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Vacuum Subdynamics in Large Quantum Systems

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We present a constructive procedure to deal with large quantum systems in the thermodynamic limit. Starting with a discrete spectrum, we perform a complete decomposition of the evolution into one-dimensional subdynamics. We then go to the limit of a continuous spectrum after collecting them into global subdynamics of given degrees of correlation. Previously obtained results for the vacuum subdynamics are justified. The procedure is applied to the problem of potential scattering.

KEY WORDS: Irreversibility; continuous spectrum; analytic continuation; subdynamics; nonunitary transformation.

1. INTRODUCTION

The question of how to reconcile the dynamical evolution of large interacting systems with the second law of thermodynamics has been of long standing interest to I. Prigogine and the Brussels group.(1) The concept of subdynamics they have defined has proved quite convenient for expressing the irreversible character of the evolution.(2) It has furthermore appeared as a major step in developing the star-unitary transformation theory, leading to the so-called physical representation.(3) While the introduction of these notions originally made use of perturbation techniques and series expansions, more formal presentations of the theory were attempted, in particular by Grecos *et al.*(4)

It is a privilege for the authors to dedicate this paper to Prof. I. Prigogine. They are both genuine offspring of the Brussels school. As such, most of the ideas they profess owe their inspiration to I. P., their mentor, colleague, and friend through fascinating teaching, stimulating discussions, and illuminating speculations, but they take full responsability for their obvious mistakes, pernicious misconceptions, and malignant deviations from the orthodoxy they have modestly helped to create.

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We intend to suggest in the present paper why these attempts did not quite achieve their purpose, which was to stir up further developments in the theory. Their authors did not properly appreciate the $i\varepsilon$-rule,[5] a well-defined procedure of analytic continuation for the resolvent formalism, introduced in the perturbative approach, and they failed to recognize its relevance in dealing, in the limit, with a continuous spectrum.

We shall give concrete content to the above-mentioned formal results for the case of a quantum system in the thermodynamic limit. Starting from a finite system, we shall precisely define the way in which to take the limit of a continuous spectrum. The constructive method we present is easily extendable to situations that, for sake of simplicity, we de not consider here, such as the presence of discrete correlations amid the continuum, degenerate levels, and so on. Due to considerations of space, we shall limit ourselves to the presentation of essentially new results obtained using this method, leaving the lengthy demonstrations for further publication.

The most striking result that we present here is the complete diagonalization of the evolution operator, together with the corresponding highly singular (of distribution-type) star-unitary transformation. Such a result might be of importance for the construction in such systems of the operator conjugate to the Liouvillian (the infinitesimal generator of the dynamical evolution), namely the internal time T, which is at the basis of recent developments of the theory.[6]

The consistency of the transition to the continuous spectrum requires that all the subdynamics with the same degree of correlation are collected into a single global subdynamics with this degree of correlation. In the particular case studied here of the global vacuum subdynamics, all well-known results concerning the vacuum subdynamics associated with the singularity at the origin in the resolvent formalism are recovered. We illustrate these considerations on the example of potential scattering.[7]

We emphasize that the classical limit of our results can only be considered after this globalization has been performed, as no Liouvillian operator with a discrete spectrum can be taken as a starting point for a classical treatment.

2. THE DYNAMICS OF CORRELATIONS

The notion of subdynamics was introduced in the study of the solution of the Liouville–von Neumann equation

$$i\frac{\partial}{\partial t}\rho = L\rho \tag{2.1}$$

describing the time evolution of the density operator ρ in terms of the Liouvillian L, which for quantum systems is the commutator with the Hamiltonian H ($\hbar = 1$).

The formal solution of (2.1) is conveniently expressed in terms of the resolvent of L:

$$\rho(t) = \frac{1}{2i\pi} \int_\gamma du\, e^{-iut} \frac{1}{u-L} \rho(0) \tag{2.2}$$

The subdynamics are related to the singularities of the resolvent $(u-L)^{-1}$ in a sense to be made more precise later in this paper.

In the general case, the analysis of these singularities relies on a perturbation scheme in which the resolvent is expressed in terms of an unperturbed Liouvillian L_0 and a perturbation δL corresponding to the decomposition of the Hamiltonian into an unperturbed part H_0 and an interaction V:

$$\frac{1}{u-L} = \frac{1}{u-L_0} \sum_{n=0}^{\infty} \left(\delta L \frac{1}{u-L_0}\right)^n \tag{2.3}$$

Such an expansion leads naturally to a description of the evolution as a dynamics of correlations.

The starting point for treating a large quantum system consists in considering it enclosed in a finite quantization box, for which at some suitable stage the infinite-volume limit will be taken.

As long as the system is finite, a basis can be constructed that is labeled by a countable set of discrete indices $|k\rangle$, to which also refer the eigenvalues of the unperturbed Hamiltonian H_0. In superspace, the correlation states are denoted by a pair of such indices $|\nu\rangle \equiv |k, k'\rangle$, which label the eigenvalues ν of the unperturbed Liouvillian L_0, and because of the discreteness one can distinguish between different correlation states. The correlation states can be classified into families according to their degree of correlation. The various vacuum states $|k, k\rangle$ are eigenstates of L_0 with vanishing eigenvalue, and the n-correlated states need at least n transitions δL to be reached starting from any vacuum. Then a theorem in dynamics of correlations (dc-theorem) can be proved[8]:

Theorem. Between two successive identical correlations, only states of higher degree of correlation may give a finite contribution when the continuous limit is taken.[2]

[2] In situations with degenerate levels or when discrete correlations are embedded in the continuum, a classification of correlations should be adopted such that the above dc-theorem remains valid.

