Scattering and intrinsic irreversibility

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The formalism of quantum systems with diagonal singularities is applied to describe scattering processes. Well defined states are obtained for infinite time, which are related to a "weak form" of intrinsic irreversibility. Real and complex generalized spectral decompositions of the Liouville-Von Neumann superoperator are computed. The physical meaning of "Gamov states" is discussed.

I. INTRODUCTION.

The search of a physical explanation for the evolution towards equilibrium of quantum systems has a great interest for quantum statistical mechanics. For many years a great number of papers were devoted to this problem.

The microscopic explanation of the approach to equilibrium was related to the so called 'intrinsic irreversibility' of quantum systems. B. Misra, I. Prigogine, M. Courbage \[1\] \[2\] pointed out the existence of a time operator for the statistical description of classical and quantum systems. The mean value of this operator is the 'age' of the system, which is a growing function of time.

A. Bohm et al. \[3\] \[4\] related the intrinsic irreversibility to the existence of generalized eigenvectors of the Hamiltonian with complex eigenvalues, corresponding to poles of the analytic extension of the scattering matrix.

Complex eigenvalues have been obtained by E. Sudarshan et al. \[5\] by analytic continuation in a generalized quantum mechanics.

The Friedrichs model, a prototype of decaying system describing the interaction between a quantum oscillator and a scalar field, was extensively analyzed in the literature for the one exited mode sector. It is an exactly solvable model, in which the quantum oscillator decays to the ground state for all initial conditions. E. Sudarshan et al. \[5\] computed the complex spectral decomposition. The spectral decomposition was also obtained by T. Petrosky, I. Prigogine, S. Tasaki \[6\] using subdynamic theory. The spectral decomposition with complex eigenvalues was interpreted in terms of Rigged Hilbert spaces by I. Antoniou, I. Prigogine in reference \[7\] and by I. Antoniou, S. Tasaki in reference \[8\].

When it is necessary to deal with systems with a huge number of particles, the standard procedure is to start with $N$ particles in a box of volume $V$, making the limit $N \to \infty$, $V \to \infty$ with $\frac{N}{V} = c < \infty$ in the last step of the calculations. This method was used in subdynamic theory (I. Antoniou, S. Tasaki \[6\], T. Petrosky, I. Prigogine \[11\]), where the collision operator, with complex eigenvalues, is responsible for the evolution to statistical equilibrium.

It is not surprising that the time evolution of Friedrichs model can be successfully described using the methods of non equilibrium statistical mechanics that can be used, for example, to describe the approach to statistical equilibrium of a quantum gas. In both cases the interaction eliminates constants of motion. In Friedrichs model the discrete eigenvalue disappear and in the gas the momentum of each particle is no more a constant of motion when the interaction is present.

In this paper we want to discuss "intrinsic irreversibility" in connection with pure scattering processes, where the total and the free Hamiltonian have the same continuous spectrum. For this purpose, it is important to use a formalism where "final" states ($t \to \infty$) are well defined.

For finite systems with continuous spectrum, the usual formalism of quantum mechanics fails to give a description of the "final" states in terms of wave functions or density operators. To overcome this difficulty we will use in this paper the formalism developed by I. Antoniou et al. for quantum systems with diagonal singularity \[10\] \[11\] \[12\]. The quantum states of this theory are functionals over the space of observables $O$. Mathematically this means that the space $S$ of states is contained in $O^\times$. Physically it means that the only thing we can really observe and measure are the mean values of the observables $O \in O$ in states $\rho \in S \subset O^\times$: namely $\langle O \rangle_\rho = \rho(O) \equiv \langle \rho|O \rangle$. This is the natural generalization of the usual trace $\text{Tr}(\rho O)$ which is ill defined in systems with continuous spectrum. For finite quantum systems with continuous spectrum, some observables (for example the Hamiltonian) are represented by operators with diagonal singularities, and as they should have well defined mean values, diagonal singularities also appears in the states.

In section 2, the resolvent formalism including creation, destruction and collision superoperators is obtained in general for quantum systems with diagonal singularities.
In section 3, we apply this formalism to the scattering problem, showing that the collision superoperator is zero, and computing the singular “final” state, and discuss its relation with a sort of ”weak intrinsic irreversibility”.

In section 4, we compute the real and the complex spectral decompositions of the time evolution with the help of the Lipmann-Schwinger vectors and its analytic extensions. Complex eigenvalues appear related to the assumed simple pole of the analytic extension of the density matrix. The physical meaning of ”Gamov states” is also discussed in this section.

II. RESOLVENT FORMALISM FOR GENERALIZED STATES.

Let us consider the Liouville-Von Neumann equation for a state ρ

\[ i \frac{d}{dt} \rho = L \rho \]  

(1)

The general solution, valid for \( t > 0 \), can be written us

\[ \rho_t = \frac{1}{2\pi i} \int_{\Gamma} dz \exp(-itz) \frac{1}{L - z} \rho_o \]  

(2)

where \( \Gamma \) is an horizontal line parallel to the real axis and located in the upper half plane.

By defining two projectors \( P \) and \( Q \) acting on the states and satisfying

\[ P^2 = P, \quad Q^2 = Q, \quad P + Q = I, \]  

(3)

(\( I \) is the identity superoperator acting on states), it is possible to decompose the resolvent as [13] [14]

\[ \frac{1}{L - z} = \left[ P + C(z) \right] \frac{1}{QLQ - z} \left[ P + D(z) \right] + \frac{1}{QLQ - z}. \]  

(4)

The superoperators \( \Psi(z) \), \( C(z) \) and \( D(z) \) of the previous expression are defined by:

\[ \Psi(z) = P \Psi(z) P = -PLQ \frac{1}{QLQ - z} QLP, \]

\[ C(z) = Q C(z) P = -1 \frac{1}{QLQ - z} QLP, \]  

\[ D(z) = P D(z) Q = -PLQ \frac{1}{QLQ - z}. \]  

(5)

They are called collision, creation and destruction operators.

