## Annales scientifiques de l'Université de Clermont-Ferrand 2 Série Probabilités et applications

# J. A. VAN CASTEREN M. DEMUTH

### On differences of heat semigroups

Annales scientifiques de l'Université de Clermont-Ferrand 2, tome 93, série Probabilités et applications, n° 8 (1989), p. 119-147

<a href="http://www.numdam.org/item?id=ASCFPA\_1989\_\_93\_8\_119\_0">http://www.numdam.org/item?id=ASCFPA\_1989\_\_93\_8\_119\_0</a>

© Université de Clermont-Ferrand 2, 1989, tous droits réservés.

L'accès aux archives de la revue « Annales scientifiques de l'Université de Clermont-Ferrand 2 » implique l'accord avec les conditions générales d'utilisation (http://www.numdam.org/conditions). Toute utilisation commerciale ou impression systématique est constitutive d'une infraction pénale. Toute copie ou impression de ce fichier doit contenir la présente mention de copyright.

NUMDAM

#### ON DIFFERENCES OF HEAT SEMIGROUPS

J.A. VAN CASTEREN - M. DEMUTH

Abstract. We describe some results on pointwise inequalities for generalized Schrödinger (or absorption/excitation or heat) semigroups. For these inequalities we use a kind of generalized Brownian bridge measure. The main topic of the present paper are some results on heat semigroup differences consisting of trace class or Hilbert-Schmidt operators. As an application stability results of essential and/or absolutely continuous spectra of quantum-mechanical Hamiltonians are obtained.

#### 1. Some properties of generalized Schrödinger semigroups.

We take a rather abstract and general point of view. Let E be a locally compact second countable Hausdorff space and let  $A_0$  be the generator of a Feller semigroup  $\{P_0(t): t \geq 0\}$  in the Banach space  $C_0(E)$ . This means that  $\{P_0(t): t \geq 0\}$  is a family of operators with the following properties:

- (i)  $P_0(s+t) = P_0(s) \circ P_0(t), s, t \ge 0, P_0(0) = I;$
- (ii)  $f \geq 0$ ,  $f \in C_0(E)$ , implies  $P_0(t)f \geq 0$  and, of course,  $P_0(t)f$  belongs to  $C_0(E)$ ;
- (iii)  $||P_0(t)f||_{\infty} \leq ||f||_{\infty}, f \in C_0(E);$
- (iv)  $\lim_{t\downarrow 0} [P_0(t)f](x) = f(x), f \in C_0(E), x \in E.$

In the presence of (i) and (iii), (iv) is equivalent to the strong continuity:

(iv')  $\lim_{t\downarrow 0} \|P_0(t)f - f\|_{\infty} = 0, f \in C_0(E).$ 

We suppose that the semigroup is given by

$$\left[P_0(t)f
ight](x)=\int f(y)p_0(t,x,y)dm(y),$$

where  $p_0(t, x, y)$  is a symmetric function which is continuous on  $(0, \infty) \times E \times E$  and where m is a given fixed strictly positive Radon measure on E. Often we write dy instead of dm(y). We also suppose

$$\lim_{x\to\Delta}\sup_{y\in K}p_0(t,x,y)=0,\quad t>0,$$

for every compact subset K of E. Here  $\triangle$  is the point at infinity of E. In addition let  $V: E \to [-\infty, \infty]$  be a Borel measurable function, defined on E.

Problem. Does some version of the operator

$$f \mapsto A_0 f - V f, \quad f \in D(A_0) \cap D(V)$$

generate a positivity preserving strongly continuous semigroup in  $C_0(E)$ ?

Regarding this kind of problem we mention the following references: Voigt [45] Simon [34] and [35], Graffi [18], Cycon et al [8], Davies and Simon [12], van Casteren [36], [38], [39] and [41]. For a concise formulation we introduce the following definition.

**1.1.** Definition. (a) A Borel measurable function  $V: E \to [0, \infty]$  belongs to  $K(E) = K(E, A_0)$  if

$$\limsup_{t\downarrow 0}\sup_{x\in E}\int_0^t\left(\int p_0(s,x,y)V(y)dm(y)\right)ds=0.$$

(b) A Borel measurable function  $V: E \to [0, \infty]$  belongs to  $K_{loc}(E) = K_{loc}(E, A_0)$  if  $1_K V$  belongs to K(E) for all compact subsets K of E.

In van Casteren [41] the following general result is proved. For more details see van Casteren [36], [38], [39] and [42].

- 1.2. Theorem. Suppose that  $V = V_+ V_-$  is a Borel measurable function defined on E such that  $V_-$  belongs to K(E) and such that  $V_+$  belongs to  $K_{loc}(E)$ .
- (a) There exists a closed, densely defined linear operator A in  $C_0(E)$ , extending  $A_0-V$ , which generates a strongly continuous positivity preserving semigroup  $\{P_V(t): t \geq 0\}$  in  $C_0(E)$ . Every operator  $P_V(t)$ , t > 0, is of the form

$$\left[P_V(t)f
ight](x)=\int p_V(t,x,y)f(y)dm(y),\quad f\in C_0(E),$$

where  $p_V(t, x, y)$  is a continuous symmetric function which verifies the identity of Chapman-Kolmogorov:

$$p_V(s+t,x,y) = \int p_V(s,x,z) p_V(t,z,y) dm(z), \quad t>0, \;\; x,y \in E.$$

- (b) The semigroup  $\{P_V(t): t \geq 0\}$  also acts as a strongly continuous semigroup in  $L^p(E,m), 1 \leq p < \infty$ .
- (c) If  $P_0(t)$  maps  $L^1(E,m)$  into  $L^{\infty}(E,m)$  for all t>0 (i.e. if  $\sup\{p_0(t,x,y):x,y\in E\}<\infty$  for all t>0), then  $P_V(t),\,t>0$ , maps  $L^p(E,m)$  into  $L^q(E,m)$ , for  $1\leq p\leq q\leq \infty$ .
- (d) In  $L^2(E,m)$  the family  $\{P_V(t): t \geq 0\}$  is a self-adjoint positivity preserving strongly continuous semigroup with a self-adjoint generator.

Remark 1. Let  $\lambda > 0$  be large enough. Using the Markov property the following equality is readily verified

$$(\lambda I - A_0)^{-1} - (\lambda I - A)^{-1} = (\lambda I - A)^{-1}V(\lambda - A_0)^{-1}.$$

From this equality the extension property in (a) easily follows.

Remark 2. If in (c) we assume that, for t > 0, the operator  $P_0(t)$  maps  $L^1(E, m)$  in  $C_0(E)$ , then we may prove that, always for t > 0, the operator  $P_V(t)$  maps  $L^p(E, m)$  in  $L^q(E, m) \cap C_0(E)$ , provided that  $1 \le p \le q \le \infty$ ,  $p \ne \infty$ . This will be explained in Theorem 1.5.(b) and Corollary 1.6. of the present paper.

Outline of a proof. Let  $(X(t), P_x)$  be the strong Markov process associated to the semigroup  $\{P_0(t): t \geq 0\}$ ; i.e. suppose

$$\left[P_{0}(t)f
ight](x)=E_{x}\left(f\left(X(t)
ight)
ight)=\int f\left(X(t)
ight)dP_{x},\quad t\geq0,\;x\in E,\;f\in C_{0}(E).$$

Define the semigroup  $\{P_V(t): t \geq 0\}$  by the Feynman-Kac formula:

$$\left[P_V(t)f\right](x)=E_x\left(\exp\left(-\int_0^tV\left(X(s)
ight)ds
ight)f\left(X(t)
ight):\zeta>t
ight),f\in C_0(E),x\in E,t\geq 0.$$

Here  $\zeta$  is the life time of the process:

$$\zeta = \inf\{s > 0 : X(s) = \triangle\}.$$

Define the function  $p_V(t, x, y)$  by:

$$p_V(t,x,y) = \lim_{s \uparrow t} E_x \left( \exp\left(-\int_0^s V\left(X(\sigma)\right) d\sigma\right) p_0(t-s,X(s),y) : \zeta > s \right).$$

Here t>0 and x and y belong to E. The various assertions in Theorem 1.3. have to be verified. The semigroup  $\{P_V(t): t \geq 0\}$  is approximated by semigroups  $\{P_{k,\ell,m}(t): t \geq 0\}$  defined by

$$\left[P_{k,\ell,m}(t)f\right](x) = E_x\left(\exp\left(-\int_0^t V_{k,\ell}(X(s))ds\right)f(X(t)): T_m > t\right).$$

Here  $-\infty < k \le \ell < \infty$ ,  $V_{k,\ell} = \max(\min(V,\ell), k)$ ,  $E = \bigcup K_m$ ,  $K_m$  is compact,  $K_m \subseteq \operatorname{int}(K_{m+1})$  and  $K_m \subseteq \operatorname{int}(K_m)$ :

$$T_m = \inf \left\{ s > 0 : X(s) \in E^{\Delta} \setminus \operatorname{int}(K_m) 
ight\}.$$

The integral kernel  $p_V(t, x, y)$  is approximated by the integral kernels of the semi-groups  $\{P_{k,\ell,m}(t): t \geq 0\}$ . In fact we have

$$\left[P_{k,\ell,m}(t)f
ight](x)=\int p_{k,\ell,m}(t,x,y)f(y)dm(y),$$

where  $p_{k,\ell,m}(t,x,y)$  is given by

$$p_{k,\ell,m}(t,x,y) = \lim_{s \uparrow t} E_x \left( \exp\left(-\int_0^s V_{k,\ell}\left(X(\sigma)\right) d\sigma \right) p_{0,m}(t-s,X(s),y) : T_m > s \right).$$

Here  $p_{0,m}(t,x,y)$  is defined by

$$p_{0,m}(t,x,y) = p_0(t,x,y) - E_x(p_0(t-T_m,X(T_m),y):T_m < t).$$

Remark 1. Throughout the text we freely use the strong Markov process  $(X(t), P_x)$  associated to the semigroup  $\{P_0(t): t \geq 0\}$ .

Remark 2. We write  $||T||_{p,q}$  for the norm of the operator T considered as an operator from  $L^p(E,m)$  to  $L^q(E,m)$ .

Remark 3. If  $\{X(t), P_x\}$  is Brownian motion, then physicists write

$$p_V(t,x,y) = \int_{\omega(0)=x}^{\omega(t)=y} D\omega \exp\left(-rac{1}{2}\int_0^t \left(|\dot{\omega}(s)|^2 + V(\omega(s))
ight)ds
ight).$$

Remark 4. Again let  $\{X(t), P_x\}$  be Brownian motion in  $\mathbb{R}^{\nu}$ , which begins in x. Fix t > 0 and  $y \in \mathbb{R}^{\nu}$ . It is useful to observe that the following processes have the same finite dimensional  $P_x$ -distributions:

$$\left(1 - \frac{s}{t}\right) X\left(\frac{st}{t-s}\right) + \frac{s}{t}y, \qquad 0 < s < t,$$
  $X(s) - \frac{s}{t}X(t) + \frac{s}{t}y, \qquad 0 < s < t.$ 

The following result can be found as Proposition 1.3. in van Casteren [41]. Estimates like the one in (a) are also interesting to find bounds for the Hilbert-Schmidt norm of the form

$$\left\|\exp\left(-t(H_0+V)\right)\right\|_{HS}^2 \leq \alpha t^{-r}\exp(\beta t).$$

- 1.4. Lemma. Let  $V \geq 0$  be in K(E). The following assertions are valid.
- (a) There exists a constant c such that

$$E_x\left(\int_0^t V(X(s))ds\right) \le \int_0^t [P_0(s)V](x)ds \le ct+1, \quad t>0, \quad x \in E,$$
 (1.1)

$$\lambda E_x \left( \int_0^\infty e^{-\lambda s} V(X(s)) ds \right) \le c + \lambda, \quad \lambda > 0, \quad x \in E;$$
 (1.2)

(b) (Khas'minskii's lemma) There exist finite constants M and  $\alpha$  such that

$$E_x\left(\exp\left(\int_0^t V(X(s))ds\right)\right) \le M\exp(\alpha t), \quad x \in E, \quad t > 0.$$
 (1.3)

The following theorem gives some interesting inequalities. A proof can be found in van Casteren [42] and if  $E = \mathbb{R}^n$  also in Demuth and van Casteren [14].