This theorem permits the unambiguous application of an analytic continuation rule that enables one to obtain separately the various contributions to the time evolution of the matrix elements of the density operator. Let us briefly recall the formulation of this $i\varepsilon$-rule:

$i\epsilon$-Rule. When evaluating the contributions coming from the singularity corresponding to a given correlation state, the propagator associated with a correlation of a higher degree must be treated as $+i\varepsilon$ ($+i\varepsilon$ has to be added to this propagator), while the propagator associated with a less correlated state is treated as $-i\varepsilon$. In the case of a correlation of equal degree, its propagator is treated as $+i\varepsilon$ or $-i\varepsilon$ when it appears, respectively, at the left or at the right (the dc-theorem prevents it from appearing on both sides) of the correlation considered.

3. THE SUBDYNAMICS

The subdynamics $\overset{v}{\Pi}$ arises from the singularity corresponding to the particular correlation v, that is, from the pole $u = v$ in the perturbation expansion. To isolate this singularity, one expresses the resolvent (2.3) in terms of functions that are regular at $u = v$. One introduces (barred) functions, which are irreducible with respect to the correlation v, i.e., do not contain the particular propagator v:

$$\bar{\psi}_v(u) = \langle v | \delta L \sum_{n=1}^{\infty} \left(\frac{1}{u - L_0} \delta L \right)^n | v \rangle_{\text{irr } v} \tag{3.1}$$

$$\bar{\mathscr{C}}_{v',v}(u) = \langle v' | \sum_{n=1}^{\infty} \left(\frac{1}{u - L_0} \delta L \right)^n | v \rangle_{\text{irr } v} \tag{3.2}$$

$$\bar{\mathscr{D}}_{v,v'}(u) = \langle v | \sum_{n=1}^{\infty} \left(\delta L \frac{1}{u - L_0} \right)^n | v' \rangle_{\text{irr } v} \tag{3.3}$$

$$\bar{\mathscr{P}}^{(v)}_{v',v''}(u) = \langle v' | \frac{1}{u - L_0} \sum_{n=0}^{\infty} \left(\delta L \frac{1}{u - L_0} \right)^n | v'' \rangle_{\text{irr } v} \tag{3.4}$$

In terms of these functions, the components of the solution (2.2) at time t can be written as

$$\begin{aligned} \rho_{v'} = \frac{1}{2i\pi} \sum_{v,v''} \int_\gamma du\, e^{-iut} \Big\{ & [\delta_{v',v} + \bar{\mathscr{C}}_{v',v}(u)] \sum_{n=0}^{\infty} \frac{[\bar{\psi}_v(u)]^n}{(u - v)^{n+1}} \\ & \times [\delta_{v,v''} + \bar{\mathscr{D}}_{v,v''}(z)]\, \rho_{v''}(0) + \bar{\mathscr{P}}^{(v)}_{v',v''}(u)\, \rho_{v''}(0) \Big\} \end{aligned} \tag{3.5}$$

or by performing the summation over n as

$$\rho_{\nu'} = \frac{1}{2i\pi} \sum_{\nu,\nu''} \int_{\gamma} du\, e^{-iut} \left\{ [\delta_{\nu',\nu} + \bar{\mathscr{C}}_{\nu',\nu}(u)] \frac{1}{u - \nu + \bar{\psi}_{\nu}(u)} \right.$$

$$\left. \times [\delta_{\nu,\nu''} + \bar{\mathscr{D}}_{\nu,\nu''}(z)]\, \rho_{\nu''}(0) + \bar{\mathscr{P}}^{(\nu)}_{\nu',\nu''}(u)\, \rho_{\nu''}(0) \right\} \tag{3.6}$$

In contrast with the usual presentation, in which ψ is an operator with diagonal and off-diagonal elements, the fact that here we consider separately each particular discrete correlation ν leads to a $\bar{\psi}$ that is a function, not an operator. As a consequence, the subdynamics we are about to construct will all be one-dimensional.

The contribution to $\rho_{\nu'}(t)$ arising from the singularity associated with the particular correlation ν is now given by

$$\overset{\nu}{\rho}_{\nu'} = \frac{1}{2i\pi} \oint_{u_\nu} du\, e^{-iut} [\delta_{\nu',\nu} + \bar{\mathscr{C}}_{\nu',\nu}(u)] \frac{1}{u - \nu - \bar{\psi}_{\nu}(u)}$$

$$\times \sum_{\nu''} [\delta_{\nu,\nu''} + \bar{\mathscr{D}}_{\nu,\nu''}(u)]\, \rho_{\nu''}(0) \tag{3.7}$$

where u_ν is the solution of

$$u_\nu - \nu - \bar{\psi}_\nu(u_\nu) = 0 \tag{3.8}$$

with the condition that it reduces to $u_\nu = \nu$ for a vanishing interaction.

At this stage, it is convenient to introduce two auxiliary parameters κ and z. The parameter κ will play a role similar to that of the coupling constant and will be set equal to 1 at the end of the calculation.[3] The parameter z will be the $i\varepsilon$ that has to be added to or subtracted from u in the propagators in order to take the $i\varepsilon$-rule into account. Equation (3.7) is thus transformed into

$$\overset{\nu}{\rho}_{\nu'} = \frac{1}{2i\pi} \oint_{u_\nu(z,\kappa)} du\, e^{-iut} [\delta_{\nu',\nu} + \bar{\mathscr{C}}_{\nu',\nu}(u, z)] \frac{1}{u - \nu - \kappa\bar{\psi}_{\nu}(u + z)}$$

$$\times \sum_{\nu''} [\delta_{\nu,\nu''} + \bar{\mathscr{D}}_{\nu,\nu''}(u, z)]\, \rho_{\nu''}(0) \tag{3.9}$$

Observe that in $\bar{\psi}_\nu$ the parameter z has been uniformly added to u, as all the correlation states in $\bar{\psi}_\nu$ are of a degree higher than ν, while in $\bar{\mathscr{C}}$ and $\bar{\mathscr{D}}$ it has to be added to or subtracted from u contained in the propagators according to the $i\varepsilon$-rule.

[3] For simplicity, we shall only introduce it here in connection with the diagonal element $\bar{\psi}$.

