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L^1-Properties of Intrinsic Schrödinger Semigroups

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We investigate the L^1-properties of the intrinsic Markov semigroup associated with a Schrödinger operator on $\mathbb{R}^N$ which possesses a positive ground state. We discover cases for which this semigroup is norm analytic for positive times, and others for which the semigroup is norm discontinuous in the strongest possible sense. In the case of the harmonic oscillator, we show that the generator of the intrinsic semigroup has totally different spectrum depending on whether one works in L^1 $(\mathbb{R}, e^{-x^2}\,dx)$ or L^2 $(\mathbb{R}, e^{-x^2}\,dx)$. In more general cases we show that the equality of the L^1 and L^2 spectrum is closely related to whether the Schrödinger semigroup is intrinsically ultracontractive. © 1986 Academic Press, Inc.

1. INTRODUCTION

Our goal is to compare the L^1 and L^2 spectral properties of certain second order elliptic operators defined on an open connected subset X of $\mathbb{R}^N$. Our starting point is an operator L defined by

$$Lf = -\sum_{i,j} \frac{\partial}{\partial x_i}\left(A_{ij}(x)\frac{\partial f}{\partial x_j}\right) + V(x)f(x)$$

where A_{ij} and V are real valued C^∞ functions on X such that V is bounded below and $A(x)$ is a strictly positive symmetric matrix for all $x \in X$ (many of the theorems in this paper are valid under much weaker local regularity

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conditions on A and V; we leave the necessary modifications to the interested reader). We define the corresponding quadratic form Q on the domain $C_0^\infty(X)$ of C^∞ functions with compact support in X by

$$Q(f)=\int_X \left(\sum_{i,j} A_{ij} \frac{\partial f}{\partial x_j}\frac{\partial \bar{f}}{\partial x_i} + V|f|^2\right) d^N x.$$

This form is semibounded, closable, and densely defined in $L^2(X, d^N x)$, so its closure is the form of a semibounded self-adjoint H on $L^2(X, d^N x)$. One has

$$Hf = Lf, \qquad f \in C_0^\infty(X)$$

and in many cases H can be identified with the operator obtained from L by imposing Dirichlet boundary conditions in the classical manner.

If φ is a strictly positive C^∞ function on X which satisfies $L\varphi = E\varphi$ for some $E \in \mathbb{R}$, then we may define the intrinsic operator $\tilde{H}$ on $L^2(X, \varphi^2\, d^N x)$ by

$$\tilde{H} = U^{-1}(H-E)\,U$$

where the unitary operator U from $L^2(X, \varphi^2\, d^N x)$ to $L^2(X, d^N x)$ is defined by $Uf = \varphi f$. A routine computation [1, 8] shows that $\tilde{H}$ is given on $C_0^\infty(X)$ by

$$\tilde{H}f = -\varphi^{-2} \sum_{i,j} \frac{\partial}{\partial x_i}\left(\varphi^2 A_{i,j} \frac{\partial f}{\partial x_j}\right)$$

and that the associated form is

$$\tilde{Q}(f) = \int_X \left(\sum_{i,j} A_{i,j} \frac{\partial f}{\partial x_i}\frac{\partial \bar{f}}{\partial x_j}\right) \varphi^2\, d^N x.$$

Since $\tilde{Q} \geqslant 0$ on $C_0^\infty(X)$, which is a form core of $\tilde{H}$, we deduce as in [1, 8] that

$$Sp(\tilde{H}) \subseteq [0, \infty)$$

The above calculation does not depend upon assuming $\varphi \in L^2$, and does not imply that $0 \in Sp(\tilde{H})$. However, we shall henceforth assume that φ lies in $L^2(X, d^N x)$, has norm one, and is the ground state of H, so that $1 \in \mathrm{Dom}\,(\tilde{H})$ and $\tilde{H}1 = 0$. Then X is a probability space with respect to the measure $\varphi^2 d^N x$, and $e^{-\tilde{H}t}$ is a self-asjoint positivity preserving semigroup on $L^2(X, \varphi^2 d^N x)$ which satisfies

$$e^{-\tilde{H}t}1 = 1$$

for all $t \geqslant 0$. It is standard [6, 8] that $e^{-\tilde{H}t}$ induces a strongly continuous one-parameter contraction semigroup on $L^p(X, \varphi^2 d^N x)$ for $1 \leqslant p < \infty$, whose generator we shall denote by $\tilde{H}_p$.

Our concern in this paper will to be study continuity properties of $e^{-\tilde{H}_p t}$ and spectral properties of $\tilde{H}_p$ with particular reference to the case $p = 1$. For other values of p the following result is known. See [7, 8] for further information when H is a Schrödinger operator.

LEMMA 1. *If e^{-Ht} is compact for $0 < t < \infty$ then $e^{-\tilde{H}_p t}$ is compact for $0 < t < \infty$ and $1 < p < \infty$, and is a norm analytic function of t for $0 < t < \infty$. Moreover $Sp(\tilde{H}_p)$ is independent of p for $1 < p < \infty$.*

Proof. The compactness of e^{-Ht} implies that of $e^{-\tilde{H}_p t}$ for $1 < p < \infty$ by an interpolation argument [4, Lemma A.5]. Norm analyticity now follows by [7, 8] and spectral independence by [4, Lemma A.5]. ∎

