Subdynamics theory in the functional approach to quantum mechanics

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The formalism of subdynamics is extended to the functional approach of quantum systems, and used for the Friedrichs model, in which diagonal singularities in states and observables are included. We compute in this approach the generalized eigenvectors and eigenvalues of the Liouville-Von Newmann operator, using an iterative scheme. As complex generalized eigenvalues are obtained, the decay rates of unstable modes are included in the spectral decomposition.

I. INTRODUCTION

For quantum system with continuous spectrum, the presence of resonances (small denominators) cause the failure of the usual perturbative methods for computing eigenvalues and eigenvectors of the time evolution generator. These difficulties have been considered as a manifestation of general limitations to computability for unstable dynamical systems [1] [2].

In the work of the Brussels-Austin groups on Large Poincare systems, we find an algorithm to overcome the problem of small denominators, which are eliminated by a "time ordering rule". This is a rule for the regularization of the perturbation terms, which can be interpreted as a generalized boundary condition where terms corresponding to excitation processes are past-oriented, while terms corresponding to the de-excitation and emission of radiation are future-oriented [1] [3].

The construction provides a new type of spectral decomposition of the Hamiltonian operator. For the Friedrichs model it was shown [1] that an appropriate mathematical framework for the time ordering construction is the theory of rigged Hilbert spaces of the Hardy class, formulated by A.Bohm and M.Gadella [4] [5] [6] [7].

For mixed states, the construction algorithm is a generalization of perturbation theory based on the subdynamics decomposition of the Liouville-Von Newmann superoperator $L$ [2] [8]. Through a non unitary transformation $Ω$, the superoperator $L$ is transformed into an operator $Θ = Ω^{-1}LΩ$, which is block diagonal in the degrees of correlations. The perturbative method to obtain the spectral decomposition of the intermediate operator $Θ$ is regularized by imposing the "time-ordering rules", which in this case means that conserving or increasing of degrees of correlations is future oriented, while decreasing of correlations is past oriented [3]. This prescription explicitly incorporates irreversibility to microscopic theories.

Usually, these perturbative algorithms are implemented in the so called "box normalization", in which the quantum system is assumed to be included in a box with periodic boundary conditions, the size of the box becoming infinite at some stage of the calculations. To perform this limit, it is necessary to consider volume dependent factors both for the diagonal components of the density operator and the observables. In this limit the recurrence time of the system is pushed to infinity.

The diagonal singularities of operators for large quantum system was discovered by Van Howe [10] [11] [12] [13]. At the same time, I. Prigogine and coworkers [14] [15] [16] [17] emphasized the importance of states with diagonal singularity in non equilibrium statistical physics.

Based in the pioneering work of I. E. Segal [18], I. Antoniou et al [19] [20] [21] developed a formalism for quantum systems with continuous spectrum without the box normalization.

The quantum states are functionals over certain space of observables $O$. Mathematically this means that the space $S$ of states is contained in $O^\ast$. Physically it means that the only thing we can really observe and measure are the mean values of the observables $O$ in states $ρ$ in $S$ $ρ ∈ S ⊂ O^\ast$ ($⟨O⟩_ρ = (ρ | O)$). This is the natural generalization of the usual trace of the product of the density operator by the observable ($Tr(ρO)$) which is not well defined for systems with continuous spectrum.

In this paper, we extend the theory of subdynamics to the case of quantum systems with diagonal singularities where, as stated in references [19] [20] [21], the states are considered as functionals acting on the space of observables. The extended formalism is applied to the Friedrichs Model.

In section II, we summarize the functional approach to quantum mechanics. The theory of subdynamics [2] [8] [3] is summarized in section III, and it is extended by us to the functional approach. In section IV, the extended formalism is applied to compute the generalized spectral decomposition and the time evolution for the Friedrichs Model.
II. FUNCTIONAL APPROACH TO QUANTUM MECHANICS

In the usual approach to quantum mechanics, a pure state is represented by a normalized vector $|\psi\rangle$ of a Hilbert space $H$. The observables of the system are represented by self adjoint operators acting on $H$. The mean value of an observable represented by the operator $O$ in a pure state represented by the vector $|\Psi\rangle$ is given by

$$\langle O \rangle_\Psi = \langle \Psi | O | \Psi \rangle$$

The time evolution of the state vector is given by the Schrödinger equation

$$i\frac{d}{dt} |\Psi_t\rangle = H |\Psi_t\rangle,$$

where the operator $H : \mathcal{H} \rightarrow \mathcal{H}$ is the Hamiltonian operator of the system. Schrödinger equation has the solution

$$|\Psi_t\rangle = e^{-iHt} |\Psi_0\rangle$$

Mixed states have no well defined state vectors, but a probabilities $p_\alpha$ $(p_\alpha \geq 0, \sum_\alpha p_\alpha = 1)$ of being in the pure states represented by normalized vectors $|\Psi_\alpha\rangle$. Therefore, the mean value of an observable $O$ is given by

$$\langle O \rangle = \sum_\alpha p_\alpha \langle \Psi_\alpha | O | \Psi_\alpha \rangle.$$}

The mixed state can be represented by the density operator $\hat{\rho} = \sum_\alpha p_\alpha |\Psi_\alpha\rangle \langle \Psi_\alpha|$, having the following properties

$$\langle O \rangle = Tr(\hat{\rho} O), \quad Tr(\hat{\rho}) = \sum_\alpha p_\alpha \langle \Psi_\alpha | \Psi_\alpha \rangle = \sum_\alpha p_\alpha = 1$$

