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Scattering and Intrinsic Irreversibility

Roberto Laura[1]

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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 "Gamow states" is discussed.

1. INTRODUCTION

The search for a physical explanation for the evolution toward equilibrium of quantum systems has been of great interest in quantum statistical mechanics, and over the years a great number of papers have been devoted to this problem.

The microscopic explanation of the approach to equilibrium was related to the so-called intrinsic irreversibility of quantum systems. Misra *et al.* (1979a, b.) 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.

Bohm *et al.* (1995; Bohm, 1995) related the intrinsic irreverisibility 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 Sudarshan *et al.* (1978) by analytic continuation in a generalized quantum mechanics.

The Friedrichs model, a prototype of a decaying system describing the interaction between a quantum oscillator and a scalar field, was extensively analyzed in the literature for the one excited mode sector. It is an exactly

[1] Departamento de Fisica, FCEIA, Universidad Nacional de Rosario, 200 Rosario, Argentina; e-mail: laura@ifir.ifir.edu.ar.

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solvable model, in which the quantum oscillator decays to the ground state for all initial conditions. Sudarshan *et al.* (1978) computed the complex spectral decomposition. The spectral decomposition was also obtained by Petrosky *et al.* (1991a) using subdynamic theory. The spectral decomposition with complex eigenvalues was interpreted in terms of rigged Hilbert spaces by Antoniou and Prigogine (1993) and by Antoniou and Tasaki (1993).

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, taking the limit $N \to \infty$, $V \to \infty$ with $N/V = c < \infty$ in the last step of the calculations. This method was used in subdynamic theory (Antoniou and Tasaki, 1993; Petrosky, and Prigogine, 1991b), where the collision operator, with complex eigenvalues, is responsible for the evolution to statistical equilibrium.

It is not surprising that the time evolution of the Friedrichs model can be successfully described using the methods of nonequilibrium statistical mechanics, which 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 the Friedrichs model the discrete eigenvalue disappears and in the gas the momentum of each particle is no longer 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 Hamiltonians 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 Antoniou *et al.* (1994, 1995, 1997) for quantum systems with diagonal singularity. The quantum states of this theory are *functionals* over the space of observables $\mathcal{O}$. Mathematically this means that the space $\mathcal{S}$ of states is contained in $\mathcal{O}^{\times}$. Physically, it means that the only thing we can really observe and measure are the mean values of the observables $O \in \mathcal{O}$ in states $\rho \in \mathcal{S} \subset \mathcal{O}^{\times}$: namely $\langle O \rangle_{\rho} = \rho[O] \equiv (\rho | O)$. This is the natural generalization of the usual trace Tr $(\hat{\rho}\hat{O})$, 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 appear 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, computing the singular "final" state, and discussing its relation with "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 "Gamow states" is also discussed in this section.

2. RESOLVENT FORMALISM FOR GENERALIZED STATES

Let us consider the Liouville–von Neumann equation for a state ρ,

$$i \frac{d}{dt} \rho = L\rho \tag{1}$$

The general solution, valid for $t > 0$, can be written as

$$\rho_t = \frac{1}{2\pi i} \int_\Gamma dz \exp(-izt) \frac{1}{L - z} \rho_o \tag{2}$$

where Γ is a 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.

$$P^2 = P, \qquad Q^2 = Q, \qquad P + Q = I \tag{3}$$

(I is the identity superoperator acting on states), it is possible to decompose the resolvent as (Grecos *et al.*, 1975; Zwanzig, 1964).

$$\frac{1}{L - z} = [P + C(z)] \frac{1}{PLP + \Psi(z) - z} [P + D(z)] = \frac{1}{QLQ - z} Q \tag{4}$$

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

$$\begin{aligned}
\Psi(z) &= P\Psi(z)P = -PLQ \frac{1}{QLQ - z} QLP \\
C(z) &= QC(z)P = -\frac{1}{QLQ - z} QLP \\
D(z) &= PD(z)Q = -PLQ \frac{1}{QLQ - z}
\end{aligned} \tag{5}$$

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 (Antoniou and Suchanecki, 1994, 1995; Antoniou *et al.*, 1997). Therefore for any observable $O \in \mathcal{O}$ and state $\rho \in \mathcal{O}^{\times}$ we have

$$\langle O \rangle_\rho = (\rho | O), \qquad (a\rho_1 + b\rho_2 | O) = a^*(\rho_1 | O) + b^*(\rho_2 | O) \tag{6}$$

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

$$(\rho | O) = (\rho | O)^* \tag{7}$$

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

$$(\rho | I) = \sum_\alpha (\rho || \alpha\rangle\langle\alpha|) = 1, \qquad (\rho || \alpha\rangle\langle\alpha|) \geq 0 \tag{8}$$

In the last expression $(\rho || \alpha\rangle\langle\alpha|)$ is the probability of the state ρ to be the pure state $|\alpha\rangle$. For continuous spectrum the sum in (8) should be replaced by an integral and $(\rho || \alpha\rangle\langle\alpha|)$ 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 (1), which can be applied to an arbitrary observable O, i.e.,

$$\left(i \frac{d}{dt} \rho | O \right) = (L\rho | O)$$

We should give a meaning to the second term of this equation. The superoperator L is defined by

$$(L\rho | O) = (\rho | L^\dagger O) = (\rho | [H, O]) \tag{9}$$

where H is the Hamiltonian of the quantum system.

