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# A Model for Absorption or Decay

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*Abstract.* We investigate the gradual absorption or decay of a single quantum-mechanical particle by means of a simple model consisting of a one-parameter contraction semigroup on a Hilbert space. As well as relating our work to quantum-mechanical measurement theory, we find the evolution equation for the particle in the classical limit.

## 1. Introduction

We study some aspects of the theory of strongly continuous one-parameter contraction semigroups $U_\lambda(t)$ on a Hilbert space $\mathscr{H}$. We suppose that the generator is

$$Z_\lambda = iH - \lambda V \qquad (1.1)$$

where $H$ is a self-adjoint operator, $V \geqslant 0$ is a well-behaved perturbation and $\operatorname{Re}\lambda \geqslant 0$. If $\operatorname{Re}\lambda = 0$, so that $U_\lambda(t)$ is a unitary group, the spectral properties of $Z_\lambda$ and its scattering theory have been intensively investigated [1, 2]. However, there are many interesting questions to be answered when $\operatorname{Re}\lambda > 0$. For example if $\lambda$ is real, one would expect that as $\lambda$ increases the semigroup would become more contractive. We show in Section 2 that in the limit $\lambda \to +\infty$ this fails in a spectacular manner, the limit $U_{+\infty}(t)$ being unitary on a subspace of $\mathscr{H}$. Subsequent sections are devoted to the probability of eventual absorption, a model for position observables, sojourn times and the classical motion, these involving the limits $\lambda \to +\infty$, $\lambda \to 0$, $t \to +\infty$ and $h \to 0$ in various combinations.

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## 2. The Strong Coupling Limit at Fixed Time

We study the limit $\lambda \to +\infty$ by analytic continuation from the unitary case very much in the spirit of [3, 4]. We shall suppose that $V$ is a relatively bounded perturbation of $H$ with relative bound zero, although the results can be extended to relatively bounded quadratic forms by the usual techniques [1, 2]. If $\operatorname{Re}\lambda \geqslant 0$ then $Z_\lambda$ is a dissipative operator with the same domain as $H$ and, by [1], $U_\lambda(t)$ is a strongly continuous one-parameter semigroup for $t \geqslant 0$. Moreover for each $t$, use of the Trotter product formula [5] shows that $U_\lambda(t)$ is an analytic function of $\lambda$ on $D = \{\operatorname{Re}\lambda > 0\}$ and strongly continuous

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for $\lambda$ in $\bar{D} = \{\mathrm{Re}\,\lambda \geqslant 0\}$. Recall from [6] that norm, strong and weak analyticity coincide for operator-valued functions of a complex variable. We shall frequently use the following proposition, which may be deduced from the scalar version.

*Proposition 2.1*: Let $\{f_\alpha(\lambda)\}_{\alpha\geqslant 0}$ be a family of uniformly bounded $\mathscr{H}$-valued analytic functions on $D$ which are norm continuous on $\bar{D}$. Suppose that

$$\lim_{\alpha\to\infty} f_\alpha(\lambda) = f(\lambda) \tag{2.1}$$

for all $\lambda \in S$, where either

i) $S$ has an accumulation point in $D$, or
ii) $S \subseteq \{z : \mathrm{Re}\, z = 0\}$ and has non-zero Lebesgue measure. Then the limit exists for all $\lambda$ in $D$ and is an analytic function on $D$.

We start our study with some results about quadratic forms. Let $\mathscr{D}$ be a subspace of $\mathscr{H}$, not necessarily dense, and let $Q$ be a non-negative quadratic form on $\mathscr{D}$. If $Q$ is closed we can associate to it a non-negative self-adjoint operator $H$ on $\bar{\mathscr{D}}$ such that $\mathscr{D} = \mathrm{Dom}(H^{1/2})$. We then define a bounded operator $A_Q(\beta)$ on $\mathscr{H}$ for all $\beta > 0$ by

$$A_Q(\beta) f = (\beta + H)^{-1} f \tag{2.2}$$

if $f \in \bar{\mathscr{D}}$ and

$$A_Q(\beta) f = 0 \tag{2.3}$$

if $f \in \bar{\mathscr{D}}^{\perp}$. These $A_Q(\beta)$ form a pseudo-resolvent family in the sense of [1]. We extend $Q$ to $\mathscr{H}$ by putting $Q(f) = +\infty$ if $f \notin \mathscr{D}$ and then write $Q_1 \leqslant Q_2$ if

$$0 \leqslant Q_1(f) \leqslant Q_2(f) \leqslant +\infty \tag{2.4}$$

for all $f \in \mathscr{H}$.

*Lemma 2.2*: If $Q_1$ and $Q_2$ are two closed non-negative quadratic forms on $\mathscr{H}$ then $Q_1 \leqslant Q_2$ if and only if $A_1(\beta) \geqslant A_2(\beta)$ for all $\beta > 0$.

*Proof*: This is a small modification of [1, p. 330].

*Corollary 2.3*: Let $Q_x$ be the form associated with $H + xV$ where $x \geqslant 0$. Then as $x \to +\infty$, $Q_x$ converges to the form $Q_\infty$ of a self-adjoint operator $H_\infty$ with

$$\mathscr{D}(H_\infty^{1/2}) = \mathscr{D}(H^{1/2}) \cap \text{Null } V. \tag{2.5}$$

For all $\beta > 0$

$$s\text{-}\lim_{x\to+\infty} A_x(\beta) = A_\infty(\beta) \tag{2.6}$$

where $A_\infty(\beta)$ is the pseudo-resolvent of $H_\infty$.

*Proof*: If we define

$$Q_\infty(f) = \lim_{x\to+\infty} Q_x(f) \tag{2.7}$$

then $Q_\infty$ is certainly a quadratic form. Since such a form is closed if and only if it is lower semi-continuous, and the limit is monotone, $Q_\infty$ is closed, and so may be associated to a self-adjoint operator $H_\infty$. Now clearly $Q_\infty$ is the smallest closed quadratic form such that $Q_\infty \geqslant Q_x$ for all $x \geqslant 0$, so by Lemma 2.2, $R_\infty(\beta)$ is the largest pseudo-resolvent family such that

$$R_\infty(\beta) \leqslant R_x(\beta) \tag{2.8}$$

for all $\beta > 0$ and $x > 0$. But $R_x(\beta)$ are monotonically decreasing in $x$ and so converge strongly, and the limit is also a pseudo-resolvent family. Therefore equation (2.6) is valid.