The proof of the above lemma cannot be extended to include the case $p = 1$, and to analyse this case it is convenient to transfer back to the space $L^1(X, d^N x)$. Thus we define the isometry V form $L^1(X, d^N x)$ to $L^1(X, \varphi^2 d^N x)$ by

$$Vf = \varphi^{-2} f$$

and define the strongly continuous positive one-parameter contraction semigroup $e^{-\hat{H}t}$ on $L^1(X, d^N x)$ by

$$e^{-\hat{H}t} f = V^{-1} e^{-\tilde{H}_1 t} Vf.$$

Since φ is C^∞ is one sees that $C_0^\infty(X)$ is contained in Dom $(\hat{H})$, and a standard calculation yields

$$\begin{aligned} \hat{H}f &= \sum_{i,j} \frac{\partial}{\partial x^i} \left(\varphi^2 A^{ij} \frac{\partial}{\partial x^j} (\varphi^{-2} f) \right) \\ &= -\sum_{i,j} \left(\frac{\partial}{\partial x^i} \left(A^{ij} \frac{\partial f}{\partial x^j} \right) + 2 \frac{\partial}{\partial x^i} \left(A^{ij} \varphi^{-1} \frac{\partial \varphi}{\partial x^j} f \right) \right) \end{aligned} \tag{1.1}$$

on this domain. The two terms on the *RHS* of this equation are called respectively the diffusion and drift terms of $\hat{H}$. Note that $\hat{H}$ is formally the adjoint of $\tilde{H}$ if we regard the latter as acting on L^∞. Note also that $e^{-\hat{H}t}$ is a Markov semigroup with $\varphi^2 \in L^1(X, dx)$ as invariant state.

We shall not make any use of the following result, but include it for completeness and reassurance.

LEMMA 2. *If H is essentially self-adjoint on the subspace $C_0^\infty(X)$ of $L^2(X, dx)$, then $C_0^\infty(X)$ is a core for the operator $\hat{H}$ on $L^1(X, dx)$.*

Proof. We first note that $C_0^\infty(X)$ is a core for $\tilde{H}_2$ because U leaves this domain invariant. Secondly $\mathrm{Dom}(\tilde{H}_2)$ is dense in $L^1(X, \varphi^2 dx)$ and invariant under $e^{-\tilde{H}t}$, and so is a core for $\tilde{H}_1$ by [2, Theorem 1.9]. But $C_0^\infty(X)$ is dense in $\mathrm{Dom}(\tilde{H}_2)$ for the graph norm wrt L^2, and hence also dense for the graph norm wrt L^1. Thus, $C_0^\infty(X)$ is a core for $\tilde{H}_1$. Since V leaves $C_0^\infty(X)$ invariant, $C_0^\infty(X)$ is also a core of $\hat{H}$. ▮

When we started this research we thought that proving

$$Sp(\tilde{H}_1) = Sp(\tilde{H}_2)$$

would be routine, wo we were rather surprised to find that even the case of the harmonic oscillator had never been analysed from this point of view. The behaviour of this example came as rather a shock.

THEOREM 3. *If*

$$H = -\frac{1}{2}\left(\frac{d^2}{dx^2} + x^2\right)$$

on $L^2(\mathbb{R}, dx)$ then

$$Sp(\tilde{H}_1) = \{z\colon \mathrm{Re}\, z \geqslant 0\}.$$

Indeed, every z with $\mathrm{Re}\, z > 0$ is an eigenvalue of multiplicity 2 of $\tilde{H}_1$. If $0 < s < t < \infty$ then

$$\|e^{-\tilde{H}_1 s} - e^{-\tilde{H}_1 t}\| = 2.$$

Proof. We start with the facts that

$$\varphi(x) = ce^{-x^2/2}$$

and that Mehler's formula [2, p. 181] states that e^{-Ht} on $L^2(\mathbb{R}, dx)$ has kernel

$$q_t(x, y) = \{\pi(1 - e^{-2t})\}^{-1/2} \exp\{-B_t(x, y)\}$$

where

$$B_t(x, y) = (1 - e^{-2t})^{-1}\left[\tfrac{1}{2}(x^2 + y^2)(1 + e^{-2t}) - 2e^{-t}xy\right].$$

Routine calculations then show that $e^{-\hat{H}t}$ on $L^1(\mathbb{R}, dx)$ has kernel

$$\hat{q}_t(x, y) = \{\pi(1 - e^{-2t})\}^{-1/2} \exp\{-\hat{B}_t(x, y)\} \tag{1.2}$$

where

$$\hat{B}_t(x, y) = \frac{(x - e^{-t}y)^2}{1 - e^{-2t}}.$$

If $\mathscr{F}$ denotes the Fourier transform map from $L^1(\mathbb{R}, dx)$ to $C_0(\mathbb{R})$ then it follows that

$$(\mathscr{F} e^{-\hat{H}t} f)(k) = e^{-c_t k^2/4} \mathscr{F} f(e^{-t} k)$$

where

$$c_t = 1 - e^{-2t}.$$

Let $X^{\pm}$ be the characteristic functions of $\pm[0, \infty)$. Letting $f_z^{\pm}$ denote the L^1 functions whose Fourier transforms are $X^{\pm}(k)\, |k|^z e^{-k^2/4}$, we see that for any $\operatorname{Re} z > 0$

$$\begin{aligned}(\mathscr{F} e^{-\hat{H}t} f_z^{\pm})(k) &= X^{\pm} e^{-c_t k^2} e^{-zt} |k|^z e^{-e^{-2t} k^2/4} \\ &= e^{-zt} (\mathscr{F} f_z^{\pm})(k).\end{aligned}$$

Hence

$$e^{-\hat{H}t} f_z^{\pm} = e^{-zt} f_z^{\pm}$$

and

$$\hat{H} f_z^{\pm} = z f_z^{\pm}.$$

We deduce the second statement of the theorem from the explicit form (1.2) of the integral kernel of $e^{-\hat{H}t}$. If f is any probability density in $L^1(\mathbb{R}, dx)$ and we put

$$f_a(x) = f(x - a)$$

then one sees that for any $0 < s < t < \infty$, $e^{-\hat{H}s} f_a$ and $e^{-\hat{H}t} f_a$ have asymptotically disjoint supports as $a \to \infty$, so

$$\begin{aligned} 2 &= \lim_{a \to \infty} \|e^{-\hat{H}s} f_a - e^{-\hat{H}t} f_a\|_1 \\ &\leqslant \|e^{-\hat{H}s} - e^{-\hat{H}t}\|. \quad \blacksquare \end{aligned}$$