As we wish to include generalized states in the formalism, it is useful to consider that the states are represented by antilinear functionals acting on the representation of the observables to give the mean value [10] [11] [12]. Therefore for any observable \( O \in \mathcal{O} \) and state \( \rho \in \mathcal{O}^\ast \) we have:

\[ \langle O \rangle_\rho = \langle \rho | O \rangle, \quad (a \rho_1 + b \rho_2 | O \rangle = a^* \langle \rho_1 | O \rangle + b^* \langle \rho_2 | O \rangle. \]  

(6)

As it is usual in quantum mechanics, the observables are represented by self adjoint operators for which we expect real mean values:

\[ \langle O \rangle = \langle \rho | O \rangle^\ast. \]  

(7)

The identity operator can be written as the sum over the projections on all the generalized pure states, i.e. \( I = \sum_\alpha | \alpha \rangle \langle \alpha | \). Therefore we should impose

\[ (\rho | I \rangle = \sum_\alpha \langle \rho | | \alpha \rangle \langle \alpha | \rangle = 1, \quad (\rho | | \alpha \rangle \langle \alpha | \rangle \geq 0. \]  

(8)

In the last expression \( (\rho | | \alpha \rangle \langle \alpha | \rangle \) is the probability of the state \( \rho \) to be the pure state \( | \alpha \rangle \). For continuous spectrum the sum in (8) should be replaced by an integral and \( (\rho | | \alpha \rangle \langle \alpha | \rangle \) is a density of probability. Expression (8) is the generalization to states represented by functionals of the concept of trace.
In this approach it is necessary to reconsider the Liouville-Von Neumann equation \( (i \frac{d}{dt}) \rho = (L \rho), \)

We should give a meaning to the second term of the previous equation. The superoperator \( L \) is defined by
\[
(L \rho | O) = (\rho | L^\dagger O) = (\rho | [H, O]),
\]
where \( H \) is the Hamiltonian of the quantum system.

From (2) and the antilinearity of the state functionals we obtain
\[
\rho_t = \int \frac{dz}{\sqrt{\pi}} \exp(-izt) (\rho_o | L^\dagger + \frac{1}{z} + O).
\]

The resolvent \( \frac{1}{L^\dagger + z} \) has the following decomposition
\[
\frac{1}{L^\dagger + z} = \left[ P^\dagger + D^\dagger(z) \right] \frac{1}{P^\dagger L^\dagger P^\dagger + \Psi^\dagger(z) + z} \left[ P^\dagger + C^\dagger(z) \right] + Q^\dagger \frac{1}{Q^\dagger L^\dagger Q^\dagger + z},
\]
where \( P^\dagger \) and \( Q^\dagger \) are defined by
\[
(\rho | P^\dagger O) = (P \rho | O), \quad (\rho | Q^\dagger O) = (Q \rho | O),
\]
and
\[
\Psi^\dagger(z) = P^\dagger \Psi^\dagger(z) P^\dagger = -P^\dagger L^\dagger Q^\dagger \frac{1}{Q^\dagger L^\dagger Q^\dagger + z} Q^\dagger L^\dagger P^\dagger,
\]
\[
C^\dagger(z) = P^\dagger C^\dagger(z) Q^\dagger = -P^\dagger L^\dagger Q^\dagger \frac{1}{Q^\dagger L^\dagger Q^\dagger + z},
\]
\[
D^\dagger(z) = Q^\dagger D^\dagger(z) P^\dagger = -\frac{1}{Q^\dagger L^\dagger Q^\dagger + z} Q^\dagger L^\dagger P^\dagger.
\]

### III. INTRINSIC IRREVERSIBILITY AND SCATTERING PROCESSES.

Now we consider the scattering of a particle by a localized single scatterer. We assume for simplicity that the matrix elements \( V_{\overline{p} \overline{p}'} = |\overline{p} \overline{p}'\rangle \langle \overline{p} | \langle \overline{p}' | \) of the potential in the basis of eigenvectors of the momentum are well behaved ordinary functions of \( \overline{p} \) and \( \overline{p}' \).

The Hamiltonian of the system is
\[
H = H_o + V = \int d\overline{p} \varepsilon_p |\overline{p}\rangle \langle \overline{p}| + \int \int d\overline{p} d\overline{p}' V_{\overline{p} \overline{p}'} |\overline{p}\rangle \langle \overline{p}'|,
\]

where \( O_{\overline{p}} \) and \( O_{\overline{p}'} \) are two independent regular functions of the variables \( \overline{p} \) and \( \overline{p}' \), satisfying
\[
O_{\overline{p}}^* = O_{\overline{p}}, \quad O_{\overline{p}'}^* = O_{\overline{p}'}.
\]

Precisely the Hamiltonian (14) is of the form given by (13).

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1 This is a suitable choice for this problem in which we have a single particle. In this case observables like momentum or energy have a diagonal part as in equation (13) and should have well defined mean values. It is not the case in the thermodynamic limit, where extensive observables have infinite mean values.
As we stated in the previous section, the states are represented by antilinear functionals acting on observables. In this case, a state $\rho$ will be represented by two regular functions $\rho_p$ and $\rho_{pp'}$. The mean value of an observable $O$ is

$$\langle \rho | O \rangle = \int d\mathcal{P} \rho_\mathcal{P} O_\mathcal{P} + \int \int d\mathcal{P} d\mathcal{P}' \rho_{\mathcal{P}\mathcal{P}'} O_{\mathcal{P}\mathcal{P}'}.$$  \hfill (16)

From the conditions of total probability and reality of the mean values, given by equations (7) and (8) we obtain:

$$\rho_p = \rho_p^* \geq 0, \quad \rho_{pp'} = \rho_{pp'}^*, \quad \int d\mathcal{P} \rho_\mathcal{P} = 1 \quad \hfill (17)$$

It is useful to use a special notation for the generalized observables expanding $O$. Therefore we define:

$$|p\rangle \equiv |p\rangle\langle p|, \quad |p\rangle' \equiv |p\rangle\langle p'|,$$

We also define the functionals $(p\rangle$ and $(p\rangle'$ satisfying

$$\langle p| k \rangle = \delta^3(p - k), \quad \langle p| k' \rangle = \delta^3(p - k) \delta^3(p' - k'), \quad \langle p| k \rangle = \langle pp'| k \rangle = 0. \quad \hfill (19)$$

These 'basis' can be used to expand states and observables

$$\rho = \int d\mathcal{P} \rho_\mathcal{P} |p\rangle\langle p| + \int \int d\mathcal{P} d\mathcal{P}' \rho_{\mathcal{P}\mathcal{P}'} |pp\rangle' \langle pp'|,$$

$$O = \int d\mathcal{P} O_{\mathcal{P}|p\rangle} + \int \int d\mathcal{P} d\mathcal{P}' O_{\mathcal{P}|p\rangle'} \langle pp'|. \quad \hfill (20)$$

With (19) and (20) we can deduce (16).