*Note*: If $\mathscr{H} = L^2(\mathbb{R}^3)$, $H$ is the Laplacian and $V \geqslant 0$ is a scalar potential whose support $S$ has smooth boundary; then $H_\infty$ is the self-adjoint operator on $L^2(\mathbb{R}^3 \backslash S)$ given by taking the Laplacian with vanishing boundary conditions.

*Theorem 2.4*: Let $f \in \mathscr{D}(H_\infty)^-$ and let $\lambda \geqslant 0$. Then

$$\lim_{\lambda \to +\infty} U_\lambda(t) f = e^{iH_\infty t} f. \tag{2.9}$$

*Proof*: We first note that by analytic continuation equation (2.6) holds for all $\mathrm{Re}\,\beta > 0$. A small modification of [1, p. 502] now yields

$$\lim_{\lambda \to +\infty} e^{it(H+\lambda V)} f = e^{itH_\infty} f \tag{2.10}$$

for all $f \in \mathscr{D}(H_\infty)^-$. If $\mathrm{Re}\,z > 0$ and we define

$$g_\lambda(z) = e^{(iH - \lambda z V)t} f \tag{2.11}$$

then

$$\lim_{\lambda \to +\infty} g_\lambda(z) = e^{itH_\infty} f \tag{2.12}$$

for all $z$ on the negative real axis and hence by Proposition 2.1 for all $\mathrm{Re}\,z > 0$. The theorem is proved by taking $z = 1$.

As an immediate consequence we see that if $f \in \mathscr{D}(H_\infty)^-$ then for all $t \geqslant 0$

$$\lim_{\lambda \to +\infty} \|U_\lambda(t) f\| = \|f\| \tag{2.13}$$

even though the generator becomes more dissipative as $\lambda \to +\infty$. We remark that similar conclusions have been reached by C. N. Friedman [7] who, however, considers the case $\lambda = +\infty$ directly using the Trotter product formula. Although at first sight paradoxical, a particular case solved by Allcock [8] shows that a wave packet suffers partial reflection at the boundary of the support of $V$ and that the reflection coefficient approaches unity as $\lambda \to +\infty$.

We mention here a related and well-known phenomenon in electromagnetic theory [9]. If an electromagnetic wave evolving according to the telegraph equation is incident upon a conducting medium then it is partially reflected and the transmitted wave is absorbed as it travels through the medium. As the conductivity is increased the absorption rate in the medium increases but so does the reflection coefficient and in the infinite conductivity limit the wave is entirely reflected.

## 3. The Probability of Eventual Absorption

We study the evolution equation

$$\psi'(t) = (iH - \lambda V)\psi(t) \tag{3.1}$$

as before. If $\|\psi\| = 1$ then according to quantum-mechanical measurement theory [10]

$$P(t) = \|e^{(iH-\lambda V)t}\psi\|^2 \tag{3.2}$$

may be interpreted as the probability of non-absorption up to time $t$ of a particle starting at time zero in the state $\psi$ and moving in a medium whose absorptive properties are represented by the operator $\lambda V$. Therefore one can say that the particle is certain to be absorbed eventually if

$$\lim_{t\to+\infty} \| e^{(iH-\lambda V)t}\psi\| = 0. \tag{3.3}$$

*Theorem 3.1*: Suppose that for small purely imaginary $\lambda$

$$s\text{-}\lim_{t\to+\infty} U_0(-t)\, U_\lambda(t) = W_+(\lambda) \tag{3.4}$$

exists. Then for all $\psi \in \mathscr{H}$ and all $\operatorname{Re}\lambda > 0$

$$P_\lambda(\infty) = \lim_{t\to+\infty} \|U_\lambda(t)\psi\|^2 \tag{3.5}$$

exists and is non-zero except possibly on a discrete set of values of $\lambda$.

*Proof*: The function

$$f_t(\lambda) = U_0(-t)\, U_\lambda(t)\psi \tag{3.6}$$

is continuous on $\bar{D}$, analytic on $D$ and uniformly bounded. We are given that it converges as $t \to +\infty$ for a certain interval on the imaginary axis. Therefore by Proposition 2.1 it converges to an analytic function $f_\infty(\lambda)$. For the given range of values of $\lambda$ on the imaginary axis $W_+(\lambda)$ is isometric so $f_\infty(\lambda)$ has non-zero boundary values. Therefore its zeros are isolated points. Finally

$$P_\lambda(\infty) = \lim_{t\to+\infty} \|U_\lambda(t)\psi\|^2 = \lim_{t\to+\infty} \|U_0(-t)\, U_\lambda(t)\psi\|^2 = \|f_\infty(\lambda)\|^2. \tag{3.7}$$

*Note*: If $\lambda$ is purely imaginary then $U_\lambda(t)$ is unitary and conditions for the existence of $W_\pm(\lambda)$ have been very extensively investigated, the case where $|\lambda|$ is small being particularly well-behaved [11]. Expressions for $W_+(\lambda)$ when $\operatorname{Re}\lambda > 0$ but $|\lambda|$ is not small may then be obtained by analytic continuation.

The following lemma shows that if $\operatorname{Re}\lambda > 0$, the existence of bound states does not prevent decay of wave-functions.

*Lemma 3.2*: Let $H$ be a self-adjoint operator with no point spectrum, let $V \geqslant 0$ be a perturbation with relative bound zero and let $\operatorname{Re}\lambda > 0$. Then any eigenvalue $\alpha$ of $iH - \lambda V$ has $\operatorname{Re}\alpha > 0$.

*Proof*: If $0 \neq \psi \in \mathscr{D}(H)$ and

$$(iH - \lambda V)\psi = \alpha\psi \tag{3.8}$$

then

$$i\langle H\psi,\psi\rangle - \lambda\langle V\psi,\psi\rangle = \alpha\langle\psi,\psi\rangle \tag{3.9}$$

and taking real parts

$$-(\operatorname{Re}\lambda)\langle V\psi,\psi\rangle = \operatorname{Re}\alpha\langle\psi,\psi\rangle. \tag{3.10}$$

Therefore either $\operatorname{Re}\alpha < 0$ or $\langle V\psi,\psi\rangle = 0$. But in the latter case, since $V \geqslant 0$, it follows that $V\psi = 0$ so that $H\psi = -i\alpha\psi$, contrary to our assumptions on $H$.