We should like to comment on the compact form, 1.2), of Mehler's formula. It says that $e^{-\hat{H}t}$ is the composition of dilation and convolution with a Gaussian. Thus if $p = -id/dx$ and $A = \frac{1}{2}(xp + px)$ is the generator of dilations, (1.2) says that

$$\exp\left[-t\left(\tfrac{1}{2} p^2 + \tfrac{1}{2} x^2 - \tfrac{1}{2}\right)\right] = e^{a(t)x^2} e^{-b(t)p^2} e^{-c(t)A} e^{-a(t)x^2}$$

for suitable functions $a(t)$, $b(0)$, $c(t)$, ($a(t)$ is constant). This presumably provides a proof of Mehler's formula using the structure of the Lie algebra $sl(Z, R)$, generated by x^2, p^2 and A. It is essentially the form arising in the Hoegh–Krohn–Simon proof of Mehler's formula, see [9, pp. 25–29; esp. Remark 2 on p. 29].

The strange behaviour of the above example suggests that the L^1 behaviour of intrinsic Schrödinger semigroups will not be very interesting. However, it turns out that this is incorrect and that such semigroups fall into two very different classes, at least in the case where $A_{ij} = \delta_{ij}$ and the potential increases in a fairly regular way at infinity. If the potential increases quadratically or slower at infinity, then the L^1 intrinsic semigroup often behaves in a qualitatively similar manner to the case of the harmonic oscillator. However, if the potential increases faster than quadratically at infinity, then e^{-Ht} is often intrinsically ultracontractive [4], and this implies that $e^{-\tilde{H}_1 t}$ is norm analytic for $0 < t < \infty$ and that $\tilde{H}_1$ and $\tilde{H}_2$ have the same spectrum. The case of bounded potentials does not fit into the above pattern, however, and a complete understanding of the possibilities remains to be obtained.

In Section 2, we use ultracontractivity to show the phenomena we just found for x^2 potentials do *not* hold for x^α potentials if $\alpha > 2$. We provide some relations to these conditions and the question of whether the continuous functions in $L^2(X, \varphi^2 dx)$ vanishing at ∂X are left invariant by $e^{-\tilde{H}t}$. In Section 3 and 4 we provide two distinct ways of seeing that the phenomena we found for x^2 potentials do hold for x^α potentials if $0 < \alpha < 2$.

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2. Ultracontractivity and invariance of $C_0(X)$

Following [4], we say that $e^{-\tilde{H}t}$ is ultracontractive if for all $t > 0$ there exists $c_t < \infty$ such that

$$\|e^{-\tilde{H}t} f\|_\infty \leqslant c_t \|f\|_2 \tag{2.1}$$

for all $f \in L^2(X, \varphi^2 dx)$ and

$$tr[e^{-\tilde{H}t}] < \infty. \tag{2.2}$$

If the eigenvalues of $\tilde{H}_2$ are denoted by $\{E_n\}_{n=0}^\infty$ and are written in increasing order, so that $E_0=0$, then the corresponding eigenfunctions φ_n satisfy

$$\|\varphi_n\|_\infty \leqslant c_t\, e^{+E_n t/3} \tag{2.3}$$

THEOREM 4. *If $e^{-\tilde{H}t}$ is ultracontractive then $e^{-\tilde{H}_1 t}$ is compact for all $t>0$ and*

$$Sp(\tilde{H}_1) = Sp(\tilde{H}_2). \tag{2.4}$$

Moreover $e^{-\tilde{H}_1 t}$ is a norm analytic function of t for $0<t<\infty$.

Proof. If $t>0$ then (2.2) and (2.3) establish that the series

$$\sum_{n=0}^{\infty} e^{-E_n t}\, |\varphi_n\rangle\langle\varphi_n|$$

is norm convergent as a series of operators on $L^1(X, \varphi^2 dx)$. But this series also converges weakly to $e^{-\tilde{H}_1 t}$ by considering test functions in $C_0^\infty(X)$. We have that

$$e^{-\tilde{H}_1 t} = \sum_{n=0}^{\infty} e^{-E_n t}\, |\varphi_n\rangle\langle\varphi_n| \tag{2.5}$$

so $\exp(-\tilde{H}_1 t)$ is a compact operator. It follows from the formula

$$(\tilde{H}_1+1)^{-1} = \int_0^\infty e^{-\tilde{H}_1 t}\, e^{-t}\, dt$$

that $\tilde{H}_1$ has compact resolvent and by the argument of [4, Lemma A.5] that (2.4) holds. The norm analyticity of $e^{-\tilde{H}_1 t}$ for $0<t<\infty$ is immediate from (2.5). ∎

We now comment that ultracontractivity should be thought of as a very strong form of recurrence, amounting to the positive probability of sample paths returning from ∂X to a compact subregion of X in a finite time. In these terms one can often anticipate whether one has ultracontractivity by looking at the drift term in the expression (1.1) for $\hat{H}$ on its own. An associated question is whether $C_0(X)$, the space of continuous functions on X which vanish on ∂X, is invariant under $(e^{-\hat{H}t})^*$.

THEOREM 5. *The space $C_0(X)$ is invariant under $(e^{-\hat{H}t})^*$ if and only if $C_0(X)\cap L^2(X, \varphi^2 dx)$ is invariant under $e^{-\tilde{H}_2 t}$. If this happens then $e^{-\tilde{H}_1 t}$ is not compact for any $t>0$, and in particular $e^{-\tilde{H}t}$ is not ultracontractive.*

Proof. The equivalence of the first two properties follows from the fact that

$$e^{-\hat{H}_2 t} f = (e^{-\hat{H}t})^* f$$

for all $f \in C_0^\infty(X)$, and that this subset is dense in $C_0(X)$ for the L^∞ norm and in $C^0(X) \cap L^2(X)$ for the L^2 norm.