From (2) and the antilinearity of the state functionals we obtain

$$(\rho_t | O) = \frac{i}{2\pi} \int_\Gamma dz \exp(-izt)(\rho_o | \frac{1}{L^\dagger + z} | O) \tag{10}$$

The resolvent $1/(L^\dagger + z)$ has the following decomposition

$$\frac{1}{L^\dagger + z} = [P^\dagger + D^\dagger(z)] \frac{1}{P^\dagger L^\dagger P^\dagger + \Psi^\dagger(z) + z} [P^\dagger + C^\dagger(z)] + Q^\dagger \frac{1}{Q^\dagger L^\dagger Q^\dagger + z} \tag{11}$$

where $P^\dagger$ and $Q^\dagger$ are defined by

$$(\rho|P^\dagger O) = (P\rho|O), \qquad (\rho|Q^\dagger O) = (Q\rho|O) \tag{12}$$

and

$$\begin{aligned}
\Psi^\dagger(z) &= P^\dagger\Psi^\dagger(z)P^\dagger = -P^\dagger L^\dagger Q^\dagger \frac{1}{Q^\dagger L^\dagger Q^\dagger + z} Q^\dagger L^\dagger P^\dagger \\
C^\dagger(z) &= P^\dagger C^\dagger(z)Q^\dagger = -P^\dagger L^\dagger Q^\dagger \frac{1}{Q^\dagger L^\dagger Q^\dagger + z} \\
D^\dagger(z) &= Q^\dagger D^\dagger(z)P^\dagger = -\frac{1}{Q^\dagger L^\dagger Q^\dagger + z} Q^\dagger L^\dagger P^\dagger
\end{aligned} \tag{13}$$

3. 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 $V_{\bar{p}\bar{p}'} = \langle\bar{p}|\hat{V}|\bar{p}'\rangle$ of the potential in the basis of eigenvectors of the momentum are well-behaved ordinary functions of $\bar{p}$ and $\bar{p}'$.

The Hamiltonian of the system is

$$H = H_o + V = \int d\bar{p}\; \epsilon_p|\bar{p}\rangle\langle\bar{p}| + \int\int d\bar{p}\; d\bar{p}'\; V_{\bar{p}\bar{p}'}|\bar{p}\rangle\langle\bar{p}'|, \qquad \epsilon_p = \frac{p^2}{2m} \tag{14}$$

Let us consider observables $O \in \mathbb{O}$ of the form

$$O = \int d\bar{p}\; O_{\bar{p}}|\bar{p}\rangle\langle\bar{p}| + \int\int d\bar{p}\; d\bar{p}'\; O_{\bar{p}\bar{p}'}|\bar{p}\rangle\langle\bar{p}'| \tag{15}$$

where $O_{\bar{p}}$ and $O_{\bar{p}\bar{p}}'$ are two independent regular functions of the variables $\bar{p}$ and $\bar{p}'$, satisfying

$$O^*_{\bar{p}} = O_{\bar{p}}, \qquad O^*_{\bar{p}\bar{p}'} = O_{\bar{p}'\bar{p}}$$

Precisely the Hamiltonian (14) is of the form given by (15).[2]

As we stated in the previous section, the states are represented by antilinear functionals acting on observables. In this case, a state ρ will be

[2] 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 (15) and should have well-defined mean values. It is not the case in the thermodynamic limit, where extensive observables have infinite mean values (Laura and Castagnino, n.d.).

represented by two regular functions $\rho_{\bar{p}}$ and $\rho_{\bar{p}\bar{p}'}$. The mean value of an observable O is

$$(\rho|O) = \int d\bar{p}\ \rho^*_{\bar{p}} O_{\bar{p}} + \int\int d\bar{p}\ d\bar{p}'\ \rho^*_{\bar{p}\bar{p}'} O_{\bar{p}\bar{p}'} \tag{16}$$

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

$$\rho^*_{\bar{p}} = \rho_{\bar{p}} \geq 0, \qquad \rho^*_{\bar{p}\bar{p}'} = \rho_{\bar{p}'\bar{p}'}, \qquad \int d\bar{p}\ \rho^*_{\bar{p}} = 1 \tag{17}$$

It is useful to use a special notation for the generalized observables expanding $\mathbb{O}$. Therefore we define

$$|\bar{p}) \equiv |\bar{p}\rangle\langle\bar{p}|, \qquad |\bar{p}\bar{p}') \equiv |\bar{p}\rangle\langle\bar{p}'| \tag{18}$$

We also define the functionals $(\bar{p}|$ and $(\bar{p}\bar{p}'|$ satisfying

$$\begin{aligned}(\bar{p}|\bar{k}) &= \delta^3(\bar{p} - \bar{k})\\ (\bar{p}\bar{p}'|\bar{k}\bar{k}') &= \delta^3(\bar{p} - \bar{k})\delta^3(\bar{p}' - \bar{k}')\\ (\bar{p}|\bar{k}\bar{k}') &= (\bar{p}\bar{p}'|\bar{k}) = 0\end{aligned} \tag{19}$$

These "bases" can be used to expand states and observables

$$\rho = \int d\bar{p}\ \rho^*_{\bar{p}}(\bar{p}| + \int\int d\bar{p}\ d\bar{p}'\ \rho^*_{\bar{p}\bar{p}'}(\bar{p}\bar{p}'| \tag{20}$$

$$O = \int d\bar{p}\ O_{\bar{p}}|\bar{p}) + \int\int d\bar{p}\ d\bar{p}'\ O_{\bar{p}\bar{p}'}|\bar{p}\bar{p}')$$

With (19) and (20) we can deduce (16).[3]

