On the existence of dynamical systems with exponentially decaying collision operators

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Abstract. The article is concerned with the time-domain collision operator ψ of the Brussels school of non-equilibrium statistical mechanics: $\psi(t) = PLQ\exp(tQLQ)QLP$, where L is the skew-adjoint Liouville operator of a dynamical system, and P and Q are complementary orthogonal projectors. Under the assumption that P is finite rank, we prove that if ψ is norm-bounded by a decreasing exponential, then L must have a certain spectral property, and that, conversely, this spectral property guarantees the existence of a projector P for which the corresponding ψ decays exponentially. We use this characterisation to show that K-systems admit exponentially decaying collision operators. We also show that this property is enjoyed by the collision operator of the Pietenpol model for a large class of interactions. This answers in the affirmative a question raised by Coveney and Penrose (*J. Phys. A: Math. Gen.* **25**, 4947–4966 (1992)).

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1. Introduction

A particularly fertile approach to the statistical mechanics of irreversible processes is based on the idea of a master equation. The first such equation is due to Pauli [29], who sought to generalise Boltzmann's kinetic equation to arbitrary quantum systems. In this endeavour he derived an equation which describes the relaxation of a macroscopic quantum system towards thermal equilibrium in terms of the occupation numbers of its quantum levels. Pauli's derivation was later generalised by van Hove [21, 22], Montroll [26], and Prigogine and Résibois [35].

The key idea of the master equation approach is that the macroscopic properties of a system can be understood in terms of a reduced description of the underlying microscopic dynamics. In this way one hopes to understand how the observed irreversible behaviour of matter in bulk arises from the fundamental reversible laws of motion governing its constituents. The reduction amounts to selecting a 'relevant' and an 'irrelevant' part of the total dynamics. A typical situation is that of a system interacting with a larger one, usually called the reservoir. The overall dynamics are given by the compound system, that is, the original system and the reservoir, and the relevant part may be chosen to be the resulting dynamics of the system itself [12, 18]. Another possibility arises if we consider a system comprising a large number of particles. In this case one can think of the relevant part as being given by the macroscopically observable quantities (the 'slow variables') [16].

Although these two set-ups are rather different from a physical point of view, they can be treated using the same mathematical method leading to the so-called 'generalised master equation'. To be precise we assume that we are given a group $\left\{ U(t) \,\middle|\, t \in \mathbb{R} \right\}$ of unitary operators acting on a Hilbert space, which describes the total dynamics of a system. Using Zwanzig's projector formalism [43, 44, 16], the separation into relevant and irrelevant parts can be modelled by a pair of complementary projectors P and Q, $P + Q = I$. A short calculation shows that the relevant part of the total evolution $V(t) := PU(t)P$ satisfies the following integro-differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}V(t) = PLPV(t) + \int_0^t \psi(t-s)V(s)\,\mathrm{d}s, \tag{1}$$

where L denotes the infinitesimal generator of the group (known as the 'Liouville operator' in this context), and $\psi(t)$ is a certain operator-valued function. This equation, first derived independently by Nakajima [27] and Zwanzig [43], is the generalised master equation. It yields a closed equation for the reduced part $V(t)$ of the total evolution, which, however, is non-local in time. This is due to the presence of the 'memory term', that is the integral involving ψ.

In order to pass from this equation to an autonomous equation resembling the kinetic equations of statistical mechanics a further idea is invoked. The Liouville operator L of the system is taken to be a perturbation of a simpler operator $L = L_0 + \lambda L_1$. Markovian master equations can then be derived in a limiting case (the 'van Hove' or 'weak coupling' limit), in which the parameter λ measuring the size of the perturbation goes to zero, while the time-variable, suitably re-scaled, goes to infinity (see [10, 11]).

Another way of thinking, associated with the Brussels school of non-equilibrium statistical mechanics, maintains that it should be possible to derive Markovian master equations that are valid not just in a limit but over a finite range of the parameter λ. At the heart of this approach is the construction of an idempotent operator which projects onto an invariant subspace of the Liouville operator L, such that the elements of this subspace obey an autonomous evolution equation, which is the desired Markovian equation (see [5, 33, 15, 34, 17]). In this version of the formalism an important role is played by the kernel ψ, termed the 'collision operator' by the Brussels school‡. This operator is also the focus of attention in an investigation by Coveney and Penrose [9], who have analysed the Brussels method from a rigorous point of view. Under the

‡ These ideas represent the key aspects of the theory as it stood in 1975. The formalism has since undergone various developments. See [3, 4] for an exposition of a current version.

assumption that P is a finite rank projector they were able to show that, if the collision operator is norm-bounded by a decreasing exponential, then at least the central part of the formalism holds.

In view of this result it is important to establish whether there exist dynamical systems with exponentially decaying collision operators — a question left open in [9]. The purpose of the present paper is to characterise and construct systems with this property. Specifically, we shall show that if P is a finite rank projector, then the existence of an exponentially decaying collision operator implies that the spectrum of the Liouville operator L of the system must have a certain property, which we call a 'Lebesgue component with full support' (see Section 3). We also prove that if a system has a generator L with a Lebesgue component with full support, then there exists a finite rank projector P for which the norm of the corresponding collision operator decays exponentially (Section 4); for brevity, we shall refer to these as systems with exponentially decaying collision operators. We then use this characterisation to show that K-systems admit exponentially decaying collision operators (Section 5). In the final section, we consider a simple quantum mechanical model of an unstable particle, the so-called Pietenpol model, and establish that the associated collision operator decays exponentially, provided that the interaction is suitably chosen.

