An open–quantum–system formulation of particle decay

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February 14, 2006

Abstract

We consider an open quantum system which contains unstable states. The time evolution of the system can be described by an effective non-hermitian Hamiltonian $H_{\text{eff}}$, in accord with the Wigner–Weisskopf approximation, and an additional term of the Lindblad form, the so-called dissipator. We show that, after enlarging the original Hilbert space by states which represent the decay products of the unstable states, the non-hermitian part of $H_{\text{eff}}$—the “particle decay”—can be incorporated into the dissipator of the enlarged space via a specific Lindblad operator. Thus the new formulation of the time evolution on the enlarged space has a hermitian Hamiltonian and is probability conserving. The equivalence of the new formulation with the original one demonstrates that the time evolution which is governed by a non-hermitian Hamiltonian and a dissipator of the Lindblad form is nevertheless completely positive, just as systems with hermitian Hamiltonians.

PACS numbers: 03.65.-w, 03.65.Yz, 13.25.Es
Key-Words: Open quantum system, Lindblad operator, particle decay, Wigner–Weisskopf approximation

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Introduction: In reality a quantum system is not isolated but always interacting with its environment and has to be considered as an open quantum system \[1, 2\]. It leads to a mixing of the states in the system—decoherence—and to an energy exchange between system and environment—dissipation \[3, 4, 5, 6\]. The decoherence/dissipation weakens or destroys the typical quantum phenomena, the interferences.

There is great interest to study such decoherence/dissipation processes for elementary particles like the “strange” K-mesons (neutral kaons) and the “beauty” B-mesons \[7, 8, 9\], in particular, the decoherence of entangled meson pairs \[10, 11, 12\] (for an overview see Ref. \[13\]). However, these particles are decaying, which leads in the framework of quantum mechanics to some difficulties. In the usual framework the decaying states evolve according to the Wigner–Weisskopf approximation (WWA) where the probability of detecting the particle is not conserved and the corresponding Hamiltonian is, for this reason, non-hermitian.

The master equation for such an open quantum system described by the density matrix $\rho(t)$ is given by

$$\frac{d\rho}{dt} = -iH_{\text{eff}}\rho + i\rho H_{\text{eff}}^\dagger - D[\rho],$$

(1)

where the dissipator has the following general structure of operators \[14, 15\]:

$$D[\rho] = \frac{1}{2} \sum_j \left( A_j^\dagger A_j \rho + \rho A_j^\dagger A_j - 2A_j \rho A_j^\dagger \right).$$

(2)

The operators $A_j$ are usually called Lindblad operators. The effective Hamiltonian of the system is given, according to the WWA, by

$$H_{\text{eff}} = H - \frac{i}{2} \Gamma,$$

(3)

where $H$ and $\Gamma$ are both hermitian and, in addition, $\Gamma \geq 0$.

In terms of open quantum systems, the time evolution of the density matrix represents a dynamical map which transform initial density matrices $\rho(0)$ on the Hilbert space of states, $H_s$, to final density matrices $\rho(t) = V_t[\rho(0)]$, while the system is interacting with an environment. Such dynamical maps are i) trace conserving, ii) convex linear, iii) completely positive. Complete positivity is a rather strong and important property. It is defined by demanding that all extensions $V_t \otimes I_n$ on the Hilbert space $H_s \otimes \mathbb{C}^n$ are positive, i.e.

$$(V_t \otimes I_n)[\rho] \geq 0 \quad \forall t \geq 0, \; \forall n = 0, 1, 2, \ldots, \; \text{and} \; \forall \rho \geq 0,$$

(4)

where $\rho$ is a density matrix on $H_s \otimes \mathbb{C}^n$. Physically, it is a reasonable condition since the extension $V_t \otimes I_n$ can be considered in quantum information as an operator on the composite quantum system Alice and Bob, which acts locally on Alice’s system without influencing Bob. Furthermore, complete positivity essentially ensures that tensor products of maps $V_t$ remain positive, an important property especially when considering entangled states.

However, extracting from a dynamical map the Hamiltonian term in the usual way \[16\] leads to a hermitian Hamiltonian in a master equation like Eq. (1). In this sense the
authors of Ref. [17] investigated recently decoherence and decay of the neutral kaons by using a dynamical map corresponding to a master equation with hermitian Hamiltonian. Nevertheless, many authors work with a non–hermitian Hamiltonian—which is a standard procedure in particle physics (see, e.g., Ref. [18])—in order to include the decay property of the particle.