The following technical lemma is needed for the proof of Theorem 3.4.

*Lemma 3.3*: Suppose the measurable function $b$ satisfies

$$0 \leqslant b(t) \leqslant \gamma \quad \text{for all} \quad 0 \leqslant t < \infty \quad \text{and} \quad \lim_{t\to+\infty} b(t) = 0.$$

Suppose $a$ is a non-negative locally bounded measurable function on $[0,\infty)$ satisfying

$$a(t) \leqslant \alpha + \int_0^t a(t-s)\, b(s)\, ds \tag{3.11}$$

for all $t \geqslant 0$. Then

$$\lim_{t\to\infty} e^{-\gamma t} a(t) = 0. \tag{3.12}$$

*Proof*: We put $\tilde{a}(t) = e^{-\gamma t} a(t)$ and $\tilde{b}(t) = e^{-\gamma t} b(t)$ so that for all $t \geqslant 0$

$$\tilde{a}(t) \leqslant \alpha e^{-\gamma t} + \int_0^t \tilde{a}(t-s)\, \tilde{b}(s)\, ds. \tag{3.13}$$

Since $\|\tilde{b}\|_1 < 1$ the equation

$$\tilde{c}(t) = \alpha e^{-\gamma t} + \int_0^t \tilde{c}(t-s)\, \tilde{b}(s)\, ds \tag{3.14}$$

can be solved by iteration in $L^1(0,\infty)$. Inspection of the equation then shows that $\tilde{c}$ is continuous and vanishes at infinity. We therefore have only to show that $\tilde{a}(t) \leqslant \tilde{c}(t)$ for all $t \geqslant 0$ to complete the proof.

The equation

$$\alpha e^{-\gamma t} + \int_0^t \tilde{a}(t-s)\, \tilde{b}(s)\, ds < (1+\varepsilon)\, \tilde{c}(t) \tag{3.15}$$

is satisfied for $t = 0$ and both sides are continuous functions. If it is not satisfied for all $t \geqslant 0$ then there is a first value $t_0$ for which it fails. But then $\tilde{a}(t) < (1+\varepsilon)\, \tilde{c}(t)$ for all $0 \leqslant t < t_0$, so

$$\alpha e^{-\gamma t_0} + \int_0^{t_0} \tilde{a}(t_0-s)\, \tilde{b}(s)\, ds < (1+\varepsilon)\, \alpha e^{-\gamma t_0} + \int_0^{t_0} (1+\varepsilon)\, \tilde{c}(t_0-s)\, \tilde{b}(s)\, ds$$
$$= (1+\varepsilon)\, \tilde{c}(t_0). \tag{3.16}$$

This contradicts the assumption that there is a first point where equation (3.15) fails. Finally $\varepsilon > 0$ is arbitrary so we get the required inequality.

*Theorem 3.4*: Suppose that $V = \gamma 1 + WX$ where $\|W\|\,\|X\| \leqslant \gamma$ and

$$\lim_{t\to+\infty} \|X e^{iHt} W\| = 0. \tag{3.17}$$

Then

$$\lim_{t\to+\infty} \|e^{(iH-V)t}\| = 0. \tag{3.18}$$

*Proof*: From the equation

$$e^{(iH+WX)t} = e^{iHt} + \int_{s=0}^{t} e^{(iH+WX)(t-s)}\, WX\, e^{iHs}\, ds \tag{3.19}$$

we obtain

$$e^{(iH+WX)t}\, W = e^{iHt}\, W + \int_{s=0}^{t} e^{(iH+WX)(t-s)}\, WX\, e^{iHs}\, W\, ds. \tag{3.20}$$

Putting

$$\|e^{(iH+WX)t}\, W\| = a(t) \tag{3.21}$$

and

$$\|X\, e^{iHs}\, W\| = b(t) \tag{3.22}$$

this yields

$$a(t) \leqslant \|W\| + \int_{s=0}^{t} a(t-s)\, b(s)\, ds \tag{3.23}$$

and so by Lemma 3.3

$$\lim_{t\to+\infty} a(t)\, e^{-\gamma t} = 0. \tag{3.24}$$

Now by equation (3.19)

$$\|e^{(iH+WX)t}\| \leqslant 1 + \int_{s=0}^{t} a(t-s)\, \|X\| ds \tag{3.25}$$

so

$$\|e^{(iH-V)t}\| \leqslant e^{-\gamma t} + \int_{s=0}^{t} e^{-\gamma t}\, a(t-s) \|X\| ds \tag{3.26}$$

which converges to zero as $t \to +\infty$.

*Theorem 3.5*: Let $H = -\Delta$ on $L^2(\mathbb{R}^n)$ and let $V$ be a bounded non-negative scalar potential

$$(V\psi)(x) = V(x)\, \psi(x) \tag{3.27}$$

such that

$$\lim_{x\to\infty} V(x) = \gamma > 0. \tag{3.28}$$

Then

$$\lim_{t\to+\infty} \|e^{(iH-V)t}\| = 0. \tag{3.29}$$

*Proof*: We let $V_\lambda(x) = V(x)$ if $0 \leqslant V(x) \leqslant \gamma$ and $V_\lambda(x) = \gamma + \lambda\{V(x) - \gamma\}$ if $V(x) > \gamma$. Then $\operatorname{Re} V_\lambda(x) \geqslant 0$ if $\lambda$ lies in the region

$$D = \{\lambda : \operatorname{Re}\lambda > 0 \text{ or } |\lambda| < \gamma\|V\|^{-1}\}. \tag{3.30}$$

If $\lambda \in D$ and $t \geqslant 0$ then by the Trotter product formula

$$A_t(\lambda) = e^{(iH-V_\lambda)t} \tag{3.31}$$

is a uniformly bounded analytic function of $\lambda$. Therefore norm convergence to zero holds for all $\lambda \in D$, and in particular for $\lambda = 1$, if it can be proved for $|\lambda| < \gamma\|V\|^{-1}$. By Theorem 3.5 it is sufficient to prove the following.