2. The generalised master equation

To derive the generalised master equation we assume that the microscopic dynamics of a system are given by a strongly continuous group $\left\{ U(t) \,\middle|\, t \in \mathbb{R} \right\}$ of unitary operators acting on a Hilbert space H. Elements of H are taken to represent the states of the system, while $\{U(t)\}$ implements the temporal evolution of the states, that is, if $f \in H$ is the state of the system at time zero, then $U(t)f$ is the state of the system at time t.

Denoting the infinitesimal (skew-adjoint) generator of this group by L and its domain by $\mathcal{D}(L)$ we have

$$\frac{\mathrm{d}}{\mathrm{d}t} U(t) f_0 = L U(t) f_0 \text{ for } f_0 \in \mathcal{D}(L),$$

so that $f(t) := U(t) f_0$, $t \in \mathbb{R}$, is a continuously differentiable solution of the equation

$$\frac{\mathrm{d}}{\mathrm{d}t} f(t) = L f(t) \tag{2}$$

subject to the initial condition $f(0) = f_0$. In this context the above equation is known as the Liouville-von Neumann equation with L being the Liouville operator of the system.

In practice, this scenario arises in the following ways.

1. *Classical statistical mechanics.* Suppose we are given a group

$$\left\{ T(t) \,\middle|\, t \in \mathbb{R} \right\}$$

of measure-preserving transformations acting on a probability space X such that the mapping $(x,t) \mapsto T(t)x$ is measurable. These conditions are satisfied in classical mechanics, where the invariant measure is guaranteed by Liouville's theorem. The

Hilbert space H my then be taken to be $L^2(X)$, the space of square-integrable functions over X, while the unitary group is given by the group $\{U(t)\}$ of Koopman operators

$$U(t)f := f \circ T(t).$$

The strong continuity of $\{U(t)\}$ follows from a theorem of von Neumann [36, Theorem VIII.9].

2. a) *Quantum mechanics.* Here H is the ordinary quantum mechanical Hilbert space and $\{U(t)\}$ the strongly continuous evolution generated by the self-adjoint Hamiltonian of the system.
   b) *Quantum statistical mechanics.* In this case the Hilbert space is given by the space of Hilbert-Schmidt density matrices, and $\{U(t)\}$ is the strongly continuous unitary group induced by the ordinary quantum mechanical evolution on the space of density matrices.

Further information on the physical content of these constructions can be found in [32, 5, 30].

As we mentioned in the introduction, the separation into relevant and irrelevant parts will be modelled by a pair of orthogonal projectors P and Q with $P + Q = I$. To derive an expression for the relevant part $Pf(t)$ of the total evolution we shall assume that

(M1) $Pf \in \mathcal{D}(L)$ and $Qf \in \mathcal{D}(L)$ for every $f \in \mathcal{D}(L)$;

(M2) PLP, PLQ, and QLP extend to everywhere-defined continuous operators;

(M3) QLQ is the infinitesimal generator of a strongly continuous quasi-bounded semigroup (see [24, p. 485] for the definition).

(M1) and (M2) are innocuous technical assumptions, while (M3) expresses the requirement that the dynamics in the Q subspace exist. Inserting P and Q in equation (2) we obtain the pair of differential equations

$$\frac{\mathrm{d}}{\mathrm{d}t} Pf(t) = PLf(t) = PLPf(t) + PLQf(t) \tag{3}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} Qf(t) = QLf(t) = QLPf(t) + QLQf(t). \tag{4}$$

The second equation is an inhomogeneous differential equation for $Qf(t)$. Since, by (M2), the function $\mathbb{R} \ni t \mapsto QLPf(t)$ is continuous, and since, by (M3), QLQ generates a strongly continuous quasi-bounded semigroup, we may invoke a theorem of Phillips (see [24, IX. Theorem 1.19]) to obtain a solution of equation (4) for positive t

$$Qf(t) = \exp(tQLQ)Qf_0 + \int_0^t \exp((t-s)QLQ)QLPf(s)\,\mathrm{d}s. \tag{5}$$

Inserting this expression into (3) yields

$$\frac{\mathrm{d}}{\mathrm{d}t} Pf(t) = PLPf(t) + PLQ\exp(tQLQ)Qf_0 + \int_0^t PLQ\exp((t-s)QLQ)QLPf(s)\,\mathrm{d}s,$$

where we used assumption (M2) to put PLQ under the integral.

If f_0 belongs to the range of P, that is, if $Pf_0 = f_0$, then the equation takes the form

$$\frac{\mathrm{d}}{\mathrm{d}t}V(t)f_0 = PLPV(t)f_0 + \int_0^t \psi(t-s)V(s)f_0\,\mathrm{d}s, \tag{6}$$

which is the desired generalised master equation. Here ψ, the (time-domain) collision operator of the Brussels school, is defined by

$$\psi(t) := PLQ\exp(tQLQ)QLP \quad (t \in \mathbb{R}^+) \tag{7}$$

and $V(t)$, the reduced evolution, is given by

$$V(t) := PU(t)P \quad (t \in \mathbb{R}^+).$$

The generalised master equation (6) is a closed integro-differential equation for the relevant part $PU(t)f_0 = Pf(t)$ of the total evolution. One method of studying this equation, which is in fact the route normally taken by the Brussels school, is to consider its Laplace transform. Denoting Laplace transforms by tildes, so that, for example,

$$\widetilde{V}(z) := \int_0^\infty \mathrm{e}^{-zt}V(t)\,\mathrm{d}t, \quad (\operatorname{Re} z > 0)$$

equation (6) is transformed into

$$z\widetilde{V}(z)f_0 - Pf_0 = PLP\widetilde{V}(z)f_0 + \widetilde{\psi}(z)\widetilde{V}(z)f_0.$$

For later use we note that $\widetilde{V}$ and $\widetilde{\psi}$ can be expressed in terms of the resolvents of L and QLQ:

$$\widetilde{V}(z) = P[z-L]^{-1}P, \quad (\operatorname{Re} z > 0) \tag{8}$$

$$\widetilde{\psi}(z) = PLQ[z-QLQ]^{-1}QLP, \quad (\operatorname{Re} z > a) \tag{9}$$

for a suitable $a \in \mathbb{R}$.