Starting from the definitions

$$L_0^\dagger O = [H_0, O], \quad L_1^\dagger O = [V, O],$$

and using the 'basis' $(|p\rangle$, $(pp\rangle)$ for the observables and $(|p\rangle$, $(pp\rangle|$ for the states, we obtain:

$$L_0^\dagger = \int d\mathcal{P} d\mathcal{P}' (\varepsilon_\mathcal{P} - \varepsilon_{\mathcal{P}'}) \langle pp'||pp\rangle|,$$

$$L_1^\dagger = \int d\mathcal{P} d\mathcal{P}' |pp\rangle V_{pp'} [|pp\rangle - (pp\rangle|$$

$$+ \int d\mathcal{P} d\mathcal{P}' |pp\rangle' V_{pp'}' [|pp\rangle' - (pp\rangle'|] \quad \hfill (21)$$

For the projectors $P^\dagger$ and $Q^\dagger$, used in the previous section to decompose the resolvent, we choose in this section the following explicit form:

$$P^\dagger O = \int d\mathcal{P} O_{\mathcal{P}|p\rangle} \langle p\rangle|,$$

$$Q^\dagger O = \int \int d\mathcal{P} d\mathcal{P}' O_{\mathcal{P}\mathcal{P}'} |pp\rangle' \langle pp'|, \quad \hfill (22)$$

or equivalently

$$P^\dagger = \int d\mathcal{P} |p\rangle\langle p|, \quad Q^\dagger = \int d\mathcal{P} d\mathcal{P}' |pp\rangle' \langle pp'|.$$
The superoperators $P^\dagger$ and $Q^\dagger$ project the observables into their diagonal and off diagonal parts. The corresponding superoperators $P$ and $Q$ project the states into their diagonal and off diagonal parts, i.e.

$$
(P\rho) = \int \! d\rho \, \rho^\dagger (P), \quad (Q\rho) = \int \! d\rho \, \rho^\dagger (P^\dagger Q).
$$

From (21) and (22) we obtain

$$
P^\dagger L^\dagger = 0, \quad \Psi^\dagger (z) = 0, \quad C^\dagger (z) = 0,
$$

and the decomposition of the resolvent reduces to

$$
\frac{1}{L^\dagger + z} = \frac{1}{z} P^\dagger + \frac{1}{z} Q^\dagger D^\dagger (z) P^\dagger + Q^\dagger \frac{1}{Q^\dagger L^\dagger Q^\dagger + z} Q^\dagger.
$$

The time evolution is given by

$$
(P\rho_t) = \frac{i}{2\pi} \int \! dz \, \frac{\exp(-i z t)}{z} (P\rho_o)
$$

$$
- \frac{i}{2\pi} \int \! dz \, \frac{\exp(-i z t)}{z} (Q\rho_o) \frac{1}{Q^\dagger L^\dagger Q^\dagger + z} Q^\dagger L^\dagger P^\dagger
$$

$$
(Q\rho_t) = \frac{i}{2\pi} \int \! dz \, \frac{\exp(-i z t)}{z} (Q\rho_o) \frac{1}{Q^\dagger L^\dagger Q^\dagger + z} Q^\dagger
$$

Equation (26) shows the influence of the diagonal part $(P\rho_o)$ and the off diagonal part $(Q\rho_o)$ of the initial state on the diagonal part of the state at time $t$. As the collision operator $\Psi^\dagger (z)$ is zero, there are no diagonal-diagonal transitions in the process.

Equation (27) shows that there is no influence of the diagonal part of the initial condition on the off diagonal part of the state at time $t$.

It is easy to show that the first factor in (26) is time independent. The integral over the horizontal line $\Gamma$ in the upper half plane can be closed over a very big semicircle in the lower half plane. The integral over this big semicircle has vanishing contribution when the radius goes to infinity. Then the closed curve can be deformed into a small circle around the simple pole at $z = 0$, to obtain

$$
\frac{i}{2\pi} \int \! dz \, \frac{\exp(-i z t)}{z} (P\rho_o) = (P\rho_o) (P^\dagger O),
$$

for all observables $O$.

To analyze the second factor it is convenient to use the complete biorthogonal system of Lipmann-Schwinger generalized eigenvectors of the Hamiltonian

$$
|k^\pm\rangle = |k\rangle + \frac{1}{\varepsilon_k \pm i 0 - H} V|k\rangle,
$$

$$
\langle k^\pm | = \langle k | + \langle k | V \frac{1}{\varepsilon_k \mp i 0 - H},
$$

for which

$$
I = \int \! d\vec{k} \, |k^\pm\rangle \langle k^\pm|, \quad H = \int \! d\vec{k} \varepsilon_k |k^\pm\rangle \langle k^\pm|, \quad \langle k^\pm | k'^\pm \rangle = \delta^3 (\vec{k} - \vec{k}')
$$

We have

$$
- \frac{i}{2\pi} \int \! dz \, \frac{\exp(-i z t)}{z} (Q\rho_o) \frac{1}{Q^\dagger L^\dagger Q^\dagger + z} Q^\dagger L^\dagger P^\dagger (O)
$$

$$
= - \frac{i}{2\pi} \int \! dz \, \frac{\exp(-i z t)}{z} \int \! d\vec{k} d\vec{k}'
$$

5
The integral over terms of the complex variable used in (33) to obtain \( \nu \), where for the last expressions we used the variables \( \varepsilon_k, \varepsilon_{k'} \) and over the angles. Using a closed curve very close to the cut we obtain

\[
\frac{\varepsilon_k - \varepsilon_{k'}}{\varepsilon_k - \varepsilon_{k'} + z} (Q \rho_o | \vec{k}^+ ) (\vec{k}'^+ ) | (\vec{k}^+ O | \vec{k}'^+ ).
\]