If $Y \geqslant 0$ is a bounded potential and $\lim_{x\to\infty} Y(x) = 0$ then

$$\lim_{t\to+\infty} \|Ye^{iHt}Y\| = 0. \tag{3.32}$$

This result holds for all bounded potentials of compact support by [11] and the class of potentials for which it holds is obviously closed under uniform limits.

## 4. Generalized Position Observables

As well as asking whether the particle is absorbed one may ask where it is absorbed. For the sake of definiteness we carry out the discussion in $L^2(\mathbb{R}^3)$ although it is clearly of a more general nature. We put $H = -\Delta$ and let $V > 0$ be a bounded scalar potential. For any Borel set $E \subseteq \mathbb{R}^3$ we define the projection $P(E)$ by

$$\{P(E)\psi\}(x) = \chi_E(x)\psi(x). \tag{4.1}$$

Following [12] we now define the probability of absorption within a region of space as a certain positive operator-valued measure.

*Theorem 4.1*: Suppose that

$$s - \lim_{t\to+\infty} e^{(iH-V)t} = 0. \tag{4.2}$$

Then if $E$ is a Borel set in $\mathbb{R}^3$ the formula

$$A(E) = 2\int_0^\infty e^{(-iH-V)t}\, V^{1/2} P(E)\, V^{1/2} e^{(iH-V)t}\, dt \tag{4.3}$$

defines a normalized positive operator-valued measure on $\mathbb{R}^3$.

*Proof*: It is shown in [10] that for all $\psi \in \mathscr{H}$

$$\frac{d}{dt}\|e^{(iH-V)t}\psi\|^2 = -2\langle Ve^{(iH-V)t}\psi, e^{(iH-V)t}\psi\rangle. \tag{4.4}$$

Therefore

$$\|\psi\|^2 = 2 \int_0^\infty \langle V e^{(iH-V)t} \psi, e^{(iH-V)t} \psi\rangle \, dt + \lim_{t\to+\infty} \|e^{(iH-V)t} \psi\|^2 \tag{4.5}$$

which proves that $A(\mathbb{R}^3) = 1$. That $A(E)$ is a countably additive positive operator-valued measure is obvious from its definition.

We now specialize further by letting $V = \frac{1}{2}\lambda 1$ where $\lambda > 0$. For $x \in \mathbb{R}^3$ we let $x \to U_x$ be the strongly continuous unitary group given for $\psi \in \mathscr{H}$ by

$$(U_x \psi)(y) = \psi(y - x). \tag{4.6}$$

*Theorem 4.2*: The positive operator-valued measure $A(E)$ is covariant in the sense that for all Borel sets $E$ and all $x \in \mathbb{R}^3$

$$U_x^* A(E) \, U_x = A(E + x). \tag{4.7}$$

*Proof*: We use the well-known fact that for all $t \in \mathbb{R}$ and all $x \in \mathbb{R}^3$

$$[U_x, e^{iHt}] = 0. \tag{4.8}$$

For the simple potential we have chosen

$$A(E) = \lambda \int_0^\infty e^{-\lambda t} e^{-iHt} P(E) \, e^{iHt} \, dt. \tag{4.9}$$

Hence

$$\begin{aligned} U_x^* A(E) \, U_x &= \lambda \int_0^\infty e^{-\lambda t} \, U_x^* \, e^{-iHt} P(E) \, e^{iHt} \, U_x \, dt \\ &= \lambda \int_0^\infty e^{-\lambda t} e^{-iHt} \, U_x^* P(E) \, U_x \, e^{iHt} \, dt \\ &= \lambda \int_0^\infty e^{-\lambda t} e^{-iHt} P(E + x) \, e^{iHt} \, dt \\ &= A(E + x). \end{aligned} \tag{4.10}$$

Introducing explicitly the dependence of $A(E)$ on $\lambda$, the relationship between it and the usual projection-valued measure is an obvious consequence of equation (4.9).

*Theorem 4.3*: For all $\psi \in \mathscr{H}$ and all $E \subseteq \mathbb{R}^3$

$$\langle P(E)\psi\psi\rangle = \lim_{\lambda\to+\infty} \langle A_\lambda(E) \, \psi, \psi\rangle. \tag{4.11}$$

Returning to the case of finite $\lambda$ we mention that covariant positive-operator valued measures have been studied in [13, 14]. The representation theorem below is a special case of a very general result in [14]. We let

$$\hat{f}(k) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} f(x) \, e^{-ix\cdot k} \, d^3 x \tag{4.12}$$

for $f \in L^2(\mathbb{R}^3)$ and let

$$\mathscr{D} = \{f \varepsilon L^2(\mathbb{R}^3) : \hat{f} \varepsilon L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)\} \tag{4.13}$$

so that $\mathscr{D}$ is a dense subspace of $L^2(\mathbb{R}^3)$ consisting entirely of continuous bounded functions.

*Theorem 4.4*: There exists a positive self-adjoint operator $T$ on $L^2(\mathbb{R}^3)$ such that $\mathscr{D} \subseteq \mathscr{D}(T^{1/2})$ and such that if one defines

$$T_x = U_x^* T U_x \tag{4.14}$$

for all $x \in \mathbb{R}^3$ then

$$\langle A(E)\psi,\psi\rangle = \int_{\mathbb{R}^3} \chi_E(x)\langle T_x\psi,\psi\rangle\, d^3x \tag{4.15}$$

for all Borel sets $E \subseteq \mathbb{R}^3$ and all $\psi \in \mathscr{D}$.