Formally solving for $\widetilde{V}(z)$ in the above yields

$$\widetilde{V}(z)f_0 = P[z - PLP - \widetilde{\psi}(z)]^{-1}Pf_0. \tag{10}$$

Taking the inverse Laplace transform of this equation, we obtain a formal solution of the generalised master equation (6) ($\gamma > 0$):

$$V(t)f_0 = \frac{1}{2\pi\mathrm{i}}\int_{\gamma-\mathrm{i}\infty}^{\gamma+\mathrm{i}\infty} \mathrm{e}^{zt}P[z - PLP - \widetilde{\psi}(z)]^{-1}Pf_0\,\mathrm{d}z \quad (t \in \mathbb{R}^+). \tag{11}$$

In their analysis of the Brussels formalism, Coveney and Penrose studied the asymptotic behaviour of $V(t)$ under the assumption that P is a finite rank operator, that is $\dim P(H) < \infty$ [9]. The central result of their paper, which is also of independent interest, shows that if the time-domain collision operator ψ has the following property

$$\exists K > 0, b > 0 \text{ such that } \|\psi(t)\| \le K\mathrm{e}^{-bt} \quad (t \in \mathbb{R}^+), \tag{12}$$

where $\|.\|$ denotes the operator norm, then $V(t)$ splits into the sum

$$V(t) = W(t) + \hat{W}(t),$$

with $W(t)$ and $\hat{W}(t)$ enjoying the following properties

(i) $\exists \hat{K} > 0$ such that $\left\|\hat{W}(t)\right\| \leq \hat{K} \mathrm{e}^{-bt/2} \quad (t \in \mathbb{R}^+)$;

(ii) $W(t) = \exp(tP\Gamma P)$, where $P\Gamma P$ is a finite rank operator whose spectrum is contained in $\left\{ z \,\middle|\, -b/2 \leq \operatorname{Re} z \leq 0 \right\}$.

Our next task is to consider the consequences of the condition (12), which we shall also refer to as 'ψ decays exponentially'.

3. Exponential decay: necessary conditions

In trying to understand what properties the system must have if it admits an exponentially decaying collision operator, we shall aim at obtaining a spectral characterisation. More precisely, we shall establish that if a system described by a unitary evolution $\{\exp(tL)\}$ admits an exponentially decaying collision operator, then the spectral representation of $\{\exp(tL)\}$ must be of a certain type.

We shall consider first the simplest case, that of an everywhere vanishing collision operator.

Proposition 1. *P commutes with L if and only if $\psi(t) = 0$ for every $t > 0$.*

Proof. The 'only if'-clause is a simple consequence of the fact that $PQ = 0$. To prove the 'if'-clause let $A := PLQ$. Then, using (M1) and (M2), the Hilbert space adjoint A^* of A is QLP. Thus, if $\psi(t) = 0$ for $t > 0$, then

$$A \exp(tQLQ) A^* f = 0 \tag{13}$$

for every $f \in H$ and every $t > 0$. Letting $t \to 0$ from above we obtain $AA^* f = 0$ for every $f \in H$ by virtue of (M2) and (M3). Thus, $AA^* = 0$, which implies $A = A^* = 0$. This means that

$$PLQf = PLf - PLPf = 0$$
$$QLPf = LPf - PLPf = 0$$

for $f \in \mathcal{D}(L)$ and we conclude that $PLf = PLPf = LPf$ for every $f \in \mathcal{D}(L)$. □

This case is uninteresting, because the decomposition into relevant and irrelevant parts is then trivial. What happens if instead the system has a non-vanishing, exponentially decaying collision operator? An immediate consequence is that the spectrum of QLQ must fill the entire imaginary axis, that is, $\sigma(QLQ) = \mathrm{i}\mathbb{R}$. To see this, we note that if the collision operator $\psi(t) = PLQ \exp(tQLQ)QLP$ decays exponentially, then so does $\exp(tQLQ)$. This, however, is known to entail that $\sigma(QLQ) = \mathrm{i}\mathbb{R}$. For a discussion of this result, as well as its connection with the problem relating to the description of exponentially decaying unstable particles, see [42, 19, 38, 13].

As we are aiming at a characterisation of systems with exponentially decaying collision operators we need a slightly sharpened version of this result. In order to formulate it we require the following terminology.

Definition 1. Let $\{U(t)\}$ be a strongly continuous unitary group acting on the Hilbert space H. If there is a closed subspace K of H such that $U(t)K \subset K$ for every $t \in \mathbb{R}$, then K is called an *invariant subspace* for $\{U(t)\}$. The group $\{U(t)\}$ is said to have a *Lebesgue-component with full support* ('LCFS' for short), if there is an invariant subspace K of $\{U(t)\}$ and a unitary transformation $W : K \to L^2(\mathbb{R}, dx)$ such that

$$WU(t)W^{-1}f = \mathrm{e}^{\mathrm{i}tx} f$$

for every $f \in L^2(\mathbb{R}, dx)$ and $t \in \mathbb{R}$.