**The formalism:** We are going to show in this letter that both approaches—each one having its own appeal—are indeed equivalent to each other for quite general quantum systems. To be more precise, we ask the following question:

*Can we work with a hermitian Hamiltonian and incorporate the decay as Lindblad operator such that the time evolution of the system represents a completely positive map? Moreover, does it describe the WWA properly without effecting decoherence and/or dissipation?*

The answer will be yes, it is possible! But we have to enlarge the Hilbert space and include formally the decay products of the unstable states.

Thus we assume that the total Hilbert space $H_{\text{tot}}$ is the direct sum

$$H_{\text{tot}} = H_s \oplus H_f,$$

(5)

where $H_s$ contains the states of the system we are interested in whereas $H_f$ is the space of the “decay states,” defined in the following way. We assume that $d_s \equiv \dim H_s < \infty$. Then the non-hermitian part $\Gamma$ of the effective Hamiltonian in Eq. (3) can be decomposed as

$$\Gamma = \sum_{j=1}^{r} \gamma_j |\varphi_j \rangle \langle \varphi_j| \quad \text{with} \quad \gamma_j > 0 \ \forall \ j,$$

(6)

with an orthonormal system $\{\varphi_j \}$ in $H_s$ and $r = \dim H_s - n_0$, where $n_0$ denotes the degeneracy of the eigenvalue zero of $\Gamma$. We demand that $\dim H_f \equiv d_f \geq r$, otherwise $H_f$ is arbitrary.

In the following, $\rho$ denotes a density matrix on $H_{\text{tot}}$, where it has the following decomposition:

$$\rho = \begin{pmatrix} \rho_{ss} & \rho_{sf} \\ \rho_{fs} & \rho_{ff} \end{pmatrix} \quad \text{with} \quad \rho_{ss}^\dagger = \rho_{ss}, \quad \rho_{ff}^\dagger = \rho_{ff}, \quad \rho_{fs}^\dagger = \rho_{sf}.$$

(7)

Now we have to define the time evolution $\rho$ on $H_{\text{tot}}$. The Hamiltonian $H$ and the Lindblad operators $A_j$ are easily extended to the total Hilbert space by

$$\mathcal{H} = \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathcal{A}_j = \begin{pmatrix} A_j & 0 \\ 0 & 0 \end{pmatrix}.$$

(8)

Note that for the definition of $\mathcal{H}$ we have used the hermitian part $H$ of $H_{\text{eff}}$.

Now we turn to the decay. We need a Lindblad operator $\mathcal{B}$ on the full space $H_{\text{tot}}$ which describes the decay in the subspace $H_s$. As we will see in the next paragraph, the decay is described by

$$\mathcal{B} = \begin{pmatrix} 0 & 0 \\ B & 0 \end{pmatrix} \quad \text{with} \quad B : H_s \to H_f$$

(9)
\[ \Gamma = B^\dagger B. \]  
(10)

Let \( \{ f_k \} \) be an orthonormal basis of \( H_f \). Then we can decompose \( B \) as
\[ B = \sum_{k=1}^{d_f} \sum_{j=1}^{r} b_{kj} |f_k\rangle \langle \varphi_j|. \]  
(11)

In order to fulfill Eq. (10), we require
\[ \sum_{k=1}^{d_f} b_{kj}^* b_{kj} = \delta_{ij} \gamma_j. \]  
(12)

For \( d_f \geq r \), such a \( d_f \times r \) matrix \( (b_{kj}) \) always exists. The simplest case is \( d_f = r \), where we can choose
\[ B = \sum_{j=1}^{d_f} \sqrt{\gamma_j} |f_j\rangle \langle \varphi_j|. \]  
(13)

In that case, each unstable decaying state \( |\varphi_j\rangle \) would decay into just one specific decay state \( |f_j\rangle \).

Then we can write the following master equation for the density matrix on \( H_{\text{tot}} \):
\[ \frac{d\rho}{dt} = -i [H, \rho] - D[\rho], \]  
(14)

with the dissipator
\[ D[\rho] = \frac{1}{2} \sum_j \left( A_j^\dagger A_j \rho + \rho A_j^\dagger A_j - 2 A_j \rho A_j^\dagger \right) + \frac{1}{2} \left( B^\dagger B \rho + \rho B^\dagger B - 2 B \rho B^\dagger \right). \]  
(15)

To prove that this master equation contains Eq. (1), we decompose it with respect to the components of \( \rho \):
\[ \hat{\rho}_{ss} = -i [H, \rho_{ss}] - \frac{1}{2} \{ B^\dagger B, \rho_{ss} \} - \frac{1}{2} \sum_j \left( A_j^\dagger A_j \rho_{ss} + \rho_{ss} A_j^\dagger A_j - 2 A_j \rho_{ss} A_j^\dagger \right), \]  
(16)
\[ \hat{\rho}_{sf} = -i H \rho_{sf} - \frac{1}{2} B^\dagger B \rho_{sf} - \frac{1}{2} \sum_j A_j^\dagger A_j \rho_{sf}, \]  
(17)
\[ \hat{\rho}_{ff} = B \rho_{ss} B^\dagger. \]  
(18)

Indeed, with Eq. (11), we immediately see that Eq. (16) for \( \rho_{ss} \) reproduces the original equation (1). Furthermore, it is obvious from Eqs. (14) and (15) that \( \text{Tr} \rho(t) = 1 \quad \forall \ t \geq 0 \).