Now the two-parameter function $u_\nu(z, \kappa)$ is the solution of

$$u_\nu(z, \kappa) - \nu - \kappa\bar{\psi}_\nu(u_\nu(z, \kappa) + z) = 0 \tag{3.10}$$

which we write explicitly

$$u_\nu(z, \kappa) = \nu + \kappa\bar{\theta}_\nu(z + \nu, \kappa) \tag{3.11}$$

and is such that

$$\bar{\theta}_\nu(y, \kappa = 0) = \bar{\psi}_\nu(y) \tag{3.12}$$

Introducing (3.11) into (3.10), one obtains the relation

$$\bar{\theta}_\nu(y, \kappa) = \bar{\psi}_\nu(y + \kappa\bar{\theta}_\nu(y, \kappa)) \tag{3.13}$$

Let us make more precise the somewhat hybrid way in which we perform the transition from the discrete to the continuous spectrum.

The states are considered discrete as long as it is convenient for their enumeration, but the continuous limit is prepared by not considering contributions that will become negligible on the basis of the dc-theorem, and by adapting, through the use of $\pm z$, the propagators associated with the various correlations. It is clear that, once the analytical continuation has been indicated, for the subdynamics corresponding to a given correlation, one can replace internal summations (over dummy indices) by integrations for all other correlations.

Let us first consider in (3.7) the element $\nu' = \nu'' = \nu$ and write

$$\begin{aligned}\frac{1}{2i\pi}\oint_{u_\nu(z,\kappa)} du \exp(-iut) \frac{1}{u - \nu - \kappa\bar{\psi}_\nu(u + z)} \\ = (\exp\{-i[\nu + \kappa\bar{\theta}_\nu(z + \nu, \kappa)]\, t\})\, \bar{A}_\nu(z + \nu, \kappa)\end{aligned} \tag{3.14}$$

where $\bar{A}_\nu(z + \nu, \kappa)$ is the residue of the function $[u - \nu - \kappa\bar{\psi}_\nu(u + z)]^{-1}$ at $u = u_\nu(z, \kappa)$. It suffices to expand the denominator around $u = u_\nu(z, \kappa)$ in (3.14) to obtain its expression in terms of the derivative $\bar{\psi}'_\nu$ of $\bar{\psi}_\nu$:

$$\bar{A}_\nu(z + \nu, \kappa) = \frac{1}{1 - \kappa\bar{\psi}'_\nu(z + \nu + \kappa\bar{\theta}_\nu(z + \nu, \kappa))} \tag{3.15}$$

An alternative form for $\bar{A}_\nu(z + \nu, \kappa)$ is obtained from an asymptotic expansion of the lhs of (3.14) (by deforming the contour around u_ν in such a way as to include the origin $u = 0$ and excluding all other singularities of the integrand)

$$\frac{1}{2i\pi}\oint_{u_\nu(z,\kappa)} du\, e^{-iut} \sum_{n=0}^{\infty} \frac{[\nu+\kappa\bar{\psi}_\nu(u+z)]^n}{u^{n+1}}$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} D_u^n\{[\nu+\kappa\bar{\psi}_\nu(u+z)]^n e^{-iut}\}_{u=0} \tag{3.16}$$

For $t=0$, one finds the required expression for $\bar{A}_\nu(z+\nu,\kappa)$:

$$\bar{A}_\nu(z+\nu,\kappa) = \sum_{n=0}^{\infty} \frac{1}{n!} D_u^n[\nu+\kappa\bar{\psi}_\nu(u+z)]_{u=0}^n$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} D_z^n[\nu+\kappa\bar{\psi}_\nu(u+z)]_{u=0}^n$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} D_z^n[\nu+\kappa\bar{\psi}_\nu(z)]^n \tag{3.17}$$

For $t\neq 0$, the identification of (3.16) with (3.14) enables one to obtain an equation for $\bar{\theta}_\nu(z+\nu,\kappa)$:

$$\nu+\kappa\bar{\theta}_\nu(z+\nu,\kappa)$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} D_u^n[\nu+\kappa\bar{\psi}_\nu(u+z)]_{u=0}\,[\nu+\kappa\bar{\theta}_\nu(z+\nu,\kappa)]^n \tag{3.18}$$

That this relation holds can be easily seen. Indeed, the rhs is an expression for the function $\nu+\kappa\bar{\psi}_\nu(u+z)$ displaced from $u=0$ to $u=\nu+\kappa\bar{\theta}_\nu(z+\nu,\kappa)$,

$$\nu+\kappa\bar{\psi}_\nu(u+\nu+\kappa\bar{\theta}_\nu(z+\nu,\kappa)+z)|_{u=0}$$
$$=\nu+\kappa\bar{\psi}_\nu(z+\nu+\kappa\bar{\theta}_\nu(z+\nu,\kappa))$$

which by virtue of (3.13) is equal to the lhs of (3.18). Note that (3.18) can also be written as

$$\nu+\kappa\bar{\theta}_\nu(z+\nu,\kappa)$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} \{D_z^n[\nu+\kappa\bar{\psi}_\nu(z)]\}[\nu+\kappa\bar{\theta}_\nu(z+\nu,\kappa)]^n \tag{3.19}$$

In this more familiar form, however, it is not easily seen that the rhs corresponds to a mere displacement, as the last factor still depends on z.

The fact that the subdynamics is one-dimensional, $\bar{\psi}$ being a function, permits one to understand the results obtained above in terms of Lagrange's theorem,[9] as in Ref. 4. This makes the mathematical formulation considerably safer than when ψ is an operator. In Section 5, we intend, however, to justify the usual results obtained from an operator formalism.