Remark 1. In the definition above and in what follows we use the convention that 'x' denotes both the variable x and the maximal operator of multiplication by x on $L^2(\mathbb{R}, dx)$, that is,

$$x : L^2(\mathbb{R}, dx) \to L^2(\mathbb{R}, dx),$$

$$(xf)(x) := xf(x),$$

with domain $\mathcal{D}(x) = \left\{ f \in L^2(\mathbb{R}, dx) \,\middle|\, \int_{\mathbb{R}} |xf(x)|^2 \,\mathrm{d}x < \infty \right\}$. Thus, in particular, $\{\mathrm{e}^{\mathrm{i}tx}\}$ denotes the strongly continuous unitary group

$$\mathrm{e}^{\mathrm{i}tx} : L^2(\mathbb{R}, dx) \to L^2(\mathbb{R}, dx),$$

$$(\mathrm{e}^{\mathrm{i}tx} f)(x) := \mathrm{e}^{\mathrm{i}tx} f(x), \quad (t \in \mathbb{R}).$$

Remark 2. It is not difficult to see that a strongly continuous unitary group $\{\exp(tL)\}$ with skew-adjoint generator L has a LCFS if and only if K is an invariant subspace for L and

$$WLW^{-1}f = \mathrm{i}xf$$

for every $f \in \mathcal{D}(x)$. In this case K belongs to the absolutely continuous subspace of L (see [24, X.1.2]) and $\sigma(L) = \mathrm{i}\mathbb{R}$.

The following preparatory lemma is well known in this context (see [42]); we include its proof for the convenience of the reader.

Lemma 1. *Let $\{U(t)\}$ be a strongly continuous unitary group on H. Suppose that there is $f_0 \in H$ such that $t \mapsto \phi(t) := (U(t)f_0, f_0)$ is non-zero on $\mathbb{R}^+$. If there exist $K > 0$ and $b > 0$ such that*

$$|\phi(t)| \le K\mathrm{e}^{-bt} \quad \textit{for } t > 0, \tag{14}$$

then there is a positive, real-analytic $h \in L^2(\mathbb{R}, dx)$ with $\operatorname{supp} h = \mathbb{R}$ (that is, the support of h is all of $\mathbb{R}$) such that

$$(U(t)f_0, f_0) = \phi(t) = \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}tx} h(x) \,\mathrm{d}x \quad \textit{for every } t \in \mathbb{R}.$$

Proof. Let μ be the spectral measure associated with f_0, so that

$$\phi(t) = \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}tx}\,\mathrm{d}\mu(x).$$

Interpreting μ and ϕ as tempered distributions we may invoke the Fourier inversion theorem to conclude that $\mu = \check{\phi}$, where $\check{}$ denotes the inverse Fourier transform for tempered distributions (see [36, Theorems IX.1 and IX.2]). Since ϕ is square-integrable we obtain $\int g\,d\mu = \int \phi\check{g}\,\mathrm{d}x = \int \check{\phi} g\,\mathrm{d}x$ for every $g \in \mathcal{S}(\mathbb{R})$. Thus, $d\mu = \check{\phi}\,dx = h\,dx$, where

$$h(x) = \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}tx}\phi(t)\,\mathrm{d}x. \tag{15}$$

We now observe that (14) implies that $|\phi(t)| \leq K\mathrm{e}^{-bt}$ for every t. This follows from $\overline{\phi(t)} = (f_0, U(t)f_0) = (U(-t)f_0, f_0) = \phi(-t)$. Thus, we conclude from (15) that h extends to an analytic function on $\left\{ z \,\middle|\, |\mathrm{Im}\, z| < b \right\}$. This means that h can only have countably many zeros, that is $\operatorname{supp} h = \mathbb{R}$. Finally, h is integrable, since μ is a finite measure. □

As a consequence, we obtain the following theorem.

Theorem 1. *If $\{U(t)\}$ satisfies the hypotheses of the previous lemma, then $\{U(t)\}$ has a LCFS.*

Proof. Let K' denote the linear span of the set $\left\{ U(t)f_0 \,\middle|\, t \in \mathbb{R} \right\}$ and let K be the closure of K'. Clearly, K is an invariant subspace of $\{U(t)\}$. On K' define a linear transformation $W : K' \to L^2(\mathbb{R}, dx)$ by

$$W : U(t)f_0 \mapsto \mathrm{e}^{\mathrm{i}tx}h^{1/2}.$$

Now observe that

$$(U(t_1)f_0, U(t_2)f_0)_H = (U(t_1 - t_2)f_0, f_0)_H = \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}(t_1-t_2)x}h(x)\,\mathrm{d}x = (\mathrm{e}^{\mathrm{i}t_1x}h^{1/2}, \mathrm{e}^{\mathrm{i}t_2}h^{1/2})_{L^2(\mathbb{R},dx)},$$

which implies that W is an isometry. Since $h > 0$ a.e. on $\mathbb{R}$, the range of W is dense in $L^2(\mathbb{R}, dx)$; thus W extends to a unitary operator from K to $L^2(\mathbb{R}, dx)$. Moreover, as

$$WU(t)W^{-1}\mathrm{e}^{\mathrm{i}t_0x} = \mathrm{e}^{\mathrm{i}tx}\mathrm{e}^{\mathrm{i}t_0x},$$

we may conclude that $WU(t)W^{-1}f = \mathrm{e}^{\mathrm{i}tx}f$ for every $f \in L^2(\mathbb{R}, dx)$ by a limiting argument. Thus, $\{U(t)\}$ has a LCFS. □

We are now able to prove the following necessary condition for the existence of a non-zero exponentially decaying collision operator.

Theorem 2. *Suppose that the time-domain collision operator*

$$\psi(t) = PLQ\exp(tQLQ)QLP$$

is non-zero. If $\psi(t)$ decays exponentially, then $\{\exp(tQLQ)\}$ has a LCFS.