At this point, some general remarks are at order. By construction, the time evolution of \( \rho_{ss} \) is independent of \( \rho_{sf} \), \( \rho_{fs} \), and \( \rho_{ff} \). Actually, the time evolution of \( \rho_{sf} \) or \( \rho_{fs} \) completely decouples from that of \( \rho_{ss} \) and \( \rho_{ff} \). The time evolution of \( \rho_{ff} \), the density matrix of the decay states, is determined solely by \( \rho_{ss}(t) \) and is the characteristic for a decay process!
With the initial condition $\rho_{ff}(0) = 0$, it is simply given by

$$
\rho_{ff}(t) = B \int_0^t dt' \rho_{ss}(t') B^\dagger.
$$

If we choose the initial condition $\rho_{sf}(0) = 0$, then $\rho_{sf}$ remains zero for all times and the same applies to $\rho_{fs}$. Anyway, these parts of $\rho$ are totally irrelevant for our discussion.

Generally, for decaying systems the following properties of the time evolution (14) are most important:

- $\rho_{ss}(t)$ and $\rho_{ff}(t)$ are positive $\forall t \geq 0$;
- The time evolution of $\rho_{ss}$ is completely positive.

**Proof:** The density matrix $\rho(t)$ obeys the time evolution given by the master equation (14), therefore, $\rho(t) \geq 0 \forall t \geq 0$. Thus, confining ourselves to vectors $v \in H_s$, we evidently have $0 \leq \langle v|\rho(t)v \rangle \equiv \langle v|\rho_{ss}(t)v \rangle$ and, therefore, $\rho_{ss}(t) \geq 0$. The same reasoning holds for $\rho_{ff}(t)$. As for complete positivity, we note that on $H_{tot} \otimes \mathbb{C}^n$ a general operator has the structure $R = \sum_k \sigma_k \otimes L_k$, with $\sigma_k$ operating on $H_{tot}$ and $L_k$ on $\mathbb{C}^n$. We know that the dynamical map $V_t$ induced by Eq. (14) is completely positive. Therefore, if $R \geq 0$, then we have $(V_t \otimes 1_n)[R] \geq 0$. We also know from Eqs. (16), (17), and (18), that $V_t$ has a well defined restriction to operators acting purely on $H_s$. Thus, $R \geq 0$ on $H_s \otimes \mathbb{C}^n$ is mapped into a positive operator on the same space by $V_t \otimes 1_n$. This concludes the proof.

The case of a non-singular $\Gamma$: Finally, it is interesting to consider the special case of a non-singular $\Gamma$, where all states of $H_s$ decay. Then, $\dim H_f \geq \dim H_s$ and, in addition to what we discussed before, the following properties of the time evolution (14) hold:

- $\lim_{t \to \infty} \rho_{sf}(t) = 0$,
- $\lim_{t \to \infty} \rho_{ss}(t) = 0$,
- $\lim_{t \to \infty} \Tr \rho_{ff}(t) = 1$.

**Proof:**

i) We consider the equation

$$
\frac{d}{dt} \omega = -iH \omega - \frac{1}{2} \Gamma' \omega, \quad \text{with} \quad \Gamma' = \Gamma + \sum_j A_j^\dagger A_j
$$

and $\omega(t) \in H_s$. From Eq. (20) we derive

$$
\frac{d}{dt} |\omega|^2 = -\langle \omega | \Gamma' \omega \rangle \leq -\gamma_0' |\omega|^2,
$$

where $\gamma_0' > 0$ is the smallest eigenvalue of $\Gamma'$. Since $|\omega|^2 \geq 0$, it follows from this equation that $|\omega(t)|^2 \leq |\omega(0)|^2 \exp(-\gamma_0' t)$ and, consequently, $\lim_{t \to \infty} \omega(t) = 0$. This leads to $\lim_{t \to \infty} \rho_{sf}(t) = 0$, because $\rho_{sf}$ is a linear combination of operators $|\omega\rangle\langle f|$ with $\omega \in H_s, f \in H_f$. 