*Proof*: We first note that $U_x : \mathscr{D} \to \mathscr{D}$ for all $x \in \mathbb{R}^3$ so if $T^{1/2}$ has domain containing $\mathscr{D}$ then so does $T_x^{1/2}$. It is sufficient to prove the theorem in the case when $E$ is a bounded Borel set. We then have

$$\langle A(E)\psi,\psi\rangle = \lambda \int_E \int_{t=0}^{\infty} e^{-\lambda t}|(e^{iHt}\psi)(x)|^2\, d^3x\, dt \tag{4.16}$$

$$= \lambda(2\pi)^{-3} \int_{t=0}^{\infty} \int_{\mathbb{R}^9} e^{-\lambda t + ik\cdot x - ik^2 t - ih\cdot x + ih^2 t}\, \chi_E(x)\,\hat{\psi}(k)\,\overline{\hat{\psi}(h)}\, dk\, dh\, dx\, dt$$

$$= (2\pi)^{-3} \int_{\mathbb{R}^9} \frac{\lambda}{\lambda + i(k^2 - h^2)} e^{i(k-h)\cdot x}\, \chi_E(x)\,\hat{\psi}(k)\,\overline{\hat{\psi}(h)}\, dk\, dh\, dx.. \tag{4.17}$$

Now if

$$\mathscr{D}_0 = \{f \varepsilon L^2 : \hat{f} \text{ has compact support}\} \tag{4.18}$$

then the formula

$$(Tf)(b) = (2\pi)^{-3} \int_{\mathbb{R}^3} \frac{\lambda}{\lambda + i(k^2 - h^2)} \hat{f}(k)\, dk \tag{4.19}$$

defines an operator $T : \mathscr{D}_0 \to L^2(\mathbb{R}^3)$. Moreover if $\psi \in \mathscr{D}_0$ then by equation (4.17)

$$\langle A(E)\psi,\psi\rangle = \int_{\mathbb{R}^3} \chi_E(x)\langle T_x\psi\psi\rangle\, dx. \tag{4.20}$$

if $S_\varepsilon$ is the sphere centre $O$, radius $\varepsilon$, then

$$\langle T\psi,\psi\rangle = \lim_{\varepsilon\to 0} (\tfrac{4}{3}\pi\varepsilon^3)^{-1} \langle A(S_\varepsilon)\psi,\psi\rangle \tag{4.21}$$

so $T \geqslant 0$ on the domain $\mathscr{D}_0$. The self-adjoint operator of the theorem is then defined as the Friedrichs extension of $T$. The domain of $T^{1/2}$ equals the domain of the closure of the quadratic form defined on $\mathscr{D}_0 \times \mathscr{D}_0$ by

$$\langle Tf, g\rangle = (2\pi)^{-3} \int_{\mathbb{R}^6} \frac{\lambda}{\lambda + i(k^2 - h^2)} \hat{f}(k)\, \overline{\hat{g}(h)}\, dk\, dh \tag{4.22}$$

and this contains $\mathscr{D}$ because the kernel is a bounded function.

## 5. Sojourn Time

We put $\mathscr{H} = L^2(\mathbb{R}^3)$ and let $P$ be the projection associated with the interior of a bounded region $D$ in $\mathbb{R}^3$. If $H$ is some Hamiltonian on $\mathscr{H}$ and $\psi \in \mathscr{H}$ is a unit vector representing the state of the particle at time zero then the length of time that the particle is within $D$, its sojourn time, is usually [15] taken to be

$$\int_0^\infty \|P e^{iHt} \psi\|^2\, dt. \tag{5.1}$$

However, the justification of this expression in terms of the quantum theory of measurement is not straightforward. One may certainly take

$$\|P e^{iHt} \psi\|^2 \tag{5.2}$$

as the probability that the particle is within $D$ at time $t$ if the particle has been allowed to evolve unobserved between times 0 and $t$. However if the particle is observed at two times $0 < s < t$ then the probability that it is inside at both times is

$$\|P e^{iH(t-s)} P e^{iHs} \psi\|^2 \tag{5.3}$$

with similar but more complicated expressions if one makes observations at frequent intervals. As Friedman [7] showed, attempts to take the limit of continuous observations in this manner lead nowhere.

The theory of quantum stochastic processes [10] allows one to describe such continuous measurements, but not in a unique way. We shall try to make clear that even for so simple a situation as asking a question corresponding to a given projection over a period of time there are various experimental methods of doing this which give rise to mathematically different equations.

In the discussion of the very similar problem of decay of an unstable particle in [16, 17] it is supposed that an unstable particle collides randomly at a rate $\lambda$ with the atoms of some medium, and at each collision the relevant atom changes its state in a manner which after amplification gives information about whether the particle has yet decayed. If $P$ is the projection onto the subspace of $\mathscr{H}$ corresponding to the undecayed particle and $Q = I - P$ the projection onto the subspace of the decay products then the evolution equation for the density matrix $\rho(t)$ of the particle is

$$\rho'(t) = i[H, \rho] - \lambda\rho + \lambda(P\rho P + Q\rho Q). \tag{5.4}$$

However, the equation in which we are interested is that for the evolution conditional on the particle not having decayed and this is

$$\rho'(t) = i[H, \rho] - \lambda\rho + P\rho P. \tag{5.5}$$

It is known [10] that if $\rho(0) \geqslant 0$ then $\rho(t) \geqslant 0$ for all $t > 0$ and that $\mathrm{tr}[\rho(t)]$ is monotonically decreasing. If $\mathrm{tr}[\rho(0)] = 1$ then $\mathrm{tr}[\rho(t)]$ is interpreted as the probability that the particle has not decayed at time $t$. Measurement theory then suggests that we should define the sojourn time $T(\lambda)$ in the unstable state by the asymptotic equation for $t \to +\infty$

$$\mathrm{tr}[\rho(t)] \simeq e^{-\lambda(t-T(\lambda))}. \tag{5.6}$$

*Theorem 5.1*: Let $\rho(0) = |\psi\rangle\langle\psi|$ where $\|\psi\| = 1$. If there exists a constant $c$ such that for all $n$

$$\int_0^\infty ds_1 \int_0^\infty ds_2 \ldots \int_0^\infty ds_n \|P e^{iHs_1} P e^{iHs_2} P \ldots P e^{iHs_n} \psi\|^2 < c^n \tag{5.7}$$

then the sojourn time $T(\lambda)$ is finite for sufficiently small $\lambda$ and

$$\lim_{\lambda \to 0} T(\lambda) = \int_0^\infty \|P e^{iHs} \psi\|^2 \, ds. \tag{5.8}$$

*Proof*: The evolution equation (5.5) may be rewritten as the integral equation

$$\rho(t) = e^{-\lambda t} e^{iHt} \rho(0) e^{-iHt} + \lambda \int_0^t e^{-\lambda s} e^{iHs} P \rho(t-s) P e^{-iHs} \, ds \tag{5.9}$$

which may then be solved by integration giving

$$\rho(t) = e^{-\lambda t} \left\{ e^{iHt} \rho(0) e^{-iHt} + \lambda \int_0^t e^{iHs} P e^{iH(t-s)} \rho e^{-iH(t-s)} P e^{-iHs} \, ds \right.$$
$$\left. + \lambda^2 \int_{s=0}^t \int_{u=0}^s e^{iH(t-s)} P e^{iH(s-u)} P e^{iHu} \rho e^{-iHu} P e^{-iH(s-u)} P e^{-iH(t-s)} \, du \, ds + \ldots \right\}. \tag{5.10}$$

