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Non-unitary scattering and capture. II. Quantum dynamical semigroup theory

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ABSTRACT. — We construct a quantum dynamical semigroup model of neutron-nucleus scattering, which incorporates irreversible effects due to γ-emission, and thus allows the possibility of neutron capture.

§ 1. INTRODUCTION

There are several situations in multibody scattering theory in which interactions of the particles with the electromagnetic field (or possibly with a phonon field) are important because they lead to irreversible effects and in particular to particle capture. For example, in low energy neutron scattering from a nucleus ([*10*], p. 411) and in electron scattering from a molecule ([*11*], p. 593) there may be sharp resonances at energies corresponding to eigenstates of the compound nucleus (or molecule) and these are associated with metastable states having a long but finite lifetime. It is clear both from the mathematical formalism of multibody, scattering theory [*1*, *13*] and from physical considerations ([*10*], p. 284; [*11*], p. 595) that true capture can only occur upon the emission of a photon which stabilises the compound nucleus (or molecule). For this reason it is desirable to obtain a mathematical model of scattering theory in which the irreversible effects due to photon emission are taken into account. It should be noted that photon emission is also of relevance in inelastic scattering ([*10*], p. 373) but it is then of less importance because it generally occurs well after the scattering event is completed.

In this paper we study the scattering of two particles (which for the sake of definiteness we call a neutron and nucleus) in a model involving both direct inelastic and compound nucleus reactions. We regard the neutron and nucleus as an open system interacting with the external electromagnetic field by a phenomenological evolution equation. Although we make systematic use of the scattering theory developed in [6, 8] for non-self-adjoint Hamiltonians involving optical potentials, our dynamics is actually specified by a quantum dynamical semigroup [5] acting on the Banach space $\mathscr{C}(\mathscr{H})$ of trace class operators. We mention some closely related work in ([7], § 6) where, however, the phenomenon of neutron capture is excluded, and a recent paper of Barchielli [2], who studies the same dynamical equations as those treated here.

§ 2. A MODEL OF NUCLEAR SCATTERING

The Hilbert space of the model in the centre of mass coordinate system is $\mathscr{H} = \mathscr{K}_0 \otimes \mathscr{K}_1$ where the neutron Hamiltonian on $\mathscr{K}_0 = L^2(\mathbb{R}^3)$ is

$$K_0 = -\frac{1}{2m}\Delta$$

and the Hamiltonian K_1 on $\mathscr{K}_1$ describes the internal dynamics of the nucleus. Since the nucleus is often very complicated we assume no more about K_1 than that $K_1 \geq 0$ and that the nucleus has a ground state Ω with $K_1\Omega = 0$. The orthogonal projection P_0 of $\mathscr{H}$ onto $\mathscr{K}_0 \otimes \Omega = \mathscr{H}_0$ commutes with

$$H_0 = K_0 + K_1.$$

We put

$$P_1 = 1 - P_0.$$

For the purposes of scattering we always assume that the nucleus is initially in its ground state, so that the ingoing state lies in $\mathscr{H}_0$.

We assume that the nucleus may relax from any excited state to the ground state by the emission of γ-radiation according to the abstract Pauli master equation

$$\frac{d\rho}{dt} = -i[K_1, \rho] - \{V_0\rho + \rho V_0\} + J(\rho) = Z_1(\rho) \tag{1}$$

where ρ is an arbitrary mixed state on $\mathscr{K}_1$, $V_0 \geq 0$ is a bounded self-adjoint operator on $\mathscr{K}_1$ with $V_0\Omega = 0$, and J is a bounded completely positive map on the space $\mathscr{C}(\mathscr{K}_1)$ of trace class operators on $\mathscr{K}_1$, satisfying

$$\mathrm{tr}\,[J(\rho)] = 2\,\mathrm{tr}\,[V_0\rho]$$

for all $\rho \in \mathscr{C}(\mathscr{K}_1)$. According to ([5], p. 83) the solution of (1) is of the form

$$\rho(t) = e^{Z_1 t}\rho$$

where $e^{Z_1 t}$ is a quantum dynamical semigroup on $\mathscr{C}(\mathscr{K}_1)$.

EXAMPLE 1. — To obtain the usual Pauli equation from (1), one puts $\mathscr{K}_1 = \mathbb{C}^2$

$$K_1 = \begin{bmatrix} \omega & 0 \\ 0 & 0 \end{bmatrix}, \quad V_0 = \begin{bmatrix} \beta & 0 \\ 0 & 0 \end{bmatrix}, \quad A = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

and

$$J(\rho) = 2\beta A\rho A^*$$

where $\beta > 0$, and then looks at the time evolution of the diagonal matrices. This case is discussed in ([9], p. 122) as a model of spin relaxation, and derivations of the master equation (1) from first principles may be found in [4], [12].

Returning to the general case, the assumption that $V_0\Omega = 0$ implies that $J(v) = 0$, $e^{Z_1 t}v = v$ for all $t \geq 0$, where $v = |\,\Omega\,\rangle\langle\,\Omega\,|$ is the ground state of the nucleus.