The terms in (3.9) containing $\mathscr{C}$ and $\bar{\mathscr{D}}$ are treated along the same lines. For instance, one has

$$\frac{1}{2i\pi}\oint_{u_\nu(z,\kappa)} du\, e^{-iut}\frac{1}{u-\nu-\kappa\bar{\psi}_\nu(u+z)}\bar{\mathscr{D}}_{\nu,\nu''}(u,z)$$
$$=[\exp(-iu_\nu t)]\,\bar{A}_\nu(z+\nu,\kappa)\,\bar{\mathscr{D}}_{\nu,\nu''}(u_\nu,z)$$
$$=(\exp\{-i[\nu+\kappa\bar{\theta}_\nu(z+\nu,\kappa)]\,t\})\,\bar{A}_\nu(z+\nu,\kappa)\,\bar{D}_{\nu,\nu''}(z,\kappa) \quad (3.20)$$

with

$$\bar{D}_{\nu,\nu''}(z,\kappa)=\bar{\mathscr{D}}_{\nu,\nu''}(u_\nu,z)=\bar{\mathscr{D}}_{\nu,\nu''}(\nu+\kappa\bar{\theta}_\nu(z+\nu,\kappa),z) \quad (3.21)$$

In the expression of the element $\bar{D}_{\nu,\nu''}$ it is the first index that refers to the subdynamics under consideration.

In the asymptotic expansion

$$\bar{A}_\nu(z+\nu,\kappa)\,\bar{D}_{\nu,\nu''}(z,\kappa)$$
$$=\sum_{n=0}^{\infty}\frac{1}{n!}D_u^n\{[\nu+\kappa\bar{\psi}_\nu(u+z)]^n\,\bar{\mathscr{D}}_{\nu,\nu''}(u,z)\}_{u=0} \quad (3.22)$$

one cannot in general replace the derivation with respect to u by a derivation with respect to z, since in $\bar{\mathscr{D}}(u,z)$ the propagators contain either $u+z$ or $u-z$ according to the $i\varepsilon$-rule.

Similar expressions are derived for the terms containing $\mathscr{C}$, with the second index referring to the subdynamics considered:

$$\bar{C}_{\nu',\nu}(z,\kappa)=\mathscr{C}_{\nu',\nu}(\nu+\kappa\bar{\theta}_\nu(z+\nu,\kappa),z) \quad (3.23)$$

and

$$\bar{C}_{\nu',\nu}(z,\kappa)\,\bar{A}_\nu(z+\nu,\kappa)$$
$$=\sum_{n=0}^{\infty}\frac{1}{n!}D_u^n\{\mathscr{C}_{\nu',\nu}(u,z)[\nu+\kappa\bar{\psi}_\nu(u+z)]^n\}_{u=0} \quad (3.24)$$

The solution (3.8) is thus given by

$$\overset{\nu}{\rho}_{\nu'}=[\delta_{\nu',\nu}+\bar{C}_{\nu',\nu}(z,\kappa)]\exp\{-i[\nu+\kappa\bar{\theta}_\nu(z+\nu,\kappa)]\,t\}$$
$$\times\bar{A}_\nu(z+\nu,\kappa)\sum_{\nu''}[\delta_{\nu,\nu''}+\bar{D}_{\nu,\nu''}(z,\kappa)]\,\rho_{\nu''}(0) \quad (3.25)$$

The operators $\overset{\nu}{\Pi}$, defined by their elements

$$\overset{\nu}{\Pi}_{\nu',\nu''} = [\delta_{\nu',\nu} + \bar{C}_{\nu',\nu}(z, \kappa)]\, \bar{A}_{\nu}(z+\nu, \kappa)[\delta_{\nu,\nu''} + \bar{D}_{\nu,\nu''}(z, \kappa)] \tag{3.26}$$

form a complete set of subdynamics. The demonstrations that they obey the usual orthonormality, completeness, and dynamical independence conditions are exactly the same as in Ref. 10 and will not be repeated here.

In the $\overset{\nu}{\Pi}$-subdynamics, the privileged component $\overset{\nu}{\rho}_{\nu} \equiv (\overset{\nu}{\Pi}\rho)_{\nu}$ evolves according to the one-dimensional equation

$$i\,\partial_t \overset{\nu}{\rho}_{\nu} = [\nu + \kappa\bar{\theta}_{\nu}(z+\nu, \kappa)]\, \overset{\nu}{\rho}_{\nu} \tag{3.27}$$

while the other components are expressed as functionals of these privileged components:

$$\overset{\nu}{\rho}_{\nu'}(t) = \bar{C}_{\nu',\nu} \overset{\nu}{\rho}_{\nu}(t) \tag{3.28}$$

In the next section we shall study in detail a particular vacuum subdynamics, before recombining all of them into the so-called Π-subdynamics familiar from previous work. Now that the role of the auxiliary parameter κ used for selecting the appropriate solution of (3.8) has been established, we may set its value equal to 1 in the following.

4. A VACUUM SUBDYNAMICS $\overset{0}{\Pi}$

By introducing an irreducibility condition with respect to all the different vacua, we shall express for the particular case of a vacuum state $|0\rangle$ the various functions appearing in the previous section in terms of the operators that were introduced in the general formalism as previously developed.

The diagonal elements of the collision operator defined as

$$\psi_{0,0}(u) \equiv \langle 0|\, \delta L \sum_{n=1}^{\infty} \left(\frac{1}{u - L_0}\, \delta L\right)^n |0\rangle_{\text{irr } V} \tag{4.1}$$

can immediately be identified with $\bar{\psi}_0(u)$,

$$\psi_{0,0} = \bar{\psi}_0(u) \tag{4.2}$$

since, due to the dc-theorem, in $\bar{\psi}_0$ all intermediate states have to be of a higher degree of correlation, thus excluding other vacuum states.

The off-diagonal elements of the collision operator ψ,

$$\psi_{0,0'}(u) \equiv \langle 0|\, \delta L \sum_{n=1}^{\infty} \left(\frac{1}{u - L_0}\, \delta L \right)^n |0'\rangle_{\mathrm{irr}\, V} \tag{4.3}$$

can serve for expressing the functions $\bar{\mathscr{D}}$ and $\bar{\mathscr{C}}$.