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ii) Taking the trace of Eq. (16), we obtain
\[ \frac{d}{dt} \text{Tr} \rho_{ss}(t) = -\text{Tr} (\Gamma \rho_{ss}(t)) \leq -\gamma_0 \text{Tr} \rho_{ss}(t). \] (22)

Here, \( \gamma_0 \) is the smallest eigenvalue of \( \Gamma \). From Eq. (22) we derive the inequality
\[ \text{Tr} \rho_{ss}(t) \leq \text{Tr} \rho_{ss}(0) \exp(-\gamma_0 t), \]
whence we find \( \lim_{t \to \infty} \text{Tr} \rho_{ss}(t) = 0 \). Since \( \rho_{ss}(t) \geq 0 \), the whole matrix must vanish in the limit \( t \to \infty \).

iii) Point ii) and \( \text{Tr} \rho(t) = \text{Tr} \rho_{ss}(t) + \text{Tr} \rho_{ff}(t) = 1 \) imply \( \lim_{t \to \infty} \text{Tr} \rho_{ff}(t) = 1 \).

The simplest possible example: We choose the minimal dimensions \( d_s = d_f = 1 \), the Hamiltonian
\[ \mathcal{H} = \begin{pmatrix} m & 0 \\ 0 & 0 \end{pmatrix}, \] (23)
and set \( A_j = 0 \), i.e. we neglect any decoherence part. Then, Eqs. (16), (18) and (19) simplify considerably, providing the result
\[ \rho(t) = \begin{pmatrix} e^{-\Gamma t} & 0 \\ 0 & 1 - e^{-\Gamma t} \end{pmatrix}, \] (24)
where we have chosen the initial conditions \( \rho_{ss}(0) = 1, \rho_{ff}(0) = \rho_{sf}(0) = 0 \). This example illustrates the general fact that, for non-singular \( \Gamma \), the probability loss of the system is balanced by the probability increase of the decay states.

Considering the mixedness of the quantum states, we can use as measure
\[ \delta(t) \equiv \text{Tr} \rho^2(t) = 1 - 2 e^{-\Gamma t} + 2 e^{-2 \Gamma t}. \] (25)
We have \( \delta(0) = 1, \lim_{t \to \infty} \delta(t) = 1 \) and \( \delta(t) < 1 \) for \( 0 < t < \infty \), i.e. in the beginning, \( \rho \) represents a pure state, then the state is mixed, whereas for large times it approaches a pure state again, when the system definitely has changed into the decay state.

The case of neutral kaons, where the Hamiltonian \( H \) and the operator \( B \) are \( 2 \times 2 \) matrices, has been investigated in detail in Ref. [17].

Kraus operators: Finally, in the case of our example, we would like to consider the time evolution of the density matrix as a dynamical map \( V_t \). In our case, \( V_t \) can be represented by a sum of operators [1, 2]:
\[ \rho(0) \to V_t[\rho(0)] = \sum_j M_j(t) \rho(0) M_j^\dagger(t) = \rho(t), \] (26)
with the normalization \( \sum_j M_j^\dagger(t) M_j(t) = 1 \) for the Kraus operators \( M_j(t) \). For the correspondence between the Lindblad and Kraus operators see Ref. [16].

The operator sum representation (26) is a very useful approach in quantum information to describe the quantum operations or the specific quantum channels. In our example, the decay of a particle corresponds to the amplitude damping channel of a quantum
operation [19], e.g., the spontaneous emission of a photon, and we can calculate the Kraus operators needed:

\[
M_0(t) = \begin{pmatrix}
\sqrt{1 - p(t)} & 0 \\
0 & 1
\end{pmatrix} \quad \text{and} \quad M_1(t) = \begin{pmatrix}
0 & 0 \\
\sqrt{p(t)} & 0
\end{pmatrix},
\]

(27)

with the probability \( p(t) = 1 - e^{-\Gamma t} \).

**Conclusions:** In this letter we have considered a time evolution given by Eq. (1), with a non-hermitian Hamiltonian \( H_{\text{eff}} \) and a dissipator of the Lindblad form (2). Assuming that the non-hermitian part of \( H_{\text{eff}} \) describes “particle decay,” we have shown that such a time evolution is completely positive. Our strategy was to add the space of “decay states” \( H_f \) to the space of states \( H_s \) and to extend the time evolution in a straightforward way to the full space \( H_s \oplus H_f \), such that this full time evolution is probability-conserving. With the initial condition that the density matrix is only non-zero on \( H_s \), the Lindblad operator \( B \) of Eq. (9), which is responsible for the decay, shifts states from \( H_s \) to \( H_f \), whereas at the same time the \( A_j \) terms cause decoherence and dissipation on \( H_s \). Thus, particle decay and decoherence/dissipation are related phenomena, which can be described by the same formalism of a completely positive time evolution.

**Acknowledgement:** The authors acknowledge financial support of EURIDICE HPRN-CT-2002-00311.
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