We assume that v is the only stable state, that is

$$\lim_{t\to\infty} e^{Z_1 t}\rho = v \operatorname{tr}[\rho] \tag{2}$$

for all $\rho \in \mathscr{C}(\mathscr{K}_1)$. In this and all similar equations convergence is taken to be in the trace norm $\|\ \|_1$. We also make the assumption, closely related to but independent of (2), that there is a constant $\beta > 0$ such that

$$\langle V_0\psi, \psi \rangle \geq \beta \langle \psi, \psi \rangle$$

for all $\psi \perp \Omega$. This implies that

$$\lim_{t\to\infty} e^{(-iK_1 - V_0)t}\phi = \langle \phi, \Omega \rangle$$

for all $\phi \in \mathscr{K}_1$.

The evolution on $\mathscr{C}(\mathscr{H})$ is given as in [2] by the quantum dynamical semigroup $T_t = e^{Zt}$ associated with the evolution equation

$$\frac{d\rho}{dt} = Z(\rho) = Z_0(\rho) + Z_1(\rho) + Z_2(\rho)$$

where the action of Z_1 on $\mathscr{C}(\mathscr{H})$ is induced in an obvious way by its action on $\mathscr{C}(\mathscr{K}_1)$ and

$$Z_0(\rho) = -i[K_0, \rho] \quad , \quad Z_2(\rho) = -i[V_1, \rho]$$

with domain precisely specified in ([5], p. 82); we assume that the interaction term V_1 on $\mathscr{H}$ is self-adjoint and relatively compact with respect to H_0. We may also write

$$Z(\rho) = -iH\rho + i\rho H^* + J(\rho)$$

where
$$H = H_0 + V_1 - iV_0$$
is the generator of a one-parameter contraction semigroup on $\mathscr{H}$ and J is extended in the natural way from $\mathscr{C}(\mathscr{K}_1)$ to $\mathscr{C}(\mathscr{K}_0 \otimes \mathscr{K}_1)$. Note that in the absence of relaxation (that is if V_0 and J vanish) the Hamiltonian H is self-adjoint and its eigenvectors describe compound nucleus bound states arising from the interaction term V_1.

Returni^r g to the general case, we define $\mathscr{H}_b$ to be the closed linear span of the eigenvectors of H associated with real eigenvalues, and put
$$\mathscr{H}_d = \{ \phi \in \mathscr{H} : \lim_{t\to\infty} \| e^{-iHt}\phi \| = 0 \}$$
We refer to [6], [8] for the definition of the absolutely continuous subspace $\mathscr{H}_{ac}$ of H. It is useful to introduce the semigroup S_t on $\mathscr{C}(\mathscr{H})$ defined by
$$S_t(\rho) = e^{-iHt}\rho e^{iH^*t}$$
for all $\rho \in \mathscr{C}(\mathscr{H})$ and $t \geq 0$, noting that
$$T_t(\rho) = S_t(\rho) + \int_0^t S_{t-s} J T_s \rho ds \tag{3}$$
for all $\rho \in \mathscr{C}(\mathscr{H})$, and hence that
$$0 \leq S_t(\rho) \leq T_t(\rho)$$
for all $0 \leq \rho \in \mathscr{C}(\mathscr{H})$ and $t \geq 0$.

For this model scattering theory must be developed at two levels. Since we shall always suppose that the nucleus is initially in its ground state we wish to prove the existence of
$$W_- f = \lim_{t\to\infty} e^{-iHt}e^{iH_0t} f$$
for all $f \in \mathscr{H}_0$, and
$$\Omega_-(\rho) = \lim_{t\to\infty} T_t(e^{iH_0t}\rho e^{-iH_0t})$$
for all $\rho \in \mathscr{C}(\mathscr{H}_0)$. The operator W_- is a contraction from $\mathscr{H}_0$ into $\mathscr{H}$, while Ω_- is a completely positive trace-preserving map from $\mathscr{C}(\mathscr{H}_0)$ into $\mathscr{C}(\mathscr{H})$. The existence of W_- and Ω_- may be shown by Cook's method.

LEMMA 2. — If
$$\int_0^\infty \| V_1 e^{iH_0t} f \| dt < \infty \tag{4}$$
for all f in a dense subspace $\mathscr{D}$ of $\mathscr{H}_0$ then $W_- f$ exists for all $f \in \mathscr{H}_0$ and $\Omega_-(\rho)$ exists for all $\rho \in \mathscr{C}(\mathscr{H}_0)$.

Proof. — The existence of W_- is standard. If
$$\tilde{\mathscr{D}} = \left\{ \sum_{r=1}^n \alpha_r | f_r \rangle \langle f_r | : \alpha_r \in \mathbb{C}, f_r \in \mathscr{D} \right\}$$

then $\tilde{\mathcal{D}}$ is dense in $\mathcal{C}(\mathcal{H}_0)$. Moreover if $\rho \in \mathcal{C}(\mathcal{H}_0)$

$$e^{(Z_0+Z_1)t}\rho = e^{Z_0 t}\rho = e^{-iH_0 t}\rho e^{iH_0 t}$$

by the Trotter product formula. To apply Cook's method it is sufficient to note that if $\rho \in \tilde{\mathcal{D}}$

$$\int_0^\infty \| Z_2(e^{iH_0 t}\rho e^{-iH_0 t}) \|_1 dt \leq 2\int_0^\infty \sum_{r=1}^{n} | \alpha_r | \| f_r \| \| V_1 e^{iH_0 t} f_r \| dt < \infty$$

The existence of the outgoing wave operators is less easy, and we prove it first at the Hilbert space level.

