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Generalized Complex Spectral Decomposition for a Quantum Decay Process

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By extending the notion of mixed states to functionals acting on the space of observables with diagonal singularity we obtain a well-defined complex spectral decomposition of the time evolution for a quantum decaying system. In this formalism, generalized Gamow states are obtained with well-defined physical properties.

KEY WORDS: complex spectral decomposition; quantum decay.

1. INTRODUCTION

In recent years, we applied functional analysis technics for the treatment of quantum systems with continuous spectrum. We considered the scattering problem and its intrinsic irreversibility (Laura, 1997), the approach to statistical equilibrium of a quantum oscillator in a thermalized field (Laura and Castagnino, 1998a), and the possibility to define norm and energy of a Gamow vector related to simple poles of the resolvent (Castagnino *et al.*, 2001a,b; Castagnino and Laura, 1997; Gadella and Laura, 2001). We also used a generalized quantum formalism suitable for the case in which the relevant quantum observables include *diagonal singularities* in the energy representation, i.e., observables represented by operators with matrix elements of the form $\langle\omega|O|\omega'\rangle = O_\omega\delta(\omega-\omega') + O_{\omega\omega'}$ (Antoniou *et al.*, 1997; Laura and Castagnino, 1998b). This formalism was developed by Antoniou and Suchanecki (1994, 1995). The need of generalized vector spaces for the description of quantum systems with continuous spectrum was emphasized by Bohm (1986, 1989, 1995) and Bohm and Gadella (1989). The identity and the Hamiltonian operators are examples of observables with diagonal singularities in the energy representation. The quantum states of this formalism are functionals over the space $\mathcal{O}$ of operators representing observables. Mathematically, this means that the space $\mathcal{S}$ of states is contained in the dual space $\mathcal{O}^\times$. Physically, it means that the only

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thing that 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 approach is a generalization of the usual $\mathrm{Tr}(\hat{\rho}\hat{O})$, which is ill defined in systems with continuous spectrum. For this formalism we developed a perturbative method to compute the generalized eigenoperators and eigenstates of the Liouville–von Neumann superoperator (Laura *et al.*, 1999). This formalism was also applied to the problem of decoherence (Castagnino and Laura, 2000).

In this paper, we analyze the generalized spectral decompositions for the time evolution of the mean value of an observable having diagonal singularity, for the case of a quantum system with a Hamiltonian having continuous spectrum and a simple pole in the analytic extension of the resolvent, a prototype model for a decay process.

In Section 2 we discuss the complex spectral decomposition of the Hamiltonian which include Gamow vectors. In Section 3 we show that this spectral decomposition cannot be used to compute mean values of observables represented by operators with diagonal singularity. Generalized states and observables already presented in Antoniou *et al.* (1997) and Laura and Castagnino (1998b) are briefly reviewed in Section 4. Sections 5 and 6 are concerned with the real and complex spectral decompositions of the Liouville–von Neumann superoperator. Generalized Gamow states are obtained in Section 6.

2. PURE STATES AND GAMOW VECTORS

Let us consider a Hamiltonian H_0 with continuous spectrum $\mathbb{R}^+ = [0, \infty)$. We represent by $|\omega\rangle(\langle\omega|)$ the right (left) eigenvector of H_0 with eigenvalue ω

$$H_0|\omega\rangle = \omega|\omega\rangle, \quad \langle\omega|H_0 = \omega\langle\omega|, \quad 0 \leq \omega < \infty. \tag{1}$$

We *assume* that the right and left eigenvectors form an orthogonal complete system, i.e.

$$I = \int_0^\infty d\omega|\omega\rangle\langle\omega|, \quad \langle\omega|\omega'\rangle = \delta(\omega - \omega'), \quad H_0 = \int d\omega\, \omega|\omega\rangle\langle\omega|, \tag{2}$$

where I is the identity operator. The eigenvectors of H_0 form the basis of what we will call the "H_0 representation" of the quantum system.

The full Hamiltonian H of the interacting system will be

$$H = H_0 + V = \int d\omega\, \omega|\omega\rangle\langle\omega| + \int d\omega \int d\omega'\, V_{\omega\omega'}|\omega\rangle\langle\omega'|, \tag{3}$$

where $V_{\omega\omega'} = \langle\omega|V|\omega'\rangle$ is a regular function of the variables ω and ω'.

Since the time evolution of the system is determined by the Hamiltonian H, it is convenient to change to a representation in terms of the eigenvectors of H (the "H representation"). For each eigenvector $|\omega\rangle$ of the Hamiltonian H_0 there is an eigenvector $|\omega^+\rangle$ of the Hamiltonian H, given by the Lippmann–Schwinger equation

$$|\omega^+\rangle = |\omega\rangle + \frac{1}{\omega + i0 - H} V|\omega\rangle. \tag{4}$$

We also assume that the vectors $|\omega^+\rangle$ generate a complete orthonormal system

$$I = \int d\omega |\omega^+\rangle\langle\omega^+|, \quad \langle\omega^+|\omega'^+\rangle = \delta(\omega - \omega'), \quad H = \int d\omega\, \omega |\omega^+\rangle\langle\omega^+|. \tag{5}$$

The probability for an initially pure state $|\varphi\rangle$ to be in the pure state $|\psi\rangle$ at the time t is

$$P(t) = |A(t)|^2,$$
$$A(t) = \langle\psi|\exp(-iHt)|\varphi\rangle = \int_0^\infty d\omega' \exp(-i\omega' t)\langle\psi|\omega'^+\rangle\langle\omega'^+|\varphi\rangle. \tag{6}$$

Let us assume that the analytic extension to the lower complex half plane ($\mathbb{C}^-$) of the integrand in $A(t)$ has a simple pole at $z = z_0$ in the lower complex half plane, very close to the positive real axis. In this case the integral in Eq. (6) may have a dominant contribution from the values of ω' close to $\omega_0 \equiv \Re(z_0)$. To describe these resonant effects, it is convenient to deform the domain of integration for $\omega' \in \mathbb{R}^+$ to a convenient curve in the complex plane. To perform this deformation, we need the analytic extensions $|z\rangle$, $\langle\tilde{z}|$, $|z^+\rangle$, and $\langle\tilde{z}^+|$, of the corresponding eigenvectors $|\omega\rangle$, $\langle\omega|$, $|\omega^+\rangle$, and $\langle\omega^+|$. All these objects are *functionals* acting over the usual wave vectors. That is, if $\varphi : \mathbb{R}^+ \to \mathbb{C}$ is a wave function in the H_0 representation, the "bra" $\langle\omega|$ is a *linear functional* whose action on φ is defined by

$$\langle\omega|\varphi\rangle \equiv \varphi(\omega).$$

Since our objects will be mainly complex, we must extend the functionals to the complex plane. In the domain of the complex plane for which the analytic extension of the function φ is well behaved, we define the linear functional $\langle\tilde{z}|$ trough the equation

$$\langle\tilde{z}|\varphi\rangle \equiv \varphi(z), \tag{7}$$

i.e. the functional $\langle\tilde{z}|$ acting on the function $\varphi : \mathbb{R}^+ \to \mathbb{C}$ gives the value of the analytic extension of the function φ at the point z of the complex plane.

