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Section A :
Physique théorique.

On the scattering theory for quantum dynamical semigroups

by

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

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

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

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

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

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 $\{ U_t ; t \in \mathbb{R}^1 \}$

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

where H_0 is a self-adjoint Hamiltonian.

The perturbed dynamics is given by the quantum dynamical semigroup

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

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

I) $W_1 : L^1(\mathscr{H}) \to L^1(\mathscr{H})$

$$W_1\sigma = \lim_{t\to\infty} \Lambda_t U_{-t}\sigma \tag{2.2}$$

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

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

$$\tilde{W}_2 a = \lim_{t\to\infty} \Lambda_t^* U_t a \tag{2.3}$$

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

We have the dual homomorphism

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

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

$$W_2^* = \tilde{W}_2^* |_{L^1(\mathscr{H})}, \qquad W_2^* : L^1(\mathscr{H}) \to L^1(\mathscr{H}). \tag{2.4}$$

Therefore we obtain the scattering matrix

$$S = W_2^* W_1$$

REMARK. — The definition of W_2^* presented here seems to be more appropriate then the strong limit $W_2^*\sigma = \lim_{t\to\infty} U_{-t}\Lambda_t\sigma$, $\sigma \in L^1(\mathscr{H})$ 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

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

where

$$\rho_{in} \in L^1(\mathscr{H}), \qquad \rho_{in} \geqslant 0, \qquad \operatorname{tr} \rho_{in} = 1, \qquad \| \varphi^{out} \| = 1.$$

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

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

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

$$W_2^* e^{\tau L_1} = e^{\tau L_0} W_2^*, \qquad \tau \geqslant 0$$

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

One can easly 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 $L^1(\mathscr{H}) \{ L^c(\mathscr{H}) \}$ such that

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

and some $s \geqslant 0$.

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

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

Here H_0 is a self-adjoint operator (free Hamiltonian), $U = U^*$ is bounded (Hamiltonian perturbation) and $\sum_\alpha V_\alpha^* V_\alpha \leqslant B$, 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 $\{ \Lambda_t = e^{tL}, t \geqslant 0 \}$ $\left(\text{conservative if } B = \sum_\alpha V_\alpha^* V_\alpha \right)$. Following Davies [*9*] the core of $L_0 = - i[H_0, \cdot\,]$ and hence of L is given by

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

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

$$\operatorname{tr}(e^{tL}\rho a) = \operatorname{tr}(\rho e^{tL_*} a) \tag{3.3}$$

where $L_* : \operatorname{dom}(L_*) \to L^c(\mathscr{H})$,

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

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

Using similar arguments one can show that

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

is a core for L_*.

It follows that

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

$a \in L^c(\mathscr{H})$ 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 $\mathscr{H}_0$ be a dense set in $\operatorname{dom}(H_0)$.

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

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

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

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 dom (H_0).

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

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

Taking $\sigma = |\psi\rangle\langle\psi|$, $\psi \in \mathscr{H}_0$ one can easly prove that *a*) implies integrability of $\|(L - L_0)e^{-tL_0}\sigma\|_1$ and similary 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 fulfiled.

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 $\mathscr{L}^2(\mathbb{R}^3)$ and

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

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

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

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

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

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

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

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 easly 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 $\{ e^{tL^{(\varepsilon)}}, t \geqslant 0 \}$ 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 $(-\infty, -s]$

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

for $\psi_t = e^{-itH_0t}\psi$, $\psi \in \mathscr{H}_0 \subset \mathrm{dom}(H_0)$ ($\mathscr{H}_0$ is dense in $\mathscr{L}^2(\mathbb{R}^3)$).

Taking $\mathscr{H}_0$ as a linear subspace spaned 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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