1.5. Theorem. Suppose the symmetric integral kernel  $p_0(t, x, y)$  has the following boundedness property. For every t > 0 the supremum

$$\sup \left\{ p_0(t,x,y) : x,y \in E \right\}$$

is finite.

(a) Let M and  $\alpha$  be constants for which

$$E_x\left(\exp\left(2\int_0^t V_-(X(s))ds\right)\right) \le M^2\exp(2\alpha t), \quad t > 0, \quad x \in E. \tag{1.4}$$

For  $1 \leq p \leq q \leq \infty$  the inequality

$$||P_V(t)||_{p,q} \le M^{1+\frac{1}{p}-\frac{1}{q}} \exp(\alpha t) \sup \left\{ p_0 \left(t/2, x, y\right)^{\frac{1}{p}-\frac{1}{q}} : x, y \in E \right\}, \quad t > 0, \quad (1.5)$$

holds true.

(b) Let  $\rho$  and  $\rho'$  be conjugate exponents:

$$\frac{1}{\rho} + \frac{1}{\rho'} = 1, \quad 1 < \rho, \quad \rho' < \infty.$$
 (1.6)

Choose constants M and  $\alpha$  such that

$$E_{x}\left(\exp\left(2\rho'\int_{0}^{\frac{1}{2}t}V_{-}(X(s))ds\right)\right) \leq M^{\rho'}\exp(\alpha t \rho'), \quad t > 0, \quad x \in E.$$
 (1.7)

For t > 0 and x, y belonging to E the following inequality is true:

$$p_V(t, x, y) \le M \exp(\alpha t) \sup \left\{ p_0(t/2, x, y)^{\frac{1}{p'}} : x, y \in E \right\} . p_0(t, x, y)^{\frac{1}{p}}.$$
 (1.8)

Before we prove this result we like to make some comments and remarks.

Remark 1. From the assumptions in the Theorem it follows that, for every t > 0, the operator  $P_0(t)$  maps  $L^1(E, m)$  in  $L^{\infty}(E, m)$ .

Remark 2. Proposition 1.4.(b) yields the existence of finite constants M and  $\alpha$  verifying inequalities like (1.4) and (1.7).

**Proof of Theorem 1.5.** (a) To prove this we suppose that  $1 \le p < q < \infty$  and we write r = p(q-1)/(q-p). Applying the Riesz-Thorin theorem twice shows, for t > 0,

$$\begin{split} \|P_{V}(t)\|_{p,q} &\leq \|P_{V}(t)\|_{1,1}^{\frac{1}{q}} \cdot \|P_{V}(t)\|_{r,\infty}^{1-\frac{1}{q}} \\ &\leq \|P_{V}(t)\|_{1,1}^{\frac{1}{q}} \left( \|P_{V}(t)\|_{1,\infty}^{\frac{1}{r}} \|P_{V}(t)\|_{\infty,\infty}^{1-\frac{1}{r}} \right)^{1-\frac{1}{q}} \\ &\leq \|P_{V}(t)\|_{1,1}^{\frac{1}{q}} \|P_{V}(t)\|_{1,\infty}^{\frac{1}{p}-\frac{1}{q}} \|P_{V}(t)\|_{\infty,\infty}^{1-\frac{1}{p}} \end{split}$$

(symmetry and semigroup property)

$$\leq \|P_{V}(t)\|_{\infty,\infty}^{1+\frac{1}{q}-\frac{1}{p}} \|P_{V}(t/2)\|_{1,2}^{\frac{1}{p}-\frac{1}{q}} \|P_{V}(t/2)\|_{2,\infty}^{\frac{1}{p}-\frac{1}{q}}$$

(symmetry)

$$\leq \|P_{V}(t)\|_{\infty,\infty}^{1+\frac{1}{q}-\frac{1}{p}} \|P_{V}(t/2)\|_{2,\infty}^{2(\frac{1}{p}-\frac{1}{q})}. \tag{1.9}$$

The Feynman-Kac formula shows

$$||P_{V}(t)||_{\infty,\infty} \leq \sup \left\{ E_{x} \left( \exp \left( \int_{0}^{t} V_{-}(X(s)) ds \right) \right) : x \in E \right\}$$

$$\leq \sup \left\{ \left( E_{x} \left( \exp \left( 2 \int_{0}^{t} V_{-}(X(s)) ds \right) \right) \right)^{\frac{1}{2}} : x \in E \right\}$$

$$\leq M \exp(\alpha t). \tag{1.10}$$

Next let x be in E and let f be in  $L^2(E, m)$ . Another estimate will show

$$|[P_{V}(t/2) f](x)|^{2} = \left| E_{x} \left( \exp\left( -\int_{0}^{\frac{1}{2}t} V(X(s)) ds \right) f(X(t/2)) : \zeta > \frac{1}{2}t \right) \right|^{2}$$

$$\leq \left| E_{x} \left( \exp\left( \int_{0}^{\frac{1}{2}t} V_{-}(X(s)) ds \right) |f(X(t/2))| : \zeta > \frac{1}{2}t \right) \right|^{2}$$

$$\leq E_{x} \left( \exp\left( 2\int_{0}^{\frac{1}{2}t} V_{-}(X(s)) ds \right) \right) . E_{x} \left( |f(X(t/2))|^{2} \right)$$

$$\leq M^{2} \exp(\alpha t) \int p_{0} (t/2, x, y) |f(y)|^{2} dy$$

$$\leq M^{2} \exp(\alpha t) \sup \left\{ p_{0} (t/2, x, y) : x, y \in E \right\} ||f||_{2}^{2}. \tag{1.11}$$

From (1.11) it follows that

$$||P_V(t/2)||_{2,\infty}^2 \le M^2 \exp(\alpha t) \sup \{p_0(t/2, x, y) : x, y \in E\}.$$
 (1.12)

From (1.9), (1.10) and (1.12) inequality (1.5) in (a) immediately follows. Among others these estimates show that for t > 0 the operator  $P_V(t)$  maps  $L^p(E, m)$  in  $L^q(E, m)$  for  $1 \le p \le q \le \infty$ .

(b) We establish inequality (1.7) with  $p_V(t,x,y)$  replaced by  $p_{V,m}(t,x,y)$  and  $p_0(t,x,y)$  replaced by  $p_{0,m}(t,x,y)$ . Taking the limit for m to infinity will give (1.7). The Feynman-Kac formula for generalized Brownian bridge (stochastic bridge) yields, for x, y belonging to int  $K_m$ ,

$$\begin{split} p_{V,m}(t,x,y) &= \lim_{s\uparrow t} E_x \left( \exp\left(-\int_0^s V(X(\sigma))d\sigma\right) p_{0,m}(t-s,X(s),y) : T_m > s \right) \\ &\leq \lim_{s\uparrow t} E_x \left( \exp\left(\int_0^s V_-(X(\sigma))d\sigma\right) p_{0,m}(t-s,X(s),y) : T_m > s \right) \end{split}$$

(Hölder's inequality)

$$\leq \lim_{s \uparrow t} E_{x} \left( \exp \left( \rho' \int_{0}^{s} V_{-}(X(\sigma)) d\sigma \right) p_{0,m}(t-s,X(s),y) : T_{m} > s \right)^{\frac{1}{\rho'}}$$

$$\times E_{x} \left( p_{0,m}(t-s,X(s),y) : T_{m} > s \right)^{\frac{1}{\rho}}$$

$$\leq \lim_{s \uparrow t} \left[ P_{-\rho'V_{-},m}(s) \left( p_{0,m}(t-s,.,y) \right) \right] (x)^{\frac{1}{\rho'}} . E_{x} \left( p_{0,m}(t-s,X(s),y) : T_{m} > s \right)^{\frac{1}{\rho}}$$

(martingale property)

$$\leq \lim_{s \uparrow t} \|P_{-\rho'V_{-},m}(s)\|_{1,\infty}^{\frac{1}{\rho'}} \cdot \left(\int p_{0,m}(t-s,z,y)dz\right)^{\frac{1}{\rho'}} \cdot p_{0,m}(t,x,y)^{\frac{1}{\rho}}$$

(symmetry and the semigroup property)

$$\leq \lim_{s \uparrow t} \|P_{-\rho'V_{-},m}(s/2)\|_{2,\infty}^{\frac{2}{\rho'}} \cdot p_{0,m}(t,x,y)^{\frac{1}{\rho}} 
\leq \|P_{-\rho'V_{-},m}(t/2)\|_{2,\infty}^{\frac{2}{\rho'}} \cdot p_{0,m}(t,x,y)^{\frac{1}{\rho}}.$$
(1.13)

With f belonging to  $L^2(E,m)$  and x in  $int(K_m)$ , the Feynman-Kac formula shows

$$| [P_{-\rho' V_{-},m}(t/2)f](x)|^{2} \leq \left( E_{x} \left( \exp\left(\rho' \int_{0}^{\frac{1}{2}t} V_{-}(X(s))ds \right) |f(X(t/2))| : T_{m} > \frac{1}{2}t \right) \right)^{2}$$

$$\leq E_{x} \left( \exp\left( 2\rho' \int_{0}^{\frac{1}{2}t} V_{-}(X(s))ds \right) : T_{m} > \frac{1}{2}t \right) \times E_{x} \left( |f(X(t/2))|^{2} : T_{m} > \frac{1}{2}t \right)$$

$$\leq M^{\rho'} \exp\left(\alpha \rho' t\right) \sup\left\{ p_{0,m}(t/2,x,y) : y \in E \right\} . ||f||_{2}^{2}. \tag{1.14}$$

The combined inequalities (1.13) and (1.14) result in inequality (1.8). This proves Theorem 1.5.

1.6. Corollary. Let the notation and hypotheses be as in Theorem 1.5. Let t > 0. The operator  $P_V(t)$  maps the space  $L^p(E,m)$  in  $L^q(E,m) \cap C_0(E)$ , provided that  $1 \le p \le q \le \infty$ ,  $p \ne \infty$ .