On the other hand if $e^{-\hat{H}t}$ were compact for some $t > 0$, then one would have

$$\lim_{t \to \infty} \| e^{-\hat{H}t} - |\varphi^2 > < 1| \| = 0$$

by [2, Theorem 2.20] and hence

$$\lim_{t \to \infty} \| (e^{-\hat{H}t})^* - |1 > < \varphi^2| \| = 0.$$

If $0 \leqslant f \in C_0(X)$ we conclude that $(e^{-\hat{H}t})^* f$ converges uniformly to a non-zero multiple of 1, so $C^0(X)$ cannot be invariant. ∎

Note 6. The invariance of $C_0(\mathbb{R})$ is an elementary consequence of the explicit formula for $(e^{-\hat{H}t})^*$ obtainable from (1.2), in the case of the harmonic oscillator.

Together with the analysis of [4] the following theorem shows that the invariance of $C_0(X)$ is quite close to being the converse of ultracontractivity. We do not claim however to have found conditions under which a precise theorem to this effect can be proved.

THEOREM 7. *Suppose $H = -\Delta + V$ on $L^2(\mathbb{R}^N)$, where $0 \leqslant V \in C^\infty$ and*

$$V(x) = o(x^2)$$

as $|x| \to \infty$. Then $C_0(\mathbb{R}^N) \cap L^2(\mathbb{R}^N, \varphi^2 dx)$ is invariant under $e^{-\hat{H}t}$, where φ denotes the ground state of H.

Proof. If follows from the Trotter formula [2, p. 119] that the integral kernel $a_t(x, y)$ of e^{-Ht} on $L^2(\mathbb{R}^N, dx)$ satisfies

$$0 \leqslant a_t(x, y) \leqslant (4\pi t)^{-N/2} e^{-(x-y)^2/4t}$$

and by subharmonic comparison inequalities [3] that

$$\varphi(x) \geqslant c_\beta e^{-\beta x^2}$$

where $c_\beta > 0$ for all $0 < \beta < \infty$. The integral kernel $\tilde{a}_t(z, y)$ of $e^{-\tilde{H}t}$ therefore satisfies

$$0 \leqslant \tilde{a}_t(x, y) = \frac{a_t(x, y)}{\varphi(x)\,\varphi(y)}$$
$$\leqslant c_\beta^{-2}\,(4\pi t)^{-N/2} \exp\left[\beta x^2 + \beta y^2 - \frac{(x-y)^2}{4t}\right]$$

from wich we see by taking β small enough that if $f \in C_0^\infty(\mathbb{R}^N)$ then

$$|e^{-\tilde{H}t} f(x)| \leqslant k_{\delta f, t}\, e^{-\delta x^2}$$

for any $0 < \delta < (4t)^{-1}$. ∎

3. Non-continuity of $e^{-\tilde{H}t}$ in One-Dimension

In this section we show that the differential operator

$$L = -\frac{d^2}{dx^2} + V(x)$$

in one dimension has similar L^1 intrinsic properties to the harmonic oscillator, provided V is reasonably well-behaved and diverges slower than quadratically as $|x| \to \infty$. Although we shall draw a similar conclusion in higher dimensions in Section 4, we have included the present section because the methods are entirely different and the results significantly more complete.

Our basic approach will be to examine the asymptotics of the eigenfunctions of $Lu = Eu$ explicitly. The key estimates involve φ_0, the ground state of L with energy, E_0, and φ, any (in particular a growing) solution of $L\varphi = E\varphi$ with $\operatorname{Re} E > E_0$. We need;

$$\int |\varphi\varphi_0|\, dx < \infty \text{ and } |\varphi'\varphi_0| \to 0 \text{ at infinity.}$$

To see why this should be true for x^α potentials with $\alpha \leqslant 2$, take E real and imagine that φ, φ_0 obey *WKB* asymptotics:

$$\varphi_0(x) \sim V^{-1/4} \exp\left(-\int_0^x (V(s) - E_0)_+^{1/2}\, ds\right),$$

$$\varphi_0'(x) \sim V^{1/4} \exp\left(-\int_0^x (V(s) - E_0)_+^{1/2}\, ds\right)$$

$$\varphi(x) \sim V^{-1/4} \exp\left(\int_0^x (V(s)-E)_+^{1/2}\, ds\right),$$

$$\varphi'(x) \sim V^{1/4} \exp\left(\int_0^x (V(s)-E)_+^{1/2}\, ds\right)$$

where $f \sim g$ means $\lim_{x\to\pm\infty} f(x)/g(x) = c_\pm$ with $c_\pm$ non-zero constants. Then, if $V(x) \sim x^\alpha$ it is always true that $\int |\varphi\varphi_0|\, dx < \infty$, albeit for very different reasons when $\alpha \leqslant 2$ or when $\alpha > 2$. $|\varphi_0'\varphi| \to 0$ requires $\alpha \leqslant 2$. Under suitable conditions on V', V'', one can verify the *WKB* asymptotics (see Theorem 2.1 on p. 193 of Olver [5]) and use these estimates to replace Lemmas 8 and 9 below. We provide these lemmas partly for the reader's convenience, partly to emphasize that only upper bounds are needed and partly because we require no bounds on V''.

Throughout this section we make the standing assumption that V is a positive C^∞ function on $\mathbb{R}$ such that

$$V(x) \sim c|x|^\alpha \text{ as } |x| \to \infty \tag{3.1a}$$

where $c > 0$ and $0 < \alpha < 2$, and also

$$V'(x) = O(|x|^{\alpha-1}) \text{ as } |x| \to \infty. \tag{3.1b}$$

Equation (3.1) is much too strong a condition. The proofs of the lemmas below are valid if (i) $V(x) \to \infty$ as $|x| \to \infty$, (ii) $V'(x)V(x)^{-1/2} \to 0$ as $|x| \to \infty$, (iii) $g(x) \equiv |\int_0^x V(s)^{-1/2} ds| \to \infty$ as $|x| \to \infty$, (iv) $e^{-g(x)} \sup_{(1/2)x \leqslant s \leqslant x} |V(x)|^{1/2} \to 0$. The theorem then requires (v) $\int e^{-g(x)}\, dx < \infty$. Rather than state (i)–(v) as our basic hypothesis, we settle for (3.1).

