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ROBERT ALICKI

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On the scattering theory for quantum dynamical semigroups

by

Robert ALICKI

Institute of Physics, Gdańsk University
PL 80-952 Gdańsk, Poland

ABSTRACT. — We consider the wave operators and scattering matrix for quantum dynamical semigroups. The dynamical semigroups with bounded perturbations are briefly studied using the Cook's method and the simplified model of heavy-ion collision is presented as an example.

1. INTRODUCTION

The purpose of this note is to clarify some ideas concerning the phenomenological approach to dissipative scattering. There exists a class of scattering phenomena for example a scattering and capture of a neutron by a nucleus or the heavy-ion collision which can be described in terms of the theory of open systems [1]-[5]. Namely we can eliminate a large number of internal degrees of freedom together with some external fields to obtain the irreversible dynamics for few fixed degrees of freedom (e. g. 3-degrees of freedom of the relative motion of two heavy-ions). Moreover because the interaction of internal degrees of freedom is strong then the relaxation time for them is short and hence one can apply the Markovian approximation [6] [7]. It follows that the dynamics of such open system can be described by quantum dynamical semigroup.

We start by introducing some preliminary mathematical definitions. Let \mathcal{H} be a Hilbert space associated with the open system with scalar

product (\cdot, \cdot) and norm $\|\cdot\| = \sqrt{(\cdot, \cdot)}$. $L^\infty(\mathcal{H})$ is a real Banach space of hermitian operators with operator norm $\|\cdot\|_\infty$ and $L^c(\mathcal{H})$ is a Banach subspace of $L^\infty(\mathcal{H})$ which contains compact operators.

$L^1(\mathcal{H})$ denote a real Banach space of hermitian trace-class operators with trace norm $\|\cdot\|_1$.

We have also the relations $L^c(\mathcal{H})^* \cong L^1(\mathcal{H})$, $L^1(\mathcal{H})^* = L^\infty(\mathcal{H})$.

Consider a one parameter strongly continuous contracting and positive semigroup $\{\Lambda_t = e^{tL}, t \geq 0\}$ on $L^1(\mathcal{H})$.

We call it *dynamical semigroup* if for all $t \geq 0$ the dual map Λ_t^* is completely positive [6]-[8] and *conservative dynamical semigroup* if moreover $\text{tr}(\Lambda_t \sigma) = \text{tr} \sigma$, for all $\sigma \in L^1(\mathcal{H})$, $t \geq 0$.

REMARKS. — The non conservative semigroups can describe the scattering if some other open channels of reaction are taken into account [3]-[9].

The complete positivity of Λ_t^* will be not used manifestly further, but this property is based on strong physical arguments and restricts the class of dynamical semigroups [6]-[8].

2. WAVE OPERATORS AND S-MATRIX

We start by assuming that the free evolution is represented by the dynamical group $\{U_t; t \in \mathbb{R}^1\}$

$$U_t \sigma = e^{-itH_0} \sigma e^{itH_0} \equiv e^{tL_0} \sigma, \sigma \in L^1(\mathcal{H}), \quad (2.1)$$

where H_0 is a self-adjoint Hamiltonian.

The perturbed dynamics is given by the quantum dynamical semigroup

$$\{\Lambda_t = e^{tL}; t \geq 0\}.$$

As in ordinary scattering theory we define the wave operators W_1 and W_2^*

$$\text{I) } W_1 : L^1(\mathcal{H}) \rightarrow L^1(\mathcal{H})$$

$$W_1 \sigma = \lim_{t \rightarrow \infty} \Lambda_t U_{-t} \sigma \quad (2.2)$$

for all $\sigma \in L^1(\mathcal{H})$

$$\text{II) } \tilde{W}_2 : L^c(\mathcal{H}) \mapsto L^\infty(\mathcal{H})$$

$$\tilde{W}_2 a = \lim_{t \rightarrow \infty} \Lambda_t^* U_t a \quad (2.3)$$

for all $a \in L^c(\mathcal{H})$.