The integral over \( \vec{k} \) and \( \vec{k}' \) can be transformed using polar coordinates into an integral over \( \varepsilon_k, \varepsilon_{k'} \) and over the angles. Looking at the integrals over the energies we can write

\[
\int d\varepsilon \frac{\exp(-iz\varepsilon)}{z} \int d\varepsilon' \frac{\exp(-iz\varepsilon')}{z} f(\varepsilon, \varepsilon') = - \int d\lambda \int d\nu \frac{\exp(-iz\varepsilon)}{z} f(\lambda, \nu)
\]

where for the last expressions we used the variables \( \nu = \varepsilon' - \varepsilon \) and \( \lambda = \frac{1}{2}(\varepsilon' + \varepsilon) \), and \( F_{\lambda}(z) \equiv \int_\lambda^\infty d\nu \frac{\exp(-iz\varepsilon)}{z} f(\lambda, \nu) \). In terms of the complex variable \( z \), \( \frac{\exp(-iz\varepsilon)}{z} F_{\lambda}(z) \) has a simple pole in \( z = 0 \) and a cut in the real interval \( (-\lambda, +\lambda) \):

\[
F_{\lambda}(x + i0) - F_{\lambda}(x - i0) = 0 \quad \text{if} \quad x \notin (-\lambda, +\lambda)
\]

As in the previous case, the integral over \( \Gamma \) can be closed in the lower half plane, surrounding the pole and the cut. Using a closed curve very close to the cut we obtain

\[
- \int_0^\infty d\lambda \int d\nu \frac{\exp(-iz\varepsilon)}{z} F_{\lambda}(z) = 2\pi i \left\{ \int_0^\infty d\lambda \int d\nu f(\lambda, \nu) + \int_0^\infty d\lambda \int d\nu \exp(-i\nu t) f(\lambda, \nu) \right\}
\]

We can now insert (31) in (30) to obtain

\[
- i \frac{1}{2\pi} \int d\varepsilon \frac{\exp(-iz\varepsilon)}{z} (Q \rho_o | \vec{k}^+ ) (\vec{k}'^+ ) | (\vec{k}^+ O | \vec{k}'^+ ).
\]

Therefore

\[
(P \rho_i | O) = (P \rho_i | P^i O) + \int \int d\vec{k} d\vec{k}' \exp\{i(\varepsilon_k - \varepsilon_{k'}) t\} (Q \rho_o | \vec{k}^+ ) (\vec{k}'^+ ) | (\vec{k}^+ O | \vec{k}'^+ ).
\]

The Lipmann-Schwinger vectors \([29]\) can also be used in expression (27)

\[
(Q \rho_i | O) = \int \int d\vec{k} d\vec{k}' \exp\{i(\varepsilon_k - \varepsilon_{k'}) t\} (Q \rho_o | \vec{k}^+ ) (\vec{k}'^+ ) | (\vec{k}^+ O | \vec{k}'^+ ).
\]

There are no singular terms in \( (Q \rho_o | \vec{k}^+ ) (\vec{k}'^+ ) | (\vec{k}^+ O | \vec{k}'^+ ) \), and therefore Riemann-Lebesgue theorem can be used in (33) to obtain
time inversion is possible in principle, although it may be very difficult to prepare the state 
\[ \rho_0 = \mathbb{P}\rho_0 \implies \rho_t = \rho_o. \]

We must isolate the singular term in \((\mathbb{Q}\rho_o|\overline{k}^+\rangle\langle\overline{k}^+|\mathbb{P}^\dagger O|\overline{k}^+\rangle\langle\overline{k}^+|)\) before using the Riemann-Lebesgue theorem to compute \(\lim_{t \to \infty}(\mathbb{P}\rho_t|O)\). Using \((29)\) we obtain:

\[
(\mathbb{Q}\rho_o|\overline{k}^+\rangle\langle\overline{k}^+|\mathbb{P}^\dagger O|\overline{k}^+\rangle\langle\overline{k}^+|) = (\mathbb{Q}\rho_o|\overline{k}^+\rangle\langle\overline{k}^+|) \times \{O_{\overline{k}^+\overline{k}^+} - \frac{1}{\varepsilon_{\overline{k}' - i0 - H}V\overline{k}'} + O_{\overline{k}^+\overline{k}^+}^+ - \frac{1}{\varepsilon_{\overline{k}' + i0 - H}V\overline{k}'} \}. \tag{35}
\]

Replacing \((35)\) in \((22)\), and using the Riemann-Lebesgue theorem we obtain:

\[
\lim_{t \to \infty}(\mathbb{P}\rho_t|O) = (\mathbb{Q}\rho_o|\overline{k}^+\rangle\langle\overline{k}^+|)O_{\overline{k}^+} = \int d\overline{k}(\mathbb{Q}\rho_o|\overline{k}^+\rangle\langle\overline{k}^+|)O_{\overline{k}^+}. \tag{36}
\]

Therefore, in weak sense:

\[
\langle \rho_o \rangle = \lim_{t \to \infty}(\rho_t) = \int d\overline{k}(\rho_o|\overline{k}^+\rangle\langle\overline{k}^+|). \tag{37}
\]

This result shows a sort of “weak intrinsic irreversibility” of the scattering process. As we mentioned, a pure state which can be represented by a normalizable wave function \(|\varphi\rangle = \int d\overline{k} \varphi_{\overline{k}}(\overline{k})\), can also be represented by the functional \(\rho = \int d\overline{p} \rho_{\overline{p}}(\overline{p})+\int d\overline{p} d\overline{p}' \rho_{\overline{p}\overline{p}'}(\overline{p}\overline{p}')\). Therefore, in this formalism, \(\rho_{\overline{k}^+} = \rho_{\overline{k}^+}^*\) is a necessary condition to have a pure state. We are used to the idea that the ‘purity’ of a state is preserved by the time evolution. However, equation \((37)\) states that, in weak sense and for all initial conditions, the evolution is not towards a pure state but towards a ‘generalized mixture’ in which \((\rho_o|\overline{k}^+\rangle\langle\overline{k}^+|)\) and \((\rho_o)_{\overline{k}^+} = 0\). This ‘final’ state is time invariant, because from \((24)\) we have

\[
(\mathbb{L}\rho_o|O) = (\mathbb{L}\rho_o|\overline{k}^+\rangle\langle\overline{k}^+|)O_{\overline{k}^+} = (\rho_o|\overline{k}^+\rangle\langle\overline{k}^+|) = 0 \implies \mathbb{L}\rho_o = 0.
\]