Analogously, if $\psi : \mathbb{R}^+ \to \mathbb{C}$ is ‘a wave function in the H_0 representation, the "ket" $|\omega\rangle$ is an *antilinear functional* defined by

$$\langle\psi|\omega\rangle \equiv \bar{\psi}(\omega),$$

where the function $\bar{\psi} : \mathbb{R}^+ \to \mathbb{C}$ is defined by $\bar{\psi}(\omega) \equiv \overline{\psi(\omega)}$. In the domain of the complex plane for which the analytic extension of the function $\bar{\psi}$ is well defined, we define the antilinear functional $|z\rangle$ through the relation

$$\langle\psi|z\rangle \equiv \bar{\psi}(z) = \overline{\psi(\bar{z})}, \tag{8}$$

i.e. the functional $|z\rangle$, acting on the function $\psi : \mathbb{R}^+ \to \mathbb{C}$ gives the value of the analytic extension of the function $\bar{\psi}$ at the point z of the complex plane.

It is easy to prove that the functionals $\langle z|$ and $|\tilde{z}\rangle$, defined by the usual relations $\langle z|\varphi\rangle \equiv \overline{\langle\varphi|z\rangle}$ and $\langle\varphi|\tilde{z}\rangle \equiv \overline{\langle\tilde{z}|\varphi\rangle}$, verify $\langle z| = \langle\tilde{\bar{z}}|$ and $|\tilde{z}\rangle = |\bar{z}\rangle$. From these results it follows that $\langle\tilde{z}| = \langle\bar{z}| \neq \langle z|$, i.e. if z is a complex number then $\langle\tilde{z}|$ is not the adjoin of $|z\rangle$. This property justifies the use of a tilde ($\sim$) in the definition given in Eq. (7), which would not be necessary for real values $z = \omega \in \mathbb{R}^+$, where $\langle\tilde{\omega} = \langle\bar{\omega} = \langle\omega|$.

The functionals defined in Eqs. (7) and (8) are generalized left and right eigenvalues of the Hamiltonian H_0 with complex eigenvalues:

$$\langle\tilde{z}|H_0 = z\langle\tilde{z}|, \quad H_0|z\rangle = z|z\rangle.$$

According to Eq. (4) it is

$$|\omega^+\rangle = |\omega\rangle + R(\omega + i0)V|\omega\rangle, \quad \langle\omega^+| = \langle\omega| + \langle\omega|VR(\omega - i0), \tag{9}$$

where the resolvent $R(z) \equiv (z - H)^{-1}$ is an analytic function of the complex variable z, except for a cut in $\mathbb{R}^+$. Therefore the analytic extensions of $|\omega^+\rangle$ and $\langle\omega^+|$ involve the analytic extension of the resolvent. We define the analytic extension $R^+(z)(R^-(z))$ of the resolvent $R(z)$ from the upper (lower) to the lower (upper) complex half plane as[3]

$$R^+(z) \equiv \begin{cases} R(z), & z \in \mathbb{C}^+ \\ \\ \mathrm{cont}_{s\in\mathbb{C}^+\to z} R(s), & z \in \mathbb{C}^- \end{cases},$$

$$R^-(z) \equiv \begin{cases} \mathrm{cont}_{s\in\mathbb{C}^-\to z} R(s), & z \in \mathbb{C}^+ \\ \\ R(z), & z \in \mathbb{C}^- \end{cases}. \tag{10}$$

With these definitions the analytic extensions of $|\omega^+\rangle$ and $\langle\omega^+|$ are

$$|z^+\rangle \equiv |z\rangle + R^+(z)V|z\rangle, \quad \langle\tilde{z}^+| \equiv \langle\tilde{z}| + \langle\tilde{z}|VR^-(z). \tag{11}$$

It can be proved that the "adjoint functionals" $\langle z^+|$ and $|\tilde{z}^+\rangle$, defined by the relations $\langle z^+|\varphi\rangle \equiv \overline{\langle\varphi|z^+\rangle}$ and $\langle\varphi|\tilde{z}^+\rangle \equiv \overline{\langle\tilde{z}^+|\varphi\rangle}$, satisfy $\langle z^+| = \langle\tilde{\bar{z}}^+|$ and $|\tilde{z}^+\rangle = |\bar{z}^+\rangle$.

[3] We use the notation $\mathrm{cont}_{s\in\mathbb{C}^+\to z}$ to indicate the analytic continuation of a function defined at a point s of the upper plane, to a point z that may be in the lower plane. The analytic extension of an operator depending on a complex variable z should always be understood in the weak sense. For example $\langle\varphi|\mathrm{cont}_{s\in\mathbb{C}^+\to z} R(s)|\psi\rangle \equiv \mathrm{cont}_{s\in\mathbb{C}^+\to z}\langle\varphi|R(s)|\psi\rangle$ where φ and ψ are suitable test functions.

For simplicity *we assume* that $R^+(z)$ has a single simple pole at $z = z_0$ in the lower complex half plane, and therefore $R^-(z)$ has a simple pole at $z = \bar{z}_0$ in the upper complex half plane. Correspondingly, $|z^+\rangle$ has a pole at z_0 and $\langle\tilde{z}^+|$ has a pole at $\bar{z}_0$.

Gamow vectors are usually defined through a contour deformation (Bohm, 1986; Bohm and Cadella, 1989). Going back to Eq. (6), we can deform the integral path over $\mathbb{R}^+$ corresponding to the variable ω' into an integral over a curve Γ in the lower complex half plane plus an integral over a closed contour surrounding clockwise the pole at z_0. Therefore, the amplitude to find the state $\varphi(t)$ in the state ψ becomes

$$\begin{aligned} A(t) &= \langle\psi|\exp(-iHt)|\varphi\rangle \\ &= \oint_C dz' \exp(-iz't)\langle\psi|z'^+\rangle\langle\tilde{z}'^+|\varphi\rangle + \int_\Gamma dz' \exp(-iz't)\langle\psi|z'^+\rangle\langle\tilde{z}'^+|\varphi\rangle, \end{aligned}$$

or equivalently

$$\begin{aligned} A(t) &= \langle\psi|\exp(-iHt)|\varphi\rangle \\ &= \exp(-iz_0t)\langle\psi|f_0\rangle\langle\tilde{f}_0|\varphi\rangle + \int_\Gamma dz' \exp(-iz't)\langle\psi|f_{z'}\rangle\langle\tilde{f}_{z'}|\varphi\rangle, \end{aligned} \tag{12}$$

where

$$\begin{aligned} \langle\tilde{f}_0|\varphi\rangle &\equiv \text{cont}_{\omega'\to z_0}\langle\omega'^+|\varphi\rangle, \\ \langle\psi|f_0\rangle &\equiv (-2\pi i)\text{cont}_{\omega'\to z_0}(\omega' - z_0)\langle\psi|\omega'^+\rangle, \\ \langle\tilde{f}_{z'}|\varphi\rangle &\equiv \text{cont}_{\omega'\to z'}\langle\omega'^+|\varphi\rangle, \\ \langle\psi|f_{z'}\rangle &\equiv \text{cont}_{\omega'\to z'}\langle\psi|\omega'^+\rangle, \quad z' \in \Gamma. \end{aligned} \tag{13}$$