LEMMA 3. — If

$$(H_0 - i)^{-1}V_1(H_0 - i)^{-1}$$

is of trace class then

$$W_+\phi = \lim_{t\to\infty} e^{iH_0 t}e^{-iHt}\phi$$

exists for all $\phi \in \mathcal{H}_{ac}$, and lies within $\mathcal{H}_0$.

Proof. — We apply ([*6*], Theorem 6.3) with

$$\tilde{B} = -iH \quad , \quad \tilde{J} = P_1$$

the ~ denoting the symbols of [*6*]. We have

$$\begin{aligned}\tilde{J}^2 + \tilde{J}^2\tilde{B} &= iH_0 - iV_1 - V_0(P_1 + P_1H_0iV_1 - V_0)\\ &= -2V_0 - i[V_1, P_1].\end{aligned}$$

Now

$$-2V_0 \leq -2\beta\tilde{J}^2$$

and

$$\begin{aligned}(1 - \tilde{B}^*)^{-1}[V_1, P_1](1 - \tilde{B})^{-1}\\ &= (1 - \tilde{B}^*)^{-1}(H_0 - i).(H_0 - i)^{-1}V_1.P_1(1 - \tilde{B})^{-1}\\ &\quad - (1 - \tilde{B}^*)^{-1}P_1.V_1(H_0 - i)^{-1}.(H_0 - i)(1 - \tilde{B})^{-1}\end{aligned}$$

which is compact since V_1 is relatively compact with respect to H_0, and V_0 is a bounded perturbation of $-iH_0$. We deduce by ([*6*], Theorem 6.3) that

$$\lim_{t\to\infty} e^{iH_0 t}P_1 e^{-iHt}\phi = 0$$

for all $\phi \in \mathcal{H}_{ac}$. On the other hand the existence of

$$\lim_{t\to\infty} e^{iH_0 t}P_0 e^{-iHt}\phi$$

for all $\phi \in \mathcal{H}_{ac}$ is an immediate consequence of ([6], Theorem 5.4) and the fact that

$$\begin{aligned}(H_0 - i)^{-1}(H_0P_0 - P_0H)(H - i)^{-1} &= (H_0 - i)^{-1}(H_0P_0 - P_0H_0 - P_0V_1 + iP_0V_0)(H - i)^{-1} \\ &= -(H_0 - i)^{-1}P_0V_1(H - i)^{-1} \\ &= -P_0.(H_0 - i)^{-1}V_1(H_0 - i)^{-1}.(H_0 - i)(H - i)^{-1}\end{aligned}$$

which is of trace class.

Although we shall systematically adopt the Hypotheses A-F of [8] and make use of the results there, slight modifications to the proofs are actually needed because V_1 is relatively compact with respect to H_0 but V_0 is not, being bounded instead. Also the wave operator W_- has domain $\mathcal{H}_0$ instead of $\mathcal{H}$, but fortunately the range of W_+ lies in $\mathcal{H}_0$ also. Moreover W_- is one-one and $\mathcal{H}_b$ lies entirely within $\mathcal{H}_0$. By Hypothesis F and Theorem 7 of [8] the scattering operator $S = W_+W_-$ maps $\mathcal{H}_0$ one-one onto $\mathcal{H}_0$ and there is a *Banach* space decomposition

$$\mathcal{H} = (\text{Range } W_-) \oplus \mathcal{H}_d \oplus \mathcal{H}_b.$$

As in [8] we define P to be the *orthogonal* projection with kernel $\mathcal{H}_d \oplus \mathcal{H}_b$. The range of P is called the set of outgoing states, and is *not* equal to Range W_- in general. The necessity for the presence of P in (5) below is connected with the possibility of neutron capture, or equivalently with the failure of asymptotic completeness.

THEOREM 4. — The modified outgoing wave operator

$$\Omega_+(\rho) = \lim_{t\to\infty} e^{iH_0t}P(T_t\rho)Pe^{-iH_0t} \tag{5}$$

exists and lies in $\mathcal{C}(\mathcal{H}_0)$ for all $\rho \in \mathcal{C}(\mathcal{H})$.

Proof. — We deduce from (3) that

$$\begin{aligned} e^{iH_0t}P(T_t\rho)Pe^{-iH_0t} &= (e^{iH_0t}Pe^{-iHt})\rho(e^{iH_0t}Pe^{-iHt})^* \\ &+ \int_0^t e^{iH_0s}(e^{iH_0(t-s)}Pe^{-iH(t-s)})(JT_s\rho)(e^{iH_0(t-s)}Pe^{-iH(t-s)})^*e^{-iH_0s}ds. \end{aligned} \tag{6}$$

By Theorem 10 of [8] we obtain

$$\lim_{t\to\infty} e^{iH_0t}Pe^{-iHt}\phi = W_+\phi$$

for all $\phi \in \mathcal{H}$, provided W_+ is extended from $\mathcal{H}_b^\perp$ to $\mathcal{H}$ by putting $W_+(\mathcal{H}_b) = 0$. The integrand of (6) therefore converges for each s to

$$e^{iH_0s}W_+(JT_s\rho)W_+^*e^{iH_0s}$$

and we obtain

$$\Omega_+(\rho) = W_+\rho W_+^* + \int_0^\infty e^{iH_0s}W_+(JT_s\rho)W_+^* e^{-iH_0s}ds \tag{7}$$

provided we justify taking the limit under the integral sign.