As each vector $|\Psi_\alpha\rangle$ evolves in time according to the Schrödinger equation, the time evolution of $\hat{\rho}$ is

$$\hat{\rho}_t = e^{-iHt} \hat{\rho}_0 e^{iHt}$$

and $\hat{\rho}_t$ satisfies the Liouville-Von Newmann equation

$$i\frac{d}{dt} \hat{\rho}_t = L \hat{\rho}_t \quad (1)$$

$$L \hat{\rho} \equiv [H, \hat{\rho}] \quad (2)$$

In a more general approach, the set of all possible observables of a quantum system is represented by an algebra $\mathcal{O}$, while the possible states are represented by a set $\mathcal{S}$ of functionals acting on $\mathcal{O}$ ($\mathcal{S} \subset \mathcal{O}^\times$).

The mean value $\langle O \rangle_\rho$ of the observable $O$ in the state $\rho$ is given by the value of the functional $\rho$ on $O$, which we denote by $(\rho|O)$

$$\langle O \rangle_\rho = (\rho | O)$$

The last expression is antilinear in $\rho$ and linear in $O$, i.e.

$$\langle \alpha_1 \rho_1 + \alpha_2 \rho_2 | O \rangle = \alpha_1^* \langle \rho_1 | O \rangle + \alpha_2^* \langle \rho_2 | O \rangle \quad (3)$$

$$\langle \rho | \alpha_1 O_1 + \alpha_2 O_2 \rangle = \alpha_1 \langle \rho | O_1 \rangle + \alpha_2 \langle \rho | O_2 \rangle \quad (4)$$

The algebra $\mathcal{O}$ is chosen to be an algebra of self adjoint operators on the vector space $\mathcal{H}$, and as the mean value of the observables should be a real number, we impose the following condition on the states

$$\langle \rho | O \rangle = (\rho | O)^*, \text{ if } O = O^\dagger \quad (5)$$

The generalization of the concept of trace is

$$Tr \rho \equiv (\rho | I) = 1 \quad (6)$$
where $I$ is the identity operator in the algebra $O$.

For the time evolution in Heisenberg representation, the states are time independent, while the observables evolve in time according to

$$O_t = e^{iHt}Oe^{-iHt}.$$  

The time evolution $\rho_t$ of the states in Schrödinger representation can be obtained from

$$\langle O \rangle_t = \langle \rho_t | O \rangle = \langle \rho_0 | e^{iHt}Oe^{-iHt} \rangle.$$  

From the previous equation we obtain

$$\langle \frac{d}{dt} \rho_t | O \rangle = i\langle \rho_0 | e^{iHt}[H,O]e^{-iHt} \rangle = i(\rho_t | [H,O])$$

Calling $L^\dagger O \equiv [H,O]$ and omitting the observable $O$ in the previous equation we obtain the generalized Liouville-Von Newmann equation

$$-i\langle \frac{d}{dt} \rho_t | L \rangle = (\rho_t | L^\dagger) \equiv (\rho_t | [H,O]).$$

III. THE FORMALISM OF SUBDYNAMICS

Let us consider a linear space of states $S$, and a linear operator $L$ on $S$ which is the generator of the time evolution of the states, i.e.

$$i\frac{d}{dt} \rho_t = L \rho_t, \quad \rho_t \in S.$$  

Let us assume that the operator $L$ can be decomposed into

$$L = L_0 + L_1$$

where $L_0$ and $L_1$ are respectively called the "free" and "interaction" parts of $L$. It is also assumed that an interaction parameter $\lambda$ is included in $L_1$ to modulate the interaction.

Starting with the projector $P_0$ on the invariant parts of the dynamics ($L_0 P_0 = P_0 L_0 = 0$), projectors $P_n$ ($n = 0, 1, \ldots$) are defined in such a way that they satisfy

$$P_n P_{n'} = \delta_{nn'} P_n, \quad L_0 P_n = P_n L_0, \quad \sum_{n=0} P_n = I, \quad P_m (L_1)^n P_0 = \begin{cases} 0 & \text{if } n < m \\ \neq 0 & \text{if } n = m \end{cases}$$

where $I$ is the identity operator on $S$. The last equation means that the transition from $P_0 \rho$ to $P_m \rho$ is a process of $m$-th order in the interaction parameter. The operator $P_m$ is called the projection on the $m$-th degree of correlation.

The main idea of subdynamics is to decompose the states through projectors $\Pi_n$ ($n = 0, 1, \ldots$) satisfying
\[ \Pi_n \Pi_{n'} = \delta_{n,n'} \Pi_n, \quad \mathbb{L} \Pi_n = \Pi_n \mathbb{L}, \quad \sum_{n=0}^{\infty} \Pi_n = \mathbb{I}, \quad \lim_{L_1 \to 0} \Pi_n = \mathbb{P}_n, \]  

(13)
i.e. projectors \( \Pi_n \) commuting with \( \mathbb{L} \) which reduce to the projectors \( \mathbb{P}_n \) on the degrees of correlation when the parameter of the interaction tends to zero.