The complex conjugate amplitude is given by

$$\begin{aligned} \overline{A(t)} &= \langle\varphi|\exp(iHt)|\varphi\rangle \\ &= \exp(i\bar{z}_0t)\langle\varphi|\tilde{f}_0\rangle\langle f_0|\psi\rangle + \int_{\bar{\Gamma}} dz\ \exp(+izt)\langle\varphi|\tilde{f}_z\rangle\langle f_z|\psi\rangle, \end{aligned} \tag{14}$$

where

$$\begin{aligned} \langle\varphi|\tilde{f}_0\rangle &\equiv \text{cont}_{\omega\to\bar{z}_0}\langle\varphi|\omega'^+\rangle, \\ \langle f_0|\psi\rangle &\equiv (+2\pi i)\text{cont}_{\omega\to\bar{z}_0}(\omega - \bar{z}_0)\langle\omega^+|\psi\rangle, \\ \langle\varphi|\tilde{f}_z|\rangle &\equiv \text{cont}_{\omega\to z}\langle\varphi|\omega^+\rangle, \\ \langle f_z|\psi\rangle &\equiv \text{cont}_{\omega\to z}\langle\omega^+|\psi\rangle, \quad z \in \bar{\Gamma}. \end{aligned} \tag{15}$$

It is easy to show that the functionals defined in Eqs. (13) and (15) are generalized eigenvectors of the Hamiltonian with complex eigenvalues, i.e.

$$
\begin{aligned}
&\langle \tilde{f}_0|H = z_0\langle \tilde{f}_0|, \quad H|f_0\rangle = z_0|f_0\rangle,\\
&\langle \tilde{f}_{z'}|H = z'\langle \tilde{f}_{z'}|, \quad H|f_{z'}\rangle = z'|f_{z'}\rangle, \quad z' \in \Gamma.\\
&H|\tilde{f}_0\rangle = \overline{z}_0|\tilde{f}_0\rangle, \quad \langle f_0|H = \overline{z}_0\langle f_0|,\\
&H|\tilde{f}_z\rangle = z|\tilde{f}_z\rangle, \quad \langle f_z|H = z\langle f_z|, \quad z \in \overline{\Gamma}.
\end{aligned} \tag{16}
$$

Moreover, for vectors ψ and φ with "H_0 representations" for which the functions $\overline{\psi}(\omega)$ and $\varphi(\omega)$ have well-defined analytic extensions to the lower complex half plane, we can write

$$
\langle\psi|\varphi\rangle = \langle\psi|f_0\rangle\langle\tilde{f}_0|\varphi\rangle + \int_\Gamma dz\langle\psi|f_z\rangle\langle\tilde{f}_z|\varphi\rangle = \langle\psi|I_{\text{ext}}|\varphi\rangle,
$$

$$
I_{\text{ext}} \equiv |f_0\rangle\langle\tilde{f}_0| + \int_\Gamma dz|f_z\rangle\langle\tilde{f}_z|.
$$

The generalized eigenvectors of H with the eigenvalues z_0 and $\overline{z}_0$, associated with the simple poles of the analytic extensions of the resolvent to the lower and the upper complex half plane, are usually called "Gamow vectors." From their definition we see that they are antilinear functionals.

It is important to note that while the amplitude $A(t)$ above is well defined, the Gamow vectors diverge for growing values of the coordinates. For instance, in the case of a one-dimensional problem in $\mathbb{R}^+$ where the potential V has compact support, in coordinate representation one obtains

$$
\langle x|f_0\rangle \sim \exp(+i\sqrt{z_0}x), \quad \langle\tilde{f}_0|x\rangle \sim \exp(+i\sqrt{z_0}x), \tag{17}
$$

i.e. an oscillating function modulated by a growing exponential. Therefore, if one attempts to define the "norm" of the functional $|f_0\rangle$ by $\langle f_0|f_0\rangle \equiv \int_0^\infty dx\langle f_0|x\rangle\langle x|f_0\rangle$, the exponentially growing integrand would give an infinite value. The "matrix element" $\langle f_0|H|f_0\rangle$ is also divergent and the internal product $\langle\tilde{f}_0|f_0\rangle$ is not defined due to the oscillatory and diverging terms. These quantities are mathematically ill defined because they are "functionals acting on functionals." Expressions like $\langle\psi|f_0\rangle$ or $\langle f_0|\varphi\rangle$ are generally well defined, at least for well-behaved "test vectors" φ and ψ. For these test vectors, Eq. (12) gives a well-defined complex spectral decomposition of the transition amplitude $A(t)$. The survival amplitude can be obtained from Eq. (12) with $\varphi = \psi$. Moreover, if $\Im z_0 \ll \Re z_0$, it can be proved that for intermediate values of the time, the complex eigenvalue z_0 gives the main contribution to the survival probability of a pure state (Khalfin, 1958), i.e. $|\langle\varphi|\exp(-iHt)|\varphi\rangle|^2 \cong \exp(-\Gamma t)$ where $\Gamma \equiv 2|\Im z_0|$.

3. MIXED STATES AND GAMOW VECTORS

In the previous section, we considered the usual definition of Gamow vectors as functionals acting on wave vectors. We saw the problems to define the norm and the energy of those vectors. Here we will proceed with an attempt to use Gamow states to describe density operators.

If we represent the initial pure state by the density operator $\rho_0 \equiv |\varphi\rangle\langle\varphi|$, the time dependent density operator is $\rho_t = \exp(-iHt)\rho_0 \exp(+iHt)$. Analogously, if we define the projector $\Pi_\psi = |\psi\rangle\langle\psi|$, the probability $P(t)$ given in Eq. (6) can also be obtained as

$$P(t) = \mathrm{Tr}(\rho_t \Pi_\psi), \tag{18}$$

and therefore using the same techniques as in the previous section we obtain

$$\begin{aligned} P(t) &= \mathrm{Tr}(\rho_t \Pi_\psi) = \langle\varphi| \exp(+iHt)|\psi\rangle\langle\psi| \exp(-iHt)|\varphi\rangle \\ &= \exp[i(\bar{z}_0 - z_0)t]\langle\varphi|\tilde{f}_0\rangle\langle f_0|\psi\rangle\langle\psi|f_0\rangle\langle\tilde{f}_0|\varphi\rangle \\ &\quad + \int_\Gamma dz' \exp[i(\bar{z}_0 - z')t]\langle\varphi|\tilde{f}_0\rangle\langle f_0|\psi\rangle\langle\psi|f_{z'}\rangle\langle\tilde{f}_{z'}|\varphi\rangle \\ &\quad + \int_{\bar{\Gamma}} dz \exp[i(z - z_0)t]\langle\varphi|\tilde{f}_z\rangle\langle f_z|\psi\rangle\langle\psi|f_0\rangle\langle\tilde{f}_0|\varphi\rangle \\ &\quad + \int_{\bar{\Gamma}} dz \int_\Gamma dz' \exp[i(z - z')t]\langle\varphi|\tilde{f}_z\rangle\langle f_z|\psi\rangle\langle\psi|f_{z'}\rangle\langle\tilde{f}_{z'}|\varphi\rangle. \end{aligned} \tag{19}$$