In order to do this we let Q denote the non-orthogonal projection with kernel $\mathcal{H}_d \oplus \mathcal{H}_b$ and range equal to range W_-. Since

$$Q(T_t\rho)Q^* = Q(S_t\rho)Q^* + \int_0^t Q(S_{t-s}JT_s\rho)Q^*ds$$

we deduce that if $\rho \geq 0$

$$\int_0^t \| Q(S_{t-s}JT_s\rho)Q^* \|_1 ds \leq \| Q \|^2 \| \rho \|_1.$$

Now by Hypothesis F and Eq. (5) of [8] there exists $\alpha > 0$ such that

$$\| Qe^{-iHt}\phi \| = \| e^{-iHt}Q\phi \| \geq \alpha \| Q\phi \|$$

for all $\phi \in \mathcal{H}$

$$\int_0^\infty \| Q(JT_s\rho)Q^* \|_1 ds \leq \alpha^{-2} \| Q \|^2 \| \rho \|_1.$$

Using the identity

$$Pe^{-iH(t-s)} = Pe^{-iH(t-s)}Q$$

we now see that the integrand of (6) is dominated in trace norm by

$$\| Pe^{-iH(t-s)}Q(JT_s\rho)Q^* e^{iH^*(t-s)}P \|_1 \leq \| Q(JT_s\rho)Q^* \|_1.$$

This is integrable so we may apply the dominated convergence theorem to complete the proof.

The fact that the projection P in (5) is orthogonal allows the following physical interpretation. If $\rho \geq 0$ and $\text{tr}\,[\rho] = 1$ then

$$\begin{aligned}\text{tr}\,[\Omega_+(\rho)] &= \lim_{t\to\infty} \text{tr}\,[e^{iH_0t}P(T_t\rho)Pe^{-iH_0t}] \\ &= \lim_{t\to\infty} \text{tr}\,[PT_t(\rho)]\end{aligned}$$

so

$$0 \leq \text{tr}\,[\Omega_+(\rho)] \leq 1$$

and this quantity may be interpreted as the probability of the neutron in the state ρ at $t = 0$ eventually escaping from the nucleus. We also define the bound states of the dynamical semigroup T_t to be those lying in

$$V_b = \{ \rho \geq 0 : \text{tr}\,[\Omega_+(\rho)] = 0 \}.$$

THEOREM 5. — The bound states of T_t are those with support in a certain closed subspace $\mathcal{L}$ of $\mathcal{H}$ satisfying

$$\mathcal{H}_b \subseteq \mathcal{L} \subseteq \mathcal{H}_b \oplus \mathcal{H}_d.$$

In the case of Example 1, $\mathscr{L}$ is the largest such subspace invariant under A and under e^{-iHt} for all $t \geq 0$.

Proof. — We first note that since Ω_+ is positivity preserving, V_b is a norm closed order ideal. By ([5], p. 54), V_b is the set of ρ with support in a certain closed subspace $\mathscr{L}$ of $\mathscr{H}$.

If $\rho \geq 0$ and tr $[PT_t(\rho)] = 0$ for all $t \geq 0$ then tr $[\Omega_+(\rho)] = 0$ so $\rho \in V_b$. Conversely if tr $[PT_a(\rho)] > 0$ for some a, then putting

$$\sigma = T_a(\rho) = \sum_{n=0}^{\infty} \lambda_n \, | f_r \rangle \langle f_r \, |$$

we obtain for $t \geq a$ that

$$\begin{aligned} \operatorname{tr}\,[PT_t(\rho)] &= \operatorname{tr}\,[PT_{t-a}\sigma] \\ &\geq \operatorname{tr}\,[PS_{t-a}\sigma] \\ &= \sum_{n=0}^{\infty} \lambda_n \, \| P e^{-iH(t-a)} f_n \|^2 . \end{aligned}$$

Now by the open mapping theorem there is a constant $0 < \delta \leq 1$ such that

$$\delta \, \| P\psi \| \leq \| Q\psi \| \leq \delta^{-1} \, \| P\psi \|$$

for all $\psi \in \mathscr{H}$. Combining this observation with Eq. (5) of [8] we obtain

$$\begin{aligned} \operatorname{tr}\,[PT_t(\rho)] &\geq \sum_{n=0}^{\infty} \lambda_n \delta^2 \, \| Q e^{-iH(t-a)} f_n \|^2 \\ &\geq \sum_{n=0}^{\infty} \lambda_n \delta^2 \alpha^2 \, \| Q f_n \|^2 \\ &\geq \sum_{n=0}^{\infty} \lambda_n \delta^4 \alpha^2 \, \| P f_n \|^2 \\ &= \delta^4 \alpha^2 \operatorname{tr}\,[P\sigma] \end{aligned}$$

so

$$\lim_{t \to \infty} \operatorname{tr}\,[\Omega_+ \rho] \geq \delta^4 \alpha^2 \operatorname{tr}\,[PT_a(\rho)] > 0$$

and $\rho \notin V_b$. Hence $\rho \in V_b$ if and only if tr $[PT_t(\rho)] = 0$ for all $t \geq 0$.