**Proof.** From Theorem 1.5.(a) it follows that the operator  $P_V(t)$  maps the space  $L^p(E,m)$  in  $L^q(E,m)$ ,  $1 \le p \le q \le \infty$ . Next suppose that  $1 , that <math>1 \le p \le q \le \infty$  and that f belongs to  $L^p(E,m)$ . We apply Theorem 1.5.(b) with  $\rho = p'$  and  $\rho' = p$ , where

 $\frac{1}{p}+\frac{1}{p'}=1.$ 

By inequality (1.8) there exist constants M and  $\alpha$  such that

$$|[P_{V}(t)f](x)| \leq \int p_{V}(t,x,y)|f(y)|dy$$

$$\leq M \exp(\alpha t) \sup \left\{ p_{0}(t/2,x,y)^{\frac{1}{p}} : x,y \in E \right\} \cdot \int p_{0}(t,x,y)^{\frac{1}{p'}}|f(y)|dy.$$
(1.15)

Put

$$M(t) = M \exp(\alpha t) \sup \left\{ p_0(t/2, x, y) : x, y \in E \right\}.$$

Let  $\epsilon > 0$ , choose g in  $C_{00}(E)$  (i.e. the function g is continuous and has compact support) in such a way that

$$||f - g||_p < \frac{\epsilon}{2M(t)} \tag{1.16}$$

and put K = supp(g). From (1.15), from (1.16) and from Hölder's inequality it follows that

$$|[P_{V}(t)f](x)| \leq M(t) \int p_{0}(t,x,y)^{\frac{1}{p'}} |f(y) - g(y)| dy + M(t) \int p_{0}(t,x,y)^{\frac{1}{p'}} |g(y)| dy$$

$$\leq M(t) \left( \int p_{0}(t,x,y) dy \right)^{\frac{1}{p'}} ||f - g||_{p} + M(t) \int |g(y)| dy. \sup_{y \in K} p_{0}(t,x,y)^{\frac{1}{p'}}$$

$$\leq \frac{1}{2} \epsilon + M(t) \int |g(y)| dy. \sup_{y \in K} p_{0}(t,x,y)^{\frac{1}{p'}}. \tag{1.17}$$

Since  $\lim_{x\to\Delta} \sup_{y\in K} p_0(t,x,y) = 0$ , we conclude from (1.17) that  $|[P_V(t)f](x)| \leq \epsilon$  for x "close" enough to  $\Delta$ . By the semigroup property and by (a) it follows that the operator  $P_V(t)$  is a mapping from  $L^p(E,m)$  to  $L^\infty(E,m) \cap C_b(E)$ : see e.g. [36] and [41]. Consequently  $P_V(t)$  maps  $L^p(E,m)$  in  $L^q(E,m) \cap C_0(E)$ . This proves Corollary 1.6. for 1 . For <math>p = 1 the proof is similar and much simpler.

## 2. Semigroup differences consisting of trace class or Hilbert-Schmidt operators.

In this section we write  $P_0(t) = \exp(-tK_0)$ , where  $-K_0$  is the generator of the semigroup  $\{P_0(t): t \geq 0\}$  viewed as a strongly continuous semigroup in  $L^2(E, m)$ , instead of  $P_V(t)$  the symbol  $P_V(t) = \exp(-t(K_0 + V))$  is employed and  $p_V(t, x, y)$  is often written as  $p_V(t, x, y) = \exp(-t(K_0 + V))(x, y)$ . If  $\Sigma$  is an open subset of E and if  $\Gamma = E \setminus \Sigma$ , then we usually write  $p_{V,\Sigma}(t, x, y) = \exp(-t(K_0 + V)_{\Sigma})(x, y)$  for the integral kernel of the semigroup killed in  $\Gamma$ . For t > 0 and  $f \in L^2(E, m)$  the following equality is valid:

$$\left[\exp\left(-t(K_0+V)_\Sigma\right)f
ight](x)=E_x\left(\exp\left(-\int_0^tV(X(s))ds
ight)f(X(t)):T>t
ight),$$

where  $T=\inf\{s>0: X(s)\in E\setminus\Sigma\}$ , the exit time from  $\Sigma$ . It is perhaps useful to notice that the semigroup  $\{\exp(-t(K_0+V)_\Sigma): t\geq 0\}$  is strongly continuous on the subspace  $\{f\in L^2(E,m): f\mid_{\Gamma}\equiv 0\}$  with a generator denoted by  $(K_0+V)_\Sigma$ . Sometimes it will be convenient to write  $J^*\exp(-t(K_0+V)_\Sigma)J$  instead of  $\exp(-t(K_0+V)_\Sigma)$ , where the operator J is defined by  $Jf=f\mid_{\Sigma}, f\in L^2(E,m)$ . Then  $[J^*f](x)=f(x)$ , for  $x\in\Sigma$  and  $[J^*f](x)=0$ , for  $x\in\Gamma$ . The set  $\Gamma$  supports a potential barrier and is called a singularity region. Another convention we use is the following. Instead of dm(x) we write dx and the inner-product of f, g in  $L^2(E,m)$  is denoted by f,  $g>=\int f(x)g(x)dx$ . Next let f be a real or complex Hilbert space and let f: f and f be a (hermitian) positive operator, i.e. suppose f and f is a trace class operator or that f belongs to f if its trace, trace f is finite. Here trace f is defined by

$$\operatorname{trace}(T) = \sum_{j=1}^{\infty} \langle T\varphi_j, \varphi_j \rangle,$$
 (2.1)

where  $\{\varphi_j: j \in \mathbb{N}\}$  is any orthonormal basis in  $\mathcal{H}$ . The expression in (2.1) is independent of the choice of the basis  $\{\varphi_j: j \in \mathbb{N}\}$ . An arbitrary operator T in  $\mathcal{L}(\mathcal{H})$  belongs to  $\mathcal{I}_1$ , if its absolute value |T| possesses a finite trace. For  $T \in \mathcal{I}_1$  we define its trace norm  $||T||_{\mathcal{I}_1}$  by  $||T||_{\mathcal{I}_1} = \operatorname{trace}(|T|)$ .

An operator T in  $\mathcal{L}(\mathcal{H})$  is a Hilbert-Schmidt operator if  $T^*T$  belongs to  $\mathcal{I}_1$ . Its Hilbert-Schmidt norm  $||T||_{\mathcal{I}_2}$  is defined by

$$||T||_{\mathcal{I}_2} = ||T^*T||_{\mathcal{I}_1}^{\frac{1}{2}} = \left(\sum_{j=1}^{\infty} ||T\varphi_j||^2\right)^{\frac{1}{2}},$$
 (2.2)

where as above  $\{ : j \in \mathbb{N} \}$  is an orthonormal basis in  $\mathcal{H}$ . If  $\mathcal{H} = L^2(E, m)$  and if T is a (hermitian) positive operator of the form

$$[Tf](x) = \int t(x,y)f(y)dm(y), \quad f \in L^2(E,m),$$

where  $t: E \times E \to [0, \infty)$  is a continuous function, then

$$\operatorname{trace}(T) = \int t(x,x) dm(x)$$
 and  $\operatorname{trace}(T^*T) = \int t(x,y)^2 dm(x) dm(y)$ . (2.3)

These facts are well-known. For example the reader may consult Reed and Simon [32].

We begin this section with an elementary proposition.

**2.1. Proposition.** Let  $v \geq u \geq 0$  be functions in  $L^2(E, m)$ . Put  $T = v \otimes v - u \otimes u$ . So that

$$Tf = \langle f, v \rangle v - \langle f, u \rangle u$$
  
=  $\langle f, v - u \rangle v + \langle f, u \rangle (v - u), \quad f \in L^2(E, m).$  (2.4)

The following assertions are valid:

(i) 
$$\operatorname{trace}(T) = \|v\|_{2}^{2} - \|u\|_{2}^{2};$$

(ii) 
$$||T||_{\mathcal{I}_1} = ||v - u||_2 ||v + u||_2 \le \sqrt{2} \sqrt{||v||_2^4 - ||u||_2^4};$$

(iii) 
$$||T||_{\mathcal{I}_2}^2 = \frac{||v||_2^4 + ||u||_2^4 - 2 < u, v >^2}{2} \le \left(||v||_2^2 - ||u||_2^2\right) ||v||_2^2.$$

**Proof.** The eigenvalues of the operator T can be computed explicitly:

$$\lambda_{1} = \frac{\|v\|_{2}^{2} - \|u\|_{2}^{2} + \|v - u\|_{2} \|v + u\|_{2}}{2};$$

$$\lambda_{2} = \frac{\|v\|_{2}^{2} - \|u\|_{2}^{2} - \|v - u\|_{2} \|v + u\|_{2}}{2}.$$
(2.5)

Then  $\lambda_1 \geq 0 \geq \lambda_2$ , so that trace $(T) = \lambda_1 + \lambda_2$ ,  $||T||_{\mathcal{I}_1} = \lambda_1 - \lambda_2$  and  $||T||_{\mathcal{I}_2}^2 = \lambda_1^2 + \lambda_2^2$ . The assertions (i), (ii) and (iii) readily follow from these equalities.

**2.2.** Theorem. Let  $V_1$  and  $V_2$  be potential functions verifying Kato's conditions, i.e. with negative (= attractive) parts in K(E) and with positive (= repulsive) parts in  $K_{loc}(E)$  and suppose  $V_1 \geq V_2$ . Also suppose that

$$\int \exp\left(-2t(K_0+V_2)\right)(x,x)(V_1(x)-V_2(x))\,dx < \infty. \tag{2.6}$$

(a) Then

$$D(t) := \exp\left(-t(K_0 + V_2)\right) - \exp\left(-t(K_0 + V_1)\right) \in \mathcal{I}_2 \tag{2.7}$$

and

$$||D(t)||_{\mathcal{I}_2}^2 \le 2t \int \exp\left(-2t(K_0+V_2)\right)(x,x)(V_1(x)-V_2(x)) dx.$$
 (2.8)

(b) If  $\|\exp(-tK_0)\|_{1,\infty} < \infty$  and if  $V_1 - V_2$  belongs to  $L^1(E, m)$ , then (2.6) is automatically satisfied.

**Proof.** (a) We shall estimate the integral:

$$\int \int (\exp(-t(K_0 + V_2))(x, y) - \exp(-t(K_0 + V_1)))^2 dxdy$$

$$= \int \left(\int \exp(-t(K_0 + V_2))(x, y)^2 dy + \int \exp(-t(K_0 + V_1))(x, y)^2 dy - 2 \int \exp(-t(K_0 + V_2))(x, y) \exp(-t(K_0 + V_1))(x, y) dy\right) dx$$

(Chapman-Kolmogorov and Feynman-Kac formula)

$$\leq \int \left( \exp\left(-2t(K_0 + V_2)\right)(x, x) + \exp\left(-2t(K_0 + V_1)\right)(x, x) - 2 \int \exp\left(-t(K_0 + V_1)\right)(x, y) \exp\left(-t(K_0 + V_1)\right)(x, y) dy \right) dx \\
= \int \left( \exp\left(-2t(K_0 + V_2)\right)(x, x) - \exp\left(-2t(K_0 + V_1)\right)(x, x) \right) dx \tag{2.9}$$

(variation of constants formula)

$$=\int\int_{0}^{2t}\int\exp\left(-u(K_{0}+V_{2})
ight)(x,z)\left(V_{1}(z)-V_{2}(z)
ight)\exp\left(-(2t-u)(K_{0}+V_{1})
ight)(z,x)\ dzdudx \ \leq \int\int_{0}^{2t}\int\exp\left(-u(K_{0}+V_{2})
ight)(x,z)\left(V_{1}(z)-V_{2}(z)
ight)\exp\left(-(2t-u)(K_{0}+V_{2})
ight)(z,x)$$

(Fubini and Chapman-Kolmogorov)

dzdudx

$$=2t\int \exp\left(-2t(K_0+V_2)\right)(z,z)(V_1(z)-V_2(z))\,dz<\infty. \tag{2.10}$$

This proves (a).