One is tempted to generalize to more general cases the expression given in Eq. (19), *which is valid to compute transition probabilities between normalized pure states*. For example, in the one-dimensional problem, we may try to compute the probability to find the particle at a distance greater than R at a time t (this is equivalent to have detected the particle passing the point R before the time t). To compute this probability using Gamow vectors, we may try to replace in Eqs. (18) and (19) the projector $\Pi_\psi = |\psi\rangle\langle\psi|$ by the projector $\Pi_{[R,\infty)} \equiv \int_R^\infty dx|x\rangle\langle x|$ onto a set of states localized at a distance greater than R, e.g. outside the potential barrier which produces the resonance. But then we find new problems: divergent terms appear. For instance $\langle f_0|\Pi_{[R,\infty)}|f_0\rangle = \int_R^\infty dx\langle f_0|x\rangle\langle x|f_0\rangle = \infty$, due to the exponentially growing factor $\langle f_0|x\rangle\langle x|f_0\rangle \sim \exp(+i[\sqrt{\bar{z}_0} - \sqrt{z_0}]x)$. The same kind of troubles appear if one tries to compute the conserved total probability $\mathrm{Tr}(\rho_t) = \mathrm{Tr}(\rho_t I) = 1$ by replacing the projector Π_ψ by $I = \int_0^\infty dx|x\rangle\langle x|$ in Eq. (19).

We thus realize that the use of Gamow vectors to compute the time evolution of mean values for observables which are not the simple projection onto a normalizable pure state, cannot be the straightforward generalization of Eq. (19). This implies that if one wants to include resonances in the time evolution of observables, a different approach is needed. In the rest of this paper we will use a suitable formalism, already introduced in Antoniou *et al.* (1997) and Laura and Castagnino (1998b), to deal with general observables and to compute their time evolution using complex eigenvalues. We will also give a precise meaning to the energy and probability of the "generalized Gamow states."

4. GENERALIZED STATES AND OBSERVABLES

The expressions given in Eqs. (2) and (3) for the operators I, H_0, and H, suggest that it is necessary to consider a general form for the self-adjoint operators representing observables of the system, namely

$$O = \int d\omega\, O_\omega |\omega\rangle\langle\omega| + \int d\omega \int d\omega'\, O_{\omega\omega'} |\omega\rangle\langle\omega'|, \tag{20}$$

where $O_\omega = \overline{O}_\omega$ and $O_{\omega\omega'} = \overline{O}_{\omega'\omega}$. The first term in this equation can be written as $\int d\omega \int d\omega' O_\omega \delta(\omega - \omega')|\omega\rangle\langle\omega'|$. Since it contains a Dirac delta, we will call it the *singular term*. The second term has no singularity because $O_{\omega\omega'}$ is a regular function, and therefore we call this the regular term.

Let $|\psi_a\rangle$ be a pure state vector and p_a the probability of the quantum system to be in this pure state ($a = 1, 2, \ldots, \Sigma_a p_a = 1, \langle\psi_a|\psi_a\rangle = 1$). In this case, the state of the system can be represented by the density operator

$$\rho \equiv \sum_a p_a |\psi_a\rangle\langle\psi_a|. \tag{21}$$

The mean value of an observable represented by an operator O of the form given in Eq. (20) is

$$\langle O\rangle_\rho = \mathrm{Tr}(\rho O) = \int d\omega \left[\sum_a p_a \langle\omega|\psi_a\rangle\langle\psi_a|\omega\rangle\right] O_\omega + \int d\omega \int d\omega' \left[\sum_a p_a \langle\omega'|\psi_a\rangle\langle\psi_a|\omega\rangle\right] O_{\omega\omega'}.$$

Defining

$$\rho_\omega \equiv \sum_a p_a \langle\omega|\psi_a\rangle\langle\psi_a|\omega\rangle, \qquad \rho_{\omega\omega'} \equiv \sum_a p_a \langle\omega'|\psi_a\rangle\langle\psi_a|\omega\rangle,$$

the mean value of the operator O can be written in the compact form

$$\langle O\rangle_\rho = \int d\omega\, \rho_\omega O_\omega + \int d\omega \int d\omega'\, \rho_{\omega\omega'} O_{\omega\omega'}. \tag{22}$$

From a more general point of view, ρ_ω and $\rho_{\omega\omega'}$ can be considered as the "components" of a *linear functional* $(\rho|$, *acting on the observable* $|O)$ which is defined by its own "components" O_ω and $O_{\omega\omega'}$. The action of the state functional on the observable provides the mean value $\langle O\rangle_\rho = (\rho|O)$. In this approach, it is convenient to *define* the "generalized observables"

$$|\omega) \equiv |\omega\rangle\langle\omega|, \quad |\omega\omega') \equiv |\omega\rangle\langle\omega'|. \tag{23}$$

in such a way that the observable O can be written as

$$|O) \equiv O = \int d\omega\, O_\omega|\omega) + \int d\omega \int d\omega'\, O_{\omega\omega'}|\omega\omega'). \tag{24}$$

Therefore $(|\omega), |\omega,\omega'))$ is the basis of the space $\mathcal{O}$ of the observables with diagonal singularity. It is also useful to *define* the generalized states $(\tilde{\omega}|$ and $(\widetilde{\omega\omega'}|$ satisfying the relations

$$(\tilde{\omega}|O) \equiv O_\omega, \quad (\widetilde{\omega\omega'}|O) \equiv O_{\omega\omega'}. \tag{25}$$

It should be emphasized that according to these definitions, $(\tilde{\omega}|O) \neq \langle\omega|O|\omega\rangle$ and $(\widetilde{\omega\omega'}|O) \neq \langle\omega|O|\omega'\rangle$. Moreover, using Eq. (20) we obtain $\langle\omega|O|\omega'\rangle = O_\omega\,\delta(\omega-\omega') + O_{\omega\omega'}$, and therefore $\langle\omega|O|\omega\rangle$ is not even defined. Using the generalized states defined in Eq. (25), the state functional reads

$$(\rho| = \int d\omega\, \rho_\omega(\tilde{\omega}| + \int d\omega \int d\omega'\, \rho_{\omega\omega')}\,(\widetilde{\omega\omega'}|. \tag{26}$$

The "states" $((\tilde{\omega}|, (\widetilde{\omega,\omega'}|)$ form a basis for the dual of the observable space, namely the state space.