Moreover, the time inversion \(\mathbb{T}\rho_o\) of the ‘final’ state is also invariant under time evolution. In fact, for any \(\rho = \int d\overline{p} \rho_{\overline{p}}(\overline{p})+\int d\overline{p} d\overline{p}' \rho_{\overline{p}\overline{p}'}(\overline{p}\overline{p}')\) we have

\[
\mathbb{T}\rho = \int d\overline{p} \rho_{\overline{p}}(\overline{p})+\int d\overline{p} d\overline{p}' \rho_{\overline{p}\overline{p}'}(\overline{p}\overline{p}'),
\]

then

\[
\mathbb{T}\rho_o = \int d\overline{k}(\rho_o|\overline{k}^+\rangle - \overline{k}^+\langle\overline{k}^+|)O_{\overline{k}^+},
\]

and

\[
\mathbb{L}\mathbb{T}\rho_o = 0.
\]

Therefore, the time evolution of the time inversion of the ‘final’ state cannot reproduce the initial state. We may say, in this sense, that the scattering process is intrinsically irreversible. But this irreversibility appears for processes involving an infinite amount of time, as the ‘final’ state is obtained with \(t \to \infty\). For a very big time \(t_o < \infty\), the time inversion is possible in principle, although it may be very difficult to prepare the state \(\mathbb{T}\rho_{t_o}\) in practice.
IV. REAL AND COMPLEX SPECTRAL DECOMPOSITIONS.

In the previous section we used the formalism of states and observables with diagonal singularities to obtain the time evolution of generalized states (equations (12) and (13)). A real spectral decomposition of the Liouville-Von Neumann superoperator is implicit in these equations.

This real spectral decomposition was enough to compute the 'final' state and to argue on the intrinsic irreversibility of the process. In this section we are going to make explicit through the spectral decomposition the influence of the resonances produced by the poles of the analytic extensions of the resolvent, which in scattering process are determined by the poles of the 'S matrix'.

Although it is possible to compute the complex spectral decomposition for the model of the previous section, we prefer to analyze a simplified model.

Let us consider a system with Hamiltonian

\[
H = H_0 + V = \int_0^\infty d\omega \omega |\omega \rangle \langle \omega | + \int_0^\infty d\omega \int_0^\infty d\omega' V_{\omega \omega'} |\omega \rangle \langle \omega' |,
\]

where the generalized right (left) eigenvectors \(|\omega \rangle (\langle \omega |)\) of \(H_0\) form a complete biorthonormal system

\[
I = \int_0^\infty d\omega |\omega \rangle \langle \omega |, \quad \langle \omega |\omega' \rangle = \delta(\omega - \omega').
\]

We also assume that the Lipmann-Schwinger generalized eigenvectors of the Hamiltonian

\[
|\omega^\pm \rangle = |\omega \rangle + \frac{1}{\omega \mp i0 - H} V |\omega \rangle
\]

\[
\langle \omega^\pm | = \langle \omega | + \langle \omega | V \frac{1}{\omega \mp i0 - H}
\]

are also a complete set:

\[
H = \int_0^\infty d\omega |\omega^\pm \rangle \langle \omega^\pm |, \quad I = \int_0^\infty d\omega |\omega^\pm \rangle \langle \omega^\pm |, \quad \langle \omega^\pm |\omega'^\pm \rangle = \delta(\omega - \omega').
\]

The vectors \(|\omega^+\rangle\) and \(|\omega^-\rangle\) are related by the "S matrix"

\[
|\omega^+ \rangle = S(\omega) |\omega^- \rangle, \quad \langle \omega^+ | = S^*(\omega) \langle \omega^- |,
\]

where

\[
S(\omega) = 1 - 2\pi i \langle \omega | V |\omega \rangle - 2\pi i \langle \omega | V \left( \frac{1}{\omega + i0 - H} \right)^+ V |\omega \rangle,
\]

\[
S^*(\omega) = 1 + 2\pi i \langle \omega | V |\omega \rangle + 2\pi i \langle \omega | V \left( \frac{1}{\omega - i0 - H} \right)^- V |\omega \rangle.
\]

We also assume that the analytic extension \(\left( \frac{1}{s - H} \right)^\pm_{s = z} \) of the resolvent \(\frac{1}{s - H} \) from the upper (lower) to the lower (upper) half plane, has a simple pole at \(z = z_0 \) \((z = z_0^*)\), where \(\text{Im} \ z_0 < 0 \) \((\text{Im} \ z_0^* > 0)\).

From (11) we can define the following analytic extensions

\[
S(z) = 1 - 2\pi i \langle z | V |z \rangle - 2\pi i \langle z | V \left( \frac{1}{s - H} \right)^+_{s = z} V |z \rangle,
\]

\[
S^*(z) = 1 + 2\pi i \langle z | V |z \rangle + 2\pi i \langle z | V \left( \frac{1}{s - H} \right)^-_{s = z} V |z \rangle.
\]

The analytic extension \(S(z) \) \((S^*(z))\) of \(S(\omega) \) \((S^*(\omega))\) has a simple pole at \(z = z_0 \) \((z = z_0^*)\).

From the Lipmann-Schwinger generalized eigenvectors of the Hamiltonian we may also construct the corresponding analytic extensions.
\[ |z^\pm\rangle = |z\rangle + \left(\frac{1}{s - H}\right)_{s=z} V|z\rangle \]
\[ \langle z^\pm | = \langle z | + \langle z | V \left(\frac{1}{s - H}\right)_{s=z}^\dagger. \]

(43)

In the previous expressions, \(|z\rangle\) and \(\langle z |\) are functionals defined by
\[ \langle z | \varphi \rangle = \varphi(z), \quad (\varphi |z\rangle = \varphi^*(z), \]
where \(\varphi(z)\) and \(\varphi^*(z)\) are the analytic extensions of \(\varphi(\omega) = \langle \omega | \varphi \rangle\) and \(\varphi^*(\omega) = \langle \varphi | \omega \rangle\).