(b) From Theorem 1.5 inequality (1.8) it follows that, for appropriate constants M and  $\alpha$ ,

$$\exp(-2t(K_0 + V_2))(z, z) \le M \exp(2\alpha t) \|\exp(-tK_0)\|_{1,\infty}^{\frac{1}{2}} \|\exp(-2tK_0)\|_{1,\infty}^{\frac{1}{2}}$$

$$\le M \exp(2\alpha t) \|\exp(-tK_0)\|_{1,\infty}^{\frac{1}{2}} \|\exp(-tK_0)\|_{1,\infty}^{\frac{1}{2}} \|\exp(-tK_0)\|_{\infty,\infty}^{\frac{1}{2}}$$

$$\le M \exp(2\alpha t) \|\exp(-tK_0)\|_{1,\infty} < \infty. \tag{2.11}$$

So (b) easily follows.

**2.3. Corollary.** Fix t > 0 and let  $V = V_+ - V_-$  be such that  $V_+$  belongs to  $K_{loc}(E)$  and such that  $V_-$  belongs to K(E). In addition let V belong to  $L^1(E, m)$  and suppose  $\|\exp(-tK_0)\|_{1,\infty} < \infty$ . Then

$$D(t) := \exp(-t(K_0 + V)) - \exp(-tK_0)$$
 (2.12)

belongs to  $\mathcal{I}_2$  and, for appropriate constants M and  $\alpha$ ,

$$||D(t)||_{\mathcal{I}_{2}}^{2} \leq 4tM \exp(2\alpha t) ||\exp(-tK_{0})||_{1,\infty} ||V||_{1}.$$
 (2.13)

**Proof.** Repeating the arguments of the previous proof with  $V_2 = V$  and  $V_1 = 0$  yields

$$||D(t)||_{\mathcal{I}_2}^2 \le 4t \int \exp\left(-2t(K_0 - V_-)\right)(z, z) |V(z)| dz.$$
 (2.14)

Then apply Theorem 1.5. to obtain (2.13).

**2.4. Theorem.** Fix t > 0 and let  $V_1 \ge V_2$  be potential functions as in Theorem 2.2. If the expression

$$M(t) :=$$

$$\int \left( \int_0^t \int \exp\left(-u(K_0 + V_2)\right)(x, z) \left(V_1(z) - V_2(z)\right) \exp\left(-(t - u)(K_0 + V_1)\right)(z, x) dz du \right)^{\frac{1}{2}} \times \left(\exp\left(-t(K_0 + V_2)\right)(x, x)\right)^{\frac{1}{2}} dx$$
(2.15)

is finite, then

$$D(t) := \exp(-t(K_0 + V_2)) - \exp(-t(K_0 + V_1))$$

belongs to  $\mathcal{I}_1$  and  $||D(t)||_{\mathcal{I}_1} \leq 2M(t)$ .

**Proof.** Notice the identity

$$\langle D(t)f, f \rangle = \int \langle T_z\left(\frac{t}{2}\right)f, f \rangle dz,$$
 (2.16)

where

$$T_{z}(t) = \exp\left(-t(K_{0} + V_{2})\right)(z,.) \otimes \exp\left(-t(K_{0} + V_{2})\right)(z,.) - \exp\left(-t(K_{0} + V_{1})\right)(z,.) \otimes \exp\left(-t(K_{0} + V_{1})\right)(z,.).$$
(2.17)

Let D(t) = U |D(t)| be the polar decomposition of D(t). Then

$$||D(t)||_{\mathcal{I}_1} = \operatorname{trace}(D(t)U^*) = \int \operatorname{trace}\left(T_z\left(\frac{t}{2}\right)U^*\right)dz$$

$$\leq \int \left\|T_z\left(\frac{t}{2}\right)\right\|_{\mathcal{I}_1}dz. \tag{2.18}$$

Next we apply Proposition 2.1, item (ii), to obtain

 $||D(t)||_{\mathcal{I}_1}$ 

$$\leq \sqrt{2} \int \left( \left( \int \exp\left(-\frac{t}{2}(K_0 + V_2)\right)(z, x)^2 dx \right)^2 - \left( \int \exp\left(-\frac{t}{2}(K_0 + V_1)\right)(z, x)^2 dx \right)^{\frac{1}{2}} dz$$

$$= \sqrt{2} \int \left( \exp\left(-t(K_0 + V_2)\right)(z, z)^2 - \exp\left(-t(K_0 + V_1)\right)(z, z)^2 \right)^{\frac{1}{2}} dz$$

$$\leq \sqrt{2} \int \left( \exp\left(-t(K_0 + V_2)\right)(z, z) - \exp\left(-t(K_0 + V_1)\right)(z, z) \right)^{\frac{1}{2}} dz$$

$$\times \left( \exp\left(-t(K_0 + V_2)\right)(z, z) + \exp\left(-t(K_0 + V_1)\right)(z, z) \right)^{\frac{1}{2}} dz$$

$$\leq 2 \int \left( \int_0^t \int \exp\left(-u(K_0 + V_2)\right)(x, z) (V_1(z) - V_2(z)) \exp\left(-(t - u)(K_0 + V_1)\right)(z, x) dz du \right)^{\frac{1}{2}}$$

$$\times \exp\left(-t(K_0 + V_2)\right)(x, x)^{\frac{1}{2}} dx. \tag{2.19}$$

This inequality yields the desired conclusion.

**2.5.** Corollary. Suppose  $E = \mathbb{R}^{\nu}$  with Lebesgue measure and let  $K_0$  be  $-\frac{1}{2}\triangle$ . Let  $V_1 \geq V_2$  be potential functions with the usual Kato properties, i.e. their negative parts belong to  $K_{\nu}$  and their positive parts are in  $K_{\nu,loc}$ . Put  $W = V_1 - V_2$  and suppose that for every  $\rho > 0$  the following integrals are finite:

$$\int \left(\int \frac{\exp\left(-\rho|z-x|^2\right)}{|z-x|^{\nu-2}} W(z) dz\right)^{\frac{1}{2}} dx < \infty, \quad \text{if } \nu \ge 3; (2.20)$$

$$\int \left(\int \left(\exp\left(-\rho|z-x|^2\right) + \log^+ \frac{1}{\rho|z-x|^2}\right) W(z) dz\right)^{\frac{1}{2}} dx < \infty, \quad \text{if } \nu = 2; (2.21)$$

$$\int \left(\int \exp\left(-\rho(z-x)^2\right) W(z) dz\right)^{\frac{1}{2}} dx < \infty, \quad \text{if } \nu = 1. (2.22)$$

Then the operators

$$D(t) := \exp\left(-t(K_0 + V_2)\right) - \exp\left(-t(K_0 + V_1)\right) \tag{2.23}$$

belong to  $\mathcal{I}_1$ .

**Proof.** Fix t > 0 and put

$$p_{0,\nu}(t,x,y) = \frac{1}{(\sqrt{2\pi t})^{\nu}} \exp\left(-\frac{|x-y|^2}{2t}\right).$$
 (2.24)

From Theorem 1.5 inequality (1.8) it follows that there are constants M and  $\alpha$  such that the expression in (2.15) is dominated by

$$\frac{M \exp(\alpha t)}{t^{\frac{1}{4}\nu}} \int \left( \int_0^t \int p_{0,\nu}(2u,x,z) W(z) p_{0,\nu}(2(t-u),z,x) dz du \right)^{\frac{1}{2}} dx.$$
 (2.25)

It is elementary to verify that the integrals

$$\int \left(\int_0^t \int p_{0,
u}(2u,x,z)W(z)p_{0,
u}(2(t-u),z,x)dzdu
ight)^{rac{1}{2}}dx$$

are dominated by constant multiples of the integrals in (2.20), (2.21) and (2.22) respectively. The constants involved (like  $\rho$ ) depend on t but not on W.

Remark 1. Let W be a non-negative Borel function, defined on  $\mathbb{R}^{\nu}$  and consider the following integrals:

$$\int \left( \int_{|y-x| \le 1} \frac{W(y)}{|y-x|^{\nu-2}} dy \right)^{\frac{1}{2}} dx, \quad \text{if } \nu \ge 3; \tag{2.20'}$$

$$\int \left( \int_{|y-x|<1} \log \frac{1}{|y-x|} W(y) dy \right)^{\frac{1}{2}} dx, \quad \text{if } \nu = 2; \tag{2.21'}$$

$$\int \left(\int_{x}^{x+1} W(y)dy\right)^{\frac{1}{2}} dx, \quad \text{if } \nu = 1.$$
 (2.22')

It is perhaps useful to observe that the integrals in (2.20), (2.21) and (2.22) are finite if and only if the integrals in respectively (2.20'), (2.21') and (2.22') are finite. The involved estimates are elementary but a little elaborous.

Remark 2. The same proof works if  $K_0$  generates a symmetric Feller semigroup of the form

$$\left[\exp\left(-tK_{0}
ight)f
ight](x)=\int p_{0}(t,x,y)f(y)dy,$$

where, for every  $t_0 > 0$  there are constants  $a_0$  and  $b_0$  such that

$$p_0(t,x,y) \le a_0 p_{0,\nu}\left(\frac{t}{b_0},x,y\right),$$
 (2.26)

for  $0 < t < t_0$  and for all x, y in  $\mathbb{R}^{\nu}$ . Here  $p_{0,\nu}(t,x,y)$  is the Gaussian kernel (2.24).

In what follows we write  $T=\inf\{s>0: X(s)\in \Gamma\}$ , whenever  $\Gamma$  is a singularity region. Quantum-mechanical particles do not penetrate singularity regions. In fact singularity regions support potential barriers. In the presence of such a potential barrier supporterd by  $\Gamma$  the Hamiltonian in its complement generates the so-called semigroup killed at  $\Gamma$ ; see the beginning of this section. Fix  $\lambda>0$  and define the function  $v_{\lambda}: E \to [0,1]$  by

$$v_{\lambda}(x) = E_{x} \left( \exp\left(-\lambda T\right) : T < \infty \right) = \lambda \int_{0}^{\infty} P_{x}(T \le \tau) \exp(-\lambda \tau) d\tau.$$
 (2.27)

We are going to describe some of the relevant properties of the function  $v_{\lambda}$ . The function  $v_{\lambda}$  is lower semi-continuous (i.e. for every  $\alpha > 0$  the set  $\{v_{\lambda} > \alpha\}$  is open), it is finely continuous in the sense that, for every  $x \in E$ , the function  $s \mapsto v_{\lambda}(X(s))$  is  $P_x$ -almost surely right-continuous and it is  $\lambda$ -excessive in the sense that, for all  $x \in E$ ,

$$\left[\exp\left(-\lambda\tau-\tau K_0\right)v_\lambda\right](x)\leq v_\lambda(x),\quad au>0,$$

and

$$\left[\exp\left(-\lambda \tau - \tau H_0\right)v_{\lambda}\right](x)$$
 increases to  $v_{\lambda}(x)$ 

if  $\tau$  decreases to 0. Moreover  $v_{\lambda}(x) = 1$ , for  $x \in \Gamma^r$ , and  $m(\Gamma \setminus \Gamma^r) = 0$ . For more details see Blumenthal and Getoor [5, p. 86, Proposition (4.4), Theorem (4.5) and Theorem (4.8)]. The function  $v_{\lambda}$  is called the  $\lambda$ -equilibrium potential of  $\Gamma$  and the quantity  $\lambda \int v_{\lambda}(x)dm(x)$  is called the  $\lambda$ -capacity of the set  $\Gamma$ . For this terminology in the context of Brownian motion see Port and Stone [30, p. 42]. The reader may also consult Demuth and van Casteren [14] for more details.