Using the expansion

$$T_t = S_t + \int_0^t S_{t-s} J S_s ds + \int_{s=0}^t \int_{u=0}^s S_{t-s} J S_{s-u} J S_u du ds + \dots$$

together with the definition of J in Example 1, we finally see that $\psi \in \mathscr{L}$, or equivalently $| \psi \rangle \langle \psi | \in V_b$, if and only if

$$Pe^{-iHt(1)}Ae^{-iHt(2)}A \dots e^{-iHt(m)}\psi = 0,$$

for all choices of $t(1), \dots$ This leads immediately to the required characterisation of $\mathscr{L}$.

The general phenomenon of neutron capture is rather complicated because $\mathscr{L}$ may be strictly larger than $\mathscr{H}_b$, but the orthogonal projection P′ of $\mathscr{H}$ onto $\mathscr{L}$ may be used to investigate it.

THEOREM 6. — If $\rho \geq 0$ and $\text{tr}\,[\rho] = 1$ then

$$p(t) = \text{tr}\,[P'T_t(\rho)]$$

is continuous and monotone increasing, with limit $p(\infty)$ which may be called the capture probability of ρ.

Proof. — By ([5], p. 18) the dynamical semigroup T_t has a dual semigroup T_t^* on $\mathscr{L}(\mathscr{H})$. Since $0 \leq P' \leq 1$ we have $0 \leq T_t^*(P') \leq 1$. By the invariance of $\mathscr{C}(\mathscr{L})$ under T_t it follows that if $\psi \in \mathscr{L}$ and $\| \psi \| = 1$

$$\langle T_t^*(P')\psi, \psi \rangle = \text{tr}\,[T_t^*(P') \,|\, \psi \rangle \langle \psi \,|] = \text{tr}\,[P'T_t(|\, \psi \rangle \langle \psi \,|)] = 1.$$

Applying the spectral theorem to $T_t^*(P')$ we deduce that

$$P' \leq T_t^*(P') \leq 1$$

for all $t \geq 0$. Now if $s \leq t$

$$\begin{aligned} p(t) &= \text{tr}\,[P'T_t(\rho)] \\ &= \text{tr}\,[T_{t-s}^*(P')T_s(\rho)] \\ &\geq \text{tr}\,[P'T_s(\rho)] = p(s). \end{aligned}$$

The continuity of $p(t)$ is obvious.

Since $PP' = P'P = 0$ we see that

$$0 \leq \text{tr}\,[PT_t(\rho)] + \text{tr}\,[P'T_t(\rho)] \leq 1$$

for all $t \geq 0$ and so

$$0 \leq \text{tr}\,[\Omega_+(\rho)] + p(\infty) \leq 1. \tag{8}$$

We conjecture that the sum actually equals 1, but have not proved this. Nevertheless even (8) allows us to give a simple sufficient condition for capture of an ingoing neutron. We state the result only for Example 1, although the method can obviously be extended.

THEOREM 7. — Suppose in Example 1 that H has a bound state ϕ_0 and that there exists $\psi \in \mathscr{H}_0$ such that $\| \psi \| = 1$ and

$$\langle W_-\psi, A^*\phi_0 \rangle \neq 0 \tag{9}$$

Then

$$\mathrm{tr}[\Omega_+\Omega_-(|\,\psi\,\rangle\langle\,\psi\,|)] < 1.$$

Proof. — By (8) and Theorem 6 we have only to show that if $\rho = \Omega_-(|\,\psi\,\rangle\langle\,\psi\,|)$ then

$$\mathrm{tr}\,[\mathrm{P}'\mathrm{T}_t(\rho)] > 0$$

for some $t \geq 0$. Now applying inequalities which follow easily from (3), we obtain

$$\begin{aligned}\mathrm{T}_t(\rho) &\geq \mathrm{T}_t(|\,\mathrm{W}_-\psi\,\rangle\langle\,\mathrm{W}_-\psi\,|)\\ &\geq \int_0^t \mathrm{S}_{t-s}\mathrm{J}\mathrm{S}_s(|\,\mathrm{W}_-\psi\,\rangle\langle\,\mathrm{W}_-\psi\,|)ds\end{aligned}$$

so

$$\begin{aligned}\mathrm{tr}\,[\mathrm{P}'\mathrm{T}_t(\rho)] &\geq \int_0^t 2\beta\,\|\,\mathrm{P}'e^{-i\mathrm{H}(t-s)}\mathrm{A}e^{-i\mathrm{H}s}\mathrm{W}_-\psi\,\|^2 ds\\ &= 2\beta\int_0^t |\,\langle\,e^{-i\mathrm{H}s}\mathrm{W}_-\psi,\ \mathrm{A}^*\phi_0\,\rangle\,|^2 ds.\end{aligned}$$

This is strictly positive by (9) and the continuity of the integrand.