Therefore if $\rho(0) = |\psi\rangle\langle\psi|$

$$e^{\lambda t} \mathrm{tr}[\rho(t)] = 1 + \lambda \int_{s=0}^t \|P e^{iHs} \psi\|^2 \, ds + \lambda^2 \int_{s=0}^t \int_{u=0}^s \|P e^{iH(s-u)} P e^{iHu} \psi\|^2 \, du \, ds + \ldots. \tag{5.11}$$

If $0 < \lambda < c^{-1}$ then $T(\lambda)$ is finite and given by

$$e^{\lambda T(\lambda)} = 1 + \lambda \int_0^\infty \|P e^{iHs} \psi\|^2 \, ds + 0(\lambda^2) \tag{5.12}$$

from which the result follows.

It is something of a joke that the standard formula for sojourn times is given by taking the weak coupling limit $\lambda \to 0$, while in the last section another equally standard formula (4.11) corresponds to $\lambda \to \infty$. As pointed out in the discussion of Eckstein and Siegert [16] the treatment above would still be correct (as far as any argument not involving a quantization of the atoms of the medium can be) even if the collisions between the undecayed particle and the atoms resulted in no macroscopically observable signal, for the reduction of the wave packet is caused by the collision and not by the efficiency of the amplification process (we stress that this statement depends on our decision not to quantize the atoms in the medium).

We consider next a somewhat different experimental arrangement, which corresponds more closely to that described by Allcock [8]. We suppose that an unstable and stationary particle is near to a counter which detects the decay products when they are emitted. The counter is spatially separated from the particle but the decay products are emitted into the counter and then detected in the same way as before. We claim that in this situation the appropriate evolution equation for the density matrix $\rho(t)$ of the particle plus decay products is [10]

$$\rho'(t) = i[H, \rho] - \tfrac{1}{2}\lambda(Q\rho + \rho Q) + \lambda Q\rho Q. \tag{5.13}$$

By [10] the equation analogous to (5.5) is

$$\rho'(t) = i[H, \rho] - \tfrac{1}{2}\lambda(Q\rho + \rho Q) \tag{5.14}$$

whose solution is

$$\rho(t) = e^{(iH - \lambda Q/2)t}\rho(0)\, e^{(-iH - \lambda Q/2)t}. \tag{5.15}$$

According to this equation, which is the one used by Allcock [8], the undecayed particle evolves without any reduction of the wave packet, but its probability decreases with time.

*Theorem 5.2*: If $\rho(0) = |\psi\rangle\langle\psi|$ where $\|\psi\| = 1$ and $P$ is a smooth perturbation of $H$, then the sojourn time is finite for sufficiently small $\lambda$ and

$$\lim_{\lambda \to 0} T(\lambda) = \int_{\infty}^{0} \|P\, e^{iHs}\psi\|^2\, ds. \tag{5.16}$$

*Proof*: By [11] if $\lambda$ is sufficiently small then the expansion

$$e^{(iH + \lambda P/2)t}\psi = e^{iHt}\psi + \tfrac{1}{2}\lambda \int_0^t e^{iH(t-s)} P\, e^{iHs}\, ds + \ldots \tag{5.17}$$

converges uniformly with respect to $t$ and one has

$$\begin{aligned} \Omega_+\psi &= \lim_{t \to +\infty} e^{-iHt} e^{(iH + \lambda P/2)t}\psi \\ &= \psi + \tfrac{1}{2}\lambda \int_0^{\infty} e^{-iHs} P\, e^{iHs}\psi\, ds + \ldots . \end{aligned} \tag{5.18}$$

Now

$$\begin{aligned} e^{\lambda t}\,\mathrm{tr}[\rho(t)] &= e^{\lambda t}\|e^{(iH - \lambda Q/2)t}\psi\|^2 \\ &= \|e^{(iH + \lambda P/2)t}\psi\|^2 \end{aligned} \tag{5.19}$$

so

$$e^{\lambda T(\lambda)} = \lim_{t\to+\infty} e^{\lambda t}\,\mathrm{tr}[\rho(t)]$$

$$= \|\Omega_+ \Psi\|^2$$

$$= 1 + \lambda \int_0^\infty \|P\, e^{iHs} \psi\|^2\, ds + 0(\lambda^2) \tag{5.20}$$

from which the result is again immediate.

An intuitive explanation of the difference between the two models is that for the first the particle may i) be observed to have decayed or ii) be observed not to have decayed, while for the second the particle may i) be observed to have decayed or ii′) be inferred not to have decayed through not having been observed decaying. Whether or not one believes that there is some philosophical distinction between ii) and ii′) it is clear that there are two mathematical models, and that which is appropriate depends on the experimental arrangement.

The above two cases are extremes but there are many intermediate situations. For example one may suppose that the particle moves through the medium but that the particle and its decay products have significantly different collision cross-sections with respect to the atoms of the medium. There are also advantages in replacing the projections by other operators for some purposes [18]. All of these possibilities can be described within the formalism of [10].

## 6. The Classical Limit

In the above sections we have described the dynamics of a quantum-mechanical particle by the use of a non-self-adjoint Hamiltonian in Hilbert space. In classical mechanics there is no possibility of following this procedure since a classical Hamiltonian can have no meaning unless it is real. It is therefore quite interesting that one can find the classical limit of the above dynamics. We follow closely the method of Hepp [19] where the unitary problem is solved.