**2.6.** Theorem. Let  $\Gamma = E \setminus \Sigma$  be a singularity region. Let V be a potential function with the usual Kato properties; i.e.  $V_- \in K(E)$  and  $V_+ \in K_{loc}(E)$ . Let  $(K_0 + V)_{\Sigma}$  be the generator of the semigroup  $\{\exp(-t(K_0 + V)_{\Sigma}) : t \geq 0\}$ . Put

$$D_{\Sigma}(t) = \exp\left(-t(K_0 + V)\right) - J^* \exp\left(-t(K_0 + V)_{\Sigma}\right) J. \tag{2.28}$$

Then  $f \geq 0$ ,  $f \in L^2(E, m)$  implies  $D_{\Sigma}(t) f \geq 0$ . Fix t > 0 and write  $\lambda = 1/(2t)$ . If

$$\int \exp\left(-2t(K_0+V)\right)(x,x)v_{\lambda}(x)dx < \infty,$$

then  $D_{\Sigma}(t)$  belongs to  $\mathcal{I}_2$  and

$$||D_{\Sigma}(t)||_{\mathcal{I}_{2}}^{2} \leq \int (\exp(-2t(K_{0}+V))(x,x) - \exp(-2t(K_{0}+V)_{\Sigma})(x,x)) dx \quad (2.29)$$

$$\leq 2 \int \exp(-2t(K_{0}+V))(x,x)v_{\lambda}(x)dx. \quad (2.30)$$

Here the function V verifies the usual Kato conditions. Before we prove this theorem we want to make the following remarks. From Theorem 2.6 it follows that the operator  $D_{\Sigma}(t)$  is a Hilbert-Schmidt operator whenever  $\Gamma$  has finite  $\lambda$ -capacity  $(\lambda = 1/(2t))$  and whenever  $\|\exp(-2t(H_0 + V))\|_{1,\infty} < \infty$ . In fact in section 3 we shall prove the following inequality:

$$\int (\exp(-t(K_0 + V))(x, x) - \exp(-t(K_0 + V)_{\Sigma})(x, x)) dx$$

$$\leq 2 \int \exp(-t(K_0 + V))(x, x) v_{1/t}(x) dx, \qquad (2.31)$$

where t>0 and where V is as in Theorem 2.6. In fact inequality (2.31) can be interpreted as saying that the quantity  $2\int \exp(-t(K_0+V))(x,x)v_{1/t}(x)dx$  dominates the trace of the operator  $D_{\Sigma}(t)$ . In [9] Davies elaborates on in the case of Brownian motion in  $\mathbb{R}^{\nu}$  ( $K_0 = \frac{1}{2}\Delta$ ) and V = 0. He considers the situation where  $\Gamma$  is a lower dimensional surface in  $\mathbb{R}^{\nu}$ .

**Proof.** Inequality (2.29) is proved in the same way as inequality (2.9) and inequality (2.30) is a consequence of inequality (2.31), which will be proved in section 3. In Demuth and van Casteren [14] a proof of (2.31) is given as well.

2.7. Theorem. Let V be a potential function verifying the usual Kato conditions and let  $\Gamma$  also be as in Theorem 2.6. Suppose that the quantity M(t) defined by

$$M(t) := \int \exp(-t(K_0 + V))(x, x)^{\frac{1}{2}}$$

$$\left(E_x \left(\exp\left(-\int_0^T V(X(s))ds\right) \exp(-(t - T)(K_0 + V))(X(T), x) : T < t\right)\right)^{\frac{1}{2}} dx$$
(2.32)

is finite. Then the operator

$$D_{\Sigma}(t) := \exp\left(-t(K_0 + V)\right) - J^* \exp\left(-t(K_0 + V)_{\Sigma}\right) J$$
 belongs to  $\mathcal{I}_1$ 

and

$$||D_{\Sigma}(t)||_{\mathcal{I}_1} \leq 2M(t).$$

**Proof.** As in the proof of Theorem 2.4. (inequality (2.19)), it follows that

$$egin{aligned} \|D_{\Sigma}(t)\|_{\mathcal{I}_{1}} &\leq \sqrt{2} \int \left(\exp\left(-t(K_{0}+V)\right)(x,x) - \exp\left(-t(K_{0}+V)_{\Sigma}\right)(x,x)
ight)^{rac{1}{2}} \ & imes \left(\exp\left(-t(K_{0}+V)\right)(x,x) + \exp\left(-t(K_{0}+V)_{\Sigma}\right)(x,x)
ight)^{rac{1}{2}} dx \ &\leq 2 \int \left(\exp\left(-t(K_{0}+V)\right)(x,x) - \exp\left(-t(K_{0}+V)_{\Sigma}\right)(x,x)
ight)^{rac{1}{2}} \ & imes \exp\left(-t(K_{0}+V)\right)(x,x)^{rac{1}{2}} dx. \end{aligned}$$

Employing the time dependent strong Markov property it may be verified that

$$\exp(-t(K_{0}+V))(x,y) - \exp(-t(K_{0}+V)_{\Sigma})(x,y)$$

$$= E_{x} \left(\exp\left(-\int_{0}^{T} V(X(s))ds\right) \exp(-(t-T)(K_{0}+V))(X(T),y) : T < t\right).$$
(2.33)

For a proof the reader is referred to Theorem 4.7 in Demuth and van Casteren [14]. If V = 0 and if  $\{X(t), P_x\}$  is Brownian motion a similar result can be found in Port and Stone [30, pp. 12-15].

2.8. Corollary. Again consider  $E = \mathbb{R}^{\nu}$  and  $K_0 = -\frac{1}{2}\triangle$ . Let V be a potential function verifying the ususal Kato conditions. Let  $\Gamma$  be a singularity region and let S be the first hitting time of  $\sqrt{2}\Gamma$ . If the expression

$$\int \left(E_x \left(p_{0,\nu}(2t-S,X(S),x):S<2t\right)\right)^{\frac{1}{4}} dx < \infty, \tag{2.34}$$

then  $D_{\Sigma}(t) := \exp\left(-t(K_0 + V)\right) - J^* \exp\left(-t(K_0 + V)_{\Sigma}\right) J$  belongs to  $\mathcal{I}_1$ .

Remark. Upon replacing the Cauchy-Schwarz inequality by the more general Hölder's inequality and by replacing  $\sqrt{2}$  by another constant a similar result is also valid for operators  $K_0$  which generate semigroups verifying (2.26).

**Proof.** By Theorem 2.7. it suffices to prove that the constant M(t) in (2.32) is finite. We apply Cauchy-Schwarz inequality to obtain

$$E_{x}\left(\exp\left(-\int_{0}^{T}V(X(s))ds\right).\exp\left(-(t-T)(K_{0}+V)\right)(X(T),x):T < t\right)^{2}$$

$$\leq E_{x}\left(\exp\left(-2\int_{0}^{T}V(X(s))ds\right).\exp\left(-(t-T)(K_{0}+V)\right)(X(T),x):T < t\right)$$

$$\times E_{x}\left(\exp\left(-(t-T)(K_{0}+V)\right)(X(T),x):T < t\right)$$

$$\leq E_{x}\left(\exp\left(2\int_{0}^{T}V_{-}(X(s))ds\right).\exp\left(-(t-T)(K_{0}-2V_{-})\right)(X(T),x):T < t\right)$$

$$\times E_{x}\left(\exp\left(-(t-T)(K_{0}-V_{-})\right)(X(T),x):T < t\right)$$

$$\times E_{x}\left(\exp\left(-(t-T)(K_{0}-V_{-})\right)(X(T),x):T < t\right)$$
(Theorem 1.5.)
$$\leq \exp\left(-t(K_{0}-2V_{-})\right)(x,x) \times M \exp(\alpha t)E_{x}\left(p_{0,\nu}(2(t-T),X(T),x):T < t\right)$$

$$\leq M^{2}\exp\left(2\alpha t\right)E_{x\sqrt{2}}\left(p_{0,\nu}(2t-S,X(S),x\sqrt{2}):S < 2t\right). \tag{2.35}$$

In the final line we used the time scaling properties of Brownian motion. From (2.32) and (2.35) we infer

$$M(t) \leq M \exp(\alpha t) \int \left( E_{x\sqrt{2}} \left( p_{0,\nu}(2t - S, X(S), x\sqrt{2}) : S < 2t \right) \right)^{\frac{1}{4}} dx$$

$$\leq \frac{M \exp(\alpha t)}{(\sqrt{2})^{\nu}} \int \left( E_{x} \left( p_{0,\nu}(2t - S, X(S), x) : S < 2t \right) \right)^{\frac{1}{4}} dx. \tag{2.36}$$

From (2.34) it follows that (2.36) is finite. Hence M(t) is finite and consequently  $D_{\Sigma}(t)$  is a trace class operator.

2.9. Corollary. Let the hypothese be as in Corollary 2.8. but with a bounded singularity region  $\Gamma$ . Then the operators  $D_{\Sigma}(t)$ , t > 0, belong to  $\mathcal{I}_1$ .

**Proof.** Let C be closed compact set containing  $\sqrt{2}\Gamma$  and let  $S_1$  be the first hitting time of C. If S is the hitting time of  $\sqrt{2}\Gamma$ , then

$$E_{x}\left(p_{0,\nu}(2t-S,X(S),y):S<2t\right)\leq E_{x}\left(p_{0,\nu}(2t-S_{1},X(S_{1}),y):S_{1}<2t\right). \tag{2.37}$$

From Lemma 21.3, p. 227 of Simon [34] we see that the right-hand side of (2.37) is dominated by the quantity

$$\frac{1}{\left(\sqrt{4\pi t}\right)^{\nu}}\exp\left(-\frac{\operatorname{dist}(x,C)^2+\operatorname{dist}(y,C)^2}{8t}\right).$$

It follows that (2.34) is dominated by

$$\int \frac{1}{\left(\sqrt{4\pi t}\right)^{\frac{\nu}{4}}} \exp\left(-\frac{\operatorname{dist}(x,C)^2}{16t}\right) dx. \tag{2.38}$$

Since C is bounded the integrals in (2.38) are finite. Hence Corollary 2.8. yields Corollary 2.9.

The following theorem gives sufficient conditions in order that  $\sigma_{ess}(K_0 + V)_{\Sigma} = \sigma_{ess}(K_0)$ .

**2.10. Theorem.** Let  $\Gamma = E \setminus \Sigma$  be a singularity region, let  $v_{\lambda}$  be the  $\lambda$ -equilibrium potential of  $\Gamma$  and let V be a potential function verifying:  $V_{+} \in K_{loc}(E)$  and  $V_{-} \in K(E)$ . In addition we suppose that, for every t > 0,

$$\int \exp\left(-t(K_0+V)\right)(x,x)v_{1/t}(x)dx < \infty;$$

$$\int \exp\left(-t(K_0+V)\right)(x,x)V_-(x)dx < \infty;$$

$$\int \exp\left(-tK_0\right)(x,x)V_+(x)dx < \infty.$$

Then, for t > 0, the operators

$$J^* \exp\left(-t(K_0+V)_{\Sigma}\right) J - \exp\left(-tK_0\right)$$

are Hilbert-Schmidt operators and

$$\sigma_{\mathrm{ess}}(K_0+V)_{\Sigma}=\sigma_{\mathrm{ess}}(K_0).$$

If for every t > 0 the quantity  $\|\exp(-tK_0)\|_{1,\infty} < \infty$ , then (a) is satisfied if  $\Gamma$  has finite 1/t-capacity and (b) and (c) are satisfied if V belongs to  $L^1(E, m)$ .