Starting from the definitions

$$L_0^\dagger O = [H_0, O], \qquad L_V^\dagger O = [V, O]$$

and using the 'bases' $|\bar{p})$, $|\bar{p}\bar{p}')$ for the observables and $(\bar{p}|$, $(\bar{p}\bar{p}'|$ for the states, we obtain

$$\begin{aligned}L_0^\dagger &= \int d\bar{p}\ d\bar{p}'\ (\epsilon_{\bar{p}} - \epsilon_{\bar{p}'})|\bar{p}\bar{p}')(\bar{p}\bar{p}'|\\ L_V^\dagger &= \int d\bar{p}\ d\bar{p}'\ |\bar{p}\bar{p}')V_{\bar{p}\bar{p}'}[(\bar{p}'| - (\bar{p}|]\\ &\quad + \int d\bar{p}\ d\bar{p}'|\bar{p}\bar{p}') \int d\bar{p}''\ [V_{\bar{p}\bar{p}''}(\bar{p}''\bar{p}'| - V_{\bar{p}''\bar{p}'}(\bar{p}\bar{p}''|]\end{aligned} \tag{21}$$

[3] At this stage the formalism may look rather exotic. To make contact with more usual things, let us mention that a pure state represented by the normalized wave function $|\varphi\rangle = \int d\bar{k}\ \varphi_{\bar{k}}|\bar{k}\rangle$ *can also be represented by the functional* $\rho = \int d\bar{p}\varphi^*_{\bar{p}}\varphi_{\bar{p}}(\bar{p}| + \int\int d\bar{p}\ d\bar{p}'\ \varphi^*_{\bar{p}}\varphi_{\bar{p}'}(\bar{p}\bar{p}'|$.

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:

$$P^\dagger O = \int d\bar{p}\; O_{\bar{p}}|\bar{p}\rangle\langle\bar{p}|, \qquad Q^\dagger O = \int\int d\bar{p}\; d\bar{p}'\; O_{\bar{p}\bar{p}'}|;\bar{p}\rangle\langle\bar{p}'|$$

or equivalently

$$P^\dagger = \int d\bar{p}\; |\bar{p})(\bar{p}|, \qquad Q^\dagger = \int d\bar{p}\; d\bar{p}'\; |\bar{p}\bar{p}')(\bar{p}\bar{p}'| \tag{22}$$

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.,

$$(P\rho| = \int d\bar{p}\; \rho^*_{\bar{p}}(\bar{p}|, \qquad (Q\rho| = \int\int d\bar{p}\; d\bar{p}'\; \rho^*_{\bar{p}\bar{p}'}(\bar{p}\bar{p}'| \tag{23}$$

From (21) and (22) we obtain

$$P^\dagger L^\dagger = 0, \qquad \Psi^\dagger(z) = 0, \qquad C^\dagger(z) = 0 \tag{24}$$

and the decomposition of the resolvent reduces to

$$\frac{1}{L^\dagger + z} = \frac{1}{z} P^\dagger + \frac{1}{z} Q^\dagger D^\dagger(z) P^\dagger + Q^\dagger \frac{1}{Q^\dagger L^\dagger Q^\dagger + z} Q^\dagger \tag{25}$$

The time evolution is given by

$$\begin{aligned}(P\rho_t| = {} & \frac{i}{2\pi}\int_\Gamma dz\, \frac{\exp(-izt)}{z}\, (P\rho_o| \\ & - \frac{i}{2\pi}\int_\Gamma dz\, \frac{\exp(-izt)}{z}\, (Q\rho_o|\, \frac{1}{Q^\dagger L^\dagger Q^\dagger + z}\, Q^\dagger L^\dagger P^\dagger\end{aligned} \tag{26}$$

$$(Q\rho_t| = \frac{i}{2\pi}\int_\Gamma dz\, \exp(-izt)(Q\rho_o|\, \frac{1}{Q^\dagger L^\dagger Q^\dagger + z}\, Q^\dagger \tag{27}$$

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 from 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 Γ 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 sinple pole at $z = 0$, to obtain

$$\frac{i}{2\pi}\int_{\Gamma} dz\,\frac{\exp(-izt)}{z}\,(P\rho_o|O) = (P\rho_o|P^{\dagger}O) \tag{28}$$

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,

$$|\bar{k}^{\pm}\rangle = |\bar{k}\rangle + \frac{1}{\epsilon_k \pm i0 - H}\,V|\bar{k}\rangle$$

$$\langle\bar{k}^{\pm}| = \langle\bar{k}| + \langle\bar{k}|V\,\frac{1}{\epsilon_k \mp i0 - H} \tag{29}$$

for which

$$I = \int d\bar{k}|\bar{k}^{\pm}\rangle\langle\bar{k}^{\pm}|, \qquad H = \int d\bar{k}\epsilon_k|\bar{k}^{\pm}\rangle\langle\bar{k}^{\pm}|, \qquad \langle\bar{k}^{\pm}|\bar{k}'^{\pm}\rangle = \delta^3(\bar{k} - \bar{k}')$$

We have

$$-\frac{i}{2\pi}\int_{\Gamma} dz\,\frac{\exp(-izt)}{z}\,(Q\rho_o|\,\frac{1}{Q^{\dagger}L^{\dagger}Q^{\dagger} + z}\,Q^{\dagger}L^{\dagger}P^{\dagger}|O)$$

$$= -\frac{i}{2\pi}\int_{\Gamma} dz\,\frac{\exp(-izt)}{z}\int\int d\bar{k}\,d\bar{k}'$$

$$(Q\rho_o|\,\frac{1}{Q^{\dagger}L^{\dagger}Q^{\dagger} + z}\,[|\bar{k}^{+}\rangle\langle\bar{k}^{+}|[H, P^{\dagger}O]|\bar{k}'^{+}\rangle\langle\bar{k}'^{+}|])$$

$$= -\frac{i}{2\pi}\int_{\Gamma} dz\,\frac{\exp(-izt)}{z}\int\int d\bar{k}\,d\bar{k}'$$

$$\frac{\epsilon_k - \epsilon_{k'}}{\epsilon_k - \epsilon_{k'} + z}\,(Q\rho_o||\bar{k}^{+}\rangle\langle\bar{k}'^{+}|)\langle\bar{k}^{+}|P^{\dagger}O|\bar{k}'^{+}\rangle \tag{30}$$