We have the dual homomorphism

$$\tilde{W}_2^* : L^\infty(\mathcal{H})^* \rightarrow L^c(\mathcal{H})^* \cong L^1(\mathcal{H}).$$

Because $L^\infty(\mathcal{H})^* \supset L^1(\mathcal{H})$ we can finally define

$$W_2^* = \tilde{W}_2^*|_{L^1(\mathcal{H})}, \quad W_2^* : L^1(\mathcal{H}) \rightarrow L^1(\mathcal{H}). \quad (2.4)$$

Therefore we obtain the scattering matrix

$$S = W_2^* W_1$$

REMARK. — The definition of W_2^* presented here seems to be more appropriate than the strong limit $W_2^* \sigma = \lim_{t \rightarrow \infty} U_{-t} \Lambda_t \sigma$, $\sigma \in L^1(\mathcal{H})$ because for the later and under the assumption that Λ_t is conservative the S-matrix preserves the trace of σ and hence cannot describe for instance the capture of particle by the potential of target which is possible in the case of dissipative scattering.

Moreover the definition (2.3)-(2.4) allows to apply the Cook's criterion. One can easily prove the following properties

i) if W_1, W_2^* exist then the following probability function

$$P(\rho_{in} \rightarrow |\varphi^{out}\rangle \langle \varphi^{out}|) := \lim_{t \rightarrow \infty} (\varphi^{out}, \{ e^{-tL_0} e^{2tL} e^{-tL_0} \rho_{in} \} \varphi^{out}) = (\varphi^{out}, (S\rho_{in})\varphi^{out}), \quad (2.6)$$

where

$$\rho_{in} \in L^1(\mathcal{H}), \quad \rho_{in} \geq 0, \quad \text{tr } \rho_{in} = 1, \quad \|\varphi^{out}\| = 1.$$

ii) W_1, W_2^* are positive contractions on $L^1(\mathcal{H})$

iii) if $\{\Lambda_t, t \geq 0\}$ is conservative then W_1 is trace preserving

iv) $e^{\tau L} W_1 = W_1 e^{\tau L_0}$

$$W_2^* e^{\tau L_1} = e^{\tau L_0} W_2^*, \quad \tau \geq 0$$

and hence $e^{\tau L_0} S = S e^{\tau L_0}$.

One can easily generalize Cook's arguments [11] [12] to prove the existence of W_1, W_2^* (see also [10]).

PROPOSITION 1. — Let $D \{ D^* \}$ be a dense set in $L^1(\mathcal{H}) \{ L^c(\mathcal{H}) \}$ such that

$$e^{-tL_0} D \subset \text{dom}(L) \cap \text{dom}(L_0) \{ e^{-tL_0} D^* \subset \text{dom}(L^*) \cap \text{dom}(L_0^*) \} \quad \text{for all } t \in [s, \infty),$$

and some $s \geq 0$.

Assume that the function $\| (L - L_0) e^{-tL_0} \sigma \|_1 \{ \| (L^* - L_0^*) e^{-tL_0} a \|_\infty \}$ is integrable on $[s, \infty)$ for $\sigma \in D \{ a \in D^* \}$.

Then $W_1 \{ \tilde{W}_2$ and therefore $W_2^* \}$ exists.

3. QUANTUM DYNAMICAL SEMIGROUPS WITH BOUNDED PERTURBATIONS

We consider a quantum mechanical Fokker-Planck equation

$$\frac{d\rho}{dt} = -i[H_0 + U, \rho] + \sum_{\alpha} V_{\alpha} \rho V_{\alpha}^* - \frac{1}{2} \{ B, \rho \} \equiv L_s \rho \quad (3.1)$$

Here H_0 is a self-adjoint operator (free Hamiltonian), $U = U^*$ is bounded (Hamiltonian perturbation) and $\sum_{\alpha} V_{\alpha}^* V_{\alpha} \leq B$, B is also bounded.