Operators \( \mathbb{C}_n \) and \( \mathbb{D}_n \), called creation and destruction of correlations are defined by

\[
\mathbb{C}_n = \mathbb{Q}_n \mathbb{C}_n \mathbb{P}_n \quad \mathbb{Q}_n \Pi_n = \mathbb{C}_n \mathbb{P}_n \Pi_n \\
\mathbb{D}_n = \mathbb{P}_n \mathbb{D}_n \mathbb{Q}_n \quad \Pi_n \mathbb{Q}_n = \Pi_n \mathbb{P}_n \mathbb{D}_n
\]

(14)

where \( \mathbb{Q}_n = \mathbb{I} - \mathbb{P}_n \). From equations (11) and (14) it is obtained

\[
i \frac{d}{dt} (\mathbb{P}_n \rho) = \Theta_n \mathbb{P}_n \rho
\]

(15)

\[
\Theta_n = \mathbb{P}_n \mathbb{L} \mathbb{P}_n + \mathbb{P}_n \mathbb{L} \mathbb{C}_n \mathbb{P}_n
\]

(16)

\[
\Pi_n = (\mathbb{P}_n + \mathbb{C}_n)(\mathbb{P}_n + \mathbb{D}_n \mathbb{C}_n)^{-1}(\mathbb{P}_n + \mathbb{D}_n)
\]

(17)

\[
[\mathbb{L}_0, \mathbb{P}_m \mathbb{C}_n] = (\mathbb{P}_m \mathbb{C}_n - \mathbb{P}_m) \mathbb{L}_1 (\mathbb{P}_n + \mathbb{C}_n)
\]

(18)

\[
[\mathbb{L}_0, \mathbb{D}_n \mathbb{P}_m] = (\mathbb{P}_n + \mathbb{D}_n) \mathbb{L}_1 (\mathbb{P}_m - \mathbb{D}_n \mathbb{P}_m).
\]

(19)

The last two equations have the form \([\mathbb{L}_0, X] = Y\), having the forward (backward) solutions

\[
X^\pm = i \int_0^{\pm \infty} dt \ e^{-i \omega_t} \ Y e^{i \omega_t}
\]

The following "time ordering rule" is chosen: +(-) sign is used for \( X = \mathbb{P}_m \mathbb{C}_n \) with \( m > n \) \((m < n)\), and for \( X = \mathbb{D}_n \mathbb{P}_m \) with \( n > m \) \((n < m)\). Therefore, the creation (destruction) of correlations, is future (past) oriented, i.e.

\[
\mathbb{P}_m \mathbb{C}_n = i \int_0^{\infty} dt \ e^{-i \omega_t} (\mathbb{P}_m \mathbb{C}_n - \mathbb{P}_m) \mathbb{L}_1 (\mathbb{P}_n + \mathbb{C}_n) e^{i \omega_t}, \quad m > n
\]

\[
\mathbb{D}_n \mathbb{P}_m = i \int_0^{\infty} dt \ e^{-i \omega_t} (\mathbb{P}_n + \mathbb{D}_n) \mathbb{L}_1 (\mathbb{P}_m - \mathbb{D}_n \mathbb{P}_m) e^{i \omega_t}, \quad m < n
\]

(20)

The two previous equations can be solved iteratively to the required order in the interaction parameter, starting with the zero order solutions

\[
\mathbb{C}^{(0)}_n = \mathbb{D}^{(0)}_n = 0.
\]

Once \( \mathbb{C}_n \) and \( \mathbb{D}_n \) are obtained, the intermediate superoperators \( \Theta_n = \mathbb{P}_n \Theta_n \mathbb{P}_n \) can be computed using (13). The block diagonal super operator \( \Theta = \sum_n \Theta_n \) satisfies

\[
\mathbb{L} = \Omega \Theta \Omega^{-1},
\]

\[
\Omega = \sum_n (\mathbb{P}_n + \mathbb{C}_n),
\]

\[
\Omega^{-1} = \sum_n (\mathbb{P}_n + \mathbb{D}_n \mathbb{C}_n)^{-1} (\mathbb{P}_n + \mathbb{D}_n),
\]

(21)

and therefore it is isospectral with the Liouville-Von Newmann operator \( \mathbb{L} \). This property can be used to obtain the spectral decomposition of \( \mathbb{L} \) in terms of the spectral decomposition of the superoperator \( \Theta \), with the same generalized eigenvalues.

The formalism of subdynamics originally stated on the space of density operators can be easily translated to the functional approach of quantum mechanics described in the previous section. All the formulas of this section are still valid, but we should remember that the superoperators are in this case defined on the space \( \mathcal{S} \) of functionals.

It is operationally more convenient to rewrite all the previous equations for the corresponding adjoint superoperators, acting on the space of observables \( \mathcal{O} \). This is easily done by using the adjoint relation
For example, equations (12) for the projections on the degrees of correlations are replaced by
\[
P_n^\dagger P_n = \delta_{nn}, \quad L_n^\dagger P_n = P_n^\dagger Q_n^\dagger, \quad \sum_n P_n^\dagger = I^\dagger, \quad P_0^\dagger (L_1^\dagger)^m P_m = \begin{cases} 0 & \text{if } n < m, \\ \neq 0 & \text{if } n = m, \end{cases}
\]
where \(I^\dagger\) is the identity superoperator on \(\mathcal{O}\).