The integral over $\bar{k}$ and $\bar{k}'$ can be transformed using polar coordinates into an integral over ϵ_k, $\epsilon_{k'}$ and over the angles. Looking at the integrals over the energies, we can write

$$\int_\Gamma dz \frac{\exp(-izt)}{z} \int_0^\infty d\epsilon \int_0^\infty d\epsilon' \frac{\epsilon - \epsilon'}{\epsilon - \epsilon' + z} f(\epsilon, \epsilon)$$

$$= -\int_\Gamma dz \frac{\exp(-izt)}{z} \int_0^\infty d\lambda \int_{-\lambda}^{\lambda} d\nu \frac{\nu}{z - \nu} f(\lambda, \nu)$$

$$= -\int_0^\infty d\lambda \int_\Gamma dz \frac{\exp(-izt)}{z} F_\lambda(z)$$

where for the last expressions we used the variables $\nu = \epsilon' - \epsilon$ and $\lambda = \frac{1}{2}(\epsilon' + \epsilon)$, and

$$F_\lambda(z) \equiv \int_{-\lambda}^{\lambda} d\nu \frac{\nu}{z - \nu} f(\lambda, \nu)$$

In terms of the complex variable z, $(e^{-izt}/z)F_\lambda(z)$ has a simple pole in $z = 0$ and a cut in the real interval $(-\lambda, +\lambda)$:

$$F_\lambda(x + i0) - F_\lambda(x - i0) = \begin{cases} 0, & \text{if} \quad x \notin (-\lambda, +\lambda) \\ -2\pi i x f(\lambda, x), & \text{if} \quad x \in (-\lambda, +\lambda) \end{cases}$$

As in the previous case, the integral over Γ 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

$$-\int_0^\infty d\lambda \int_\Gamma dz \frac{\exp(-izt)}{z} F_\lambda(z)$$

$$= 2\pi i \left\{ \int_0^\infty d\lambda \int_0^\infty d\nu\, f(\lambda, \nu) + \int_0^\infty d\lambda \int_0^\infty d\nu \exp(-i\nu t)\, f(\lambda, \nu) \right\} \quad (31)$$

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

$$-\frac{i}{2\pi} \int_\Gamma dz \frac{\exp(-izt)}{z} (Q\rho_o| \frac{1}{Q^\dagger L^\dagger Q^\dagger + z} Q^\dagger L^\dagger P^\dagger |O)$$

$$= \int \int d\bar{k}\, d\bar{k}' \exp\{i(\epsilon_k - \epsilon_{k'})t\} (Q\rho_o||\bar{k}^+\rangle\langle\bar{k}^+|P^\dagger O|\bar{k}'^+\rangle\langle\bar{k}'^+|)$$

Therefore

$$(P\rho_t|O) = (P\rho_o|P^\dagger O)$$

$$+ \int \int d\bar{k}\, d\bar{k}' \exp\{i(\epsilon_k - \epsilon_{k'})t\} (Q\rho_o||\bar{k}^+\rangle\langle\bar{k}^+|P^\dagger O|\bar{k}'^+\rangle\langle\bar{k}'^+|) \quad (32)$$

The Lipmann–Schwinger vectors (29) can also be used in expression (27),

$$(Q\rho_t|O) = \int\int d\bar{k}\, d\bar{k}'\, \exp\{i(\epsilon_k - \epsilon_{k'})t\}(Q\rho_o||\bar{k}^+\rangle\langle\bar{k}^+|Q^\dagger O|\bar{k}'^+\rangle\langle\bar{k}'^+|) \tag{33}$$

There are no singular terms in $(Q\rho_o||\bar{k}^+\rangle\langle\bar{k}^+|Q^\dagger O|\bar{k}'^+\rangle\langle\bar{k}'^+|)$, and therefore the Riemann–Lebesgue theorem can be used in (33) to obtain

$$\lim_{t\to\infty} (Q\rho_t|O) = 0 \tag{34}$$

From equations (32) and (33) it is easy to show that there is no time evolution for a diagonal initial condition, i.e.,

$$\rho_o = P\rho_o \Rightarrow \rho_t = \rho_o$$

We must isolate the singular term in $(Q\rho_o||\bar{k}^+\rangle\langle\bar{k}^+|P^\dagger O|\bar{k}'^+\rangle\langle\bar{k}'^+|)$ before using the Riemann–Lebesgue theorem to compute $\lim_{t\to\infty}(P\rho_t|O)$. Using (29), we obtain

$$\begin{aligned}
&(Q\rho_o||\bar{k}^+\rangle\langle\bar{k}^+|P^\dagger O|\bar{k}'^+\rangle\langle\bar{k}'^+|)\\
&=(Q\rho_o||\bar{k}^+\rangle\langle\bar{k}'^+|) \times \{O_{\bar{k}}\delta^3(\bar{k} - \bar{k}') + O_{\bar{k}}\langle\bar{k}| \frac{1}{\epsilon_{k'} + i0 - H} V|\bar{k}'\rangle\\
&+ \langle\bar{k}|V \frac{1}{\epsilon_{\bar{k}'} - i0 - H} |\bar{k}'\rangle O_{\bar{k}'}\\
&+ \langle\bar{k}|V \frac{1}{\epsilon_{\bar{k}'} - i0 - H} |\bar{k}''\rangle O_{\bar{k}''}\langle\bar{k}''| \frac{1}{\epsilon_{k'} + i0 - H} V|\bar{k}'\rangle\}
\end{aligned} \tag{35}$$