Proof. Since $\psi(t)$ is non-zero, there exists a $t_0 \in \mathbb{R}$ such that $\psi(t_0) \neq 0$. Thus, there is $f_0 \in H$ such that $(\psi(t_0)f_0, f_0) \neq 0$. Since $t \mapsto \psi(t)$ is strongly continuous, the function $t \mapsto (\psi(t)f_0, f_0) = (\exp(tQLQ)QLPf_0, QLPf_0)$ is non-zero. Observing that $|(\psi(t)f_0, f_0)| \leq \|\psi(t)\| \, \|f_0\|^2$ and using the fact that $\psi(t)$ decays exponentially, we conclude that $\{\exp(tQLQ)\}$ has a LCFS by theorem 1. □

If P is finite rank we can conclude more.

Theorem 3. *Suppose that $\psi(t)$ is non-zero and decays exponentially. If P is a finite rank projector, then the full evolution $\{\exp(tL)\}$ has a LCFS.*

Proof. By hypothesis and the previous theorem $\{\exp(tQLQ)\}$ has a LCFS. Since $L = QLQ + (PLP + PLQ + QLP)$ and P is a finite rank projector, L is a finite rank — and hence *a fortiori* a trace class — perturbation of QLQ. By the Kato-Rosenblum Theorem (see [24, X. Theorem 4.4]) the absolutely continuous subspaces of L and QLQ are unitarily equivalent. Thus, $\{\exp(tL)\}$ has a LCFS by Remark 2. □

4. Exponential decay: sufficient conditions

In the previous section we saw that the existence of an exponentially decaying collision operator imposes certain restrictions on the spectral properties of the full evolution of the system. In particular, we showed that a decaying collision operator implies that the full evolution $\{\exp(tL)\}$ has a LCFS, provided that P is a finite rank projector. We shall presently establish that the converse is true in the following sense: if $\{\exp(tL)\}$ has a LCFS, then it is possible to choose a rank-1 projector P such that the corresponding collision operator decays exponentially.

We shall prove this in two steps. First we assume that the full evolution is given by $\{e^{itx}\}$ on $L^2(\mathbb{R}, dx)$ and show that in this case an appropriate P can be chosen. In the next step we shall extend this procedure to the case where $\{U(t)\}$ has a LCFS.

Step 1. Let $U(t) := e^{itx}$, so that the infinitesimal generator L of $\{U(t)\}$ is ix. Let $f_0 \in L^2(\mathbb{R}, dx)$ be defined as

$$f_0(x) := \sqrt{\frac{2r^3}{\pi}} \frac{1}{(x + ir)^2} \quad (r > 0).$$

Since $\|f_0\| = 1$, the operator P given by

$$Pf := (f, f_0)f_0$$

is an orthogonal projection onto the subspace spanned by f_0. We note that ixf_0 is square-integrable, so that $f_0 \in \mathcal{D}(L)$, which implies that the assumptions (M1) and (M2) of Section 2 hold. Furthermore, (M3) is also satisfied, since QLQ is a finite-rank perturbation of L (see [24, IX. Theorem 2.1]).

As P is a rank-1 projector, the operators $V(t)$, PLP, and $\psi(t)$ must be of the form

$$V(t) = \alpha(t)P; \quad PLP = \beta P; \quad \psi(t) = \gamma(t)P,$$

where

$$\begin{aligned}\alpha(t) &:= (U(t)f_0, f_0)\ ;\\ \beta &:= (Lf_0, f_0)\ ,\end{aligned}$$

and $\gamma(t)$ is the function to be determined. The unknown $\gamma(t)$ may be calculated from a perturbation expansion of $\exp(tQLQ)$, which, however, turns out to be very cumbersome. It is much easier to proceed using Laplace transforms (denoted by tildes). To do this, we note that

$$\begin{aligned}\widetilde{V}(z) &= \widetilde{\alpha}(z)P,\\ \widetilde{\psi}(z) &= \widetilde{\gamma}(z)P,\end{aligned}$$

where

$$\widetilde{\alpha}(z) = \left([z-L]^{-1}f_0, f_0\right)\ ,$$

by virtue of equation (8). In order to determine $\widetilde{\gamma}(z)$ from $\widetilde{\alpha}(z)$ and β we recall the identity (10):

$$\widetilde{V}(z) = P[z - PLP - \widetilde{\psi}(z)]^{-1}P. \tag{16}$$

The term on the right hand side is of the form

$$P[z - a(z)P]^{-1}P,$$

with

$$a(z) := \beta + \widetilde{\gamma}(z). \tag{17}$$

Since

$$(I - aP)(I - \frac{a}{a-1}P) = (I - \frac{a}{a-1}P)(I - aP) = I,$$

which follows from $P^2 = P$, we have

$$(z - aP)^{-1} = z^{-1}(I - \frac{a}{z}P)^{-1} = z^{-1}(I - \frac{a}{a-z}P),$$

whence

$$P(z - aP)^{-1}P = \frac{1}{z-a}P.$$

The last equation together with equations (16) and (17) imply that

$$\widetilde{\alpha}(z) = (z - \beta - \widetilde{\gamma}(z))^{-1}$$

which yields

$$\widetilde{\gamma}(z) = z - \beta - \widetilde{\alpha}(z)^{-1}. \tag{18}$$

Having obtained an equation for $\widetilde{\gamma}(z)$ we only need to calculate $\widetilde{\alpha}(z)$ and β. To do this we observe that $(z-L)^{-1}f = (z - \mathrm{i}x)^{-1}f$ for $f \in L^2(\mathbb{R}, dx)$. Thus, $\widetilde{\alpha}(z)$ and β are given by

$$\widetilde{\alpha}(z) = \frac{2r^3}{\pi}\int_{-\infty}^{\infty}\frac{1}{(z-\mathrm{i}x)(x+\mathrm{i}r)^2(x-\mathrm{i}r)^2}\,\mathrm{d}x = \frac{z+2r}{(z+r)^2} \quad (\mathrm{Re}\, z > 0);$$

$$\beta = \frac{2r^3}{\pi}\int_{-\infty}^{\infty}\frac{\mathrm{i}x}{(x+\mathrm{i}r)^2(x-\mathrm{i}r)^2}\,\mathrm{d}x = 0.$$

Using equation (18), we get an expression for the collision operator

$$\widetilde{\psi}(z) = -\frac{r^2}{z+2r}P \quad (\mathrm{Re}\, z > 0),$$

which, on taking the inverse Laplace transform, yields the time-domain collision operator

$$\psi(t) = -r^2\mathrm{e}^{-2rt}P \quad (t \in \mathbb{R}^+).$$

Since $r > 0$, the collision operator is indeed bounded by a decreasing exponential.