§ 3. SCATTERING WITH SLOW DECAY

In this section we consider the asymptotic form for small $\alpha > 0$ of the scattering operators of the last section, where V_0, J are replaced by $\alpha\mathrm{V}_0$, $\alpha\mathrm{J}$ everywhere, so that α measures the rate of decay of the nucleus to its ground state. Physically it is clear that as $\alpha \to 0$ direct nuclear scattering and radiative decay operate on different time scales and become independent processes. If S^0 is the unitary scattering operator on $\mathcal{H}$ for the self-adjoint Hamiltonian $\mathrm{H}_0 + \mathrm{V}_1$, and if the relaxation of the nucleus to its ground state $v = |\,\Omega\,\rangle\langle\,\Omega\,|$ is described by the map

$$\mathrm{E}(\rho) = \mathrm{tr}_1\,[\rho] \otimes v$$

from $\mathcal{T}(\mathcal{H})$ to $\mathcal{T}(\mathcal{H})$, then one expects that

$$\lim_{\alpha\to 0} \Omega_+^\alpha\Omega_-^\alpha\rho = \mathrm{E}(\mathrm{S}^0\rho\mathrm{S}^{0*})$$

The proof of this is surprisingly difficult, mathematically because we cannot suppose that W_-^α has closed range for *all* small $\alpha > 0$ because of the comments in [*8*], § 4, and physically because of the long lifetimes associated with compound nuclear scattering. We therefore make rather different technical assumptions in this section on the operator V_1 and apply Kato's smooth perturbation theory. We replace the hypothesis of Lemmas 2 and 3 by the assumptions that the self-adjoint operator V_1 on $\mathcal{H}$ is of the form

$$\mathrm{V}_1 = (\mathrm{A} \otimes 1)\mathrm{X}(\mathrm{B} \otimes 1)$$

where $\| X \| = 1$ and the bounded operators A, B on $\mathscr{K}_0$ satisfy

$$\int_0^\infty \| Ae^{-iK_0t}B \| \, dt = c < 1. \tag{10}$$

We also suppose, probably unnecessarily, that

$$\int_{-\infty}^\infty \| Be^{-iK_0t}\phi \| \, dt < \infty \tag{11}$$

for all ϕ in a dense subspace $\mathscr{D}$ of $\mathscr{K}_0$. All the other assumptions are as before, the dependence of various operators on α being indicated by superscripts.

As usual the dependence of the ingoing wave operators on α is easy to handle.

THEOREM 8. — If $\psi \in \mathscr{H}_0$ and $\rho \in \mathscr{C}(\mathscr{H}_0)$ then

$$\lim_{\alpha \to 0} W_-^\alpha \psi = W_-^0 \psi$$

and

$$\lim_{\alpha \to 0} \Omega_-^\alpha(\rho) = W_-^0 \rho W_-^{0*} \tag{12}$$

Proof. — Since (11) implies Cook's condition we see that the wave operators W_-^α exist and are given by

$$W_-^\alpha \psi = \psi - i \int_0^\infty e^{-iH^\alpha s} V_1 e^{iH_0 s} \psi \, ds$$

for all $\psi \in \mathscr{D}$. Now $e^{-iH^\alpha s}$ converges strongly to $e^{-i(H_0+V_1)s}$ as $\alpha \to 0$, so by the dominated convergence theorem

$$\lim_{\alpha \to 0} W_-^\alpha \psi = \psi - i \int_0^\infty e^{-i(H_0+V_1)s} V_1 e^{iH_0 s} \psi \, ds$$
$$= W_-^0 \psi .$$

The result for general $\psi \in \mathscr{H}_0$ is obtained by density arguments. The proof of (12) depends upon the observation that if $0 \le \rho \in \mathscr{C}(\mathscr{H}_0)$ then

$$0 \le S_t^\alpha(e^{iH_0 t} \rho e^{-iH_0 t}) \le T_t^\alpha(e^{iH_0 t} \rho e^{-iH_0 t})$$

so

$$0 \le W_-^\alpha \rho W_-^{\alpha *} \le \Omega_-^\alpha(\rho).$$

Therefore

$$\| \Omega_-^\alpha(\rho) - W_-^\alpha \rho W_-^{\alpha *} \|_1 = \operatorname{tr} [\Omega_-^\alpha(\rho) - W_-^\alpha \rho W_-^{\alpha *}]$$
$$= \operatorname{tr} [\rho] - \operatorname{tr} [W_-^\alpha \rho W_-^{\alpha *}]$$

Since W_-^α converges strongly to W_-^0 as $\alpha \to 0$, where W_-^0 is unitary, we see that

$$\lim_{\alpha \to 0} \| \Omega_-^\alpha(\rho) - W_-^0 \rho W_-^{0*} \|_1 = \operatorname{tr} [\rho] - \lim_{\alpha \to 0} \operatorname{tr} [W_-^\alpha \rho W_-^{\alpha *}] = 0.$$

Before stating the next theorem we note that W_+^0 is a unitary operator on $\mathscr{H}$ under the condition (10).

THEOREM 9. — The limit

$$\Omega_+^\alpha \rho = \lim_{t \to \infty} e^{iH_0 t}(T_t^\alpha \rho) e^{-iH_0 t}$$

exists for all $\rho \in \mathscr{C}(\mathscr{H})$ and $\alpha > 0$, and defines a completely positive trace-preserving map Ω_+^α from $\mathscr{C}(\mathscr{H})$ into $\mathscr{C}(\mathscr{H}_0)$. Moreover

$$\lim_{\alpha \to 0} \Omega_+^\alpha \rho = E(W_+^0 \rho W_+^{0*})$$

for all $\rho \in \mathscr{C}(\mathscr{H})$.

Before starting the proof we use the theory of dilations of dynamical semigroups as in ([3], § 6) to reduce to a Hilbert space problem.