Let φ_0 be the (strictly positive) eigenfunction of H corresponding to its lowest eigenfunction E_0, and let φ be *any* solution of the differential equation

$$-\varphi'' + V\varphi = E\varphi \tag{3.2}$$

with $\mathrm{Re}(E) > E_0$.

LEMMA 8. *If $E_0 < F_1$ there exists a constant $c_1 > 0$ such that*

$$|\varphi_0(x)| + |\varphi_0'(x)| \leqslant c_1 \exp\left[-\int_0^x V(s)^{1/2}\, ds + \frac{1}{2} F_1 \int_0^x V(s)^{-1/2}\, ds\right]$$

for all $x \geqslant 0$.

Proof. If

$$W(x)=\int_0^x V(s)^{1/2}\,ds-\frac{1}{2}F\int_0^x V(s)^{-1/2}\,ds$$

and $\psi=e^{-W}$, then using (3.1):

$$\begin{aligned}\psi''/\psi &= (W')^2-W''\\ &= (V^{1/2}-\tfrac{1}{2}FV^{-1/2})^2\\ &\quad -\tfrac{1}{2}V'V^{-1/2}-\tfrac{1}{4}FV'V^{-3/2}\\ &= V-F+o(1)\end{aligned}$$

as $x\to\infty$. The upper bound on $\varphi_0(x)$ now follows by the subharmonic comparison lemma [3]. To bound $\varphi_0'(x)$ we note that φ_0 is convex (and positive) for large x, so

$$\begin{aligned}x^{-\alpha/2}\,|\varphi_0'(x)| &\leqslant \varphi_0(x-x^{-\alpha/2})\\ &\leqslant c_2\exp\left[-\int_0^{x-x^{-\alpha/2}} V(s)^{1/2}\,ds+\frac{1}{2}F_2\int_0^{x-x^{-\alpha/2}} V(s)^{-1/2}\,ds\right]\end{aligned}$$

where $E_0<F_2<F_1$. Therefore

$$\begin{aligned}|\varphi_0'(x)| &\leqslant c_2\,x^{\alpha/2}\exp\left[-\int_0^x V(s)^{1/2}\,ds\right.\\ &\qquad\left.+\int_{x-x^{-\alpha/2}}^x V(s)^{1/2}\,ds+\frac{1}{2}F_2\int_0^x V(s)^{-1/2}\,ds\right]\\ &\leqslant \frac{1}{2}c_1\exp\left[-\int_0^x V(s)^{1/2}\,ds+1\frac{2}{}F_1\int_0^x V(s)^{-1/2}\,ds\right]\end{aligned}$$

because

$$\left|\int_{x-x_{-\alpha/2}}^x V(s)^{1/2}\,ds\right|\leqslant x^{-\alpha/2}\sup_{x/2\leqslant s\leqslant x}|V(s)|^{1/2}$$

is bounded as $x\to\infty$ and $x^{\alpha/2}$ is dominated by

$$\exp\left[\frac{1}{2}(F_1-F_2)\int_0^x V(s)^{-1/2}\,ds\right]$$

as $x\to\infty$, by virtue of (3.1). ∎

LEMMA 9. *If* $F_3 < \mathrm{Re}(E)$ *then there exists* $c_3 > 0$ *such that*

$$|\varphi(x)| + |\varphi'(x)| \leqslant c_3 \exp\left[\int_0^x V(s)^{1/2}\, ds - \frac{1}{2} F_3 \int_0^x V(s)^{-1/2}\, ds\right]$$

for all $x \geqslant 0$.

Proof. We put

$$X = V^{1/2} - \tfrac{1}{2} F V^{-1/2}$$

and

$$\psi = X^{-1} \varphi'$$

for large $x > 0$. Then

$$\psi' = X^{-1} (V - E) \varphi - X^{-2} X' \varphi'$$

so

$$\begin{aligned} \varphi' &= X\psi, \\ \psi' &= X^{-1} (V - E) \varphi - X^{-1} X' \psi. \end{aligned}$$

Putting $\xi = (\varphi, \psi)$ and using the L^1 norm on $\mathbb{C}^2$ we deduce that

$$\|\xi\|' \leqslant \|\xi'\| \leqslant \|B\|\, \|\xi\|$$

where the norm of the 2×2 matrix B satisfies

$$\|B\| = \mathrm{Max}\, \{(X^{-1}(V - E)|, |X^{-1} X'| + |X|\}.$$

If $F_3 < F_4 < F < \mathrm{Re}(E)$ then

$$\begin{aligned} |X^{-1} X'| + |X| &= V^{1/2} - \tfrac{1}{2} F V^{-1/2} + o(x^{-1}) \\ &\leqslant V^{1/2} - \tfrac{1}{2} F_4 V^{-1/2} \end{aligned}$$

for large $x > 0$. Also

$$\begin{aligned} |X^{-1}(V - E)| &= V^{1/2} |(1 - \tfrac{1}{2} F V^{-1})^{-1} (1 - E V^{-1})| \\ &= V^{1/2} |1 + (\tfrac{1}{2} F - E) V^{-1} + O(V^{-2})| \\ &\leqslant V^{1/2} (1 + (\tfrac{1}{2} F - \mathrm{Re}(E)) V^{-1} + O(V^{-2}) \\ &\leqslant V^{1/2} - \tfrac{1}{2} F_4 V^{-1/2} \end{aligned}$$