**Proof.** The result follows by considering the differences of (pseudo-)resolvents:

$$R_{\Sigma}(\lambda)f - R(\lambda)f := J^* (\lambda I - (K_0 + V)_{\Sigma})^{-1} Jf - (\lambda I - K_0)^{-1} f$$

$$= \int e^{-\lambda t} (J^* \exp(-t(K_0 + V)_{\Sigma}) J - \exp(-tK_0)) f dt, \qquad (2.41)$$

for  $\lambda > 0$  sufficiently large. These differences are compact operators because by Theorem 2.2. and Theorem 2.6. the differences

$$J^* \exp(-t(K_0 + V)_{\Sigma}) J - \exp(-tK_0) = \exp(-t(K_0 + V)) - \exp(-t(K_0 + V_+)) + \exp(-t(K_0 + V_+)) - \exp(-tK_0) + J^* \exp(-t(K_0 + V)_{\Sigma}) J - \exp(-t(K_0 + V)),$$

are Hilbert-Schmidt operators. The claim in the theorem on the stability of the essential spectra then follows from a general two space criterion as exhibited in Brüning,

Demuth and Gesztesy [6]; see also Theorem 4.1. below. We have to employ this theorem twice. A first time with T=I,  $\mathcal{H}_1=\mathcal{H}_2=L^2(E,m)$ ,  $A_1=K_0$  and  $A_2+K_0+V$ . A second time with T defined by  $Tf=f|_{\Sigma}$ ,  $\mathcal{H}_1=L^2(E,m)$ ,  $\mathcal{H}_2=L^2(\Sigma,m)$ ,  $A_1=K_0+V$  and  $A_2=(K_0+V)_{\Sigma}$ . To apply this result we need the compactness of the operators  $1_{\Gamma} \exp(-t(K_0+V))$ , t>0. Since, by (a),

$$\int \int 1_{\Gamma}(x) \exp\left(-t(K_0+V)\right)(x,y)^2 dx dy = \int_{\Gamma} \exp\left(-2t(K_0+V)\right)(x,x) dx < \infty,$$

these operators are in fact Hilbert-Schmidt operators. So certainly they are compact.

We also have an application to the stability of the absolutely continuous parts of the spectra. As in Theorem 2.10. T is the first hitting time of  $\Gamma$ .

**2.11. Theorem.** Let V and  $\Gamma$  be as in Theorem 2.10. Suppose in addition that, for all t > 0, the quantities

$$\left( a \right) \int \exp\left( -t(K_0 + V) \right) (x, x)^{\frac{1}{2}}$$

$$\left( E_x \left( \exp\left( -\int_0^T V(X(s)) ds \right) \exp\left( -(t - T)(K_0 + V) \right) (X(T), x) : T < t \right) \right)^{\frac{1}{2}} dx,$$

$$(b) \int \exp\left( -t(K_0 + V) \right) (x, x)^{\frac{1}{2}}$$

$$\left( \int_0^t \int \exp\left( -u(K_0 + V) \right) (x, z) V_-(z) \exp\left( -(t - u)(K_0 + V) \right) (z, x) dz du \right)^{\frac{1}{2}} dx$$
and
$$(c) \int \exp\left( -tK_0 \right) (x, x)^{\frac{1}{2}} \left( \int_0^t \int \exp\left( -uK_0 \right) V_+(z) \exp\left( -(t - u)K_0 \right) (z, x) dz du \right)^{\frac{1}{2}} dx$$

are finite. Then, for all t > 0, the operators

$$J^* \exp(-t(K_0 + V)_{\Sigma}) J - \exp(-tK_0)$$
 (2.42)

are trace class operators and

(i) 
$$\sigma_{\operatorname{ess}}(K_0+V)_{\Sigma} = \sigma_{\operatorname{ess}}(K_0)$$
 and (ii)  $\sigma_{\operatorname{ac}}(K_0+V)_{\Sigma} = \sigma_{\operatorname{ac}}(K_0).$ 

Proof. From Theorem 2.4. and Theorem 2.7. it indeed follows that the operators in (2.42) are trace class operators; see the proof of the Hilbert-Schmidt analogue in the previous theorem. For the sake of completeness we repeat here a version of the two space trace class condition for the existence of wave operators due to Pearson: see e.g. Reed and Simon [32, p. 24].

**2.12.** Lemma. Let  $K_0$  and  $(K_0 + V)_{\Sigma}$  be as above. Then  $K_0$  is a selfadjoint generator in  $L^2(E, m)$  and  $(K_0 + V)_{\Sigma}$  is a selfadjoint generator in  $L^2(\Sigma, m)$ . Let the

operator J be defined by  $Jf = f \mid_{\Sigma}$ . Here f belongs to  $L^2(E, m)$ . Suppose that the operator

$$\exp\left(-(K_0+V)_{\Sigma}\right)J-J\exp\left(-K_0\right)$$

is a trace class operator. Then the wave operator

$$W_{+}(\exp(-(K_{0}+V)_{\Sigma}), J, \exp(-K_{0}))$$
:= s-  $\lim_{t\to\infty} \exp(+it \exp(-(K_{0}+V)_{\Sigma})) J \exp(-it \exp(-K_{0})) P_{ac} (\exp(-K_{0}))$ 

exists. Here  $P_{ac}(\exp(-K_0))$  denotes the projection onto the absolutely continuous subspace of  $\exp(-K_0)$ . Moreover by the invariance principle for wave operators (see also [32, p. 31] or for the two-space situation Baumgärtel and Wollenberg [4, pp. 246 ff.] the existence of the wave operator

$$W_+((K_0+V)_\Sigma,J,K_0)= ext{s-}\lim_{t o\infty}\exp\left(it(K_0+V)_\Sigma
ight)J\exp\left(-itK_0
ight)P_{ ext{ac}}(K_0)$$

follows. If, additionally, the operator

$$\exp\left(-(K_0+V)\right)-\exp\left(-K_0\right)$$

is of trace class and if for all f in  $L^2(E, m)$ ,

$$\lim_{t \to \infty} \|1_{\Gamma} \exp(-it(K_0 + V)) P_{ac}(K_0 + V) f\|_2 = 0$$
 (2.43)

then the wave operator  $W_+((K_0+V)_{\Sigma}, J, K_0)$  is complete. This implies the stability of the absolutely continuous spectra, i.e.

$$\sigma_{\rm ac}(K_0+V)_{\Sigma}=\sigma_{\rm ac}(K_0).$$

For the latter the reader may consult Demuth [13, p. 17 ff.]. In order to prove (2.43) observe that w- $\lim_{t\to\infty} \exp(-it(K_0+V))P_{ac}(K_0+V)=0$ . So by an approximation argument it suffices to show that for every s>0 fixed the operator  $1_{\Gamma}\exp(-s(K_0+V))$  is compact. From (a) it follows that it is a Hilbert-Schmidt operator: again see the proof of Theorem 2.10. and notice that the quantity in (a) dominates  $\int_{\Gamma} \exp(-t(K_0+V))(x,x)dx$ . In order to see that (2.43) suffices indeed for completeness we first may verify that  $W_+(K_0+V,I,K_0)$  exists and is complete and that the same is true for  $W_+((K_0+V)_{\Sigma},J,K_0+V)$  provided (2.43) is valid. Consequently, the claims on the invariance of the absolutely continuous and essential spectra follow from an invariance and stability result in mathematical scattering theory. For more details the reader is referred to Demuth and van Casteren [14, section 5].

Condition (b) (condition (c)) in Theorem 2.10 is valid if  $\|\exp(-tK_0)\|_{1,\infty} < \infty$  for all t > 0 and if  $V_-$  ( $V_+$ ) belongs to  $L^1(E, m)$ . In Demuth and van Casteren [14] similar results are obtained if E is replaced with  $\mathbb{R}^n$ . The proofs in [14] to verify (a)

and (b) are the same in the present situation. In these verifications the inequalities in Theorem 1.5. are important.

**Problem.** Theorem 2.10. shows how to change the original state (=configuration) space E to  $\Sigma = E \setminus \Gamma$ , without changing the essential spectra of the Hamiltonian. Are such stability results true in spaces other than  $L^2(E, m)$ ? For example is such kind of stability true in  $L^1(E, m)$ .

#### 3. A proof of inequality (2.29)

A proof of inquality (2.29) is contained in the following theorem.

3.1. Theorem. Let  $\Gamma = E \setminus \Sigma$  be a singularity region, let T be the first hitting time of  $\Gamma$  and let  $v_{\lambda}$  be the  $\lambda$ -equilibrium potential of  $\Gamma$ . Suppose that V is a potential function verifying the standard hypotheses (i.e.  $V_{-}$  is a member of K(E) and  $V_{+}$  belongs to  $K_{loc}(E)$ ). Then

$$\int E_{x} \left( \exp\left(-\int_{0}^{T} V(X(\tau))d\tau\right) \exp\left(-(t-T)(K_{0}+V)\right) (X(T),x) : T < t \right) dx$$

$$= \int \left( \exp\left(-t(K_{0}+V)\right) (x,x) - \exp\left(-t(K_{0}+V)_{\Sigma}\right) (x,x) \right) dx \qquad (3.1)$$

$$\leq 2 \int \exp\left(-t(K_{0}+V)\right) (x,x) v_{\lambda}(x) dx, \qquad (3.2)$$

where  $t\lambda = 1$ .

**Proof.** Equality (3.1) is a consequence of the strong Markov property: see Theorem 4.6 in [14]. A proof of inequality (3.2) can be obtained as follows. Suppose that V is bounded and continuous. An approximation argument will yield the required inequality for general V. For brevity we write  $v = v_{\lambda}$ ,  $t_{\lambda} = 1$ ,  $m = 2^n$ ,  $m_{\lambda} = t$  and we introduce the hitting times  $T_{\xi}$ ,  $\xi > 0$ , by

$$T_{\xi} = \inf \left\{ s > 0 : v(X(s)) > \xi 
ight\}.$$

We also write

$$ho(\omega)(\sigma) = \omega\left(\left[rac{\sigma}{s}
ight]s
ight), \quad \sigma \geq 0, \; \omega \in \Omega, \quad ext{and} \quad E_{m{x}}^{m{s}}(Y) = E_{m{x}}\left(Y \circ 
ho_{m{s}}
ight),$$

whenever Y is an appropriate random variable. The function  $h_s(\xi, x, z)$  is defined as follows:

$$h_{s}(\xi, x, z) = E_{x}^{s} \left( \exp\left(-\int_{0}^{t-s} V(X(\tau)) d\tau\right) p_{0}(s, X(t-2s), z) \min\left(T_{\xi}, t-2s\right) \right)$$
(3.3)

and notice that  $h_s(\xi, x, z) = 0$  if  $v(x) > \xi$ .