The generalized states $(\tilde{\omega}|, (\widetilde{\omega,\omega'}|$ and observables $|\omega), |\omega\omega')$ form a complete biorthonormal system to describe observables and states of the form given in Eqs. (24) and (26). It is straightforward to verify the orthogonality and completeness conditions

$$(\tilde{\omega}|\omega') = \delta(\omega-\omega'),\ (\widetilde{\omega\omega'}|\varepsilon\varepsilon') = \delta(\omega-\varepsilon)\delta(\omega'-\varepsilon'),\ (\tilde{\omega}|\varepsilon\varepsilon') = (\widetilde{\omega\omega'}|\varepsilon) = 0, \tag{27}$$

$$(\rho|\mathbb{I} = (\rho|O) = (\rho|\mathbb{I}|O),\ \mathbb{I} \equiv \int d\omega|\omega)(\tilde{\omega}| + \int d\omega \int d\omega'|\omega\omega')(\widetilde{\omega\omega'}|, \tag{28}$$

where $\mathbb{I}$ is the *identity superoperator* (not to be confused with the identity operator $I = \int d\omega|\omega\rangle\langle\omega|$).

Up to this point, we have only presented an alternative mathematical framework for the description of states that can be also described in terms of the well-known density operator given in Eq. (21). However, we will show in what follows that the spectral decomposition of the time evolution of a quantum system with continuous spectrum includes generalized states which are functionals, and which can not be described by the usual density operators. The well-known conditions $\mathrm{Tr}\rho = 1$ and $\rho^\dagger = \rho$ for the density operator, must be replaced in this formalism by the conditions of *total probability* and *reality* on the state functionals (see

Antoniou *et al.*, 1997; Laura and Castagnino, 1998b, for details)

$$(\rho|I) = 1, \quad (\rho|O^{\dagger}) = \overline{(\rho|O)}.$$

From these two conditions one obtains that the components of the states should satisfy $\int d\omega\, \rho_\omega = 1$, $\rho_\omega = \overline{\rho_\omega}$, and $\rho_{\omega'\omega} = \overline{\rho_{\omega\omega'}}$. The *positivity* condition remains the usual one, i.e. $\rho_\omega = \overline{\rho_\omega} \geq 0$.

The time evolution of the state functionals is obtained from the equation

$$\begin{aligned}(\rho_t|O) \equiv (\rho_0|O_t) &= (\rho_0|\exp(+iHt)O\ \exp(-iHt)) \\ &= (\rho_0|\exp(+i\mathbb{L}t)O), \quad \mathbb{L}O \equiv [H, O],\end{aligned} \tag{29}$$

relating Schrödinger and Heisenberg representations.

The basis given in Eqs. (23) and (25) can be used to represent the Liouville–von Neuman superoperators corresponding to the Hamiltonians H_0 and H. We easily obtain

$$\mathbb{L}_0 \equiv [H_0,\ \ ] = \int d\omega \int d\omega'(\omega - \omega')|\omega\omega')(\widetilde{\omega\omega'}|.$$

From this expression we conclude that the basis of Eqs. (23) and (25) are generalized eigenvectors of $\mathbb{L}_0$:

$$\mathbb{L}_0|\omega\omega') = (\omega - \omega')|\omega\omega'), \quad (\widetilde{\omega\omega'}|\mathbb{L}_0 = (\widetilde{\omega\omega'}|(\omega - \omega'),$$
$$\mathbb{L}_0|\omega) = 0, \quad (\tilde{\omega}|\mathbb{L}_0 = 0.$$

There is a more complicated expression for the superoperator $\mathbb{L}$.

$$\begin{aligned}\mathbb{L} \equiv [H,\ \ ] &= \int d\omega \int d\omega'(\omega - \omega')|\omega\omega')(\widetilde{\omega\omega'}| \\ &+ \int d\omega \int d\omega'|\omega\omega')\{V_{\omega\omega'}[(\tilde{\omega}'| - (\tilde{\omega}|] \\ &+ \int d\omega''[V_{\omega\omega''}(\widetilde{\omega''\omega'}| - V_{\omega''\omega'}(\widetilde{\omega\omega''}|]\}.\end{aligned}$$

In the next section we will construct a basis of generalized left and right eigenvectors of $\mathbb{L}$.

5. GENERALIZED REAL SPECTRAL DECOMPOSITION OF THE TIME EVOLUTION

If we compute the matrix elements of an operator O of the form given in Eq. (20) in the H_0 representation, we obtain $\langle\omega|O|\omega'\rangle = \delta(\omega - \omega')O_\omega + O_{\omega\omega'}$ (where the singular and the regular term appear naturally). If one uses the H representation, the matrix element $\langle\omega^+|O|\omega'^+\rangle$ also include the singular term

$\delta(\omega-\omega')O_\omega$, and therefore there is a term of the form $\int d\omega\, O_\omega|\omega^+\rangle\langle\omega^+|$ in the operator O. This term is time independent in the Heisenberg representation.

Since Gamow vectors are exponentially decaying states they cannot be contained in the time-independent term. We, therefore, separate the time-independent from the time-dependent part of the observables, hoping to find the generalized Gamow states in the time-dependent part. To do this we define the invariant and the noninvariant or "fluctuating" parts of O as follows

$$O_{\text{inv}} \equiv \int d\omega\, O_\omega|\omega^+\rangle\langle\omega^+|, \qquad O_{\text{fluc}} \equiv O - O_{\text{inv}}. \tag{30}$$

The matrix elements of O_{fluc} are

$$\begin{aligned}\langle\omega^+|O_{\text{fluc}}|\omega'^+\rangle &= \int d\varepsilon[\langle\omega^+|\varepsilon\rangle\langle\varepsilon|\omega'^+\rangle - \delta(\omega-\varepsilon)\,\delta(\varepsilon-\omega')]\,(\tilde{\varepsilon}|O)\\ &\quad + \int d\varepsilon\int d\varepsilon'\,\langle\omega^+|\varepsilon\rangle\langle\varepsilon'|\omega'^+\rangle\,(\varepsilon\varepsilon'|O).\end{aligned} \tag{31}$$

The time-dependent contribution to the mean value is given by the fluctuating part since it is

$$\begin{aligned}\langle O\rangle_t &= (\rho_0|e^{+iHt}Oe^{-iHt})\\ &= (\rho_0|O_{\text{inv}}) + (\rho_0|e^{+iHt}O_{\text{fluc}}e^{-iHt}) = \int d\omega(\rho_0||\omega^+\rangle\langle\omega^+|)O_\omega\\ &\quad + \int d\omega\int d\omega' e^{i(\omega-\omega')t}(\rho_0||\omega^+\rangle\langle\omega'^+|)\langle\omega^+|O_{\text{fluc}}|\omega'^+\rangle.\end{aligned} \tag{32}$$