The destruction element $\bar{\mathscr{D}}_{0,v}(u)$ is irreducible only with respect to the vacuum $|0\rangle$ and contains other vacua. In particular, the element $\bar{\mathscr{D}}_{0,0'}(u)$ admits the expansion

$$\begin{aligned} \bar{\mathscr{D}}_{0,0'}(u) = {} & \psi_{0,0'}(u) \frac{1}{u - \psi_{0',0'}(u)} \\ & + \sum_{0''} \psi_{0,0''}(u) \frac{1}{u - \psi_{0'',0''}(u)}\, \psi_{0'',0'}(u) \frac{1}{u - \psi_{0',0'}(u)} \\ & + \cdots \end{aligned} \tag{4.4}$$

Defining

$$\mathscr{D}_{0'',0'}(u) = \psi_{0'',0'}(u) \frac{1}{u - \psi_{0',0'}(u)} \tag{4.5}$$

one may write an integral equation for $\bar{\mathscr{D}}_{0,0'}(u)$:

$$\bar{\mathscr{D}}_{0,0'}(u) = \mathscr{D}_{0,0'}(u) + \sum_{0''} \bar{\mathscr{D}}_{0,0''}(u)\, \mathscr{D}_{0'',0'}(u) \tag{4.6}$$

Similarly, for the creation elements, one obtains

$$\bar{\mathscr{C}}_{0',0}(u) = \mathscr{C}_{0',0}(u) + \sum_{0''} \mathscr{C}_{0',0''}(u)\, \bar{\mathscr{C}}_{0'',0}(u) \tag{4.7}$$

where $\mathscr{C}_{0',0}(u)$ is defined as

$$\mathscr{C}_{0',0}(u) = \frac{1}{u - \psi_{0',0'}(u)}\, \psi_{0',0}(u) \tag{4.8}$$

The $\bar{\mathscr{D}}_{0,c}$ and $\bar{\mathscr{C}}_{c,0}$, where the index c refers to any correlated state different from a vacuum, can be expressed in a similar way:

$$\bar{\mathscr{D}}_{0,c}(u) = \mathscr{D}_{0,c}(u) + \sum_{0''} \bar{\mathscr{D}}_{0,0''}(u)\, \mathscr{D}_{0'',c}(u) \tag{4.9}$$

$$\bar{\mathscr{C}}_{c,0}(u) = \mathscr{C}_{c,0}(u) + \sum_{0''} \mathscr{C}_{c,0''}(u)\, \bar{\mathscr{C}}_{0'',0}(u) \tag{4.10}$$

in which $\mathscr{D}_{0,c}$ and $\mathscr{C}_{c,0}$ are elements of the usual destruction and creation operators irreducible with respect to all vacuum states. In terms of these elements, the solution for the various vacuum components of $\overset{0}{\rho}(t)$ is given by

$$\overset{0}{\rho}_{0'}(t)=(\delta_{0',0}+\bar{C}_{0',0})[\exp(-i\bar{\theta}_0 t)]\,\bar{A}_0\sum_{0'',c}(\delta_{0,0''}+\bar{D}_{0,0''})(\rho_{0''}+\overset{0}{D}_{0'',c}\rho_c) \tag{4.11}$$

and for the correlated components by

$$\overset{0}{\rho}_c(t)=\sum_{0'}\overset{0}{C}_{c,0'}\overset{0}{\rho}_{0'}(t) \tag{4.12}$$

where

$$\bar{D}_{0,0''}=\bar{\mathscr{D}}_{0,0''}(u,z)|_{u=\bar{\theta}_0(z)}=\bar{\mathscr{D}}_{0,0''}(\bar{\theta}_0(z),z) \tag{4.13}$$

$$\bar{C}_{0',0}=\bar{\mathscr{C}}_{0',0}(u+z)|_{u=\bar{\theta}_0(z)}=\bar{\mathscr{C}}_{0',0}(z+\bar{\theta}_0(z)) \tag{4.14}$$

$$\overset{0}{D}_{0'',c}=\mathscr{D}_{0'',c}(u+z)|_{u=\bar{\theta}_0(z)}=\mathscr{D}_{0'',c}(z+\bar{\theta}_0(z)) \tag{4.15}$$

$$\overset{0}{C}_{c,0'}=\bar{\mathscr{C}}_{c,0'}(u+z)|_{u=\bar{\theta}_0(z)}=\mathscr{C}_{c,0'}(z+\bar{\theta}_0(z)) \tag{4.16}$$

Expressions (4.14)–(4.16) are functions of $u+z$, as all the propagators correspond either to correlation or to vacuum states at the left of the vacuum 0. This is not the case for $\bar{D}_{0,0''}$ in (4.13), in which vacuum states appear at the right of 0 and one must treat them $u-z$.

More explicitly, in the expression (4.7), using the definition (4.8), one replaces u by $u+z$ everywhere, including the propagators present due to (4.8):

$$\bar{\mathscr{C}}_{0',0}(u+z)=\frac{1}{u+z-\psi_{0',0'}(u+z)}\times\left[\psi_{0',0}(u+z)+\sum_{0''}\psi_{0',0''}(u+z)\,\bar{\mathscr{C}}_{0'',0}(u+z)\right] \tag{4.17}$$

By contrast, with the use of (4.5), one replaces u by $u+z$ in (4.6) everywhere except in the vacuum propagators, in which u is replaced by $u-z$:

$$\bar{\mathscr{D}}_{0,0'}(u,z)=\left[\psi_{0,0'}(u+z)+\sum_{0''}\bar{\mathscr{D}}_{0,0''}(u,z)\,\psi_{0'',0'}(u+z)\right]\times\frac{1}{u-z-\psi_{0',0'}(u+z)} \tag{4.18}$$