As in section 3, we consider observables of the form
\[ O = \mathbb{P}^1 O + Q^1 O = \int d\omega O_\omega |\omega\rangle + \int \int d\omega d\omega' O_{\omega\omega'} |\omega\omega'\rangle, \]
(44)
\[ |\omega\rangle \equiv |\omega\rangle \langle \omega |, \quad |\omega\omega'\rangle \equiv |\omega\rangle \langle \omega |, \quad O_\omega = O^*_\omega, \quad O_{\omega\omega'} = O^*_{\omega\omega'}. \]

If we define the functionals \((\omega |\omega\rangle\) and \((\omega\omega' |\omega\rangle\) by the following equations
\[ (\omega |\omega'\rangle = \delta(\omega - \omega') \]
\[ (\omega\omega' |\omega\rangle = (\omega\omega' |\omega\rangle = 0 \]
\[ (\omega\omega' |\omega\omega'\rangle = \delta(\omega - \zeta)\delta(\omega' - \zeta'), \]
they can be used to represent the state functionals
\[ \rho = \int d\omega \rho^*_\omega (\omega |\omega\rangle + \int \int d\omega d\omega' \rho^*_{\omega\omega'} (\omega\omega' |\omega\omega'\rangle \]
\[ \rho^*_\omega = \rho_\omega \geq 0, \quad \rho^*_{\omega\omega'} = \rho_{\omega\omega'}, \quad \int d\omega \rho^*_\omega = 1. \]

The mean value of an observable \(O\) in the state \(\rho\) is given by
\[ \langle O \rangle \rho = (\rho |O\rangle = \int d\omega \rho^*_\omega O_\omega + \int \int d\omega d\omega' \rho^*_{\omega\omega'} O_{\omega\omega'}, \]

with the following time evolution
\[ (\rho_t |O\rangle = (U_t \rho_0 |O\rangle = (\rho_0 |U^*_t O = (\rho_0 | \exp(iHt)O \exp(-iHt). \]

The observable given in (44) can be written as
\[ O = O_{\text{diag}} + O_{\text{reg}} \]
\[ O_{\text{diag}} = \int d\omega O_\omega |\omega\rangle \langle \omega | \]
\[ O_{\text{reg}} = \int \int d\omega d\omega' O_{\omega\omega'} |\omega \langle \omega |. \]

Using the Lipmann-Schwinger vectors \([3]\), we have
\[ O_{\text{diag}} = O_{\text{inv}} + \Delta O_{\text{diag}}, \]

where
\[ O_{\text{inv}} = \int d\omega O_\omega |\omega^+\rangle \langle \omega^+ | \]
\[ \Delta O_{\text{diag}} = \int d\omega O_\omega (|\Delta \omega\rangle \langle \Delta \omega | + |\Delta \omega\rangle \langle \omega^+ | + |\omega^+ \rangle \langle \Delta \omega | \]
\[ |\Delta \omega \rangle = |\omega\rangle - |\omega^+\rangle = -\frac{1}{\omega + i0 - H} V|\omega\rangle. \]
Therefore the observable \( O \) can be decomposed into an invariant (\( \text{inv} \)) and a fluctuating (\( \text{fluc} \)) part

\[
O = O_{\text{inv}} + O_{\text{fluc}}
\]

\[
O_{\text{fluc}} = O_{\text{reg}} + \Delta O_{\text{diag}}.
\] (45)

The fluctuating part \( O_{\text{fluc}} \) has no diagonal singularity ((\( O_{\text{fluc}} \)) = 0), and \( O_{\text{inv}} \) is time independent (\( U_t^\dagger O_{\text{inv}} = O_{\text{inv}} \)).

The real spectral decomposition of the time evolution can be obtained using the decomposition \( O = O_{\text{inv}} + O_{\text{fluc}} \) of the observables and the Lipmann-Schwinger vectors (49):

\[
\rho_t |O\rangle = (\rho_0 |O_{\text{inv}}\rangle + (\rho_0 |\exp[iHt]O_{\text{fluc}}\exp[-iHt]|)
\]

\[
= \int_0^\infty d\omega (\rho_0 |\omega^+\rangle \langle \omega^+|)O_\omega +
\]

\[
+ \int_0^\infty d\omega \int_0^\infty d\omega' e^{i(\omega-\omega')t} (\rho_0 |\omega^+\rangle \langle \omega^+|O_{\text{fluc}}|\omega'^+\rangle \langle \omega'^+|)
\] (46)

The last term will vanish when \( t \to \infty \) and therefore, in weak sense

\[
(\rho_\infty) = \lim_{t\to\infty} (\rho_t) = \int_0^\infty d\omega (\rho_0 |\omega^+\rangle \langle \omega^+|)\langle \omega|^.
\] (47)

Expression (46) correspond to the following real spectral decomposition of the identity (\( \mathbb I^\dagger \)) and Liouville-Von Neumann (\( \mathbb L^\dagger \)) superoperators

\[
\mathbb I^\dagger = \int_0^\infty d\omega |\Phi_\omega\rangle \langle \Phi_\omega| + \int_0^\infty d\omega \int_0^\infty d\omega' |\Phi_{\omega\omega'}\rangle \langle \Phi_{\omega\omega'}|,
\]

\[
\mathbb L^\dagger = \int_0^\infty d\omega \int_0^\infty d\omega' (\omega - \omega') |\Phi_{\omega\omega'}\rangle \langle \Phi_{\omega\omega'}|
\] (48)

where

\[
|\Phi_\omega\rangle = |\omega^+\rangle \langle \omega^+|)
\]

\[
(\Phi_\omega) = (\omega)
\]

\[
|\Phi_{\omega\omega'}\rangle = |\omega^+\rangle \langle \omega'^+|)
\] (49)

\[
(\Phi_{\omega\omega'}) = \int dy \{(\omega^+|y\rangle \langle y'|\omega'^+\rangle - \delta(\omega - y)\delta(\omega' - y')\}|y\rangle +
\]

\[
+ \int dy dy' (\omega^+|y\rangle \langle y'|\omega'^+\rangle)(yy')
\]

It is easy to prove that the generalized right and left eigenvectors of \( \mathbb L^\dagger \) given in (49) satisfy the orthogonality conditions

\[
(\Phi_\omega |\Phi_{\omega'}\rangle) = \delta(\omega - \omega')
\]

\[
(\Phi_\omega |\Phi_{yy'}\rangle) = (\Phi_{\omega\omega'} |\Phi_y\rangle) = 0
\]

\[
(\Phi_{\omega\omega'} |\Phi_{yy'}\rangle) = \delta(\omega - y)\delta(\omega' - y').
\]