Replacing (35) in (32), and using the Riemann–Lebesgue theorem, we obtain

$$\begin{aligned}
\lim_{t\to\infty} (P\rho_t|O) &= (P\rho_o|P^\dagger O) + \int d\bar{k}\, (Q\rho_o||\bar{k}^+\rangle\langle\bar{k}^+|)O_{\bar{k}}\\
&= \int d\bar{k}\, (\rho_o||\bar{k}^+\rangle\langle\bar{k}^+|)O_{\bar{k}}
\end{aligned} \tag{36}$$

Therefore, in the weak sense

$$(\rho_\infty| = \lim_{t\to\infty} (\rho_t| = \int d\bar{k}\, (\rho_o||\bar{k}^+\rangle\langle\bar{k}^+|)(\bar{k}| \tag{37}$$

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 $|\varphi\rangle = \int d\bar{k}\ \varphi_{\bar{k}}|\bar{k}\rangle$ can also be represented by the functional

$$\rho = \int d\bar{p}\ \varphi_{\bar{p}}^{*}\varphi_{\bar{p}}(\bar{p}| + \int\int d\bar{p}\ d\bar{p}'\ \varphi_{\bar{p}}^{*}\varphi_{\bar{p}'}(\bar{p}\bar{p}'|$$

Therefore, in this formalism, $\rho_{\bar{k}}^{*} = \rho_{\bar{k}\bar{k}'}^{*}$ 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 the weak sense and for all initial conditions, the evolution is not toward a pure state, but toward a 'generalized mixture' in which $(\rho_{\infty})_{\bar{k}}^{*} = (\rho_{o}||\bar{k}^{+})(\bar{k}^{+}|)$ and $(\rho_{\infty})_{\bar{k}\bar{k}'}^{*} = 0$. This 'final' state is time invariant, because from (24) we have

$$(L\rho_{\infty}|O) = (LP\rho_{\infty}|O) = (\rho_{\infty}|P^{\dagger}L^{\dagger}O) = 0 \Rightarrow L\rho_{\infty} = 0$$

Moreover, the time inversion $T\rho_{\infty}$ of the 'final' state is also invariant under time evolution. In fact, for any

$$\rho = \int d\bar{p}\ \rho_{\bar{p}}^{*}(\bar{p}| + \int\int d\bar{p}\ d\bar{p}'\ \rho_{\bar{p}\bar{p}'}^{*}(\bar{p}\bar{p}'|$$

we have

$$T\rho = \int d\bar{p}\ \rho_{-\bar{p}}(\bar{p}| + \int\int d\bar{p}\ d\bar{p}'\ \rho_{-\bar{p}-\bar{p}'}(\bar{p}\bar{p}'|$$

then

$$T\rho_{\infty} = \int d\bar{k}\ (\rho_{o}|| - \bar{k}^{+})(-\bar{k}^{+}|)^{*}(\bar{k}|$$

and

$$LT\rho_{\infty} = 0$$

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 $T\rho_{t_o}$ in practice.

4. 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 (32) and (33)]. 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 for 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 the 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

$$H = H_0 + V = \int_0^\infty d\omega\ \omega|\omega\rangle\langle\omega| + \int_0^\infty d\omega \int_0^\infty d\omega'\ V_{\omega\omega'}|\omega\rangle\langle\omega'| \qquad (38)$$

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

$$I = \int_0^\infty d\omega\ |\omega\rangle\langle\omega|, \qquad \langle\omega|\omega'\rangle = \delta(\omega - \omega')$$

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

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

$$\langle\omega^{\pm}| = \langle\omega| + \langle\omega|V\frac{1}{\omega \mp i0 - H} \qquad (39)$$

are also a complete set:

$$H = \int_0^\infty d\omega\ \omega|\omega^{\pm}\rangle\langle\omega^{\pm}|, \qquad I = \int_0^\infty d\omega\ |\omega^{\pm}\rangle\langle\omega^{\pm}|, \qquad \langle\omega^{\pm}|\omega'^{\pm}\rangle = \delta(\omega - \omega')$$

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

$$|\omega^+\rangle = S(\omega)|\omega^-\rangle, \qquad \langle\omega^+| = S^*(\omega)\rangle\omega^-| \qquad (40)$$

where

$$S(\omega) = 1 - 2\pi i\langle\omega|V|\omega\rangle - 2\pi i\langle\omega|V\frac{1}{\omega + i0 - H} V|\omega\rangle$$

$$S^*(\omega) = 1 + 2\pi i\langle\omega|V|\omega\rangle + 2\pi i\langle\omega|V\frac{1}{\omega - i0 - H} V|\omega\rangle \qquad (41)$$

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

From (41) we can define the following analytic extensions:

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

$$S^*(z) = 1 + 2\pi i\langle z|V|z\rangle + 2\pi i\langle z|V\left(\frac{1}{s - H}\right)^{-}_{s=z} V|z\rangle \tag{42}$$

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

$$|z^{\pm}\rangle = |z\rangle + \left(\frac{1}{s - H}\right)^{\pm}_{s=z} V|z\rangle$$

$$\langle z^{\pm}| = \langle z| + \langle z|V\left(\frac{1}{s - H}\right)^{\mp}_{s=z} \tag{43}$$