Let us define the following *generalized* states and observables

$$\begin{aligned}|\Phi_\omega) &\equiv |\omega^+\rangle\langle\omega^+|,\\ (\tilde{\Phi}_\omega| &\equiv (\tilde{\omega}|,\\ |\Phi_{\omega\omega'}) &\equiv |\omega^+\rangle\langle\omega'^+|,\\ (\tilde{\Phi}_{\omega\omega'}| &\equiv \int d\varepsilon[\langle\omega^+|\varepsilon\rangle\langle\varepsilon|\omega'^+\rangle - \delta(\omega-\varepsilon)\delta(\varepsilon-\omega')](\tilde{\varepsilon}|\\ &\quad + \int d\varepsilon\int d\varepsilon'\langle\omega^+|\varepsilon\rangle\langle\varepsilon'|\omega'^+\rangle(\widetilde{\varepsilon\varepsilon'}|.\end{aligned} \tag{33}$$

From Eqs. (30)–(33), one gets the compact form

$$\begin{aligned}\langle O\rangle_t = (\rho_t|O) &= \int d\omega\,(\rho_0|\Phi_\omega)(\tilde{\Phi}_\omega|O)\\ &\quad + \int d\omega\int d\omega' e^{i(\omega-\omega')t}(\rho_0|\Phi_{\omega\omega'})(\tilde{\Phi}_{\omega\omega'}|O).\end{aligned} \tag{34}$$

In the next section we will see that the Gamow vectors are contained in the analytic continuation of the last term.

The generalized states and observables defined in Eq. (33) have interesting properties.

(i) *They form a complete biorthogonal system for observables and states.*

It is easy to use the orthogonality and completeness relations given in Eqs. (27) and (28) to prove that the generalized states and observables just defined by Eq. (33) satisfy

$$(\tilde{\Phi}_{\omega}|\tilde{\Phi}_{\omega'}) = \delta(\omega-\omega'), \quad (\tilde{\Phi}_{\omega\omega'}|\tilde{\Phi}_{\varepsilon\varepsilon'}) = \delta(\omega-\varepsilon)\delta(\omega'-\varepsilon'),$$
$$(\tilde{\Phi}_{\omega}|\tilde{\Phi}_{\varepsilon\varepsilon'}) = (\tilde{\Phi}_{\varepsilon\varepsilon'}|\tilde{\Phi}_{\omega'}) = 0. \tag{35}$$

The identity superoperator $\mathbb{I}$, already defined in Eq. (27), can be written in the form

$$\mathbb{I} = \int d\omega|\Phi_{\omega})(\tilde{\Phi}_{\omega}| + \int d\omega \int d\omega'|\Phi_{\omega\omega'})(\tilde{\Phi}_{\omega\omega'}|. \tag{36}$$

(ii) *They provide the spectral decomposition of the time evolution generator.*

In the Heisenberg representation the time evolution of an observable O of the form given in Eq. (20) is given by $O_t = \exp(+iHt)O\exp(-iHt) = \exp(+i\mathbb{L}t)O$, where $\mathbb{L}$ is the Liouville–von Neumann superoperator, defined by $\mathbb{L}O \equiv HO - OH$. It is

$$\mathbb{L} = \int d\omega \int d\omega'(\omega-\omega')|\Phi_{\omega\omega'})(\tilde{\Phi}_{\omega\omega'}|. \tag{37}$$

Therefore $|\Phi_{\omega})((\tilde{\Phi}_{\omega}|)$ is a right (left) eigenvector of $\mathbb{L}$ with zero eigenvalue, and $|\Phi_{\omega\omega'})((\tilde{\Phi}_{\omega\omega'}|)$ is a right (left) eigenvector of $\mathbb{L}$ with eigenvalue $(\omega-\omega')$. Gamow vectors will be also eigenvectors of $\mathbb{L}$ but with complex eigenvalues.

(iii) *The generalized states $(\tilde{\Phi}_{\omega}|$ and $(\tilde{\Phi}_{\omega\omega'}|$ have well defined physical properties.*

Any state functional can be written as the linear combination

$$(\rho| = (\rho|\mathbb{I} = \int d\omega(\rho|\Phi_{\omega})(\tilde{\Phi}_{\omega}| + \int d\omega \int d\omega'(\rho|\Phi_{\omega\omega'})(\tilde{\Phi}_{\omega\omega'}|,$$

and therefore $(\tilde{\Phi}_{\omega}|$ and $(\tilde{\Phi}_{\omega\omega'}|$ can be considered as a basis of generalized states.

The generalized state $(\tilde{\Phi}_{\omega}|$ satisfies

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

$$(\tilde{\Phi}_\omega|H) = (\tilde{\Phi}_\omega|\left[\int d\omega'\omega'|\omega') + \int d\omega' \int d\omega'' V_{\omega'\omega''}|\omega'\omega'')\right]$$

$$= \int d\omega'\omega'(\tilde{\omega}|\omega'|) + \int d\omega' \int d\omega'' V_{\omega'\omega''}(\tilde{\omega}|\omega'\omega'')$$

$$= \int d\omega'\omega'\delta(\omega - \omega') = \omega.$$

Therefore $(\tilde{\Phi}_\omega|$ verifies the total probability condition $(\tilde{\Phi}_\omega|I) = 1$ (the generalization of the condition $\mathrm{Tr}\rho = 1$ for usual density operators). The mean value of the energy is $\langle H\rangle = \tilde{\Phi}_\omega|H) + \omega$. Moreover, one can show that $\langle H^n\rangle = (\tilde{\Phi}_\omega|H^n) = \omega^n (n = 1, 2, \ldots)$, which implies $\langle(H - \langle H\rangle)^n\rangle = 0$. In summary, the mean value ω of the energy has no dispersion, and one can say that the generalized state $(\tilde{\Phi}_\omega|$ *has* energy ω. It is clear from the definition that this is a generalized state that cannot be represented neither by a normalized wave function nor by a density operator.

The generalized state $(\tilde{\Phi}_{\omega\omega'}|$ satisfies

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

$$= \int d\varepsilon[\langle\omega^+|\varepsilon\rangle\langle\varepsilon|\omega'^+\rangle - \delta(\omega - \varepsilon)\,\delta(\varepsilon - \omega')](\tilde{\varepsilon}| \int d\varepsilon'|\varepsilon')$$

$$= \int d\varepsilon[\langle\omega^+|\varepsilon\rangle\langle\varepsilon|\omega'^+\rangle - \delta(\omega - \varepsilon)\delta(\varepsilon - \omega')]$$

$$= \int d\varepsilon\langle\omega^+|\varepsilon\rangle\langle\varepsilon|\omega'^+\rangle - \int d\varepsilon\,\delta(\omega - \varepsilon)\delta(\varepsilon - \omega')$$

$$= \delta(\omega - \omega') - \delta(\omega - \omega') = 0.$$

$$(\tilde{\Phi}_{\omega\omega'}|H) = \int d\varepsilon[\langle\omega^+|\varepsilon\rangle\langle\varepsilon|\omega'^+\rangle - \delta(\omega - \varepsilon)\delta(\varepsilon - \omega')]\varepsilon$$

$$+ \int d\varepsilon \int d\varepsilon'\langle\omega^+|\varepsilon\rangle\langle\varepsilon'|\omega'^+\rangle V_{\varepsilon\varepsilon'}$$

$$= \langle\omega^+|\left[\int d\varepsilon\,\varepsilon|\varepsilon\rangle\langle\varepsilon|\right.$$

$$\left. + \int d\varepsilon \int d\varepsilon' V_{\varepsilon\varepsilon'}|\varepsilon\rangle\langle\varepsilon'|\right]|\omega'^+\rangle - \delta(\omega - \omega')\omega$$

$$= \langle\omega^+|H|\omega'^+\rangle - \delta(\omega - \omega')\omega = 0.$$

As we obtained $(\tilde{\Phi}_{\omega\omega'}|I) = 0$ and $(\tilde{\Phi}_{\omega\omega'}|H) = 0$, we conclude that this functional cannot represent by itself a physical state, since it has zero probability and zero energy. Gamow vectors will inherit these rigorous mathematical properties as we will see in the next section.