Equations (20) for the creation and destruction of correlations transform into
\[
C_n^\dagger P_m = -i \int_0^{\pm \infty} dt e^{-it} (P_m^\dagger + C_n^\dagger) L_1^\dagger (C_n^\dagger P_m^\dagger - P_m^\dagger) e^{it} t, \quad m > n
\]
and
\[
P_m^\dagger D_n^\dagger = -i \int_0^{\pm \infty} dt e^{-it} (P_m^\dagger - P_m^\dagger D_n^\dagger) L_1^\dagger (P_m^\dagger + D_n^\dagger) e^{it} t, \quad m < n,
\]
where now
\[
C_n^\dagger = P_m^\dagger C_n^\dagger Q_m^\dagger, \quad D_n^\dagger = Q_n^\dagger D_n^\dagger P_m^\dagger, \quad Q_n^\dagger = I^\dagger - P_n^\dagger
\]
Equations (23) and (24) can be written in a form which is more suitable for calculations. Let us consider the generalized left and right eigenvectors \((\alpha|\) and \(|\beta)\) of \(L_0^\dagger\), having degrees of correlation \(n_\alpha\) and \(n_\beta\), i.e.
\[
(\alpha|L_0^\dagger = \omega_\alpha (\alpha|, \quad L_0^\dagger |\beta) = \omega_\beta |\beta), \quad (\alpha| = (\alpha|P_n^\dagger, \quad |\beta) = (|P_n^\dagger |\beta).
\]
From equation (23) we obtain
\[
(\alpha|C_n^\dagger |\beta) = -i \int_0^{\pm \infty} dt e^{it} (\alpha| (P_m^\dagger + C_n^\dagger) L_1^\dagger (C_n^\dagger - Q_n^\dagger) |\beta), \quad n_\beta > n_\alpha
\]
If we use in the previous expression the identity
\[
\int_0^{\pm \infty} dt e^{i\theta t} = \frac{i}{\omega_\beta - \omega_\alpha + i0}
\]
we obtain
\[
(\alpha|C_n^\dagger |\beta) = \frac{1}{\omega_\beta - \omega_\alpha + i0} (\alpha| (P_m^\dagger + C_n^\dagger) L_1^\dagger (C_n^\dagger - Q_n^\dagger) |\beta), \quad n_\beta > n_\alpha
\]
In the same way we obtain
\[
(\alpha|D_n^\dagger |\beta) = \frac{1}{\omega_\beta - \omega_\alpha + i0} (\alpha| (Q_n^\dagger - D_n^\dagger) L_1^\dagger (P_m^\dagger + D_n^\dagger) |\beta), \quad n_\beta > n_\alpha
\]
The intermediate operator \(\Theta^\dagger\) is
\[
\Theta^\dagger = \sum_n \Theta_n^\dagger, \quad \Theta_n^\dagger = P_n^\dagger L_1^\dagger + P_n^\dagger C_n^\dagger L_1^\dagger
\]
The intermediate operator \(\Theta^\dagger\) is isospectral with \(L^\dagger\)
\[
L^\dagger = (\Omega^\dagger)^{-1} \Theta^\dagger \Omega^\dagger
\]
\[
\Omega^\dagger = \sum_n (P_n^\dagger + C_n^\dagger)
\]
\[
(\Omega^\dagger)^{-1} = \sum_n (P_n^\dagger + D_n^\dagger)(P_n^\dagger + C_n^\dagger D_n^\dagger)^{-1}
\]
For \((P_n^\dagger + C_n^\dagger D_n^\dagger)^{-1}\) we can use the following expansion
\[
(P_n^\dagger + C_n^\dagger D_n^\dagger)^{-1} = P_n^\dagger + \sum_{j=1}^{\infty} (-1)^j (C_n^\dagger D_n^\dagger)^j
\] (30)

The spectral decomposition of the intermediate operator \(\Theta_n^\dagger\), i.e. a set of right (left) generalized eigenvectors \(|\tilde{u}_{n\alpha}\rangle\), \((|u_{n\alpha}\rangle)\) satisfying
\[
(\tilde{u}_{n\alpha}|u_{m\beta}\rangle) = \delta_{nm}\delta_{\alpha\beta}, \quad \Theta_n^\dagger = \sum_{\alpha} z_{n\alpha}|\tilde{u}_{n\alpha}\rangle(u_{n\alpha}|, \quad P_n^\dagger = \sum_{\alpha} |\tilde{u}_{n\alpha}\rangle(u_{n\alpha}|.
\] (31)

where \(\alpha\) and \(\beta\) are discrete or continuous indexes. In the later case the sums in the previous expression should be replaced by integrals and the Kronecker by Dirac deltas.

The spectral decomposition of \(L_n^\dagger\) can be obtained from the spectral decomposition of the intermediate operator \(\Theta_n^\dagger\). From equations (29) and (31) it follows that
\[
L_n^\dagger = \sum_{n\alpha} z_{n\alpha} |\hat{f}_{n\alpha}\rangle (f_{n\alpha}|,
\] (32)

where
\[
|\hat{f}_{n\alpha}\rangle = (\Omega^\dagger)^{-1}|\tilde{u}_{n\alpha}\rangle \quad (f_{n\alpha}| = (u_{n\alpha}| \Omega^\dagger.
\] (33)

The time evolution of a state functional, governed by the generalized Liouville-Von Neumann equation
\[
-i\frac{d}{dt}(\rho_t) = (\rho_t| L_n^\dagger,
\] (34)

is given by
\[
(\rho_t) = \sum_{n\alpha} e^{iz_{n\alpha}t} (\rho_0|\hat{f}_{n\alpha}\rangle(f_{n\alpha}|.
\] (35)