In the previous expressions, $|z\rangle$ and $\langle z|$ are functionals defined by

$$\langle z|\varphi\rangle = \varphi(z), \qquad \langle\varphi|z\rangle = \varphi^*(z)$$

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

$$O = P^{\dagger}O + Q^{\dagger}O = \int d\omega\, O_{\omega}|\omega) + \int\int d\omega\, d\omega'\, O_{\omega\omega'}|\omega\omega') \tag{44}$$

$$|\omega) \equiv |\omega\rangle\langle\omega|, \qquad |\omega\omega') \equiv |\omega\rangle\langle\omega'|, \qquad O_{\omega} = O^*_{\omega}, \qquad O_{\omega\omega'} = O^*_{\omega'\omega}$$

If we define the functionals $(\omega|$ and $(\omega\omega'|$ by the equations

$$(\omega|\omega') = \delta(\omega - \omega')$$

$$(\omega|\omega'\omega'') = (\omega'\omega''|\omega) = 0$$

$$(\omega\omega'|\varsigma\varsigma') = \delta(\omega - \varsigma)\delta(\omega' - \varsigma')$$

they can be used to represent the state functionals

$$\rho = \int d\omega\ \rho^*_\omega\ (\omega| + \int\int d\omega\ d\omega'\ \rho^*_{\omega\omega'}(\omega\omega'|$$

$$\rho^*_\omega = \rho_\omega \geq 0, \qquad \rho^*_{\omega\omega'} = \rho_{\omega'\omega}, \qquad \int d\omega\ \rho^*_\omega = 1$$

The mean value of an observable O in the state ρ is given by

$$\langle O\rangle_\rho = (\rho|O) = \int d\omega\ \rho^*_\omega O_\omega + \int\int d\omega\ d\omega'\ \rho^*_{\omega\omega'} O_{\omega\omega'}$$

with the following time evolution:

$$(\rho_t|O) = (U_t\rho_0|O) = (\rho_0|U_t^\dagger O) = (\rho_0|\exp(iHt)O\exp(-iHt))$$

The observable given in (44) can be written as

$$O = O_{\text{diag}} + O_{\text{reg}}$$

$$O_{\text{diag}} = \int d\omega\ O_\omega|\omega\rangle\langle\omega|$$

$$O_{\text{reg}} = \int\int d\omega\ d\omega'\ O_{\omega\omega'}|\omega\rangle\langle\omega'|$$

Using the Lipmann–Schwinger vectors (39), 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 (inv) and a fluctuating (fluc) part,

$$O = O_{\text{inv}} + O_{\text{fluc}}$$

$$O_{\text{fluc}} = O_{\text{reg}} + \Delta O_{\text{diag}} \tag{45}$$

The fluctuating part O_{fluc} has no diagonal singularity $[(O_{\text{fluc}})_\omega = 0]$, and O_{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 (39):

$$(\rho_t|O) = (\rho_0|O_{\text{inv}}) + (\rho_0|\exp[iHt]O_{\text{fluc}}\exp[-iHt])$$
$$= \int_0^\infty d\omega(\rho_0||\omega^+\rangle\langle\omega^+|)O_\omega$$
$$+ \int_0^\infty d\omega \int_0^\infty d\omega'\, e^{i(\omega-\omega')t}(\rho_0||\omega^+\rangle\langle\omega^+|O_{\text{fluc}}|\omega'^+\rangle\langle\omega'^+|) \tag{46}$$

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

$$(\rho_\infty| = \lim_{t\to\infty}(\rho_t| = \int_0^\infty d\omega\, (\rho_0||\omega^+\rangle\langle\omega^+|)(\omega| \tag{47}$$

Expression (46) corresponds to the following real spectral decomposition of the identity ($I^\dagger$) and Liouville–von Neumann ($L^\dagger$) superoperators:

$$I^\dagger = \int_0^\infty d\omega\, |\Phi_\omega)\,(\tilde{\Phi}_\omega| + \int_0^\infty d\omega \int_0^\infty d\omega'\, |\Phi_{\omega\omega'})\,(\tilde{\Phi}_{\omega\omega'}|$$
$$L^\dagger = \int_0^\infty d\omega \int_0^\infty d\omega'\, (\omega - \omega')|\Phi_{\omega\omega'})(\tilde{\Phi}_{\omega\omega'}| \tag{48}$$

where

$$|\Phi_\omega) = ||\omega^+\rangle\langle\omega^+|)$$
$$(\tilde{\Phi}_\omega| = (\omega|$$
$$|\Phi_{\omega\omega'}) = ||\omega^+\rangle\langle\omega'^+|) \tag{49}$$
$$(\tilde{\Phi}_{\omega\omega'}| = \int dy\,\{\langle\omega^+|y\rangle\langle y|\omega'^+\rangle - \delta(\omega - y)\delta(y - \omega')\}(y|$$
$$+ \int\int dy\,dy'\,\langle\omega^+|y\rangle\langle y'|\omega'^+\rangle(yy'|$$

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

$$(\tilde{\Phi}_\omega|\Phi_{\omega'}) = \delta(\omega - \omega')$$
$$(\tilde{\Phi}_\omega|\Phi_{yy'}) = (\tilde{\Phi}_{\omega\omega'}|\Phi_y) = 0$$
$$(\tilde{\Phi}_{\omega\omega'}|\Phi_{yy'}) = \delta(\omega - y)\delta(\omega' - y')$$

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

$$\rho = \int_0^\infty d\omega\ (\rho|\Phi_\omega)(\tilde{\Phi}_\omega| + \int_0^\infty d\omega \int_0^\infty d\omega'\ (\rho|\Phi_{\omega\omega'})(\tilde{\Phi}_{\omega\omega'}|$$