(iv) *For very long times, they provide a suitable representation for the "final" state.*

If $(\rho_0|\Phi_{\omega\omega'})$ and $(\tilde{\Phi}_{\omega\omega'}|O)$ are regular functions of the variables ω and ω', the second factor of the expression given in Eq. (34) for the time-dependent mean value $\langle O\rangle_t$ of the observable tends to vanish for very long times, due to the rapidly oscillating factor $e^{i(\omega-\omega')t}$ inside the double integral. Therefore, we obtain $\lim_{t\to\infty}(\rho_0|O) = \int d\omega(\rho_0|\Phi_\omega)(\tilde{\Phi}_\omega|O)$, or (in the weak sense)

$$(\rho_\infty| \equiv \lim_{t\to\infty}(\rho_t \;= \int d\omega(\rho_0|\Phi_\omega)(\tilde{\Phi}_\omega|.$$

Therefore, the components $(\tilde{\Phi}_{\omega\omega'}|$ of the state are eliminated during the time evolution, and the apparently "unphysical" properties $(\tilde{\Phi}_{\omega\omega'}|H) = 0$ and $(\tilde{\Phi}_{\omega\omega'}|I) = 0$ discussed above, are now found to be essential for energy and probability conservation, i.e.

$$\langle H\rangle = (\rho_0|H) = (\rho_t|H) = (\rho_\infty|H), \quad \langle I\rangle = (\rho_0|I) = (\rho_t|I) = (\rho_\infty|I), = 1.$$

6. GENERALIZED COMPLEX SPECTRAL DECOMPOSITION OF THE TIME EVOLUTION AND GAMOW STATES

We obtained in Eq. (34), the spectral decomposition of the mean value of an observable, i.e.

$$\langle O\rangle_t = (\rho_t|O) = \int_0^\infty d\omega(\rho_0|\Phi_\omega)(\tilde{\Phi}_\omega|O) + \int_0^\infty d\omega \int_0^\infty d\omega'\, e^{i(\omega-\omega')t}(\rho_0|\Phi_{\omega\omega'})(\tilde{\Phi}_{\omega\omega'}|O). \tag{38}$$

We wish to deform the integral over $\mathbb{R}^+$ for the variable $\omega'(\omega)$ into a curve $\Gamma(\overline{\Gamma})$ in the lower (upper) complex half plane. Therefore, we need the following analytic extensions

$$(\rho_0|\Phi_{zz'}) \equiv \text{cont}_{\omega\to z}\text{cont}_{\omega'\to z'}(\rho_0|\Phi_{\omega\omega'}), \tag{39}$$

$$(\tilde{\Phi}_{zz'}|O) \equiv \text{cont}_{\omega\to z}\text{cont}_{\omega'\to z'}(\tilde{\Phi}_{\omega\omega'}|O). \tag{40}$$

If $z \in \mathbb{C}^+$ and $z' \in \mathbb{C}^-$, the definitions of $|\Phi_{\omega\omega'})$ and $(\tilde{\Phi}_{\omega\omega'}|$ given in Eq. (33) enable to prove that $(\rho_0|\Phi_{zz'})$ is analytic and $(\tilde{\Phi}_{zz'}|O)$ has simple poles for $z = \overline{z_0}$ and $z' = z_0$. These are the simple poles of the extensions $R^-(z)$ and $R^+(z)$ of the resolvent, already defined in Eq. (10). It is, therefore, possible to deform the integrals over the real variables ω' and ω into the integrals over the curves Γ and

$\overline{\Gamma}$, plus the contributions of the residues of the simple poles. Finally, the following expression is obtained for the time evolution of the mean value

$$\begin{aligned}(\rho_t|O) = &\int_0^\infty d\omega(\rho_0|\Phi_\omega)(\tilde{\Phi}_\omega|O) \\ &+ e^{i(\overline{z}_0 - z_0)t}(\rho_0|\Phi_{00})(\tilde{\Phi}_{00}|O) \\ &+ \int_\Gamma dz' e^{i(\overline{z}_0 - z')t}(\rho_0|\Phi_{0z'})(\tilde{\Phi}_{0z'}|O) \\ &+ \int_{\overline{\Gamma}} dz\, e^{i(z - z_0)t}(\rho_0|\Phi_{z0})(\tilde{\Phi}_{z0}|O) \\ &+ \int_{\overline{\Gamma}} dz \int_\Gamma dz' e^{i(z - z')t}(\rho_0|\Phi_{zz'})(\tilde{\Phi}_{zz'}|O).\end{aligned} \tag{41}$$

To obtain this last expression, the following functionals were introduced

$$\begin{aligned}(\rho_0|\Phi_{00}) &\equiv \mathrm{cont}_{\omega\to\overline{z}_0}\mathrm{cont}_{\omega'\to z_0}(\rho_0|\Phi_{\omega\omega'}) = (\rho_0||\tilde{f}_0\rangle\langle\tilde{f}_0|), \\ (\tilde{\Phi}_{00}|O) &\equiv \mathrm{cont}_{\omega\to\overline{z}_0}\mathrm{cont}_{\omega'\to z_0}4\pi^2(\omega - \overline{z}_0)(\omega' - z_0)(\tilde{\Phi}_{\omega\omega'}|O) \\ &= \langle f_0|(O - O_{\mathrm{inv}})|f_0\rangle, \\ (\rho_0|\Phi_{0z'}) &\equiv \mathrm{cont}_{\omega\to\overline{z}_0}\mathrm{cont}_{\omega'\to z'}(\rho_0|\Phi_{\omega\omega'}) = (\rho_0||\tilde{f}_0\rangle\langle\tilde{f}_{z'}|), \\ (\tilde{\Phi}_{0z'}|O) &\equiv \mathrm{cont}_{\omega\to\overline{z}_0}\mathrm{cont}_{\omega'\to z'}(2\pi i)(\omega - \overline{z}_0)(\tilde{\Phi}_{\omega\omega'}|O) \\ &= \langle f_0|(O - O_{\mathrm{inv}})|f_{z'}\rangle, \\ (\rho_0|\Phi_{z0}) &\equiv \mathrm{cont}_{\omega\to z}\mathrm{cont}_{\omega'\to z_0}(\rho_0|\Phi_{\omega\omega'}) = (\rho_0||\tilde{f}_z\rangle\langle\tilde{f}_0|), \\ (\tilde{\Phi}_{z0}|O) &\equiv \mathrm{cont}_{\omega\to z}\mathrm{cont}_{\omega'\to z_0}(-2\pi i)(\omega =' -z_0)(\tilde{\Phi}_{\omega\omega'}|O) \\ &= \langle f_z|(O - O_{\mathrm{inv}})|f_0\rangle, \\ (\rho_t|\Phi_{zz'}) &\equiv \mathrm{cont}_{\omega\to z}\mathrm{cont}_{\omega'\to z'}(\rho_0|\Phi_{\omega\omega'}) = (\rho_0||\tilde{f}_z\rangle\langle\tilde{f}_{z'}|), \\ (\tilde{\Phi}_{zz'}|O) &\equiv \mathrm{cont}_{\omega\to z}\mathrm{cont}_{\omega'\to z'}(\tilde{\Phi}_{\omega\omega'}|O) = \langle f_z|(O - O_{\mathrm{inv}})|f_{z'}\rangle.\end{aligned} \tag{42}$$