A. Perturbative solutions and \(\lambda^2t\) approximation.

If we replace the zero order approximation for \(C_n^\dagger\) and \(D_n^\dagger\) (i.e. \(C_n^{(0)} = D_n^{(0)} = 0\)) in the right hand side of equations (26) and (27), we can obtain the first order approximations:
\[
(\alpha|C_n^{(1)}|\beta) = \frac{-1}{\omega_\beta - \omega_\alpha + i0} (\alpha| P_n^\dagger L_n^\dagger Q_n^\dagger | \beta), \quad n_\beta > n_\alpha
\] (36)
\[
(\alpha|D_n^{(1)}|\beta) = \frac{1}{\omega_\beta - \omega_\alpha + i0} (\alpha| Q_n^\dagger L_n^\dagger P_n^\dagger | \beta), \quad n_\beta < n_\alpha
\] (37)

With \(C_n^{(1)}\) and \(D_n^{(1)}\) it is possible to obtain the intermediate operators \(\Theta_n^\dagger\) up to second order, using equation (28)
\[
\Theta_n^{(2)} = P_n^\dagger L_n^\dagger P_n^\dagger + P_n^\dagger C_n^{(1)} L_n^\dagger P_n^\dagger
\] (38)

From equations (29), (30), (36) and (37), we can compute \(\Omega^\dagger\) and \((\Omega^\dagger)^{-1}\) up to first order
\[
\Omega^{(1)} = \sum_n (P_n^\dagger + C_n^{(1)})
\]
\[
(\Omega^\dagger)^{-1} = \sum_n (P_n^\dagger + D_n^{(1)})
\] (39)

The first order expressions for \(C_n^\dagger\) and \(D_n^\dagger\) given in equations (36) and (37) can be replaced in the right hand side of equations (26) and (27) to obtain the next order approximation. In this way, through the computation of the
eigenvalues and eigenvectors of the intermediate operator $\Theta^\dagger$, it is possible to obtain the eigenvalues and eigenvectors of $L^\dagger$ as a power expansion in the interaction parameter $z_n^\alpha = z_n^{(0)} + z_n^{(1)} + z_n^{(2)} + \cdots$

$$|f_{n\alpha}\rangle = |f_{n\alpha}^{(0)}\rangle + |f_{n\alpha}^{(1)}\rangle + |f_{n\alpha}^{(2)}\rangle + \cdots$$  

$$|\tilde{f}_{n\alpha}\rangle = |\tilde{f}_{n\alpha}^{(0)}\rangle + |\tilde{f}_{n\alpha}^{(1)}\rangle + |\tilde{f}_{n\alpha}^{(2)}\rangle + \cdots$$  

Taking into account equations (33) and (39) relating the eigenvectors of $\Theta^\dagger$ and $L^\dagger$ we obtain

$$|\tilde{f}_{n\alpha}\rangle = |\tilde{u}_{n\alpha}^{(0)}\rangle + D_n^{(1)}|\tilde{u}_{n\alpha}^{(1)}\rangle + \cdots$$  

$$|f_{n\alpha}\rangle = |u_{n\alpha}^{(0)}\rangle + (u_{n\alpha}^{(0)}|C_n^{(1)} + (u_{n\alpha}^{(0)}|C_n^{(1)} + \cdots$$

Replacing (40) and (41) in (35) we obtain the following expression for the time evolution

$$(\rho_t) \approx \sum_{n\alpha} \exp \left[ i(z_{n\alpha}^{(0)} + z_{n\alpha}^{(1)} + z_{n\alpha}^{(2)} + \cdots) t \right] \times (\rho_0) \left[ |\tilde{u}_{n\alpha}^{(0)}\rangle(u_{n\alpha}^{(0)}| + |\tilde{u}_{n\alpha}^{(1)}\rangle(u_{n\alpha}^{(1)}| + \cdots \right].$$

If we omit first order contributions coming from the eigenvectors and third order contributions from the eigenvalues, the previous expression has the following approximated form

$$(\rho_t) \approx \sum_{n\alpha} \exp \left[ i(z_{n\alpha}^{(0)} + z_{n\alpha}^{(1)} + z_{n\alpha}^{(2)} + \cdots) t \right] \langle \rho_0|u_{n\alpha}^{(0)}\rangle(u_{n\alpha}^{(0)}|.$$  

As we omitted first order terms in the eigenvectors, a necessary condition for equation (42) to be valid is

$$\lambda << 1,$$  

where $\lambda$ is the interaction parameter. Moreover, as we considered the eigenvalues up to second order, a second condition involving the possible values of time is necessary for equation (42) to be valid

$$\lambda^3 t << 1,$$  

which together with (43) gives

$$t < \lambda^{-2}.$$  

In summary, the time evolution is given by the equation (42) if the interaction is small ($\lambda << 1$) and the time is not too large ($t < \lambda^{-2}$). Conditions (43) and (45) appear in the literature as the ”$\lambda^2$ approximation”.

IV. FRIEDRICHS MODEL

A. Observables, states and degrees of correlation

The Hamiltonian of Friedrichs model is

$$H = H_0 + V,$$

$$H_0 = m|1\rangle \langle 1| + \int_0^\infty d\omega \omega |\omega\rangle \langle \omega|,$$  

$$V = \int_0^\infty d\omega V_\omega (|\omega\rangle \langle 1| + |1\rangle \langle \omega|).$$

Where the vectors $|1\rangle$ and $|\omega\rangle$ form a complete orthonormal set.
Let us consider the following definitions

\[
|1\rangle \equiv |1\rangle \langle 1|, \quad |\omega\rangle \equiv |\omega\rangle \langle \omega|, \quad |1\rangle \equiv |1\rangle \langle 1|, \quad |\omega\rangle \equiv |\omega\rangle \langle \omega|.
\]

(48)

Any element \(O\) belonging to the space of observables \(\mathcal{O}\), can be written in terms of the operators defined in (48)

\[
|O\rangle = O_1|1\rangle + \int d\omega O_{\omega}|\omega\rangle + \int d\omega O_{1\omega}|1\rangle + \int d\omega \int d\omega' O_{\omega\omega'}|\omega\omega'|.
\]

(49)

Notice that we explicitly included a diagonal singularity through the term \(\int d\omega O_{\omega}|\omega\rangle\).