Step 2. Suppose now that $\{\bar{U}(t)\}$ is a strongly continuous unitary group with infinitesimal generator $\bar{L}$ acting on H and that $\{\bar{U}(t)\}$ has a LCFS. Then there is an invariant subspace $K \subset H$ of $\{\bar{U}(t)\}$ and a unitary transformation $W : K \to L^2(\mathbb{R}, dx)$ such that

$$W\bar{U}W^{-1} = U(t) = \mathrm{e}^{\mathrm{i}tx}.$$

Letting $\bar{P} : H \to H$ denote the orthogonal projection onto the subspace spanned by $W^{-1}f_0$, and putting $\bar{Q} := I - \bar{P}$, we see that K is an invariant subspace for $\bar{P}$, $\bar{Q}$, and $\bar{L}$. Thus

$$W(\bar{P}\bar{L}\bar{Q}\exp(t\bar{Q}\bar{L}\bar{Q})\bar{Q}\bar{L}\bar{P})W^{-1} = PLQ\exp(tQLQ)QLP = \psi(t).$$

Denoting the collision operator of the system $\{\bar{U}(t)\}$ corresponding to the projection $\bar{P}$ by $\bar{\psi}(t)$ the previous equation implies that

$$\bar{\psi}(t)f = W^{-1}\psi(t)Wf \quad \text{for } f \in K.$$

Since $\bar{\psi}(t)f = 0$ for $f \in K^{\perp}$, we conclude that $\bar{\psi}(t)$ must also decay exponentially.

Summarising these results, we have proved the following.

Theorem 4. *Let $\{U(t)\}$ be a strongly continuous unitary group which has a LCFS. Then there is a rank-1 projection P satisfying (M1) and (M2) of Section 2, such that the corresponding collision operator is non-zero and decays exponentially.*

We note that $V(t)$, which can be obtained from the inverse Laplace transform of $\widetilde{\alpha}(z)$,

$$V(t) = (1+rt)\mathrm{e}^{-rt}P \text{ for } t \in \mathbb{R}^+,$$

is a solution of the generalised master equation (6). In this case, the remainder term $\hat{W}(t)$ given by Coveney and Penrose vanishes and $V(t)$ itself is the asymptotic operator $W(t)$.

5. K-systems

As an application of the results of the previous section, we shall now show that a class of dynamical systems known as K-systems can give rise to exponentially decaying collision operators.

Suppose that $\left\{ T(t) \,\middle|\, t \in \mathbb{R} \right\}$ is a group of measure-preserving transformations acting on a probability space $(X, \mathcal{A}, \mu)$ ($\mathcal{A}$ denotes the σ-algebra of measurable sets and μ the probability measure) such that the mapping $(x, t) \mapsto T(t)x$ is measurable.

The group $\{T(t)\}$ is called a K-system (see [8]) if there exists a sub-σ-algebra $\mathcal{A}_0$ of $\mathcal{A}$ such that

(i) $T_{-t}\mathcal{A}_0 \subset \mathcal{A}_0$ for $t > 0$;

(ii) $\bigwedge_{t=0}^{\infty} T_{-t}\mathcal{A}_0 = \mathcal{N}$;

(iii) $\bigvee_{t=0}^{\infty} T_t\mathcal{A}_0 = \mathcal{A}$,

where $\mathcal{N}$ denotes the trivial algebra. K-systems may be interpreted to be abstractions of regular identically distributed stochastic processes, thus representing a class of highly chaotic systems.

Systems of physical interest which have been shown to be K-systems include abstract systems like the geodesic flow on a manifold of negative curvature [2, 28]; certain billiard systems, that is, dynamical systems describing the motion of a point particle in a region undergoing elastic reflections at the boundary, amongst them the Sinai billiard [37] and the Bunimovich stadion [6]; a number of hard ball systems, that is, dynamical systems describing the motion of a number of hard spheres in a region undergoing elastic reflections at the boundary and collisions amongst each other, for example, the motion of four balls on a three-torus [25], the motion of an arbitrary number of balls on a ν-torus with ν sufficiently large [39, 40], or the motion of an arbitrary number of balls with restricted interactions [7] (for an excellent review of the state-of-art of hard balls and billiard systems see [41]); and finally, a number of infinite-particle systems, including the infinite ideal gas [8] or the hard rods system [1].

In order to apply Theorem 4 to K-systems we only need to know whether the associated group $\{U(t)\}$ of Koopman operators on $L^2(X, \mathcal{A}, \mu)$ has a LCFS. This, however, is the case, since $\{U(t)\}$ is known to have countable Lebesgue spectrum on the orthocomplement of the constant functions (see [8]).

Summarising, we have the following.