PROPOSITION 10. — There exists a Hilbert space $\mathscr{K}_2$ and a one-parameter group of isometries on $\mathscr{K}_1 \otimes \mathscr{K}_2$ with generator K^α such that

$$e^{Z_1^\alpha t}(\mathrm{tr}_2\,[\rho]) = \mathrm{tr}_2\left[e^{-iK^\alpha t} \rho e^{iK^{\alpha*} t}\right] \tag{13}$$

for all $\rho \in \mathscr{C}(\mathscr{K}_1 \otimes \mathscr{K}_2)$. Moreover there is a one-parameter group of isometries $e^{-iK_2 t}$ on $\mathscr{K}_2$ such that

$$\lim_{\alpha \to 0} e^{-iK^\alpha t}\psi = e^{-i(K_1 + K_2 t)}\psi \tag{14}$$

for all $\psi \in \mathscr{K}_1 \otimes \mathscr{K}_2$.

Proof. — The basic construction is that of Theorem 5 of [3], whose method may be extended to more general states ρ than considered there. The limit $\alpha \to 0$ is easily taken, the isometries $e^{-iK_2 t}$ on $\mathscr{K}_2 = L^2(Y_\infty)$ corresponding to simple shifts on the time parameters of the elements $\omega \in Y_\infty$ without change of length of ω as time passes.

Proof of theorem. — Using the Trotter product formula we obtain

$$T_t^\alpha(\mathrm{tr}_2\,[\rho]) = \mathrm{tr}_2\,[e^{-i(K_0 + K^\alpha + V_1)t} \rho e^{i(K_0 + K^{\alpha*} + V_1)t}].$$

We expand the exponential terms of this in powers of V_1, obtaining

$$\begin{aligned} e^{-i(K_0+K^\alpha+V_1)x}\psi &= e^{-i(K_0+K^\alpha)x}\psi \\ &- i\int_{s=0}^{x} e^{-i(K_0+K^\alpha)(x-s)} V_1 e^{-i(K_0+K^\alpha)s}\psi ds \\ &- \int_{s=0}^{x}\int_{u=0}^{s} e^{-i(K_0+K^\alpha)(x-s)} V_1 e^{-i(K_0+K^\alpha)(s-u)} V_1 e^{-i(K_0+K^\alpha)} u du ds + \dots \end{aligned}$$

If ψ lies in the algebraic tensor product

$$\mathscr{D}' = \mathscr{D} \otimes \mathscr{K}_1 \otimes \mathscr{K}_2$$

we deduce from (10) and (11) that

$$\int_0^\infty \| V_1 e^{-i(K_0+K^\alpha+V_1)x}\psi \| dx < \infty \tag{15}$$

where the integral converges uniformly with respect to α. We denote the integrand of (15) by ψ_x^α.

If $\rho = | \phi \rangle \langle \psi |$ where $\phi, \psi \in \mathcal{D}'$ then

$$e^{iK_0t}T_t^\alpha(\mathrm{tr}_2[\rho])e^{-iK_0t} = \mathrm{tr}_2\left[\int_{x=0}^t\int_{y=0}^t dxdy \; e^{-iK^\alpha(t-x)}e^{iK_0x} | \phi_x^\alpha \rangle \langle \psi_y^\alpha | e^{-iK_0y}e^{iK^{\alpha*}(t-y)}\right]$$

$$= \mathrm{tr}_2\left[\int_{0\le x\le y\le t} \dots + \int_{0\le y\le x\le t} \dots\right]$$

$$= \int_{0\le x\le y\le t} e^{Z_1(t-y)}\,\mathrm{tr}_2\,[e^{-iK^\alpha(y-x)}e^{iK_0x} | \phi_x^\alpha \rangle \langle \psi_y^\alpha | e^{-iK_0y}]dxdy$$

$$+ \int_{0\le y\le x\le t} e^{Z_1(t-x)}\,\mathrm{tr}_2\,[e^{iK_0x} | \phi_x^\alpha \rangle \langle \psi_y^\alpha | e^{-iK_0y}e^{iK^{\alpha*}(x-y)}]dxdy$$

by (13). We deduce using (2) and (15) that

$$\Omega_+^\alpha(\mathrm{tr}_2[\rho]) = \lim_{t\to\infty} e^{iK_0t}T_t^\alpha(\mathrm{tr}_2[\rho])e^{-iK_0t}$$

$$= \int_{0\le x\le y<\infty} \mathrm{tr}_{12}\,[e^{-iK^\alpha(y-x)}e^{iK_0x} | \phi_x^\alpha \rangle \langle \psi_y^\alpha | e^{-iK_0y}]dxdy \otimes v$$

$$= \int_{0\le y\le x<\infty} \mathrm{tr}_{12}\,[e^{iK_0x} | \phi_x^\alpha \rangle \langle \psi_y^\alpha | e^{-iK_0y}e^{iK^{\alpha*}(x-y)}]dxdy \otimes v$$

We next use (14) and exploit the uniformity of the convergence with respect to α, to obtain

$$\lim_{\alpha\to 0} \Omega_+^\alpha\,(\mathrm{tr}_2[\rho])$$

$$= \int_{0\le x\le y<\infty} \mathrm{tr}_{12}\,[e^{-i(K_1+K_2)(y-x)}e^{iK_0x} | \phi_x^0 \rangle \langle \psi_y^0 | e^{-iK_0y}]dxdy \otimes v$$

$$+ \int_{0\le y\le x<\infty} \mathrm{tr}_{12}\,[e^{iK_0x} | \phi_x^0 \rangle \langle \psi_y^0 | e^{-iK_0y}e^{i(K_1+K_2)(x-y)}]dxdy \otimes v.$$