We also consider the states as functionals acting on the operators. For this purpose it is convenient to define a set of functionals \(|1\rangle, |\omega\rangle, |1\omega\rangle, (\omega 1)\rangle and (\omega \omega')\rangle with the following properties

\[
(1)|O\rangle = O_1, \quad (\omega)|O\rangle = O_{\omega}, \quad (1\omega)|O\rangle = O_{1\omega}, \quad (\omega 1)|O\rangle = O_{\omega 1}, \quad (\omega \omega')|O\rangle = O_{\omega \omega'}.
\]

(50)

or equivalently

\[
(1)|1\rangle = 1, \quad (1)|\omega\rangle = (1)|1\omega\rangle = (1)|\omega 1\rangle = (1)|\omega \omega'\rangle = 0,
\]

(51)

\[
(\omega)|\omega\rangle = \delta(\omega - \omega'), \quad (\omega)|1\rangle = (\omega)|1\omega\rangle = (\omega)|\omega 1\rangle = (\omega)|\omega \omega'\rangle = 0,
\]

\[
(1\omega)|\omega\rangle = \delta(\omega - \omega'), \quad (1\omega)|1\rangle = (1\omega)|1\omega\rangle = (1\omega)|\omega 1\rangle = (1\omega)|\omega \omega'\rangle = 0,
\]

\[
(\omega \omega'|\alpha\alpha') = \delta(\omega - \alpha)\delta(\omega' - \alpha'), \quad (\omega \omega' 1)|1\rangle = (\omega \omega' 1)|\alpha\rangle = (\omega \omega'|1\alpha) = (\omega \omega'|\alpha) = 0.
\]

In terms of these functionals, we assume that any element \((\rho)\) of the space of states \(\mathcal{S} \subset \mathcal{O}^*\) can be written as

\[
(\rho) = \rho_1^*|1\rangle + \int d\omega \rho_{\omega}^*|\omega\rangle + \int d\omega \rho_{1\omega}^*|1\rangle + \int d\omega \int d\omega' \rho_{\omega\omega'}^*|\omega\omega'|.
\]

(52)

where

\[
\rho_1^* = \rho_1, \quad \rho_{\omega}^* = \rho_{\omega}, \quad \rho_{1\omega}^* = \rho_{1\omega}, \quad \rho_{\omega\omega'}^* = \rho_{\omega\omega'},
\]

(53)

\[
\rho_1^* + \int d\omega \rho_{\omega}^* = 1.
\]

(54)

Equations (52) are the conditions for \(\rho\) to be a positive functional, while (54) is a consequence of the total probability condition \((\rho|I) = 1\). In what follows \((\rho|I)\) will be called the generalized trace of the state \(\rho (|I| \equiv |1\rangle + \int d\omega |\omega\rangle)\) is the identity operator in \(\mathcal{O}\).

By using the basis for states and observables, defined through (48) and (50), we can also write

\[
\mathbb{L}_0 = \int d\omega (m - \omega)|1\omega\rangle\langle 1\omega| + \int d\omega (m - \omega)|\omega 1\rangle\langle \omega 1| + \int d\omega \int d\omega' (\omega - \omega')|\omega\omega'\rangle\langle \omega\omega'|,
\]

(55)

\[
\mathbb{L}_1 = \int d\omega V_{\omega}|1\omega\rangle - |1\omega\rangle\langle 1| + \int d\omega V_{\omega}|1\omega\rangle - |1\omega\rangle\langle \omega 1| + \int d\omega [-V_{\omega}|1\rangle + \int d\omega' V_{\omega'}|\omega'\rangle\langle \omega'| + \int d\omega V_{\omega'}|\omega'\rangle\langle \omega'| + \int d\omega V_{\omega'}|\omega'\rangle\langle \omega'|,
\]

where \(\mathbb{L}_0^+\) and \(\mathbb{L}_1^+\) are the "free" and "interaction" parts of the Liouville-Von Newmann operator acting on \(\mathcal{O}\), i.e.

\[
\mathbb{L}_0^+ O \equiv [H_0, O], \quad \mathbb{L}_1^+ O \equiv [V, O] \quad O \in \mathcal{O}
\]

(56)

The diagonal and off-diagonal projectors, acting on \(\mathcal{O}\), are defined by
\[ P_0^\dagger \equiv |1\rangle(1) + \int d\omega |\omega\rangle(\omega), \]

\[ Q_0^\dagger \equiv \int d\omega |1\omega\rangle(1\omega) + \int d\omega |1\omega 1| + \int d\omega d\omega' |\omega\omega'\rangle(\omega\omega'). \] (57)

The off-diagonal projector \( Q_0^\dagger \) can be decomposed into

\[ Q_0^\dagger = P_1^\dagger + P_2^\dagger, \quad P_1^\dagger \equiv \int d\omega |1\omega\rangle(1\omega) + \int d\omega |1\omega 1|, \quad P_2^\dagger \equiv \int d\omega \int d\omega' |\omega\omega'\rangle(\omega\omega'). \] (58)