Proposition 2. *Let $\{U(t)\}$ be the group of Koopman operators associated with a K-system. Then there is a rank-1 projector P such that the collision operator is bounded by a decreasing exponential.*

6. The Pietenpol model

We shall now consider a generalisation of a simple quantum mechanical model of an unstable state originally due to Pietenpol [31] in this context. The unstable state is described by an eigenstate embedded in the continuous spectrum of an unperturbed Hamiltonian which dissolves into the continuous part under the influence of an interaction. The state space H of this model is the direct sum

$$H = \mathbb{C} \oplus L^2(\mathbb{R}, dx),$$

while the generator of the unitary evolution is given by the family of operators

$$L_\lambda = L_0 + \lambda L_I \quad (\lambda \in \mathbb{R}),$$

with

$$L_0(u \oplus f) = \mathrm{i}(\epsilon u \oplus xf);$$
$$L_I(u \oplus f) = \mathrm{i}((f, v)_{L^2} \oplus uv).$$

Here, ϵ is a real number, v belongs to $L^2(\mathbb{R}, dx)$, and x again denotes the maximal operator of multiplication on $L^2(\mathbb{R}, dx)$. We note that the generator of the free evolution L_0 is skew-adjoint and has a simple eigenvalue $i\epsilon$ embedded in the continuous spectrum which fills the entire imaginary axis. The spectral properties of the perturbed operator L_λ $(\lambda \neq 0)$ are easily obtained using standard arguments. Observing that L_I is a skew-adjoint rank-2 perturbation we see that L_λ is skew-adjoint ([24, V. Theorem 4.3]) and that $\sigma(L_\lambda) = \mathrm{i}\mathbb{R}$ ([24, IV. Theorem 5.35]). The point spectrum of L_λ depends on the interaction v. Under certain conditions (for example, if v is continuous and everywhere non-zero) the point spectrum of L_λ is empty for every $\lambda \neq 0$. It is this property which suggests the interpretation of the Pietenpol model as that of an unstable system: the eigenstate $u \oplus 0$ corresponding to the eigenvalue $i\epsilon$ vanishes once the perturbation is switched on.

The Pietenpol model§ is similar to the Friedrichs model [14, 20, 13] but differs from it in that the spectrum of the Hamiltonian $\mathrm{i}L_\lambda$ is not bounded below. Although this feature is unrealistic, the model may be considered to approximate a physical system in which the energy level ϵ is far above the threshold, as was suggested by Pietenpol [31, p.1302].

Let us remark that L_λ has a LCFS; as in Section 3, this follows from the Kato-Rosenblum Theorem [24, X. Theorem 4.4] and the fact that L_λ is a finite rank perturbation of the operator L_0 which has a LCFS. Thus, as we have shown in Section 4, there must be a projection P for which the corresponding collision operator decays exponentially.

For the rest of this section, however, we shall consider the existence of exponentially decaying collision operators for this model from a different perspective. We shall keep P fixed, that is, we choose P to project onto the unstable state

$$P(u \oplus f) = u \oplus 0,$$

and we shall show that, provided that the interaction v satisfies certain additional assumptions, the time-domain collision operator ψ is bounded by a decreasing exponential for every $\lambda \in \mathbb{R}$.

§ In Pietenpol's original paper v is chosen to be $v(x) = \sqrt{r^3/4\pi}(x + \mathrm{i}r)^{-1}$ $(r > 0)$.

In order to do this we consider the Laplace transformed collision operator $\widetilde{\psi}$ given by (9)

$$\widetilde{\psi}(z) = PLQ[z - QLQ]^{-1}QLP \quad (\mathrm{Re}\, z > 0).$$

Here and in what follows we write 'L' instead of 'L_λ' to avoid cluttered notation.

Since P commutes with the free evolution

$$PL_0 \subset L_0 P$$

and

$$QL_1Q = 0,$$

$\widetilde{\psi}$ simplifies to

$$\widetilde{\psi}(z) = \lambda^2 PL_1Q[z - L_0]^{-1}QL_1P.$$

A straightforward calculation using the above expression yields

$$\widetilde{\psi}(z) = -\lambda^2 \widetilde{\gamma}(z)P,$$

where

$$\widetilde{\gamma}(z) = \int_{-\infty}^{\infty} \frac{|v(x)|^2}{z - \mathrm{i}x}\,\mathrm{d}x \quad (\mathrm{Re}\, z > 0).$$

To determine the original function $\gamma(t)$ from this expression we put $w(x) := |v(x)|^2$ and observe that, since $w \in L^1(\mathbb{R}, dx)$, we have

$$\int_{-\infty}^{\infty} \frac{w(x)}{z - \mathrm{i}x}\,\mathrm{d}x = \int_{-\infty}^{\infty} w(x) \int_0^{\infty} \mathrm{e}^{-zt}\mathrm{e}^{\mathrm{i}xt}\,\mathrm{d}t\, dx = \int_0^{\infty} \mathrm{e}^{-zt} \int_{-\infty}^{\infty} w(x)\mathrm{e}^{\mathrm{i}xt}\,\mathrm{d}x\,\mathrm{d}t$$

for $\mathrm{Re}\, z > 0$ by virtue of Fubini's theorem. Thus

$$\widetilde{\gamma}(z) = \int_0^{\infty} \widehat{w}(t)\mathrm{e}^{-zt}\,\mathrm{d}t, \tag{19}$$

where $\widehat{w}$ denotes the Fourier transform of w

$$\widehat{w}(t) = \int_{-\infty}^{\infty} w(x)\mathrm{e}^{\mathrm{i}xt}\,\mathrm{d}x. \tag{20}$$

Equations (19) and (20) imply that $\widehat{w}(t) = \gamma(t)$.

A sufficiently rich class of interactions $|v|^2 = w$ yielding an exponentially decaying collision operator $\psi(t) = -\lambda^2\gamma(t)P$ is given by the following Paley-Wiener-type theorem

Theorem 5. *Let β be a positive real number. Suppose that w is a function with an analytic continuation to the set $\{\zeta \mid 0 \le \mathrm{Im}\,\zeta \le \beta\}$ such that*

(i) for each η with $0 \le \eta \le \beta$ the function $w(\cdot + \mathrm{i}\eta)$ belongs to $L^1(\mathbb{R}, dx)$;

(ii) $\sup_{0\le\eta\le\beta} \|w(\cdot + \mathrm{i}\eta)\|_{L^1} = K < \infty$.