Next let U be an open subset of E and let  $T_U$  be its hitting time:  $T_U = \inf\{s > 0 : X(s) \in U\}$ . Since the measure

$$dx_0 \dots dx_{m-1} \prod_{j=1}^m p_0(s, x_{j-1}, x_j)$$
 (3.4)

(where  $x_0 = x_m$ ) is invariant under cyclic permutations we have:

$$\int E_{x} \left( \exp\left(-s \sum_{k=0}^{m-1} V(X(ks))\right) p_{0}(s, X((m-1)s), x) \max_{1 \leq j \leq m-1} 1_{U}(X(js)) \right) dx$$

$$= \int_{U} E_{x} \left( \exp\left(-s \sum_{k=0}^{m-1} V(X(ks))\right) p_{0}(s, X((m-1)s), x) \right)$$

$$\times \min\left(\min\left(1 \leq j < \infty, X(js) \in U\right), m-1\right) dx. \tag{3.5}$$

Hence

$$\int E_{x} \left( \exp\left(-s \sum_{k=0}^{m-1} V(X(ks))\right) p_{0}(s, X((m-1)s), x) \max_{1 \leq j \leq m-1} 1_{U}(X(js)) \right) dx$$

$$= \int_{U} E_{x} \left( \exp\left(-s \sum_{k=0}^{m-1} V(X(ks))\right) p_{0}(s, X((m-1)s), x) \right) dx$$

$$+ \int_{U} \exp\left(-sV(x)\right) E_{x} \left( \exp\left(-s \sum_{k=0}^{m-2} V(X((k+1)s))\right) p_{0}(s, X((m-1)s), x)$$

$$\times \min\left(\min\left(0 \leq j < \infty, X((j+1)s) \in U\right), m-2\right) dx$$
(3.6)

Consequently, by the definition of  $E_x^s(Y)$ , we get

$$\int E_{x} \left( \exp\left(-s \sum_{k=0}^{m-1} V(X(ks))\right) p_{0}(s, X((m-1)s), x) \max_{1 \leq j \leq m-1} 1_{U}(X(js)) \right) dx$$

$$= \int_{U} E_{x}^{s} \left( \exp\left(-\int_{0}^{t} V(X(\tau)) d\tau\right) p_{0}(s, X(t-s), x) \right) dx$$

$$+ \frac{1}{s} \int_{U} \exp\left(-sV(x)\right) E_{x} \left( E_{X(s)}^{s} \left( \exp\left(-\int_{0}^{t-s} V(X(\tau)) d\tau\right) p_{0}(s, X(t-2s), x) \right) \right) dx$$

$$\times \min\left(T_{U}, t-2s\right) dx$$

$$= \int_{U} E_{x}^{s} \left( \exp\left(-\int_{0}^{t} V(X(\tau)) d\tau\right) p_{0}(s, X(t-s), x) dx$$

$$+ \frac{1}{s} \int_{U} \exp\left(-sV(x)\right) \left[ \exp\left(-sK_{0}\right) E_{(.)} \left( \exp\left(-\int_{0}^{t-s} V(X(\tau)) d\tau\right) p_{0}(s, X(t-s), x) \right) dx$$

$$\times \min\left(T_{U}, t-2s\right) dx. \tag{3.7}$$

From (3.7) we infer

$$\begin{split} \int E_{x} \left( \exp\left(-s \sum_{k=0}^{m-1} V(X(ks))\right) p_{0}(s, X((m-1)s), x) \max_{1 \leq j \leq m-1} v(X(js)) \right) dx \\ &\leq \int E_{x}^{s} \left( \exp\left(-\int_{0}^{t} V(X(\tau)) d\tau\right) p_{0}(s, X(t-s), x) \max_{1 \leq j \leq m-1} \int_{0}^{\infty} 1_{\{v>\xi\}} (X(js)) d\xi \right) dx \\ &\leq \int \int_{0}^{\infty} E_{x}^{s} \left( \exp\left(-\int_{0}^{t} V(X(\tau)) d\tau\right) p_{0}(s, X(t-s), x) \max_{1 \leq j \leq m-1} 1_{\{v>\xi\}} (X(js)) d\xi \right) dx \\ &\leq \int \int_{0}^{v(x)} E_{x}^{s} \left( \exp\left(-\int_{0}^{t} V(X(\tau)) d\tau\right) p_{0}(s, X(t-s), x) \right) \frac{\max_{1 \leq j \leq m-1} 1_{\{v>\xi\}} (X(js)) d\xi \right) dx \\ &+ \frac{1}{s} \int \int_{0}^{v(x)} \exp\left(-sV(x)\right) \left[ \exp\left(-sK_{0}\right) E_{(\cdot)}^{s} \left( \exp\left(-\int_{0}^{t-s} V(X(\tau)) d\tau\right) p_{0}(s, X(t-2s), x) \right. \\ &\times \min\left(T_{\xi}, t-2s\right) \right) \right] (x) d\xi dx \\ &= \int v(x) E_{x}^{s} \left( \exp\left(-\int_{0}^{t} V(X(\tau)) d\tau\right) p_{0}(s, X(t-s), x) \right) dx \\ &+ \int \exp\left(-sV(x)\right) \left[ \frac{\exp\left(-sK_{0}\right)}{s} E_{(\cdot)}^{s} \left( \exp\left(-\int_{0}^{t-s} V(X(\tau)) d\tau\right) p_{0}(s, X(t-2s), x) \right. \\ &\times \int_{0}^{v(x)} \min\left(T_{\xi}, t-2s\right) d\xi \right) \right] (x) dx \\ &= \int v(x) E_{x}^{s} \left( \exp\left(-\int_{0}^{t} V(X(\tau)) d\tau\right) p_{0}(s, X(t-s), x) \right) dx \\ &+ \int \left[ \frac{\exp\left(-sK_{0}\right)}{s} \exp\left(-sV(\cdot)\right) E_{x}^{s} \left( \exp\left(-\int_{0}^{t-s} V(X(\tau)) d\tau\right) p_{0}(s, X(t-2s), x) \right. \\ &\times \int_{0}^{v(\cdot)} \min\left(T_{\xi}, t-2s\right) d\xi \right) \right] (x) dx \\ &= \int v(x) E_{x}^{s} \left( \exp\left(-\int_{0}^{t} V(X(\tau)) d\tau\right) p_{0}(s, X(t-s), x) \right) dx \\ &+ \int \left[ \frac{\exp\left(-sK_{0}\right)}{s} \exp\left(-sV(\cdot)\right) \int_{s(x)}^{v(\cdot)} h_{s}(\xi, x, \cdot) d\xi \right] (x) dx. \end{aligned} \tag{3.8}$$

Hence we may conclude

$$\int E_x^s \left( \exp\left( - \int_0^t V(X(\sigma)) d\sigma \right) p_0(s, X(t-s), x) \max_{s \le \sigma \le t-s} v(X(\sigma)) \right) dx$$

$$\leq \int v(x)E_{x}^{s}\left(\exp\left(-\int_{0}^{t}V(X(\tau))d\tau\right)p_{0}(s,X(t-s),x)\right)dx \\
+ \int \left[\frac{\exp(-sK_{0})}{s}\exp(-sV(.))\int_{v(x)}^{v(.)}h_{s}(\xi,x,.)d\xi\right](x)dx \\
= \int v(x)E_{x}^{s}\left(\exp\left(-\int_{0}^{t}V(X(\tau))d\tau\right)p_{0}(s,X(t-s),x)\right)dx \\
+ \int E_{x}\left(\exp(-sV(X(s)))\frac{\int_{v(x)}^{v(X(s))}h_{s}(\xi,x,X(s))d\xi}{s}\right)dx \\
= \int v(x)E_{x}^{s}\left(\exp\left(-\int_{0}^{t}V(X(\tau))d\tau\right)p_{0}(s,X(t-s),x)\right)dx \\
+ \int E_{x}\left(\frac{\exp(-sV(X(s))) - \exp(-sV(x))}{s}\int_{v(x)}^{v(X(s))}h_{s}(\xi,x,X(s))d\xi\right)dx \\
+ \int \exp(-sV(x))\frac{E_{x}\left(\int_{0}^{v(X(s))}\left(h_{s}(\xi,x,X(s)) - h_{s}(v(x)+,x,x)\right)d\xi\right)}{s}dx \\
+ \int \exp(-sV(x))h_{s}(v(x)+,x,x)\frac{E_{x}(v(X(s)) - v(x)}{s}dx. \tag{3.9}$$

Since

$$E_x(v(X(s)) = [\exp(-sK_0)v](x) \le \exp\left(\frac{s}{t}\right)v(x),$$

since V is bounded and continuous, since  $\lim_{s\downarrow 0} v(X(s)) = 0$ ,  $P_x$ -almost surely, since

$$h_s(\xi, x, z) \leq t \exp\left(t \left\|V_-\right\|_{\infty}\right) p_0(t - s, x, z)$$

and since

$$\lim_{s\downarrow 0}h_s(\xi(s),x,z(s))=\lim_{s\downarrow 0}h_s(\xi+,x,z)\leq t\exp(-t(K_0+V))(x,z),$$

whenever  $\xi(s)$  decreases to  $\xi$  and whenever z(s) tends to z in E, we deduce from (3.9) and from standard arguments in integration theory that

$$\lim_{s\downarrow 0} \int E_x \left( \exp\left( -\int_0^{t-s} V(X(\sigma)) d\sigma \right) \max_{0<\tau < t} v_{1/t}(X(\tau)) \right) dx$$

$$\leq 2 \int \exp(-t(K_0 + V))(x, x) v_{1/t}(x) dx. \tag{3.10}$$

Since the measure of  $\Gamma \setminus \Gamma^r$  is zero and since  $v_{\lambda}(x) = 1$  for  $x \in \Gamma^r$  inequality (3.2) and therefore (2.29) follows from inequality (3.10). Strictly speaking we only proved (3.1) for continuous and bounded functions V. Employing standard approximation arguments will show that inequality (3.10) remains valid for arbitrary Borel measurable functions V which take values in  $[-\infty, \infty]$  and which verify the usual Kato properties.

#### 4. A two space criterion for invariance of essential spectra.

The following general two space criterion, as exhibited in Brüning, Demuth and Gesztesy [6], was used in the proof of Theorem 2.10.

4.1. Theorem. Let  $A_1$  and  $A_2$  be two selfadjoint operators in some complex, separable Hilbert spaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$  respectively. Let T be bounded operator from  $\mathcal{H}_1$  to  $\mathcal{H}_2$  and let  $\lambda$  be a point in the resolvent set of  $A_1$  as well as  $A_2$ . If, for some p,  $q, r \in \mathbb{N}$ ,

$$(\lambda Id_2 - A_2)^{-p}T - T(\lambda Id_1 - A_1)^{-p} \in \mathcal{I}_{\infty} (\mathcal{H}_1, \mathcal{H}_2)$$
  
 $(Id_1 - T^*T)(\lambda Id_1 - A_1)^{-q} \in \mathcal{I}_{\infty} (\mathcal{H}_1, \mathcal{H}_1)$   
 $(Id_2 - TT^*)(\lambda Id_2 - A_2)^{-r} \in \mathcal{I}_{\infty} (\mathcal{H}_2, \mathcal{H}_2),$ 

then

$$\sigma_{\mathtt{ess}}(A_1) = \sigma_{\mathtt{ess}}(A_2).$$

Here  $\mathcal{I}_{\infty}(\mathcal{H}_i, \mathcal{H}_j)$  denotes the space of compact operators between  $\mathcal{H}_i$  and  $\mathcal{H}_j$ .

As a consequence we have the following result, which is applicable in the present situation. We use the notation and convention of section 2 and 3. In addition the operator  $J: L^2(E,m) \to L^2(\Sigma,m)$  is defined by  $Jf = f \mid_{\Sigma}, f \in L^2(E,m)$ .

**4.2.** Corollary. Suppose that, for some  $\lambda > 0$ , the operators

$$(\lambda I + (K_0 + V)_{\Sigma})^{-1} J - J (\lambda I + K_0 + V)^{-1}, \quad 1_{\Gamma} (\lambda I + K_0 + V)^{-1}$$

and

$$(\lambda I + K_0 + V)^{-1} - (\lambda + K_0)^{-1}$$

are compact. Then  $\sigma_{ess}(K_0) = \sigma_{ess}(K_0 + V)_{\Sigma}$ .

Here, as above,  $(K_0 + V)_{\Sigma}$  is the generator in  $L^2(\Sigma, m)$  of the semigroup  $\{\exp(-t(K_0 + V)_{\Sigma}): t \geq 0\}$ , defined by

$$\left[\exp\left(-t(K_0+V)_\Sigma\right)f\right](x)=E_x\left(\exp\left(-\int_0^tV(X(s))ds
ight)f(X(t)):T>t
ight),$$

where f belongs to  $L^2(\Sigma, m)$ .