Any state can be expanded in terms of the complete biorthonormal system (49)

\[
\rho = \int_0^\infty d\omega (\rho |\Phi_\omega\rangle \langle \Phi_\omega| + \int_0^\infty d\omega \int_0^\infty d\omega' (\rho |\Phi_{\omega\omega'}\rangle \langle \Phi_{\omega\omega'}|)
\]

and therefore it is important to give a physical meaning to the generalized states (\( \Phi_\omega \)) and (\( \Phi_{\omega\omega'} \)). For the mean value of the total energy we obtain

\[
(\Phi_\omega |H) = (\omega |H) = \omega
\]

\[
(\Phi_{\omega\omega'} |H) =
\]
\[= \int dy\{\omega^+|y\rangle\langle y|\omega'^+) - \delta(\omega - y)\delta(y - \omega')\}y + \int \int dydy'\langle \omega^+|y\rangle V_{gy'}\langle y'|\omega'^+\rangle = 0,\]

and for the "trace"

\[
(\Phi_{\omega}|I) = (\omega|I) = (\omega|\int d\omega'\delta(\omega - \omega') = \int d\omega'\delta(\omega - \omega') = 1
\]

\[
(\Phi_{\omega\omega'}|I) =
\]

\[= \int dy\{\omega^+|y\rangle\langle y|\omega'^+) - \delta(\omega - y)\delta(y - \omega')\} = \langle \omega^+|\omega'^+\rangle - \delta(\omega - \omega') = 0.\]

The generalized state \((\Phi_{\omega})\) is a physical state with energy \(\omega\) and "trace" 1, and \((\Phi_{\omega\omega'})\) has zero energy and zero "trace". Clearly, it is impossible to realize a physical state including only \((\Phi_{\omega\omega'})\) components.

The complex number \(z_0\), where the analytic extension of \(S^*(\omega)\) has a simple pole, can be introduced in the spectral decomposition if, in equation (50), we deform the \(\omega\) integral over \(\mathbb{R}^+\) into an integral over a curve in the upper half plane, i.e.

\[
\int_0^\infty d\omega e^{i\omega t}|\omega^+)\langle \omega'^+| = \int_0^\infty d\omega e^{i\omega t}|\omega^+)\langle \omega'^+| \rightarrow \rightarrow e^{iz_0 t}|f_0\rangle\langle f_0| + \int_0^{-\infty} d\omega e^{i\omega t}|(\omega + i0)^+\rangle\langle (\omega + i0)^+|
\]

\[|f_0\rangle = [2\pi i(ResS^*)z_0]^{1/2}|z_0^+\rangle, \quad \langle f_0| = [2\pi i(ResS^*)z_0]^{1/2}\langle z_0^-|.
\]

The complex numbers \(z_0\), where the analytic extension of \(S(\omega')\) has a simple pole, can be introduced in the spectral decomposition if, in equation (51), we deform the \(\omega'\) integral over \(\mathbb{R}^+\) into an integral over a curve in the lower half plane, i.e.

\[
\int_0^\infty d\omega e^{-i\omega t}|\omega'^+)\langle \omega'^+| = \int_0^\infty d\omega e^{-i\omega t}S(\omega')|\omega'^-)\langle \omega'^+| \rightarrow \rightarrow e^{-iz_0 t}|\bar{f}_0\rangle\langle \bar{f}_0| + \int_0^{-\infty} d\omega e^{-i\omega t}|(\omega' - i0)^+\rangle\langle (\omega' - i0)^+|
\]

\[|\bar{f}_0\rangle = [-2\pi i(ResS)z_0]^{1/2}|z_0^-\rangle, \quad \langle \bar{f}_0| = [-2\pi i(ResS)z_0]^{1/2}\langle z_0^+|.
\]

Replacing (50) and (51) in (46) we obtain

\[
(\rho_t|O) = \int_0^\infty d\omega(\rho_0|\omega^+)\langle \omega^+|O_\omega + e^{i(z_0 - z_0)t}(\rho_0|f_0\rangle\langle f_0|O_{fluc}|f_0\rangle\langle f_0|) + \int_0^{-\infty} d\omega e^{i(z_0 - \omega)t}(\rho_0|f_0\rangle\langle f_0|O_{fluc}|(\omega' - i0)^+\rangle\langle (\omega' - i0)^+|) + \int_0^{-\infty} d\omega e^{i(\omega - z_0)t}(\rho_0|(\omega + i0)^+\rangle\langle (\omega + i0)^+|O_{fluc}|f_0\rangle\langle f_0|) + \int_0^{-\infty} d\omega \int_0^{-\infty} d\omega' e^{i(\omega - \omega')t} \times \times(\rho_0|(\omega + i0)^+\rangle\langle (\omega + i0)^+|O_{fluc}|(\omega' - i0)^+\rangle\langle (\omega' - i0)^+|)
\]

(52)
The changes indicated in equations (50) and (51) are possible if we impose on the states and observables the condition that \( \rho_{\omega'} \) and \( O_{\omega'} \) have well defined analytic extensions to the upper (lower) half plane in the variable \( \omega \) (\( \omega' \)). In this case it is possible to prove that \( (O_{\omega'c})_{\omega'} \) has also a well defined analytic extension to the upper (lower) half plane in the variable \( \omega \) (\( \omega' \)). Expression (52) correspond to the following complex spectral decomposition of the identity \( (\mathbb{I}) \) and Liouville-Von Neumann \( (L^i) \) superoperators

\[
\mathbb{I}^i = \int_0^\infty d\omega |\Psi_\omega \rangle \langle \Psi_\omega | + \int_0^{-\infty} d\omega' |\Psi_{0,\omega'} \rangle \langle \Psi_{0,\omega'} |
+ \int_0^\infty d\omega |\Psi_{\omega,0} \rangle \langle \Psi_{\omega,0} | + \int_0^{-\infty} d\omega' \int_0^\infty d\omega |\Psi_{\omega,\omega'} \rangle \langle \Psi_{\omega,\omega'} |
\]

\[
L^i = (z_0^+ - z_0) |\Psi_{0,0} \rangle \langle \Psi_{0,0} | + \int_0^{-\infty} d\omega (z_0^+ - \omega') |\Psi_{0,\omega'} \rangle \langle \Psi_{0,\omega'} |
+ \int_0^\infty d\omega |\Psi_{\omega,0} \rangle \langle \Psi_{\omega,0} | + \int_0^{-\infty} d\omega \int_0^{\infty} d\omega' (\omega - \omega') |\Psi_{\omega,\omega'} \rangle \langle \Psi_{\omega,\omega'} |
\]