Multiplying both sides by the denominator and taking the value at $u=\bar{\theta}_0(z)$, one obtains the following equations:

$$[z+\bar{\theta}_0(z)-\psi_{0',0'}(z+\bar{\theta}_0(z))]\,\bar{C}_{0',0}$$
$$=\psi_{0',0}(z+\bar{\theta}_0(z))+\sum_{0''}\psi_{0',0''}(z+\bar{\theta}_0(z))\,\bar{C}_{0'',0} \tag{4.19}$$

$$\bar{D}_{0,0'}[-z+\bar{\theta}_0(z)-\psi_{0',0'}(z+\bar{\theta}_0(z))]$$
$$=\psi_{0,0'}(z+\bar{\theta}_0(z))+\sum_{0''}\bar{D}_{0,0''}\psi_{0'',0'}(z+\bar{\theta}_0(z)) \tag{4.20}$$

It is quite clear from these expressions that the transformation of $\bar{C}$ into $\bar{D}$ through a *-conjugation cannot be accomplished without explicit reference to the $i\varepsilon$-rule.

5. THE VACUUM SUBDYNAMICS $\Pi=\sum_0 \overset{0}{\Pi}$

In going to the continuous spectrum limit, one gives up the idea of discriminating between the different vacuum states. Let us thus proceed to the summation over the corresponding vacuum subdynamics. For this summation to be performed, and once it has been, the vacuum indices can be treated as continuous integration variables.

By summation over 0 one obtains

$$\tilde{\rho}_{0'}(t)=\sum_0(\delta_{0',0}+\bar{C}_{0',0})[\exp(-i\bar{\theta}_0 t)]\,\bar{A}_0$$
$$\times\sum_{0'',c}(\delta_{0,0''}+\bar{D}_{0,0''})(\rho_{0''}+D_{0'',c}\rho_c) \tag{5.1}$$

Let us first consider the initial time contribution:

$$\tilde{\rho}_{0'}(0)=\sum_{0,0'',c}(1+\bar{C})_{0',0}\,\bar{A}_0(1+\bar{D})_{0,0''}\,(\rho_{0''}+\overset{0}{D}_{0'',c}\rho_c) \tag{5.2}$$

In terms of the operators irreducible with respect to all vacuum states, the same expression was given as

$$\tilde{\rho}_{0'}(0)=\sum_{0'',c}A_{0',0''}(\rho_{0''}+D_{0'',c}\rho_c) \tag{5.3}$$

so that one obtains by direct identification

$$A_{0',0''}=\sum_0(1+\bar{C})_{0',0}\,\bar{A}_0(1+\bar{D})_{0,0''} \tag{5.4}$$

One also has the relation

$$\sum_{0''} A_{0',0''} D_{0'',c} = \sum_{0,0''} (1+\bar{C})_{0',0}\, \bar{A}_0 (1+\bar{D})_{0,0''} \overset{0}{D}_{0'',c} \tag{5.5}$$

from which one cannot easily obtain a closed form for D, as the last factor of the rhs still depends on the summation index 0.

For the correlated components, $\tilde{\rho}_c$, one has on the one hand

$$\tilde{\rho}_c = \sum_{0,0',0'',c'} \overset{0}{C}_{c,0'} (1+\bar{C})_{0',0}\, \bar{A}_0 (1+\bar{D})_{0,0''}\, (\rho_{0''} + \overset{0}{D}_{0'',c'} \rho_{c'}) \tag{5.6}$$

and on the other

$$\tilde{\rho}_c = \sum_0 C_{c,0} \tilde{\rho}_0 \tag{5.7}$$

which enables one to define C through the identity

$$(CA)_{c,0''} = \sum_{0,0'} \overset{0}{C}_{c,0'} (1+\bar{C})_{0',0}\, \bar{A}_0 (1+\bar{D})_{0,0''} \tag{5.8}$$

Before showing that this is indeed the usual expression for C,[2] let us go back to the contribution to $\tilde{\rho}_{0'}$ at time t, which is usually cast into the form

$$\tilde{\rho}_{0'} = \sum_{\underline{0},0''} (e^{-i\theta t})_{0',\underline{0}} \left[A_{\underline{0},0''} \rho_{0''}(0) + \sum_c (AD)_{\underline{0},c} \rho_c(0) \right] \tag{5.9}$$

By comparison with (5.1) and using (5.4), one sees that $\theta_{0',\underline{0}}$ is given by

$$\theta_{0',\underline{0}} = \sum_0 (1+\bar{C})_{0',0}\, \bar{\theta}_0 (1+\bar{C})^{-1}_{0,\underline{0}} \tag{5.10}$$

where we have formally introduced the inverse of the operator $(1+\bar{C})$. Now by (4.16), one can write

$$\begin{aligned} \overset{0}{C}_{c,0'} &= \mathscr{C}_{c,0'}(u + z + \bar{\theta}_0(z))|_{u=0} \\ &= \sum_n \frac{1}{n!} [D_u^n \mathscr{C}_{c,0'}(u+z)]_{u=0}\, [\bar{\theta}_0]^n \\ &= \sum_n \frac{1}{n!} [D_z^n \mathscr{C}_{c,0'}(z)]\, [\bar{\theta}_0]^n \end{aligned} \tag{5.11}$$

The expression (5.8) becomes

$$(CA)_{c,0''} = \sum_{\mathrm{Q}} C_{c,\mathrm{Q}} A_{\mathrm{Q},0''}$$

$$= \sum_{n} \sum_{0'} \frac{1}{n!} [D_z^n \mathscr{C}_{c,0'}(z)] \sum_{0} (1 + \bar{C})_{0',0} [\bar{\theta}_0]^n \bar{A}_0 (1 + \bar{D})_{0,0''}$$

Using (5.4), $A_{\mathrm{Q},0''}$ is made to appear at the right in the rhs of the above expression. Then using (5.10), one recovers the usual definition of C:

$$C_{c,\mathrm{Q}} = \sum_{n} \sum_{0'} \frac{1}{n!} [D_z^n \mathscr{C}_{c,0'}(z)](\theta^n)_{0',\mathrm{Q}} \tag{5.12}$$

We shall not give here the corresponding expression for D, which would require the introduction of the mirror-image operator of θ (see Ref. 2).