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

$$(\tilde{\Phi}_\omega|H) = (\omega|H) = \omega$$

$$(\tilde{\Phi}_{\omega\omega'}|H) = \int dy\ \{\langle\omega^+|y\rangle\langle y|\omega'^+\rangle - \delta(\omega - y)\delta(y - \omega')\}y$$
$$+ \int\int dy\, dy'\ \langle\omega^+|y\rangle V_{yy'}\langle y'|\omega'^+\rangle = 0$$

and for the "trace"

$$(\tilde{\Phi}_\omega|I) = (\omega|I) = (\omega| \int d\omega' |\omega') = \int d\omega'\ \delta(\omega - \omega') = 1$$

$$(\tilde{\Phi}_{\omega\omega'}|I) = \int dy\ \{\langle\omega^+|y\rangle\langle y|\omega'^+\rangle - \delta(\omega - y)\delta(y - \omega')\}$$
$$= \langle\omega^+|\omega'^+\rangle - \delta(\omega - \omega') = 0$$

The generalized state $(\tilde{\Phi}_\omega|$ is a physical state with energy ω and "trace" 1, and $(\tilde{\Phi}_{\omega\omega'}|$ has zero energy and zero "trace." Clearly, it is impossible to realize a physical state including only $(\tilde{\Phi}_{\omega\omega'}|$ 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 (46) we deform the ω integral over R^+ into an integral over a curve in the lower half-plane, i.e.,

$$\int_0^\infty d\omega\ e^{i\omega t}|\omega^+\rangle\langle\omega^+|$$
$$= \int_0^\infty d\omega\ e^{i\omega t}|\omega^+\rangle\langle\omega^-|S^*(\omega)$$
$$\to e^{iz_0^* t}|\tilde{f}_0\rangle\langle f_0| + \int_0^{-\infty} d\omega\ e^{i\omega t}|(\omega + i0)^+\rangle\langle(\omega + i0)^+|$$

$$|\tilde{f}_0\rangle = [2\pi i(\mathrm{Res}\ S^*)_{z_0^*}]^{1/2}|z_0^{*+}\rangle, \qquad \langle f_0| = [2\pi i(\mathrm{Res}\ S^*)_{z_0^*}]^{1/2}\langle z_0^{*-}| \qquad (50)$$

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

(46), we deform the ω' integral over R^+ into an integral over a curve in the lower half-plane, i.e.,

$$\begin{aligned}
&\int_0^\infty d\omega'\; e^{-i\omega' t}|\omega'^{+}\rangle\langle\omega'^{+}| \\
&\quad = \int_0^\infty d\omega'\; e^{-i\omega' t}S(\omega')|\omega'^{-}\rangle\langle\omega'^{+}| \\
&\quad \to e^{-iz_0 t}|f_0\rangle\langle\tilde{f}_0| + \int_0^{-\infty} d\omega'\; e^{-i\omega' t}|(\omega' - i0)^{+}\rangle\langle(\omega' - i0)^{+}|
\end{aligned}$$

$$|f_0\rangle = [-2\pi i(\mathrm{Res}\, S)_{z_0}]^{1/2}|z_0^{-}\rangle, \qquad \langle\tilde{f}_0| = [-2\pi i(\mathrm{Res}\, S)_{z_0}]^{1/2}\langle z_0^{+}| \tag{51}$$

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

$$\begin{aligned}
(\rho_t|O) = &\int_0^\infty d\omega\; (\rho_0||\omega^{+}\rangle\langle\omega^{+}|)O_\omega \\
&+ e^{i(z_0^* - z_0)t}(\rho_0||\tilde{f}_0\rangle\langle f_0|O_{\text{fluc}}|f_0\rangle\langle\tilde{f}_0|) \\
&+ \int_0^{-\infty} d\omega'\; e^{i(z_0^* - \omega')t}(\rho_0||\tilde{f}_0\rangle\langle f_0|O_{\text{fluc}}|(\omega' - i0)^{+}\rangle\langle(\omega' - i0)^{+}|) \\
&+ \int_0^{-\infty} d\omega\; e^{i(\omega - z_0)t}(\rho_0||(\omega + i0)^{+}\rangle\langle(\omega + i0)^{+}|O_{\text{fluc}}|f_0\rangle\langle\tilde{f}_0|) \\
&+ \int_0^{-\infty} d\omega \int_0^{-\infty} d\omega'\; e^{i(\omega - \omega')t} \\
&\times (\rho_0||(\omega + i0)^{+}\rangle\langle(\omega + i0)^{+}|O_{\text{fluc}}|(\omega' - i0)^{+}\rangle\langle(\omega' - i0)^{+}|)
\end{aligned} \tag{52}$$

The changes indicated in equations (50) and (51) are possible if we impose on the states and observables the condition that $\rho^*_{\omega\omega'}$ and $O_{\omega\omega'}$ have well-defined analytic extensions to the upper (lower) half-plane in the variable $\omega(\omega')$.[4] In this case it is possible to prove that $(O_{\text{fluc}})_{\omega\omega'}$ also has a well-defined analytic extension to the upper (lower) half-plane in the variable $\omega(\omega')$. Expression (52) corresponds to the following complex spectral decomposition of the identity ($I^\dagger$) and Liouville–von Neumann ($L^\dagger$) superoperators:

[4]Equations (50) and (51) require 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 $e^{i\omega t}(e^{-i\omega' t})$, with $t > 0$, makes it easier to satisfy the requirement.

