2}$ when $|\Omega_1-\omega_1| \ll \omega_1$, $i\Theta \ll \omega_1$).

Let us now turn to the interpretation of $W_{kk'}$. This is a difference between two positive definite quantities :

$$ w_{kk'} = 2\pi\,\delta(\omega_k-\omega_{k'})\,\lambda^4\,\frac{|v_k|^2\,|v_{k'}|^2}{|\eta^{+}(\omega_k)|^2} \qquad \text{(A4.14)} $$

$$ u_{kk'} = -\frac{W_{k1}\,W_{1k'}}{W_{11}} \qquad \text{(A4.15)} $$

In order to discuss the scattering problem, let us consider an initial condition where all the elements ${}^{\flat}\rho_{11}$, ${}^{\flat}\rho_{kk}$ are of the same order of magnitude $o(L^{-3})$. Then, we have to keep the full equations (7.11), (7.12). The

solution of (7.11) may be written :

$$ {}^{\flat}\rho_{11}(t) = e^{W_{11}t}\,{}^{\flat}\rho_{11}(0) + \int_0^t d\tau\, e^{W_{11}\tau} \sum_k W_{1k}\,{}^{\flat}\rho_{kk}(t-\tau) \qquad \text{(A4.16)} $$

If we introduce this in (7.12) and use (14.14) and (A4.15), we obtain :

$$ \frac{\partial\,{}^{\flat}\rho_{kk}(t)}{\partial t} = W_{kk}\,{}^{\flat}\rho_{kk}(t) + W_{k1}\,e^{W_{11}t}\,{}^{\flat}\rho_{11}(0) $$

$$ + \sum_{k'} \Big\{ w_{kk'}\,{}^{\flat}\rho_{kk'}(t) - u_{kk'}\Big[{}^{\flat}\rho_{k'k'}(t) + W_{11}\int_0^t d\tau\, e^{W_{11}\tau}\,{}^{\flat}\rho_{k'k'}(t-\tau)\Big]\Big\} \qquad \text{(A4.17)} $$

For times much larger than the life time of the unstable state, i.e. such that (A4.6) is satisfied, (A4.16) and (A4.17) become (see also [15]) :

$$ {}^{\flat}\rho_{11}(t) = -\sum_k \frac{W_{1k}}{W_{11}}\,{}^{\flat}\rho_{kk}(t) \qquad \text{(A4.18)} $$

$$ \frac{\partial\,{}^{\flat}\rho_{kk}(t)}{\partial t} = W_{kk}\,{}^{\flat}\rho_{kk}(t) + \sum_{k'} w_{kk'}\,{}^{\flat}\rho_{k'k'}(t) \qquad \text{(A4.19)} $$

which leads quite naturally to the interpretation of $w_{kk'}$ as the <u>total</u> cross section.

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References.

1) I. Prigogine, Nobel Lecture 1977, Stockholm, to be reproduced in Science.
A preliminary presentation of the results to be discussed here has been given by I. Prigogine and C. George, Int. Journ. of Quantum Chemistry 1978.

2) I. Prigogine, F. Mayné, C. George, M. de Haan, Proc. Natl. Acad. Sci. (U.S.A.) 74 (1977) 4152.

3) see i.e. G. Barton, Introduction to Advanced Field Theory, Interscience 1963.

4) W. Heitler, Quantum Theory of Radiation, Clarendon (1954).

5) I. Prigogine, C. George, F. Henin & L. Rosenfeld, Chemica Scripta 4, 5 (1973).

6) M. Jammer, The Philosophy of Quantum Mechanics, Wiley (1974).

7) A. Grecos & I. Prigogine, Physica 59 (1972) 77.

8) M. de Haan and F. Henin, Physica 67 (1973) 197.

9) see i.e. M. Goldberger and K. Watson, Collision Theory, Wiley 1964.

10) B. Misra and I. Prigogine, (to be published).

11) C. George, Physica 65 (1973) 277.

12) I. Prigogine, C. George, J. Rae, Physica 56 (1971) 25.

13) I. Prigogine and C. George, Physica 56 (1971) 329.

14) M. de Haan, C. George and F. Mayné, Physica (1978).

15) M. de Haan, Thesis U.L.B. (1973).