Including the diagonal elements in (4.7),

$$(1 - \mathscr{C})(1 + \bar{\mathscr{C}}) = 1 \tag{5.13}$$

one obtains the equation

$$[z + \bar{\theta}(z) - \psi(z + \bar{\theta}(z))](1 + \bar{C}) = z + \bar{\theta}(z) - \bar{\psi}(z + \bar{\theta}(z)) \tag{5.14}$$

which generalizes Eq. (4.19). Observe that, in the explicit expressions for the different elements, the index of $\bar{\theta}$ is everywhere the same as the right index of $(1 + \bar{C})$, the notation ψ now summarizing both diagonal and off-diagonal elements. Due to (3.13), the rhs of (5.14) reduces to z. By multiplying both sides at the right by $(1 + \bar{C})^{-1}$, with its left index the same as that of $\bar{\theta}$, and using (5.10), one recasts (5.14) into the form

$$\theta - \psi(z + \bar{\theta}(z))(1 + \bar{C})(1 + \bar{C})^{-1} = z[(1 + \bar{C})^{-1} - 1] \tag{5.15}$$

Following the same procedure used to obtain (5.12) from (5.8), the second term of the lhs leads to the usual expansion of θ in terms of the derivatives of the ψ operator. However, the identification

$$\theta(z) = \sum_{n} \frac{1}{n!} [D_z^n \psi(z)]\, \theta^n(z) \tag{5.16}$$

is not possible analytically for all z, but only strictly in the limit $z = i0$ where the rhs of (5.15) vanishes.

The same remark holds for the usual expansion

$$A(z) = \sum_{n} \frac{1}{n!} [D_z^n \psi^n(z)] \tag{5.17}$$

for which a general proof will not be given even in the limit $z = i0$.

In the next section, however, we shall indicate how this equality is verified at the lowest orders in an expansion in the inverse of the volume (L^{-3}).

6. POTENTIAL SCATTERING

This problem has been treated extensively in Ref. 7 and we shall apply the above considerations to the particular one-particle sector that was labeled 1–1 in that article.

Many simplifications will occur when the orders of magnitude of the various elements with respect to the volume are taken into account explicitly. In particular, one has

$$\bar{\psi}_0(u) = \psi_{0,0}(u) = O(1/L^3) \tag{6.1}$$

From the definition (3.13) for $\bar{\theta}_0$,

$$\bar{\theta}_0(z) = \bar{\psi}_0(z + \bar{\theta}_0(z)) \tag{6.2}$$

one sees that as all the propagators inside $\bar{\psi}_0$ correspond to more correlated states and are thus of the form $1/(z + \bar{\theta}_0 - v)$, $\bar{\theta}_0$ can be neglected in front of v. Therefore $\bar{\theta}_0$ can be identified with $\bar{\psi}_0$ and also through (4.2) with the diagonal element of ψ:

$$\bar{\theta}_0(z) = \bar{\psi}_0(z) = \psi_{0,0}(z) = (\psi_d(z))_{0,0} \tag{6.3}$$

Similarly, one gets from (4.15)–(4.16)

$$\overset{0}{D}_{0'',c} = \mathscr{D}_{0'',c}(z + \bar{\theta}_0) = \mathscr{D}_{0'',c}(z) = D_{0'',c} \tag{6.4}$$

$$\overset{0}{C}_{c,0'} = \mathscr{C}_{c,0'}(z + \bar{\theta}_0) = \mathscr{C}_{c,0'}(z) = C_{c,0'} \tag{6.5}$$

In the creation and destruction of correlations, the explicit reference to the subdynamics $\overset{0}{\Pi}$ disappears when orders of magnitude in the volume are taken into account; the expressions for these operators are hence considerably simplified, as they are reduced to a single term instead of a series.

By contrast, in spite of the fact that

$$\psi_{0',0''} = (\psi_{nd}(u))_{0',0''} = O(1/L^6) \tag{6.6}$$

the creation and destruction elements from one vacuum to another still obey integral equations. Indeed, from (4.17),

$$\bar{C}_{0',0} = \bar{\mathscr{C}}_{0',0}(u + z + \bar{\theta}_0(z))]_{u=0}$$

satisfies, using (6.3),

$$\bar{C}_{0',0}=\frac{1}{z+\psi_{0,0}(z)-\psi_{0',0'}(z)}\left[\psi_{0',0}(z)+\sum_{0''}\psi_{0',0''}(z)\,\bar{C}_{0'',0}\right] \tag{6.7}$$

and is of order L^{-3} due to the volume dependence of the numerator and denominator (the limit $z\to i0$ is understood in all that follows).

Multiplying both sides by the denominator and adding $\psi_{0',0'}$ to both sides for diagonal elements, one gets

$$((1+\bar{C})\,\psi_d(z))_{0',0}=(\psi_d(z)(1+\bar{C}))_{0',0}+(\psi_{nd}(z)(1+\bar{C}))_{0',0} \tag{6.8}$$

which also reads

$$(1+\bar{C})\,\bar{\theta}(z)=\psi(z)(1+\bar{C}) \tag{6.9}$$

where the index of $\bar{\theta}$ is the same as the right index of $\bar{C}$ and $\psi(z)$ summarizes the ψ_d and ψ_{nd} elements.