By standard theorems [11] and using Lindblad results one can prove that the equation (3.1) generates the quantum dynamical semigroup $\{ \Lambda_t = e^{tL}, t \geq 0 \}$ (conservative if $B = \sum_{\alpha} V_{\alpha}^* V_{\alpha}$). Following

Davies [9] the core of $L_0 = -i[H_0, \cdot]$ and hence of L is given by

$$\mathcal{D} = (1 + iH_0)^{-1} L^1(\mathcal{H})(1 + iH_0)^{-1} \quad (3.2)$$

One can check that for $\rho \in L^1(\mathcal{H})$ and $a \in L^c(\mathcal{H})$

$$\text{tr}(e^{tL}\rho a) = \text{tr}(\rho e^{tL^*}a) \quad (3.3)$$

where $L_* : \text{dom}(L_*) \rightarrow L^c(\mathcal{H})$,

$$L_* a = i[H_0 + U, a] + \sum_{\alpha} V_{\alpha}^* a V_{\alpha} - \frac{1}{2} \{ B, a \}. \quad (3.4)$$

REMARK. — In this paper we denote by $i[H, \cdot]$ the closure of a commutator (in a suitable Banach space of operators) which is a generator of one parameter group $X \rightarrow e^{itH} X e^{-itH}$.

Using similar arguments one can show that

$$\mathcal{D}_* = (1 + iH_0)^{-1} L^c(\mathcal{H})(1 - iH_0)^* \quad (3.5)$$

is a core for L_* .

It follows that

$$\tilde{W}_2 a \equiv W_2 a = \lim_{t \rightarrow \infty} e^{tL^*} e^{tL_0} a$$

$a \in L^c(\mathcal{H})$ and $\tilde{W}_2^* = W_2^*$ in this case (if W_2 exists of course).

Now one can prove the simple form of Cook's criterion valid for the dynamical semigroup governed by (3.1).

PROPOSITION 2. — Let \mathcal{H}_0 be a dense set in $\text{dom}(H_0)$.

Assume that the following functions are integrable on $[s, \infty)$, $s \geq 0$ for all $\psi \in \mathcal{H}_0$.

$$a) \quad \sum_{\alpha} \| V_{\alpha} e^{-itH_0} \psi \|^2, \quad \| B e^{-itH_0} \psi \|^2, \quad \| U e^{-itH_0} \psi \|^2, \quad (3.6)$$

$$b) \quad \sum_{\alpha} \| V_{\alpha}^* e^{itH_0} \psi \|^2, \quad \| B e^{itH_0} \psi \|^2, \quad \| U e^{itH_0} \psi \|^2, \quad (3.7)$$

Then a) implies the existence of W_1 and

b) implies the existence of W_2^* .

Proof. — Let D be a set of all finite rank hermitian operators whose eigenvectors lie in $\text{dom}(H_0)$.

D is dense in $L^1(\mathcal{H})$, $L^2(\mathcal{H})$ and $D \subset \mathcal{D} \cap \mathcal{D}_*$.

Therefore D can be used as a set D and D^* in Proposition 1.

Taking $\sigma = |\psi\rangle\langle\psi|$, $\psi \in \mathcal{H}_0$ one can easily prove that $a)$ implies integrability of $\|(L - L_0)e^{-tL_0}\sigma\|_1$ and similiary for $a = |\psi\rangle\langle\psi|$ and $\|(L^* - L_0^*)e^{tL_0^*}a\|_\infty$ under the assumption $b)$.

Taking linear combinations we extend the above results to σ , $a \in D$ and therefore all assumptions of Proposition 1 are fulfilled.

4. SIMPLE MODEL OF HEAVY-ION COLLISION

In paper 5 one can find the heuristic derivation based on the simple model of heavy-ion collision of the quantum Fokker-Planck equation describing the relative motion of two nuclei. The final result is the following

$$\frac{d\rho}{dt} = -i[H_0 + U, \rho] + \frac{1}{2} \sum_{k=1}^3 \{ [V_k, \rho V_k^*] + [V_k \rho, V_k^*] \} \equiv L_\delta \quad (4.1)$$