$$I^{\dagger} = \int_0^{\infty} d\omega\ |\Psi_\omega)(\tilde{\Psi}_\omega| + |\Psi_{00})(\tilde{\Psi}_{00}| + \int_0^{-\infty} d\omega'\ |\Psi_{0\omega'})(\tilde{\Psi}_{0\omega'}|$$
$$+ \int_0^{-\infty} d\omega\ |\Psi_{\omega 0})(\tilde{\Psi}_{\omega 0}| + \int_0^{-\infty} d\omega \int_0^{-\infty} d\omega'\ |\Psi_{\omega\omega'})(\tilde{\Psi}_{\omega\omega'}|$$
$$L^{\dagger} = (z_0^* - z_0)|\Psi_{00})(\tilde{\Psi}_{00}| + \int_0^{-\infty} d\omega'\ (z_0^* - \omega')|\Psi_{0\omega'})(\tilde{\Psi}_{0\omega'}|$$
$$+ \int_0^{-\infty} d\omega\ (\omega - z_0)|\Psi_{\omega 0})(\tilde{\Psi}_{\omega 0}|$$
$$+ \int_0^{-\infty} d\omega \int_0^{-\infty} d\omega'\ (\omega - \omega')|\Psi_{\omega\omega'})(\tilde{\Psi}_{\omega\omega'}| \tag{53}$$

where

$$\begin{aligned}
|\Psi_\omega) &= ||\omega^+\rangle\langle\omega^+|) \\
(\tilde{\Psi}_\omega| &= (\omega| \\
|\Psi_{00}) &= ||\tilde{f}_0\rangle\langle\tilde{f}_0|) \\
(\tilde{\Psi}_{00}| &= [2\pi i(\mathrm{Res}\ S^*)_{z_0^*}]^{-1/2}[-2\pi i(\mathrm{Res}\ S)_{z_0}]^{-1/2} \\
&\quad \times (2\pi i \mathrm{Res}_{\omega=z_0^*})(-2\pi i \mathrm{Res}_{\omega'=z_0})(\tilde{\Psi}_{\omega\omega'}| \\
|\Psi_{0\omega'}) &= ||\tilde{f}_0\rangle\langle(\omega' - i0)^+|) \\
(\tilde{\Psi}_{0\omega'}| &= [2\pi i(\mathrm{Res}\ S^*)_{z_0^*}]^{-1/2}(2\pi i \mathrm{Res}_{\omega=z_0^*})(\tilde{\Phi}_{\omega\omega'}| \\
|\Psi_{\omega 0}) &= ||(\omega + i0)^+\rangle\langle\tilde{f}_0|) \\
(\tilde{\Psi}_{\omega 0}| &= [-2\pi i(\mathrm{Res}\ S)_{z_0}]^{-1/2}(-2\pi i \mathrm{Res}_{\omega'=z_0})(\tilde{\Phi}_{\omega\omega'}| \\
|\Psi_{\omega\omega'}) &= ||(\omega + i0)^+\rangle\langle(\omega' - i0)^+|) \\
(\tilde{\Psi}_{\omega\omega'}| &= (|(\omega + i0)^+\rangle\langle(\omega' - i0)^+||
\end{aligned} \tag{54}$$

From these equations it is easy to prove that $(\tilde{\Psi}_{00}|$, $(\tilde{\Psi}_{0\omega'}|$, $(\tilde{\Psi}_{\omega 0}|$, and $(\tilde{\Psi}_{\omega\omega'}|$ have no energy or "trace," i.e.,

$$(\tilde{\Psi}_{00}|H) = (\tilde{\Psi}_{0\omega'}|H) = (\tilde{\Psi}_{\omega 0}|H) = (\tilde{\Psi}_{\omega\omega'}|H) = 0$$
$$(\tilde{\Psi}_{00}|I) = (\tilde{\Psi}_{0\omega'}|I) = (\tilde{\Psi}_{\omega 0}|I) = (\tilde{\Psi}_{\omega\omega'}|I) = 0$$

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

5. 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 classes of states are not representable by wave functions or by trace class density operators.

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 ($\rho_\infty = P\rho_\infty$), which is a mixture of generalized eigenvectors of the free Hamiltonian H_0:

$$\rho_\infty = \lim_{t\to\infty} \rho_t = \int d\bar{k}\, (\rho_o \| \bar{k}^+\rangle \langle \bar{k}^+ |)(\bar{k}| \tag{55}$$

$$(\bar{k}|\bar{k}') = \delta(\bar{k} - \bar{k}'), \qquad |\bar{k}) = |\bar{k}\rangle\langle\bar{k}|, \qquad H_0|\bar{k}\rangle = |\bar{k}\rangle$$

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

The final state depends 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

$$\rho = \int d\bar{p}\, \rho^*_{\bar{p}}(\bar{p}| + \int\int d\bar{p}d\bar{p}'\, \rho^*_{\bar{p}\bar{p}'}(\bar{p}\bar{p}|$$

$$T\rho = \int d\bar{p}\, \rho_{-\bar{p}}(\bar{p}| + \int\int d\bar{p}d\bar{p}'\, \rho_{-\bar{p}-\bar{p}'}(\bar{p}\bar{p}'|$$

and a "weak intrinsic irreversibility" appears: as

$$T\rho_\infty = \int d\bar{k}(\rho_o \| -\bar{k}^+\rangle\langle -\bar{k}^+ |)^*(\bar{k}|$$

and

$$U_t T\rho_\infty = e^{-iL_t}T\rho_\infty = T\rho_\infty$$

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 Lippmann–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 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 Gamow 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 "Gamow states" expand the time-dependent part of the physical states, which goes to zero for infinite time. Therefore, in this formalism, the "Gamow 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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