In $L^2(\mathbb{R})$ we consider the equation

$$\psi'(t) = Z_\lambda \psi(t) \tag{6.1}$$

where

$$Z_\lambda = -\frac{i}{2} p^2 - i\lambda^{-1} V(\lambda^{1/2} q) - B(\lambda^{1/2} q). \tag{6.2}$$

Here $p, q$ are the usual operators on $L^2(\mathbb{R})$, $V$ is real, twice differentiable and satisfies

$$|V''(x) = V''(y)| \leqslant C|x-y|^\delta + C|x-y|^{1/\delta} \tag{6.3}$$

for some $\delta > 0$ and all $x, y \in \mathbb{R}$, while $B \geqslant 0$ satisfies

$$|B(x) - B(y)| \leqslant C|x-y|^\delta + C|x-y|^{1/\delta}. \tag{6.4}$$

It is shown in [19] that the growth condition for large $|x-y|$ may be greatly weakened, and it may easily be seen that the same is true of the growth condition for small

$|x-y|$. In connection with the technique of analytic continuation it is significant that $B$ and $V$ have different scaling factors and that different degrees of smoothness are needed for $B$ and $V$ in the proof of the theorem below.

We suppose that $U_\lambda(t)$ is a one-parameter contraction semigroup on $L^2(\mathbb{R})$ for all sufficiently small $\lambda > 0$ and that its generator is an extension of $Z_\lambda$ defined on Schwartz space $\mathcal{S}$. For any complex $\alpha = 2^{-1/2}(\xi + i\pi)$ the Weyl operator

$$U(\alpha) = \exp i(\pi q - \xi p) \tag{6.5}$$

is well defined and

$$U(\alpha)^* p U(\alpha) = p + \pi, \quad U(\alpha)^* q U(\alpha) = q + \xi. \tag{6.6}$$

We define the classical evolution by

$$\xi'(t) = \pi(t), \quad \pi'(t) = -V'\{\xi(t)\} \tag{6.7}$$

with initial conditions $\xi(0) = \xi$ and $\pi(0) = \pi$, and suppose that these equations have a solution for $0 \leqslant t \leqslant T$. We then put

$$\alpha(t) = 2^{-1/2}(\xi(t) + i\pi(t)). \tag{6.8}$$

We also let

$$\beta(t,s) = \int_t^s B\{\xi(x)\}\, dx \tag{6.9}$$

so $e^{-2\beta(t,s)}$ represents the probability that a particle starting at time $s$ and moving along the classical trajectory is not absorbed at time $t$, when the absorption rate at position $x$ is $2B(x)$.

*Theorem 6.1*: If $r, s \in \mathbb{R}$ then

$$\begin{aligned} s-\lim_{\lambda\to 0} U(\lambda^{-1/2}\alpha)^* U_\lambda(t)^* \exp\{ir\lambda^{1/2}q + is\lambda^{1/2}p\} U_\lambda(t) U(\lambda^{-1/2}\alpha) \\ = \exp\{ir\xi_t + is\pi_t - 2\beta_{t,0}\} \end{aligned} \tag{6.10}$$

uniformly for $0 < t < T$. Consequently if $\|\psi\| = 1$ and

$$\psi_\lambda(t) = U_\lambda(t) U(\lambda^{-1/2}\alpha)\psi \tag{6.11}$$

then

$$\lim_{\lambda\to 0} \langle \exp\{ir\lambda^{1/2}q + is\lambda^{1/2}p\}\psi_\lambda(t), \psi_\lambda(t)\rangle = \exp\{ir\xi_t + is\pi_t - 2\beta_{t,0}\}. \tag{6.12}$$

*Proof*: We define the unitary operators $V_\lambda(t)$ on $L^2(\mathbb{R})$ by

$$\frac{\partial}{\partial t} V_\lambda(t)\psi = i\lambda^{-1/2} V_\lambda(t)(\pi_t' q - \xi_t' p)\psi \tag{6.13}$$

where $\psi \in \mathcal{S}$ and $V_\lambda(0) = U(\lambda^{-1/2}\alpha)$. Then for all $t \geqslant 0$

$$V_\lambda(t) = U(\lambda^{-1/2}\alpha_t) \exp i\theta(\lambda, t) \tag{6.14}$$

where the form of the phase factor $\theta(\lambda, t)$ does not concern us. We also define

$$W_\lambda(t,s) = V_\lambda(t)^* \, U_\lambda(t-s) \, V_\lambda(s) \exp i\lambda^{-1} \gamma_{t,s} \tag{6.15}$$

where

$$\gamma_{t,s} = \int_s^t \{\tfrac{1}{2}\pi_x^2 + V(\xi_x)\} \, dx. \tag{6.16}$$

Then if $\psi \in L^2(\mathbb{R})$

$$\begin{aligned} &\|U(\lambda^{-1/2}\alpha)^* \, U_\lambda(t)^* \exp\{ir\lambda^{1/2}q + is\lambda^{1/2}p\} \, U_\lambda(t) \, U(\lambda^{-1/2}\alpha)\psi \\ &\quad - \exp\{ir\xi_t + is\pi_t - 2\beta_{t,0}\}\psi\| \\ &\quad = \|V_\lambda(0)^* \, U_\lambda(t)^* \exp\{ir\lambda^{1/2}(q - \lambda^{-1/2}\xi_t) + is\lambda^{1/2}(p - \lambda^{-1/2}\pi_t)\}. \\ &U_\lambda(t) \, V_\lambda(0)\psi - e^{-2\beta(t,0)}\psi\| \\ &\quad = \|W_\lambda(t,0)^* \exp\{ir\lambda^{1/2}q + is\lambda^{1/2}p\} \, W_\lambda(t,0)\psi - e^{-2\beta(t,0)}\psi\|. \end{aligned} \tag{6.17}$$

Since

$$s - \lim_{\lambda \to 0} \exp\{ir\lambda^{1/2}q + is\lambda^{1/2}p\} = 1 \tag{6.18}$$

it is sufficient to prove that

$$s - \lim_{\lambda \to 0} W_\lambda(t,0) = W(t,0) \, e^{-\beta(t,0)} \tag{6.19}$$

and

$$s - \lim_{\lambda \to 0} W_\lambda(t,0)^* = W(t,0)^* \, e^{-\beta(t,0)} \tag{6.20}$$

where $W(t,s)$ is the unitary propagator such that for $\psi \in \mathscr{S}$

$$\frac{\partial}{\partial t} W(t,s)\psi = -iH(t) \, W(t,s)\psi \tag{6.21}$$

and

$$H(t) = \tfrac{1}{2}p^2 + \tfrac{1}{2}V''(\xi_t)q^2 \tag{6.22}$$

with the usual boundary condition that $W(t,t) = 1$ for all $t \in \mathbb{R}$.