(53)

where

\[
|\Psi_\omega \rangle = |\omega^+ \rangle \langle \omega^+ |
\]

\[
(\bar{\Psi}_\omega) = (\omega^+)
\]

\[
|\Psi_{0,0} \rangle = |\tilde{f}_0 \rangle \langle \tilde{f}_0 |
\]

\[
(\bar{\Psi}_{0,0}) = [2\pi i (Res S)^* z_0^+ - \frac{i}{2} [-2\pi i (Res S) z_0] - \frac{i}{2} (2\pi i Res \omega = z_0)] \langle \Phi_{\omega,\omega'} |
\]

\[
|\Psi_{\omega,\omega'} \rangle = |\tilde{f}_0 \rangle \langle \omega' - i0^+ |
\]

\[
(\bar{\Psi}_{0,\omega}) = [2\pi i (Res S)^* z_0^+ - \frac{i}{2} (2\pi i Res \omega = z_0)] \langle \Phi_{\omega,\omega'} |
\]

\[
|\Psi_{\omega} \rangle = |\omega + i0^+ \rangle \langle \omega + i0^+ |
\]

\[
(\bar{\Psi}_{\omega}) = [-2\pi i (Res S) z_0] - \frac{i}{2} (-2\pi i Res \omega' = z_0) \langle \Phi_{\omega,\omega'} |
\]

\[
|\Psi_{\omega'} \rangle = |\omega + i0^+ \rangle \langle \omega' - i0^+ |
\]

(54)

From these equations it is easy to prove that \( (\bar{\Psi}_{0,0}) \), \( (\bar{\Psi}_{0,\omega}) \), \( (\bar{\Psi}_{\omega,0}) \) and \( (\bar{\Psi}_{\omega,\omega'}) \) have no energy nor "trace", i.e.

\[
(\bar{\Psi}_{0,0}) H = (\bar{\Psi}_{0,\omega}) H = (\bar{\Psi}_{\omega,0}) H = (\bar{\Psi}_{\omega,\omega'}) H = 0
\]

\[
(\bar{\Psi}_{0,0}) I = (\bar{\Psi}_{0,\omega}) I = (\bar{\Psi}_{\omega,0}) I = (\bar{\Psi}_{\omega,\omega'}) I = 0,
\]

and therefore these generalized states cannot have an independent physical meaning.

V. CONCLUSIONS.

For a quantum scattering problem, the continuous spectrum requires the existence of well defined values of observables with diagonal singularities. The Hamiltonian of the system, in momentum representation, is an example of this class of observables.

Defining the states as functionals acting on the operators representing the observables, more general states are allowed in the formalism. These new class of states are not represenable by wave functions nor by trace class density operators.

---

3Equations (50) and (51) requires the vanishing of the integrals over a very big semicircle in the upper (lower) half plane in the variable \( \omega \) (\( \omega' \)). The presence of the exponential factor \( e^{iut} (e^{-i\omega'}) \), with \( t > 0 \), makes the requirement easier to be satisfied.
The main conclusion of this paper is that the functional approach can give a more complete description of the process. We proved that, even for initial conditions representable by wave functions, the "final" state \( (t = \infty) \) is a well defined diagonal functional \( \rho_{\infty} = \mathbb{P}\rho_{\infty} \), which is a mixture of generalized eigenvectors of the free Hamiltonian \( H_0 \):

\[
\rho_{\infty} = \lim_{t \to \infty} \rho_t = \int d\vec{k} \rho_o(\vec{k}) \langle \hat{\pi}^+ | \hat{\pi}^+ \rangle (\hat{\pi}^-),
\]

\[(\hat{\pi}^- | \hat{\pi}^+) = \delta(\vec{k} - \vec{k}'), \quad |\vec{k}\rangle = |\vec{k}\rangle (\hat{\pi}^-), \quad H_0 |\vec{k}\rangle = |\vec{k}\rangle.
\]

This state cannot be represented by a wave function or by a trace class operator.

The final state depend on the initial condition, although different initial conditions may converge into the same final state.

The time inversion of a state is well defined in the formalism

\[
\rho = \int d\vec{p} \rho^*_{\vec{p}}(\vec{p}) + \int \int d\vec{p} d\vec{p'} \rho^*_{\vec{p} \vec{p}'} (\vec{p} \vec{p}'),
\]

\[T\rho = \int d\vec{p} \rho_{-\vec{p}}(\vec{p}) + \int \int d\vec{p} d\vec{p'} \rho_{-\vec{p} - \vec{p}'} (\vec{p} \vec{p}'),
\]

and a "weak intrinsic irreversibility" appears as

\[T \rho_{\infty} = \int d\vec{k} \rho_o(\vec{k}) \langle \hat{\pi}^- | \hat{\pi}^- \rangle (\hat{\pi}^+) (\hat{\pi}^-)^* (\hat{\pi}^-),
\]

and

\[U_t T \rho_{\infty} = e^{-itL} T \rho_{\infty} = T \rho_{\infty},
\]

the time evolution of the time inverted 'final' state cannot reproduce the initial state. But this irreversibility appears for processes involving an infinite amount of time, as the 'final' state is obtained with \( t \to \infty \). For a very big time \( t_o < \infty \), the time inversion is possible in principle, although it may be very difficult to prepare the state \( T \rho_{t_o} \) in practice.

It is interesting to emphasize that it is not necessary to consider the analytic extensions of the "components" of the states to obtain these results. Only regularity of the functions representing the off diagonal parts of states and observables is required to expand the observables in terms of the Lipmann-Schwinger eigenvectors, and to use the Riemann-Lebesgue theorem for the deduction of (55).

If, in addition, we assume that the "components" of states and observables have well defined analytic extensions, as it is the case if Hardy class functions are involved, a complex spectral decomposition of the time evolution is possible. In section 4, we constructed a complex spectral decomposition including "generalized Gamov states" related to the poles of the "S matrix". However, we proved that these generalized states have zero energy and zero "trace". This is an expected result, consistent with energy and probability conservation, because the "Gamov states" expand the time dependent part of the physical states, which goes to zero for infinite time. Therefore, in this formalism, the "Gamov states" cannot exist as autonomous states, but only in a linear combination which should include the time independent component (an eigenvector of the Liouville-Von Neumann superoperator with zero eigenvalue).

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