\( P_0^\dagger, P_1^\dagger \) and \( P_2^\dagger \) are the projectors corresponding to degrees of correlation zero, one and two respectively, i.e.

\[ P_0^\dagger (L_1^1)^0 P_0^\dagger = P_0^\dagger \neq 0, \quad P_0^\dagger (L_1^1)^0 P_1^\dagger = P_0^\dagger P_1^\dagger = 0, \quad P_0^\dagger L_1^1 P_1^\dagger \neq 0, \quad P_0^\dagger (L_1^1)^2 P_1^\dagger = 0, \quad P_0^\dagger (L_1^1)^2 P_2^\dagger \neq 0. \] (59)

### B. Creation, Destruction and Intermediate Operators

Using the equation (34) and (35) for the Friedrichs model we obtain for the creation and destruction operator up to second order are:

\[ C_{0}^{(1)} = \int d\omega V_\omega \left[ \frac{|1\rangle(1)}{m - \omega + i0} - \frac{|1\rangle(1)}{m + \omega + i0} \right], \]

\[ C_{1}^{(1)} = \int d\omega V_\omega \left[ \frac{|1\omega\rangle(1)}{m - \omega + i0} - \frac{|1\omega\rangle(1)}{m + \omega + i0} \right] + \int d\omega d\omega' \left[ \frac{V_\omega |\omega\rangle|\omega\rangle|\omega\rangle}{m - \omega' + i0} - \frac{V_\omega |\omega\rangle|\omega\rangle|\omega\rangle}{m - \omega + i0} \right], \]

\[ C_{2}^{(1)} = \int d\omega d\omega' \left[ V_\omega |\omega\rangle(\omega\omega')(1\omega) + \frac{V_\omega |\omega\rangle(\omega\omega')(1\omega)}{\omega' - m + i0} \right], \]

\[ D_{0}^{(1)} = \int d\omega V_\omega \left[ \frac{|1\omega\rangle(1)}{m - \omega + i0} + \frac{|1\omega\rangle(1)}{m - \omega - i0} \right] - \int d\omega V_\omega \left[ \frac{|1\omega\rangle(1)}{m - \omega + i0} + \frac{|1\omega\rangle(1)}{m - \omega - i0} \right], \]

\[ D_{1}^{(1)} = \int d\omega V_\omega \left[ \frac{|1\omega\rangle(1)}{m - \omega + i0} - \frac{|1\omega\rangle(1)}{m - \omega - i0} \right] + \int d\omega d\omega' V_\omega \left[ \frac{|\omega\omega\rangle|\omega\rangle|\omega\rangle}{m - \omega' + i0} - \frac{|\omega\omega\rangle|\omega\rangle|\omega\rangle}{m - \omega' - i0} \right], \]

\[ D_{2}^{(1)} = \int d\omega d\omega' \left[ V_\omega |\omega\rangle(\omega\omega')(\omega\omega') + V_\omega |\omega\rangle(\omega\omega')(\omega\omega') \right]. \] (60)

Then, the intermediate operator \( \Theta_{0}^{(2)} \), up to second order, can be obtained using equation (38)

\[ \Theta_{0}^{(2)} = 2\pi i V_m^2 |1\rangle(1 - |m\rangle), \quad |m\rangle(1 - |m\rangle) \equiv (\omega)_{\omega=m}, \]

\[ \Theta_{1}^{(2)} = \int d\omega [m - \omega - \beta]|1\omega\rangle(1\omega) + \int d\omega [m - \omega - \beta^*]|1\omega\rangle(1\omega) + \int d\omega d\omega' V_\omega V_\omega' \left[ \frac{|1\omega\rangle(1\omega)}{m - \omega' + i0} + \frac{|1\omega\rangle(1\omega)}{m - \omega' - i0} + \frac{|1\omega\rangle(1\omega)}{m - \omega + i0} + \frac{|1\omega\rangle(1\omega)}{m - \omega - i0} \right] + \int d\omega d\omega' V_\omega V_\omega' \left[ \frac{|\omega\omega\rangle|\omega\rangle|\omega\rangle}{m - \omega' + i0} + \frac{|\omega\omega\rangle|\omega\rangle|\omega\rangle}{m - \omega' - i0} + \frac{|\omega\omega\rangle|\omega\rangle|\omega\rangle}{m - \omega + i0} + \frac{|\omega\omega\rangle|\omega\rangle|\omega\rangle}{m - \omega - i0} \right], \]

\[ \beta = \int_0^\infty \frac{d\omega}{\omega - m + i0}, \quad \Re \beta = \int_0^\infty d\omega V_\omega^2 P \left( \frac{1}{\omega - m} \right), \quad \Im \beta = -\pi \cdot V_m^2 \]

\[ \Theta_{2}^{(2)} = \int d\omega d\omega' (\omega' - \omega)|\omega\omega')(\omega'\omega') + \int d\omega d\omega' d\omega'' \left[ V_\omega V_\omega' V_\omega'' |\omega\omega')(\omega\omega') - V_\omega V_\omega' V_\omega'' |\omega\omega')(\omega\omega') \right]. \] (61)
C. Generalized spectral decomposition and time evolution.