for large $x > 0$. The estimate

$$\|\xi\|' \leqslant (V^{1/2} - \tfrac{1}{2} F_4 V^{-1/2}) \|\xi\|$$

for large $x > 0$ leads immediately to

$$\|\xi\| \leqslant c_4 \exp\left[\int_0^x V(s)^{1/2}\, ds - \frac{1}{2} F_4 \int_0^x V(s)^{-1/2}\, ds\right]$$

for all $x \geqslant 0$, and hence

$$\begin{aligned} &|\varphi(x)| + |\varphi'(x)| \\ &\leqslant c_4(1+X) \exp\left[\int_0^x V(s)^{1/2}\, ds - \frac{1}{2} F_4 \int_0^x V(s)^{-1/2}\, ds\right] \\ &\leqslant c_5(1+x^\alpha) \exp\left[\int_0^x V(s)^{1/2}\, ds - \frac{1}{2} F_4 \int_0^x V(s)^{-1/2}\, ds\right] \\ &\leqslant c_3 \exp\left[\left(\int_0^x V(s)^{1/2} F_3 \int_0^x V(s)^{-1/2}\, ds\right]. \quad \blacksquare \end{aligned}$$

THEOREM 10. *The function* $\tilde{\varphi} = \varphi/\varphi_0$ *lies in the domain of* $\tilde{H}_1$ *and satisfies*

$$\tilde{H}_1 \tilde{\varphi} = (E - E_0)\, \tilde{\varphi} \tag{3.3}$$

Hence every $z \in \mathbb{C}$ *with* $\operatorname{Re} z > 0$ *lies in the point spectrum of* H_1 *and thus* $\operatorname{spec}(\tilde{H}_1) = \{z \mid \operatorname{Re} z \geqslant 0\}$.

Proof. Since φ satisfies (3.2) the function $\tilde{\varphi}$ satisfies

$$-\tilde{\varphi}'' + b\, \tilde{\varphi}' = (E - E_0)\, \tilde{\varphi} \tag{3.4}$$

where

$$b = 2\varphi_0'/\varphi_0.$$

Moreover if $E_0 < F_1 < F_3 < \operatorname{Re}(E)$ then

$$\begin{aligned} \int_0^\infty |\tilde{\varphi}|\, \varphi_0^2\, dx &= \int_0^\infty |\varphi\varphi_0|\, dx \\ &\leqslant c_1 c_1 \int_0^\infty \exp\left[-\frac{1}{2}(F_3 - F_1) \int_0^x V(s)^{-1/2}\, ds\right] dx \\ &< \infty \end{aligned}$$

and a similar calculation on $(-\infty, 0)$ implies $\tilde{\varphi} \in L^1(\mathbb{R}, \varphi_0^2\, dx)$.

Altough $\tilde{\varphi}$ lies in L_1 and satisfies the differential equation (3.4) this does not immediately imply that $\tilde{\varphi}$ lies in the domain of $\tilde{H}_1$. Using the bounds of Lemmas 9 and 10 and the corresponding estimates on $(-\infty, 0)$ we obtain

$$\int_{-\infty}^{\infty} |\tilde{\varphi}'| \, \varphi_0^2 \, dx$$

$$= \int_{\infty}^{\infty} |\varphi' \varphi_0 - \varphi \varphi_0'| \, dx < \infty$$

and

$$\int_{-\infty}^{\infty} |b\tilde{\varphi}| \, \varphi_0^2 \, dx$$

$$= \int_{-\infty}^{\infty} |2\varphi_0' \varphi| \, dx < \infty$$

so $\tilde{\varphi}$, $\tilde{\varphi}'$ and $b\tilde{\varphi}$ all lie in $L^1(\mathbb{R}, \varphi_0^2 \, dx)$.

Now let $f \in C_0^\infty(\mathbb{R})$ satisfy $f(x) = 1$ for $|x| \leqslant 1$ and put

$$\tilde{\varphi}_n(x) = \tilde{\varphi}(x) f_n(x) = \tilde{\varphi}(x) f(x/n).$$

Then $\tilde{\varphi}_n \in C_0^\infty(\mathbb{R})$ so $\tilde{\varphi}_n \in \operatorname{Dom}(\tilde{H}_1)$ and

$$\tilde{H}_1 \tilde{\varphi}_n = -\varphi_n'' + b\tilde{\varphi}_n'$$

$$= -\left(\tilde{\varphi}'' f_n + \frac{2}{n} \tilde{\varphi}' f_n' + \frac{1}{n^2} \tilde{\varphi} f_n'' \right)$$

$$+ b\tilde{\varphi}' f_n + \frac{1}{n} \tilde{\varphi} f_n'$$

$$= (E - E_0) \, \tilde{\varphi} f_n + \frac{2}{n} \tilde{\varphi}' f_n' + \frac{1}{n^2} \tilde{\varphi} f_n'' + \frac{1}{n} b \, \tilde{\varphi} f_n'$$

which converges in the $L_1(\mathbb{R}, \varphi_0^2 \, dx)$ norm to

$$(E - E_0) \, \tilde{\varphi}$$

as $n \to \infty$. Since $\tilde{H}_1$ is a closed operator (3.3) follows. ∎

In the above, f_n' and f_n'' stand for $f'(x/n)$ and $f''(x/n)$ and not for $(d/dx)(f_n)$, $(d^2/dx^2) f_n$. Note that since f_n is supported in $(-an, an)$ for some a, we do not require that $\tilde{\varphi}'$ and $b\tilde{\varphi}$ lie in $L^1(\mathbb{R}, \varphi_0^2 \, dx)$ but only that

$$\frac{1}{n} \int_{-n}^{n} [|\tilde{\varphi}'| + |b\tilde{\varphi}|] \, dx \to 0$$

and, as above, this holds if $|\varphi'\varphi_0| + |\varphi_0'\varphi| \to 0$ at $\pm\infty$. This remark is important if one wanted to discuss the x^2 potential from this point of view.