Here ρ is a density matrix on Hilbert space $\mathcal{L}^2(\mathbb{R}^3)$ and

$$(H_0\psi)(\vec{x}) = -\frac{1}{2m} \Delta\psi(\vec{x}), \quad \vec{x} = (x_1, x_2, x_3). \quad (4.2)$$

$$(U\psi)(\vec{x}) = U(\vec{x})\psi(\vec{x}) \quad (4.3)$$

$$(V_k\psi)(\vec{x}) = W(\vec{x}) \left(x_k + \alpha \frac{\partial}{\partial x_k} \right) \psi(\vec{x}), \quad k = 1, 2, 3 \quad (4.4)$$

$$\lim_{|\vec{x}| \rightarrow \infty} W(\vec{x}) = \lim_{|\vec{x}| \rightarrow \infty} U(\vec{x}) = 0, \quad \alpha > 0$$

To give the physical motivation of (4.1) we write down the formal Heisenberg evolution equations for position and momentum operators $(\hat{x}_k, \hat{p}_k) k = 1, 2, 3)$

$$\frac{d\hat{x}_k}{dt} = \frac{1}{m} \hat{p}_k + \alpha^2 \frac{\partial}{\partial \hat{x}_k} W^2(\hat{x}) - \alpha W^2(\hat{x}) \hat{x}_k \quad (4.5)$$

$$\frac{d\hat{p}_k}{dt} = -\frac{\partial}{\partial \hat{x}_k} U(\hat{x}) - \frac{\alpha}{2} \{ W^2(\hat{x}), \hat{p}_k \}, \quad k = 1, 2, 3 \quad (4.6)$$

For large $|\langle \hat{p}_k \rangle|$ or small α (4.5) (4.6) correspond to the classical Newton equation with a friction force $-\alpha W^2(x)\vec{p}$ describing the « nuclear friction » in heavy-ion collisions [4].

Under some technical conditions one can construct rigorously the dynamical semigroup generated by (4.1) using the method of minimal solution [9] but unfortunately the domain of obtained generator is not manifestly defined and then we cannot easily adopt the methods presented in Section 3.

However one can introduce the « regularized version » of equation (4.1). Namely we assume that

- A) $U(\vec{x})$, $W(\vec{x})$, $x_k W(\vec{x})$ are bounded and continuous functions on \mathbb{R}^3 ,
 B) operator V_k is replaced by

$$(V_k^{(\varepsilon)}\psi)(\vec{x}) = W(\vec{x})x_k\psi(\vec{x}) + \alpha W(\vec{x})\frac{1}{\varepsilon} [\psi(\vec{x} + \varepsilon\vec{e}_k) - \psi(\vec{x})] \quad (4.7)$$

The regularized generator $L^{(\varepsilon)}$ belongs to the class described in Section 4 and $\{e^{tL^{(\varepsilon)}}, t \geq 0\}$ is a conservative dynamical semigroup.

PROPOSITION 3. — Assume that A) B) hold and moreover

$$\int_{\mathbb{R}^3} \{U^2(\vec{x}) + \vec{x}^2 W^2(\vec{x})\} d^3\vec{x} < \infty \quad (4.8)$$

Then the wave operators W_1 and W_2^* exist for the generator $L^{(\varepsilon)}$.

Proof. — Taking into account the structure of $L^{(\varepsilon)}$, $V_k^{(\varepsilon)}$ and Proposition 2 it is sufficient to prove that the following functions are integrable on $[s, \infty)$ and $(-\infty, -s]$

$$\|U\psi_t\|, \quad \|W\psi_t\|, \quad \|W\hat{x}_k\psi_t\|, \quad k = 1, 2, 3 \quad (4.9)$$

for $\psi_t = e^{-itH_0}\psi$, $\psi \in \mathcal{H}_0 \subset \text{dom}(H_0)$ (\mathcal{H}_0 is dense in $\mathcal{L}^2(\mathbb{R}^3)$).

Taking \mathcal{H}_0 as a linear subspace spanned by all Gaussian functions

$$\exp\left\{-\frac{|\vec{x} - \vec{\xi}|^2}{2a^2}\right\}$$

we apply the standard method [13] to prove the integrability of (4.9).

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