From the explicit form of $\Theta_n^\dagger$ given up to second order in equations (61) for Friedrichs model, the generalized eigenvectors and eigenvalues can be computed up to zero and second order respectively. The results are shown in the following table

| $\Theta_n^\dagger$ | $z_{na}$ | $|u_{na}\rangle$ | $|u_{na}\rangle$ |
|-------------------|---------|----------------|----------------|
| $\Theta_0^0$     | $z_0 = m$ | $|u_{m}\rangle = \delta(\omega - m)|1\rangle + |\omega\rangle$ | $(u_{m}) = (\omega)$ |
| $\Theta_1^1$     | $z_1 = 2\pi i V^2_m$ | $|u_{1\omega}\rangle = |1\omega\rangle$ | $(u_{1\omega}) = (1\omega)$ |
| $\Theta_2^1$     | $z_{1\omega} = m - \omega - \beta$ | $|u_{1\omega}\rangle = |1\omega\rangle$ | $(u_{1\omega}) = (1\omega)$ |
| $\Theta_2^2$     | $z_{2\omega'} = \omega - \omega'$ | $|u_{2\omega'}\rangle = |\omega\omega'\rangle$ | $(u_{2\omega'}) = (\omega\omega')$ |

The generalized eigenvalues and eigenvectors given in the previous expression can be replaced in the equation (62), to obtain the following time evolution

$$(\rho_t|1\rangle \approx e^{-2\pi V^2_m t} (\rho_0|1\rangle),$$

$$(\rho_t|\omega\rangle \approx (\rho_0|\omega\rangle + [1 - e^{-2\pi V^2_m t}] (\rho_0|1\rangle \delta(\omega - m),$$

$$(\rho_t|1\omega\rangle \approx e^{i(m-\omega-\beta)t} (\rho_0|1\omega\rangle),$$

$$(\rho_t|\omega1\rangle \approx e^{i(\omega-m-\beta)t} (\rho_0|\omega1\rangle),$$

$$(\rho_t|\omega\omega'\rangle \approx e^{i(\omega-\omega')t} (\rho_0|\omega\omega'\rangle).$$

The first equation shows the decay of the discrete component $(\rho_t|1\rangle$ of the state, with a rate $2\pi V^2_m$. Simultaneously, there is a growing term in the continuous distribution $(\rho_t|\omega\rangle$, with a sharp peak for the energy $\omega = m$ of the decaying mode.

V. CONCLUSIONS

We extended the formalism of subdynamics to the functional approach of quantum mechanics, in which the states are represented by functionals acting on the operators representing observables.

The generalized spectral decomposition is obtained through an intermediate superoperator $\Theta^\dagger$ isospectral to the Liouville-Von Newmann superoperator $L^\dagger$ ($L^\dagger = \Omega^\dagger \Theta^\dagger \Omega^{-1}\dagger$). The small denominators appearing in the perturbative expansions due to the continuous spectrum are regularized by the "$i\epsilon$-rule" (a time ordering prescription in which increasing (decreasing) of correlations is future (past) oriented). Due to this time ordering rule, $\Theta^\dagger$ and therefore $L^\dagger$ may have complex eigenvalues.

Considering eigenvalues up to second order and eigenvectors up to zero order, the time evolution is given by

$$(\rho_t|1\rangle \approx \sum_{n\alpha} \exp \left[ i(z_{na}^{(0)} + z_{na}^{(1)} + z_{na}^{(2)}t) \right] (\rho_0|\tilde{u}_{na}^{(0)}\rangle)(\tilde{u}_{na}^{(0)}|),$$

where $|\tilde{u}_{na}^{(0)}\rangle$ and $|\tilde{u}_{na}^{(0)}\rangle$ are generalized right and left eigenvector of $\Theta_n^\dagger$ computed up to zero order. For the previous expression to be valid, it is necessary that the interaction parameter be small and the time not too large, i.e. $\lambda \ll 1$ and $t \ll \lambda^{-2}$.

When this procedure is applied to the Friedrichs model, we obtain

$$(\rho_t|1\rangle \approx e^{-2\pi V^2_m t} (\rho_0|1\rangle),$$

$$(\rho_t|\omega\rangle \approx (\rho_0|\omega\rangle + [1 - e^{-2\pi V^2_m t}] (\rho_0|1\rangle \delta(\omega - m),$$

$$(\rho_t|1\omega\rangle \approx e^{i(m-\omega-\beta)t} (\rho_0|1\omega\rangle),$$

$$(\rho_t|\omega1\rangle \approx e^{i(\omega-m-\beta)t} (\rho_0|\omega1\rangle),$$

$$(\rho_t|\omega\omega'\rangle \approx e^{i(\omega-\omega')t} (\rho_0|\omega\omega'\rangle).$$

The first equation shows the decay of the discrete component $(\rho_t|1\rangle$ of the state, with a rate $2\pi V^2_m$. Simultaneously, there is a growing term in the continuous distribution $(\rho_t|\omega\rangle$, with a sharp peak for the energy $\omega = m$ of the decaying mode.
It is interesting to note that both decaying and growing terms are purely exponential. This may appear at first sight as a contradiction with the well known Zeno and Khalin effects, which are deviations from exponential decays for small and big times. However, the previous expressions are not valid approximations for very big times. Moreover, Zeno effect implies \( \frac{d}{dt}(\rho(t)|1)_{t=0} \). In our approximation, if we compute this derivative we obtain that it is of second order in the interaction parameter. As we neglected this order in the approximation, this result is not in contradiction with Zeno effect.

In spite of the fact that the complex spectral decomposition can be obtained analytically for the Friedrichs model \[23\] [24], this paper shows that this approach is potentially suitable to deal with more complicated decaying processes where it is impossible to obtain exact solutions.

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