Naively, one might suppose that all this fooling around with derivatives is a purely technically nicety and that surely any $\varphi \in L^1(\mathbb{R}, \varphi_0^2\, dx)$ obeying $H\varphi = E\varphi$ must lie in $D(\tilde{H}_1)$. However, if $V(x) = x^\alpha$ with $\alpha > 2$, as we remarked above, *WKB* asymtotics and $(V(x)+1)^{-1/2} \in L^1(\mathbb{R}, dx)$ imply that φ is in $L_1(\mathbb{R}, \varphi_0^2\, dx)$ for *any* solution of $H\varphi = E\varphi$. By Theorem 4, not all such φ lie in $D(\tilde{H}_1)$. In this case, $|\varphi'\varphi_0|$ is bounded but not vanishing at infinity!

COROLLARY 11. *If* $0 < s < t < \infty$ *then*

$$\|e^{-\hat{H}s} - e^{-\hat{H}t}\| = 2.$$

Proof. We have shown that if $\operatorname{Re} z > 0$ there exists $f_z \in L_1(\mathbb{R}, dx)$ such that

$$\hat{H} f_z = z f_z.$$

Given $0 < s < t < \infty$ and $\varepsilon >$ we put

$$z = \frac{\varepsilon}{2} + \frac{i\pi}{t-s}$$

to get

$$\begin{aligned} \|e^{-\hat{H}t} - e^{-\hat{H}s}\| &\geqslant \|e^{-\hat{H}t} f_z - e^{-\hat{H}s} f_z\| / \|f_z\| \\ &= |e^{-zt} - e^{-zs}| \\ &= |e^{-zs}|\, |e^{-z(t-s)} - 1| \\ &= e^{-\varepsilon}(e^{-\varepsilon(t-s)/s} + 1) \\ &\to 2 \end{aligned}$$

as $\varepsilon \to 0$. Thus

$$\begin{aligned} 2 &\leqslant \|e^{-\hat{H}t} - e^{-\hat{H}s}\| \\ &\leqslant \|e^{-\hat{H}t}\| + \|e^{-\hat{H}s}\| \leqslant 2. \quad \blacksquare \end{aligned}$$

4. NON-CONTINUITY OF $e^{-\hat{H}t}$ IN HIGHER DIMENSIONS

In this section, we use an entirely different method to show that for a large class of operators $\tilde{H}_2$ which have compact resolvent but are not ultracontractive, the semigroup $e^{-\tilde{H}t}$ is not norm continuous. Although we deal with a much wider class of operators than in Section 3, we do not obtain such detailed spectral information about $\tilde{H}_1$ as in Theorem 10.

We start with some abstract considerations. If e^{-At} and e^{-Bt} are one-parameter contraction semigroups on a Banach space $\mathcal{B}$, we say that B lies in the limit class of A if there exists a sequence of invertible isometries V_n on $\mathcal{B}$ such that B is the limit of $V_n^{-1} A V_n$ in the strong resolvent sense. By [2, Theorem 3.17] this is equivalent to e^{-Bt} being the limit of $V_n^{-1} e^{-At} V_n$ in the strong operator topology, uniformly on all intervals $[0, T]$. We also write $\mathcal{U}(A)$ for the component of $\mathbb{C}\backslash Sp(A)$ which contains the left-hand half-plane. As far as we know, the following proposition is new in the form written down.

Proposition 12. *If B lies in the limit class of A then*

$$\|e^{-As}-e^{-At}\| \geqslant \|e^{-Bs}-e^{-Bt}\| \tag{4.1}$$

for all $0 \leqslant s < t < \infty$, and $\mathcal{U}(A) \subset \mathcal{U}(B)$.

Proof. If $f \in \mathcal{B}$ then

$$\begin{aligned}\|e^{-Bs}f-e^{-Bt}f\| &= \lim_{n\to\infty} \|V_n^{-1} e^{-As}V_n f - V_n^{-1} e^{-At}V_n f\| \\ &= \lim_{n\to\infty} \|(e^{-As}-e^{-At})\, V_n f\| \\ &\leqslant \|e^{-As}-e^{-At}\|\; \|V_n f\| \\ &= \|e^{-As}-e^{-At}\|\; \|f\|\end{aligned}$$

and this establishers (3.1). A similar calculation to that of [2, Theorem 3.17] shows that

$$\|(\lambda-A)^{-1}\| \geqslant \|(\lambda-B)^{-1}\|$$

for all

$$\lambda \notin Sp(A) \cup Sp(B)$$

and so in particular for all $\operatorname{Re}\lambda < 0$. The second statement of the theorem now follows from the fact [2, Corollary 2.3] that $\|(\lambda-B)^{-1}\|$ becomes infinite as λ approaches the boundary of $\mathcal{U}(B)$. ∎

Corollary 13. *Let B lie in the limit class of A, and let B generate a one-parameter group of isometries on $\mathcal{B}$ such that*

$$\|e^{-Bt}-1\| = 2$$

for all $t \neq 0$. *Then* $Sp(A) \supseteq Sp(B)$ *and*

$$\|e^{-As} - e^{-At}\| = 2 \tag{4.2}$$

for all $0 < s < t < \infty$.