Multiplying at the right by $(1+\bar{C})^{-1}$, one then finds that the asymptotic collision operator θ reduces to the collision operator itself as

$$\theta(z)=(1+\bar{C})\,\bar{\theta}(z)(1+\bar{C})^{-1}=\psi(z) \tag{6.10}$$

To complete the comparison, we need the expression for A. From (3.15), one has

$$\bar{A}_0=\frac{1}{1-\psi_0'(z+\bar{\theta}_0)}=\frac{1}{1-(\psi_d'(z))_{0,0}}=1+O\left(\frac{1}{L^3}\right) \tag{6.11}$$

From (5.5) and (6.11), one can write at the dominant order in the volume

$$A=(1+\bar{C})(1+\bar{D}) \tag{6.12}$$

The diagonal elements are thus given by

$$(A_d)_{0,0}=1 \tag{6.13}$$

and for the off-diagonal elements one has

$$(A_{nd})_{0,0'}=\bar{C}_{0,0'}+\bar{D}_{0,0'}+\sum_{0''}\bar{C}_{0,0''}\bar{D}_{0'',0'} \tag{6.14}$$

Using the Poincaré–Bertrand identity,

$$\lim_{z\to i0}\left[\frac{1}{z+a}\frac{1}{z+b}-\frac{1}{z+a+b}\left(\frac{1}{z+a}+\frac{1}{z+b}\right)\right]=0 \tag{6.15}$$

one finds that all terms in (6.14) vanish[4] at order L^{-3}.

[4] When these calculations are consistently performed up to the next order in the volume, it is found, using repeatedly (6.15), that $(A_{nd})_{0,0'}=(\psi'_{nd})_{0,0'}=O(L^{-6})$. This result agrees at that order with the usual general expansion (5.17).

Thus, at the dominant order in the volume, one has for the case of potential scattering,

$$A = 1 \tag{6.16}$$

and an explicit expression for the inverse of $(1 + \bar{C})$ is obtained,

$$(1 + \bar{C})^{-1} = (1 + \bar{D}) \tag{6.17}$$

As a consequence, the evolution equation in the Π-subdynamics reads

$$i\,\partial_t \tilde{\rho}_0 = \psi_{0,0}(z)\,\tilde{\rho}_0 + \sum_{0'} \psi_{0,0'}(z)\,\tilde{\rho}_{0'} \tag{6.18}$$

Let us briefly recall that, in the present case, due to the fact that $A = 1$, it is possible to identify $\tilde{\rho}_0$ with the diagonal component ${}^{P}\rho_0$ in the physical representation, which is obtained, in the general theory,[3] through the star-unitary transformation. Also, ϕ is equal to ψ,

$$\psi_{0,0} = \phi_{kk,kk} = 2i \operatorname{Im} t^{+}_{kk}(\omega_k) \tag{6.19}$$

is related to the forward scattering, and

$$\psi_{0,0'} = \phi_{kk,k'k'} = 2\pi i\, \delta(\omega_k - \omega_{k'})\, |t^{+}_{kk'}(\omega_k)|^2 \tag{6.20}$$

to the cross-sections for the $k \to k'$ process. The optical theorem ensures the conservation of the norm.

7. CONCLUDING REMARKS

In this paper, we have succeeded in obtaining a complete decomposition of the evolution of a large quantum system into one-dimensional subdynamics. Using a less restrictive irreducibility criterion than in previous work, we have introduced different barred elements in connection with each particular correlation.

The previous (unbarred) operators serve to define subdynamics of a given degree rather than that of a given correlation. For instance, the diagonal elements of the collision operator ψ are identical with $\bar{\psi}$, while off-diagonal ones of ψ are now included in creation or destruction elements $\bar{\mathscr{C}}$, $\bar{\mathscr{D}}$ relating different states of the same degree of correlation.

In the case of the complete decomposition, the generators of the evolution $\bar{\theta}$ are identical with the diagonal elements of the evolution generator θ of the collected subdynamics. In particular, for the vacuum subdynamics

$$\bar{\theta}_0 = \theta_{0,0}$$

As a consequence of the well-known dissipative properties of these elements, all privileged components of the states in the various subdynamics decay to zero in the course of time.

This fact, however, does not preclude the existence of collisional invariants, although these only come into view after globalization into the Π-subdynamics.

This can be most easily seen in the case of potential scattering (Section 6), where the collisional invariants are functions of the unperturbed energy ω_k due to (6.18)–(6.20).

As usual, the operators entering in the theory are highly singular, and the transformation that diagonalizes the θ operator, i.e., carries out the decomposition of Π into the $\{\Pi\}$ subdynamics, indeed contains distributions. Furthermore, as can be seen, for instance, for the elements involved in (4.4), one cannot limit oneself to a finite number of terms in an expansion in the volume or in the coupling constant, but one must deal with the entire series.

These remarks are of prime importance for the justification of our procedure in the general case, the consequences of which are still under intensive investigation.

When one compares the results we have obtained with previous ones, one cannot help noticing the fact that the collision operator has, in general, a continuous spectrum. Starting with an unperturbed Liouvillian with a discrete spectrum, we first get a discrete spectrum for $\bar{\theta}$. But in the thermodynamic limit, in which L_0 becomes continuous, we obtain a continuous collision operator θ. This contrasts with the viewpoint of Ref. 4, which insists on a continuous spectrum Liouvillian *ab initio* coupled with the much less exacting assumption that the collision operator has a discrete spectrum.

The new situation created by the constructive method we have proposed ought to revive interest in the complete subdynamics decomposition of the evolution, with the prospect of a better understanding of the advent of dissipativity at the limit of a continuous spectrum.

As far as the choice of a unique star-unitary transformation is concerned, which leads to the physical transformation, we gave an example for the case of potential scattering. In this problem, the χ operator, which is made up of the vacuum–vacuum elements of the star-unitary operator, reduces quite naturally to the identity. It is thus obvious that the role of this χ operator cannot be the diagonalization of the collision operator. In the building up of the general formalism, successive criteria have been proposed to fix uniquely the χ operator, among which is the diagonalization of the energy superoperator.[11] This criterion is nicely fulfilled for potential scattering. It has been used in several other problems,[12] but its general validity remains an open question.

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