Then

$$|\widehat{w}(t)| = |\gamma(t)| \le K\mathrm{e}^{-\beta t} \quad (t > 0).$$

Proof. Fix $t > 0$ and let α be a positive real number. Let Γ_α be the rectangular path with vertices at $\pm\alpha$ and $\pm\alpha + \mathrm{i}\beta$. By Cauchy's theorem we have

$$\int_{\Gamma_\alpha} w(z)\mathrm{e}^{\mathrm{i}zt}\,\mathrm{d}z = 0.$$

Thus

$$\int_{-\alpha}^{\alpha} w(u)\mathrm{e}^{\mathrm{i}ut}\,\mathrm{d}u = \mathrm{e}^{-\beta t}\int_{-\alpha}^{\alpha} w(u+\mathrm{i}\beta)\mathrm{e}^{\mathrm{i}ut}\,\mathrm{d}u + \\ + \mathrm{i}\mathrm{e}^{-\mathrm{i}\alpha t}\int_0^{\beta} w(-\alpha+\mathrm{i}u)\mathrm{e}^{-ut}\,\mathrm{d}u - \mathrm{i}\mathrm{e}^{\mathrm{i}\alpha t}\int_0^{\beta} w(\alpha+\mathrm{i}u)\mathrm{e}^{-ut}\,\mathrm{d}u.$$

Taking the modulus on both sides of this inequality and using (ii) we obtain the estimate

$$\left|\int_{-\alpha}^{\alpha} w(u)\mathrm{e}^{\mathrm{i}ut}\,\mathrm{d}u\right| \le \mathrm{e}^{-\beta t}\int_{-\alpha}^{\alpha} |w(u+\mathrm{i}\beta)|\,\mathrm{d}u + \Phi(\alpha) + \Phi(-\alpha) \\ \le K\mathrm{e}^{-\beta t} + \Phi(\alpha) + \Phi(-\alpha), \tag{21}$$

where $\Phi(\alpha)$ is defined as

$$\Phi(\alpha) := \int_0^{\beta} |w(\alpha+\mathrm{i}u)|\,\mathrm{d}u.$$

By (i), (ii), and Fubini's theorem we have

$$\int_{-\infty}^{\infty} \Phi(\alpha)\,\mathrm{d}\alpha \le K\beta,$$

so that $\Phi(\alpha) + \Phi(-\alpha) \to 0$ as $\alpha \to \infty$. Thus, letting $\alpha \to \infty$ in (21) we obtain the desired inequality

$$|\widehat{w}(t)| \le K\mathrm{e}^{-\beta t} \quad (t > 0).$$

□

Corollary 1. *Suppose the interaction v is chosen so that $|v|^2$ satisfies the hypotheses of the previous theorem. Then the time-domain collision operator of the Pietenpol model decays exponentially for any value of the perturbation parameter $\lambda \in \mathbb{R}$.*

To illustrate this result we choose

$$v(x) = \frac{1}{x + \mathrm{i}r} \quad (r > 0).$$

Clearly, $|v|^2$ satisfies the hypotheses of the previous theorem and

$$\widetilde{\gamma}(z) = \int_{-\infty}^{\infty} \frac{1}{(z - \mathrm{i}x)(x^2 + r^2)}\,\mathrm{d}x = \frac{\pi}{r(z + r)}.$$

Thus,

$$\gamma(t) = \frac{\pi}{r}\mathrm{e}^{-rt} \quad (t > 0),$$

so that the time-domain collision operator ψ

$$\psi(t) = -\lambda^2\frac{\pi}{r}\mathrm{e}^{-rt}P \quad (t > 0)$$

is indeed bounded by a decreasing exponential.

7. Discussion

We saw that the condition that the collision operator of a system be norm-bounded by a decreasing exponential, which played an important role in the analysis of the Brussels formalism presented in [9], imposes certain restrictions on the Liouville operator of the system. More precisely, we have shown that the existence of a projection P, for which the associated collision operator is non-vanishing and decays exponentially, forces the generator of the reduced evolution QLQ to exhibit a Lebesgue spectrum with full support, which — provided that P is a finite rank projection — implies that L itself must have a Lebesgue component with full support. Our result can be viewed as a sharpened version of the well known observation that the quantum-mechanical Hamiltonians of systems describing exponentially decaying states must have spectra which are unbounded from below (see, for example, [38, 42]).

We were also able to provide a converse of the above characterisation, in the sense that, for every system with a generator which has a Lebesgue spectrum with full support, there is a finite rank projection for which the corresponding collision operator is non-vanishing and decays exponentially. This characterisation is likely to be of limited practical use, because the construction of P requires detailed knowledge of the spectral representation of L, which is generally difficult to obtain. Moreover, in concrete applications, the projection P is determined by physical considerations, and is thus fixed in advance. On the other hand, our characterisation serves the main purpose of this article, which was to show that the class of systems admitting non-trivial exponentially decaying collision operators is not empty: it contains, for example, all K-systems.

Using different methods we were able to show that this class also contains the Pietenpol model provided that the interaction is suitably chosen and provided that P projects onto the unstable state. As the spectrum of the Pietenpol Hamiltonian is not bounded below, and thus unphysical, it would be desirable to find more realistic models giving rise to exponentially decaying collision operators. Good candidates might be found amongst the spin-boson models describing the interaction of a spin system with a free Bose gas, which have received much attention lately (see [23] and references therein).

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