Since K_2 commutes with K_0, K_1 and V_1 we see that

$$\phi_x^0 = V_1 e^{-i(K_0+K_1+K_2+V_1)x}\phi$$

$$= e^{-iK_2x}V_1 e^{-i(K_0+K_1+V_1)x}\phi$$

which implies that

$$\lim_{\alpha\to 0} \Omega_+^\alpha\,(\mathrm{tr}_2[\rho]) = \int_{x=0}^\infty\int_{y=0}^\infty \mathrm{tr}_{12}\,[e^{i(K_0+K_1)x}V_1 e^{-i(K_0+K_1+V_1)x} | \phi \rangle \langle \psi | \; e^{i(K_0+K_1+V_1)y}V_1 e^{-i(K_0+K_1)y}]dxdy \otimes v$$

$$= \mathrm{tr}_{12}\,[W_+^0\rho W_+^{0*}] \otimes v$$

$$= E\{ W_+^0\,\mathrm{tr}_2[\rho]W_+^{0*} \}$$

We conclude by noting that the set of states on $\mathscr{H}$ of the form $\mathrm{tr}_2\,[\rho]$ for $\rho = | \phi \rangle \langle \psi |$ and $\phi, \psi \in \mathscr{D}'$, is dense in $\mathscr{C}(\mathscr{H})$.

We use Theorem 9 to investigate the time dependence of the energy of the system. By the conservation of energy, the coupling of the nucleus to the electromagnetic field, and the fact that the nucleus is initially in its ground state, one would expect that

$$\mathrm{tr}\,[\mathrm{H}_0\Omega_+\Omega_-(\rho)] \leq \mathrm{tr}\,[\mathrm{H}_0\rho]$$

for all $0 \leq \rho \in \mathscr{C}(\mathscr{H}_0)$. We have not been able to prove this and believe that it is at best approximately true. The following is relevant to this conjecture for small α.

THEOREM 11. — Under the hypothesis of this section

$$\lim_{\alpha\to 0} \Omega_+^\alpha \Omega_-^\alpha \rho = \sigma$$

exists for all $0 \leq \rho \in \mathscr{C}(\mathscr{H}_0)$ and lies in $\mathscr{C}(\mathscr{H}_0)$. Moreover

$$0 \leq \mathrm{tr}\,[\mathrm{H}_0\sigma] \leq \mathrm{tr}\,[\mathrm{H}_0\rho].$$

Proof. — By Theorems 8 and 9

$$\lim_{\alpha\to 0} \Omega_+^\alpha \Omega_-^\alpha \rho = \mathrm{E}(\mathrm{S}^0\rho\mathrm{S}^{0*})$$

where $\mathrm{S}^0 = \mathrm{W}_+^0\mathrm{W}_-^0$ is unitary and commutes with H_0. Therefore

$$\begin{aligned}\mathrm{tr}\,[\mathrm{H}_0\sigma] &= \mathrm{tr}\,[\mathrm{H}_0\mathrm{E}(\mathrm{S}^0\rho\mathrm{S}^{0*})]\\ &\leq \mathrm{tr}\,[\mathrm{H}_0(\mathrm{S}^0\rho\mathrm{S}^{0*})]\\ &= \mathrm{tr}\,[\mathrm{H}_0\rho].\end{aligned}$$

REFERENCES

[1] W. O. AMREIN, J. M. JAUCH, K. B. SINHA, *Scattering theory in quantum mechanics*, W. A. Benjamin, Inc., 1977.

[2] A. BARCHIELLI, Quantum dynamical semigroups and nucleon-nucleus scattering, *Il Nuovo Cimento*, t. **47** A, 1978, p. 187-199.

[3] E. B. DAVIES, Some contraction semigroups in quantum probability, *Z. Wahrscheinlichkeitstheorie*, t. **23**, 1972, p. 261-273.

[4] E. B. DAVIES, Markovian master equations, *Commun. Math. Phys.*, t. **39**, 1974, p. 91-110.

[5] E. B. DAVIES, *Quantum theory of open systems*, Academic Press, 1976.

[6] E. B. DAVIES, Two-channel Hamiltonians and the optical model of nuclear scattering, *Ann. Inst. H. Poincaré*, t. **29** A, 1978, p. 395-413.

[7] E. B. DAVIES, Scattering from a spatially restricted atom. I, *Adv. Math.*, t. **34**, 1979, p. 28-45.

[8] E. B. DAVIES, Non-unitary scattering and capture. I. Hilbert space theory, *Commun. Math. Phys.*, t. **71**, 1980, p. 277-288.

[9] F. HAAKE, Statistical treatment of open systems by generalized master equations, *Springer Tracts in Modern Physics*, vol. **66**, 1973.
[10] P. E. HODGSON, *Nuclear reactions and nuclear structure*, Oxford Univ. Press, 1971.
[11] R. G. NEWTON, *Scattering theory of waves and particles*, McGraw-Hill, 1966.
[12] J. V. PULÈ, The Bloch equations, *Commun. Math. Phys.*, t. **38**, 1974, p. 241-256.
[13] M. REED and B. SIMON, *Methods of modern mathematical physics*, vol. **3**, Academic Press, 1979.

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