It is important to notice that in the definitions of these functionals the analytic continuations should be understood in the weak sense, i.e., *the analytic continuations must be performed after the application of the functionals* $|\Phi_{\omega\omega'})$ and $(\tilde{\Phi}_{\omega\omega'}|$, *depending on the real parameters* ω *and* ω', *to suitable test functions* $(\rho|$ and $|O)$. This is clear from the fact that the new spectral decomposition given in Eq. (41) was obtained using the Cauchy theorem.

Equation (41) provides an alternative spectral decomposition to the one given by Eq. (38), where the resonances at z_0 and $\overline{z}_0$ explicitly appear. Since $\overline{z}_0 - z_0 = -2i\Im z_0$, and by definition $\Im z_0 < 0$, $(\tilde{\Phi}_{00}|$ is an exponentially decaying mode and therefore a generalized Gamow state. This decomposition has the same properties as the one in the previous section, namely

(i) *They form a basis for observables and states.*

The identity superoperator $\mathbb{I}$ can be written in the form

$$\mathbb{I} = \int d\omega|\Phi_\omega)(\tilde{\Phi}_\omega| + |\Phi_{00})(\tilde{\Phi}_{00}| + \int_\Gamma dz'|\Phi_{0z'})(\tilde{\Phi}_{0z'}| + \int_{\bar{\Gamma}} dz|\Phi_{z0})(\tilde{\Phi}_{z0}| + \int_\Gamma dz \int_{\Gamma'} dz'|\Phi_{zz'})(\tilde{\Phi}_{zz'}|. \tag{43}$$

(ii) *They provide the spectral decomposition of the time evolution generator.*

$$\mathbb{L} = (\overline{z}_0 - z_0)|\Phi_{00})(\tilde{\Phi}_{00}| + (\overline{z}_0 - z')\int_\Gamma dz'|\Phi_{0z'})(\tilde{\Phi}_{0z'}| + \int_{\bar{\Gamma}} dz(z - z_0)|\Phi_{z0})(\tilde{\Phi}_{z0}| + \int_{\bar{\Gamma}} dz \int_\Gamma dz'(z - z')|\Phi_{zz'})(\tilde{\Phi}_{zz'}|. \tag{44}$$

Therefore $|\Phi_{00})((\tilde{\Phi}_{00}|)$ is a right (left) eigenvector of $\mathbb{L}$ with eigenvalue $\overline{z}_0 - z_0 = -2i\Im z_0$, $|\Phi_{0z'})((\tilde{\Phi}_{0z'}|)$ is a right (left) eigenvector of $\mathbb{L}$ with eigenvalue $(\overline{z}_0 - z')$, $|\Phi_{z0})((\tilde{\Phi}_{z0}|)$ is a right (left) eigenvector of $\mathbb{L}$ with eigenvalue $(z - z_0)$, and $|\Phi_{zz'})((\tilde{\Phi}_{zz'}|)$ is a right (left) eigenvector of $\mathbb{L}$ with eigenvalue $(z - z')$. Gamow state $(\tilde{\Phi}_{00}|$ will give the exponentially decaying term of the evolution.

(iii) *The generalized states have well defined physical properties.*

We have proved in the previous section that $(\tilde{\Phi}_{\omega\omega'}|H) = (\tilde{\Phi}_{\omega\omega'}|I) = 0$, i.e., that the generalized states $(\tilde{\Phi}_{\omega\omega'}|$ have zero probability and zero energy. This property is also verified by the new generalized states $(\tilde{\Phi}_{00}|$, $(\tilde{\Phi}_{0z'}|$, $(\tilde{\Phi}_{z0}|$, and $(\tilde{\Phi}_{zz'}|$, as they are obtained by analytic extensions of the functional $(\tilde{\Phi}_{\omega\omega'}|$ (the analytic extension of zero is zero!). As $(\tilde{\Phi}_{00}|I) = 0$ and $(\tilde{\Phi}_{00}|H) = 0$, we conclude that the generalized Gamow state cannot represent by itself a physical state since it has zero probability and zero energy.[4] They are just *useful mathematical tools in the spectral decomposition*. Then their nature is *purely mathematical* and it is not strange that their properties look unphysical.

(iv) *They provide a suitable representation to describe the asymptotic (in time) behavior of a state.*

As in the previous section, only the first term of Eq. (41) remains when $t \to \infty$, and we also obtain $W \lim_{t\to\infty}(\rho_t| = \int d\omega|\Phi_\omega)(\tilde{\Phi}_\omega|$.

[4] The rigorous property $(\tilde{\Phi}_{00}|I) = 0$ substitute in our formalism the dubious one $\langle f_0|f_0\rangle = 0$.

7. CONCLUSIONS

We have shown the difficulties of the complex spectral decomposition of pure states to compute the mean values of an observable with diagonal singularity, and therefore the problems to give a meaning to the probability and the energy of the Gamow vectors. The problem remains with the usual mixed states.

However, the key for the solution of the problem is to search for the generalized left and right and right eigenvectors of the Liouville–von Neumann superoperator (in other words the generalized "eigenstates" and "eigenobservables" of the quantum system), in a formalism where observables with diagonal singularity are included. The states of this formalism are not the usual density operators, but functionals acting on the space of observables. The eigenvectors corresponding to the zero eigenvalue expand the time-independent part of the mean values of an observable. In this formalism, we obtain what we call *generalized Gamow states,* generalized left eigenvectors of the Liouville–von Neumann superoperator with complex eigenvalue. These generalized states have no component in the time invariant space, and therefore they have zero energy and zero probability. In other words, in this formalism the complex eigenstates are correlations, and can not appear as single physical states. A physical state may have a generalized Gamow state as a component, but it should always include time invariant part.

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