Just as $H(t)$ lies in the Lie algebra of quadratic Hamiltonians for all $t$, it may be shown by explicit calculations that $W(t,s)$ lies in a certain Lie group of unitary operators on $L^2(\mathbb{R})$.

It follows that $W(t,s)$ leaves $\mathscr{S}$ invariant and that if $\psi \in \mathscr{S}$ then $t, s \to W(t,s)\psi$ is a continuous function when $\mathscr{S}$ is given its usual Frechet space topology.

If $\psi \in \mathscr{S}$ then

$$
\begin{aligned}
&\|W_\lambda(t,0)\psi - e^{-\beta(t,0)}W(t,0)\psi\|^2 \\
&= \|U_\lambda(t)V_\lambda(0)\psi - e^{-i\lambda^{-1}\gamma(t,0)-\beta(t,0)}V_\lambda(t)W(t,0)\psi\|^2 \\
&= \left\| \int_0^t \frac{\partial}{\partial s} U_\lambda(t-s)e^{-i\lambda^{-1}\gamma(s,0)-\beta(s,0)}V_\lambda(s)W(s,0)\psi\, ds \right\|^2 \\
&\leqslant t^2 \max_{0\leqslant s\leqslant t} \left\| \frac{\partial}{\partial s} U_\lambda(t-s)e^{-i\lambda^{-1}\gamma(s,0)-\beta(s,0)}V_\lambda(s)W(s,0)\psi \right\|^2 \\
&= t^2 \max_{0\leqslant t\leqslant s} \Big\| U_\lambda(t-s)(-z_\lambda)e^{-i\lambda^{-1}\gamma(s,0)-\beta(s,0)}V_\lambda(s)W(s,0)\psi \\
&\qquad + U_\lambda(t-s)\{-i\lambda^{-1}\tfrac{1}{2}\pi_s^2 - i\lambda^{-1}V(\xi_s) - B(\xi_s)\}e^{-i\lambda^{-1}\gamma(s,0)-\beta(s,0)}V_\lambda(s)W(s,0)\psi \\
&\qquad + U_\lambda(t-s)e^{-i\lambda^{-1}\gamma(s,0)-\beta(s,0)}V_\lambda(s)\{i\lambda^{-1/2}\pi_s' q - i\lambda^{-1/2}\xi_s' p\}W(s,0)\psi \\
&\qquad + U_\lambda(t-s)e^{-i\lambda^{-1}\gamma(s,0)-\beta(s,0)}V_\lambda(s)\left\{-\frac{i}{2}p^2 - \frac{i}{2}V''(\xi_s)q^1\right\}W(s,0)\psi \Big\|^2 \\
&\leqslant T^2 \max_{0\leqslant s\leqslant T} \Big\| \Big[\frac{i}{2}(p+\lambda^{-1/2}\pi_s)^2 + i\lambda^{-1}V(\xi_s+\lambda^{1/2}q) + B(\xi_s+\lambda^{1/2}q) \\
&\qquad - i\lambda^{-1/2}V'(\xi_s)q - i\lambda^{-1/2}\pi_s p - i\lambda^{-1}\tfrac{1}{2}\pi_s^2 - i\lambda^{-1}V(\xi_s) \\
&\qquad - B(\xi_s) - \frac{i}{2}p^2 - \frac{i}{2}V''(\xi_s)q^2\Big]W(s,0)\psi \Big\|^2 \\
&= T^2 \max_{0\leqslant s\leqslant T} \Big\| \Big[ i\lambda^{-1}V(\xi_s+\lambda^{1/2}q) - i\lambda^{-1}V(\xi_s) - i\lambda^{-1/2}V'(\xi_s)q \\
&\qquad - \frac{i}{2}V''(\xi_s)q^2 + B(\xi_s+\lambda^{1/2}q) - B(\xi_s)\Big]W(s,0)\psi \Big\|^2 \\
&\leqslant T^2 \max_{0\leqslant s\leqslant T} \int_{\mathbf{R}} \Big| i\lambda^{-1}V(\xi_s+\lambda^{1/2}x) - i\lambda^{-1}V(\xi_s) - i\lambda^{-1/2}V'(\xi_s)x \\
&\qquad - \frac{i}{2}V''(\xi_s)x^2 + B(\xi_s+\lambda^{1/2}x) - B(\xi_s)\Big|^2 |\{W(s,0)\psi\}(x)|^2\, dx \\
&\leqslant T^2 \max_{0\leqslant s\leqslant T} \int_{\mathbf{R}} \{C\lambda^{\delta/2}x^{2+\delta} + C\lambda^{1/2\delta}x^{2+1/\delta} + C\lambda^{\delta/2}x^{\delta} + C\lambda^{2/\delta}x^{1/\delta}\}^2. \\
&|\{W(s,0)\psi\}(x)|^2\, dx. \qquad (6.23)
\end{aligned}
$$

This converges to 0 as $\lambda \to 0$ because $W(s,0)\psi \in \mathscr{S}$ uniformly for $0 \leqslant s \leqslant T$.

The proof of equation (6.20) is similar. If $\psi \in \mathcal{S}$ then

$$\begin{aligned}
&\|W_\lambda(t,0)^* \psi - e^{-\beta(t,0)} W(t,0)^* \psi\| \\
&\quad = \|V_\lambda(0)^* U_\lambda(t)^* V_\lambda(t) e^{-i\lambda^{-1}\gamma(t,0)} \psi - e^{-\beta(t,0)} W(t,0)^* \psi\| \\
&\quad = \|U_\lambda(t)^* V_\lambda(t) \psi - e^{i\lambda^{-1}\gamma(t,0)-\beta(t,0)} V_\lambda(0) W(t,0)^* \psi\| \\
&\quad = \left\| \int_0^t \frac{\partial}{\partial s} U_\lambda^*(s) V_\lambda(s) e^{i\lambda^{-1}\gamma(t,s)-\beta(t,s)} W(t,s)^* \psi \, ds \right\|
\end{aligned} \tag{6.24}$$

after which we proceed as before, using

$$\frac{\partial}{\partial s} W(t,s)^* \psi = -iH(s) W(t,s)^* \psi \tag{6.25}$$

instead of equation (6.21).

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