A corresponding stability result for the absolutely continuous parts of the spectrum reads as follows. A combination of Theorem XI.7 (Pearson's Theorem) in Reed and Simon [32, p. 24], the two space invariance principle [32, pp. 30-32], Proposition 4 [32, p. 34] and Proposition 5, assertion (c), [32, pp. 35-36] yields the following stability result. Another valuable source of information is Bamgärtel and Wollenberg [4].

4.3. Theorem. Suppose that the operator

$$\exp\left(-(K_0+V)_{\Sigma}\right)J-J\exp\left(-K_0\right)$$

is a trace class operator and suppose that, for some  $\lambda > 0$ , the operator

$$1_{\Gamma} \left(\lambda I + K_0 + V\right)^{-1}$$

is compact. Then the wave operator

$$W_+\left((K_0+V)_\Sigma,J,K_0\right):=\operatorname{s-}\lim_{t\to\infty}\exp\left(it(K_0+V)_\Sigma\right)J\exp\left(-itK_0\right)P_{\operatorname{ac}}(K_0)$$

exists and its restriction to  $\mathcal{H}_{ac}(K_0)$  is surjective and injective from  $\mathcal{H}_{ac}(K_0)$  to  $\mathcal{H}_{ac}((K_0+V)_{\Sigma})$ . Moreover the restriction  $K_0\mid_{\mathcal{H}_{ac}(K_0)}$  is unitarily equivalent to  $(K_0+V)_{\Sigma}\mid_{\mathcal{H}((K_0+V)_{\Sigma})}$ . In particular  $\sigma_{ac}(K_0+V)_{\Sigma}=\sigma_{ac}(K_0)$ .

Remark. Examples of applications of differences of heat semigroups in scattering theory are among others:

A general formulation of the invariance principle (see Baumgärtel and Wollenberg [4, p. 341] or the completeness of certain scattering systems due to the Enss method (see e.g. [4, p. 331]). Other examples of spectral properties depending on semigroup behaviour can be found in Reed and Simon [33] or for Schrödinger operators in [35] or [1].

Acknowledgement. The authors want to thank several people who in one way or another were involved during the preparation of the present paper. First of all thanks are due to A. Badrikian of the University of Clermont-Ferrand for his kind hospitality while the second author was visiting Clermont-Ferrand and Saint-Flour. the authors are also grateful to H. Langer of the Technische Universität Dresden for giving them the opportunity to present some of their work at the seminar ISAM 88 in Gaussig. The second author is obliged to the University of Antwerp (UIA) and to the Belgian National Fund for Scientific Research (NFWO) for their material support. Both authors want to thank the Akademie der Wissenschaften der DDR for giving the opportunity of this collaboration during the symposium on "Partial Differential Equations" held at Holzhau, GDR, from April 24 until April 30, 1988.

#### References.

This list contains more relevant titles than actual references.

- M. Aizenman and B. Simon, Brownian motion and Harnack inequality for Schrödinger operators, Comm. Pure and Appl. Math. Vol. XXXV, 1982, 209-273.
- 2. S. Albeverio et al (editors), Feynman path integrals, Lecture Notes in Physics 106, Springer Verlag, Berlin 1979.
- 3. H. Baumgärtel and M. Demuth, Decoupling by a projection, Rep. Math. Physics 15, 1979, 173-186.
- 4. H. Baumgärtel and M. Wollenberg, Mathematical scattering theory, Birkhäuser, Boston, Basel 1983.
- 5. R.M. Blumenthal and R.K. Getoor, Markov processes and potential theory, Academic Press, London, New York 1968.
- 6. E. Brüning, M. Demuth and F. Gesztesy, Invariance of the essential spectra for perturbations with unbounded hard cores, Letters Math. Physics 13, 1987, 69-77.
- 7. R.H. Cameron and D.A. Storvick, A simple definition of the Feynman path integral with applications, Memoirs Amer. Math. Soc. no. 288, Providence 1983.
- 8. H.L. Cycon, R.G. Froese, W. Kirsch and B. Simon, Schrödinger operators with applications to quantum mechanics and global geometry, Textbooks in Mathematical Physic, Springer Verlag 1986.
- 9. E.B. Davies, Structural isomers, double wells, resonances, and Dirichlet decoupling, Annals of Physics Vol. 157, N, 1984, 166-182.
- 10. E.B. Davies, Heat kernel bounds for second order elliptic operators on Riemannian manifolds, Amer. J. Math. 109, 1987, no. 3, 545-569.
- 11. E.B. Davies, Explicit constants for Gaussian upper bounds on heat kernels, Amer. J. of Math. to appear.
- 12. E.B. Davies and B. Simon, Ultracontractivity and the heat kernel for Schrödinger operators and Dirichlet Laplacians, J. of Functional Analysis. 59,1984,335-394.
- 13. M. Demuth, Zeitabhängige Streutheorie für Erzeuger von Markov Prozessen mit anisotropen und singulären Potentialen, Report Karl-Weierstrass Institut der Mathematik, Berlin, R-Math-04/85, 1985.
- 14. M. Demuth and J.A. van Casteren, On spectral theory for Feller generators, Research report University of Antwerp 88-13, 1988.
- 15. R. Durrett, Brownian motion and martingales in analysis, Wadsworth Advanced Books and Software, Belmont 1984.
- 16. A. Friedman, Stochastic differential equations and applications, Vol. 1, Academic Press, New York, London 1976.
- 17. M. Fukushima, Dirichlet forms and Markov processes, North-Holland, Amsterdam 1980.
- 18. S. Graffi (editor), Schrödinger operators, Proceedings of a Conference (CIME) in Como (1984), Lecture Notes in Math. 1159, Springer Verlag, Berlin 1986.
- 19. R. Hempel and J. Voigt, On the  $L_p$ -spectrum of Schrödinger operators, J. of Math. Anal. and Applic. Vol. 121, 1987, 138-159.

- 20. G.W. Johnson, Feynman's paper revisited, in supplemento ai Rendiconti del Circolo matematico di Palermo, 1987, 249-270, special issue containing the Proceedings of the Workshop on Functional Integration with an emphasis on the Feynman integral, held at the University of Sherbrooke, Canada, July 21-30, 1986.
- 21. G.W. Johnson and M.L. Lapidus, Generalized Dyson series, generalized Feynman diagrams, the Feynman integral and Feynman's operational calculus, Memoirs Amer. Math. Soc. no. 351, Providence 1986.
- 22. G.W. Johnson and D.L. Skoug, Notes on the Feynman integral I, Pac. J. of Math. Vol. 93, no.2, 1981, 313-324.
- 23. G.W. Johnson and D.L. Skoug, Notes on the Feynman integral II, J. of Functional Analysis, 41, 1981, 277-289.
- 24. G.W. Johnson and D.L. Skoug, Notes on the Feynman integral III, Pac. J. of Math. Vol. 105, no.2, 1983, 321-358.
- 25. K. Jörgens, Lineare Integraloperatoren, B.G. Teubner, Stuttgart 1970.
- 26. T. Kato, Remarks on the self-adjointness and related topics for differential operators, in "Spectral theory for differential operators", J.W. Knowles and R.T. Lewis (editors), North-Holland, Amsterdam, 1982, p. 253.
- 27. M.L. Lapidus, Perturbation theory and a dominated convergence theorem for Feynman integrals, Integral Equations and Operator Theory, Vol.8, 1985, 36-62.
- 28. M.L. Lapidus, Product formula for imaginary resolvents with applications to a modified Feynman integral, J. of Functional Analysis, 63, 1985, 261-275.
- 29. M.L. Lapidus, The Feynman-Kac formula with a Lebesgue-Stieltjes measure and Feynman's operational calculus, Studies in Applied Mathematics, Vol. 76, no.2, 1987, 93-132.
- 30. S.C. Port and C.J. Stone, Brownian motion and potential theory, Academic Press, London, New York 1978.
- 31. M. Reed and B. Simon, Methods of modern mathematical physics, Vol. 2, Fourier analysis, self-adjointness; Academic Press, New York, London, 1975.
- 32. M. Reed and B. Simon, Methods of Modern mathematical physics, Vol. 3, Scattering theory; Academic Press, New York, London 1979.
- 33. M. Reed and B. Simon, Methods of modern mathematical physics, Vol. 4, Analysis of operators; Academic Press, New York, London 1978.
- 34. B. Simon, Functional integration and quantum physics, Academic Press, New York 1979.
- 35. B. Simon, Schrödinger semigroups, Bull. Amer. Math. Soc. Vol. 7, 1982, no.3, 447-526.
- 36. J.A. van Casteren, Generators of strongly continuous semigroups, Research Notes in Math. 115, Pitman, London 1985.
- 37. J.A. van Casteren, Integral kernels and Schrödinger type equations, in Rendiconti del Circolo Matematica de Palermo, special issue containing the proceedings of the Summer School on Functional Integration held at the University of Sherbrooke, Canada, July 21-July 30, 1986, 393-421.
- 38. J.A. van Casteren, Integral kernels and the Feynman-Kac formalism, in Aspects

- of Positivity in Functional Analysis, R.Nagel, U.Schlotterbeck and M.P.H. Wolff (editors), North-Holland, Amsterdam 1986, 179-185.
- 39. J.A. van Casteren, Semigroupes de Schrödinger généralizés, Lectures for a seminar in Clermont-Ferrand, handwritten manuscript, 1987.
- 40. J.A. van Casteren, Pointwise inequalities for Schrödinger semigroups, to appear in the Proceedings of the meeting "Trends in Semigroup Theory and Applications" held at Trieste, Italy, Sept. 28 Oct. 2, 1987, to be published by Marcel Dekker Inc. in "Lecture Notes in Pure and Applied Mathematicss.
- 41. J.A. van Casteren, On generalized Schrödinger semigroups, to be published in the proceedings of the ISAM 88, Markovsche Prozesse und Steuerungstheorie, held at Gaussig, GDR, 11-15 January 1988 under auspices of the Technical University of Dresden, Teubner, Leipzig.
- 42. J.A. van Casteren, A pointwise inequality for generalized Schrödinger semigroups, University of Antwerp prerint 88-10, to be published in the proceedings of the conference "Partial Differential Operators" held from April 24 until April 30, 1988, at Holzhau, GDR.
- 43. M. van den Berg, On the spectrum of the Dirichlet Laplacian for horn-shaped regions in  $\mathbb{R}^n$  with infinite volume, J. Funct. Anal. 58, 1984, 150-156.
- 44. M. van den Berg, On the asymptotics of the heat equation and bounds on traces associated with the Dirichlet Laplacian, J. Funct. Anal. 71, 1987, 279-293.
- 45. J. Voigt, Absorption semigroups, their generators and Schrödinger semigroups, J. of Functional Analysis Vol.67, 1986, 167-205.
- 46. N. Wielens, The essential self-adjointness of generalized Schrödinger operators, J. Funct. Anal. 61, 1985, 98-115.
- 47. K. Yosida, Functional analysis, 6th printing, Springer Verlag, Berlin 1980.

J.A. VAN CASTEREN
University of Antwerp (UIA)
Department of Mathematics and
Computer Science
Universiteitsplein 1,
2610 WILRIJK/ANTWERP

BELGIUM

M. DEMUTH
Akademie der Wissenschaften der DDR
Karl-Weierstrass Institut für
Mathematik
Mohrenstrasse 39
DDR-1086 BERLIN