Proof. Since $Sp(B) \subset i\mathbb{R}$ and

$$\{z: \operatorname{Re} z < 0\} \subset \mathscr{U}(A) \subset \mathscr{U}(B) \subset \mathbb{C} \backslash Sp(B)$$

we see that $Sp(B)$ lies in the frontier of $\mathscr{U}(A)$ and so is a subset of $Sp(A)$. To prove (3.2) we merely note that

$$\begin{aligned}\|e^{-As} - e^{-At}\| &\geqslant \|e^{-Bs} - e^{-Bt}\| \\ &= \|e^{-B(s-t)} - 1\| = 2\end{aligned}$$

and that the reverse inequality is trivial. ∎

We apply Corollary 13 to the semigroup $e^{-\hat{H}t}$ on $L^1(\mathbb{R}^N, dx)$ by making an explicit choice of V_n for which B can be computed. In this section, we assume that $\hat{H}$ is given by (1.1) on the domain $C_0^\infty(\mathbb{R}^N)$ and that $X = \mathbb{R}^N$. We do not need to assume that C_0^∞ is a core of $\hat{H}$, but only that $\hat{H}$ has some extension which is the generator of a one-parameter contraction semigroup on $L^1(\mathbb{R}^N)$. We rewrite (1.1) in the form

$$\hat{H}f = -\sum_{i,j} \frac{\partial}{\partial x^i}\left(A^{ij} \frac{\partial f}{\partial x^j}\right) + \sum_i \frac{\partial}{\partial x^i}(b^i f)$$

where $b^i = 2\sum_j A^{ij} \varphi^{-1} (\partial\varphi/\partial x^j)$.

We now define the isometries V_n on $L_1(\mathbb{R}^N, dx)$ by

$$V_n f(x) = n^{-N} f\left(\frac{x - u_n}{n}\right)$$

where u_n is some sequence in $\mathbb{R}^N$. It is evident that V_n leaves C_0^∞ invariant and if we put

$$\hat{H}_n = V_n^{-1} \hat{H} V_n$$

then a straightforward compution establishes that

$$\hat{H}_n f = -\sum \frac{\partial}{\partial x^i}\left(A_n^{ij} \frac{\partial f}{\partial x^j}\right) + \sum_i \frac{\partial}{\partial x^i}(b_n^i f)$$

where

$$A_n^{ij}(x) = n^{-2} A^{ij}(u_n + nx)$$
$$b_n^i(x) = n^{-1} b^i(u_n + nx).$$

THEOREM 14. *Suppose there exists a sequence u_n and a vector $0 \neq c \in \mathbb{R}^N$ such that*

$$\lim_{n \to \infty} A_n^{ij}(x) = 0,$$

$$\lim_{n \to \infty} \sum_i \frac{\partial}{\partial x^i} A_n^{ij}(x) = 0,$$

$$\lim_{n \to \infty} b_n^i(x) = c,$$

$$\lim_{n \to \infty} \sum_i \frac{\partial}{\partial x^i} b_n^i(x) = 0$$

all locally uniformly on $\mathbb{R}^N$. Then

$$\|e^{-\hat{H}s} - e^{-\hat{H}t}\| = 2$$

for all $0 \leqslant s < t < \infty$, and

$$Sp(\hat{H}) \supseteq i\mathbb{R}.$$

Proof. If we define the operator B on C_0^∞ by

$$Bf = \sum_i c_i \frac{\partial f}{\partial x^i}$$

then the conditions above are precisely those needed to ensure that

$$\lim_{n \to \infty} \|\hat{H}_n f - Bf\|_1 = 0$$

for all $f \in C_0^\infty$. But the group e^{-Bt} is given explicitly by

$$e^{-Bt} f(x) = f(x - ct)$$

so $\hat{H}_n$ converges in the strong resolvent sense to B by [2, Theorem 3.17], which only requires C_0^∞ to be a core for B; this fact follows from the invariance of C_0^∞ under e^{-Bt} by [2, Theorem 1.9]. The Theorem now follows directly from Corollary 13. ∎

Note 15. In some cases, such as that of Theorem 10, we can prove that

$$Sp(\hat{H}) = \{z\colon \operatorname{Re} z \geqslant 0\}$$

but we are not able to prove this in general.

In order to get a feeling for the circumstances where Theorem 14 is applicable, we now specialize to the case where $H = -\Delta + V$ and where the ground state φ is rewritten as e^{-W}.

THEOREM 16. *If there is a sequence u_n with $n^{-1}|u_n| \to \infty$ as $n \to \infty$, and a non-zero vector $c \in \mathbb{R}^N$ such that*

$$\lim_{n \to \infty} 2n^{-1} \nabla W(u_n + nx) = -c$$

locally uniformly on $\mathbb{R}^N$, and

$$\lim_{|y| \to \infty} \Delta W = 0$$

then the conditions of Theorem 14 *are satisfied.*

Proof. We see that in this case $A^{ij}(x) = \delta^{ij}$ so the first two conditions of Theorem 14 are immediate, and

$$b(x) = -2\nabla W(x).$$

Also

$$\begin{aligned} \sum_i \frac{\partial}{\partial x^i} b_n^i(x) &= \nabla \cdot b(u_n + nx) \\ &= -2\Delta W(u_n + nx) \end{aligned}$$

and this goes to zero locally uniformly as $n \to \infty$ because

$$|u_n + nx| \geqslant |u_n| - n|x|$$

and $n^{-1}|u_n| \to \infty$ as $n \to \infty$ hypothesis. ∎

Unfortunately we do not have explicit conditions of a general nature on the potential V which ensure that W satisfies the hypotheses of Theorem 16, but we believe that they are valid if V increases sufficiently regularly at infinity and is $o(x^2)$ for large $|x|$. However, one may regare the operator as determined by W instead of V, because of the relationship

$$V = |\nabla W|^2 - \Delta W \tag{4.3}$$

and from this point of view, which is quite natural probabilistically, the conditions on W may be explicitly verified in many cases. For example, if

$$W(x) = c(1 + x^2)^{\alpha/2} + d$$

then the conditions of Theorem 16 hold if and only if $0 < \alpha < 2$. This contrasts with the condition for intrinsic ultracontractivity, which is $2 < \alpha < \infty$.

In spite of our above comments about the potentials V for which Theorem 16 might be applicable, the following theorem shows that the situation is not entirely straightforward. Because of the identity (4.3), the conditions of the following theorem can only hold if the potential V is bounded. We actually expect them to hold for all bounded potentials which are sufficiently regular at infinity.

THEOREM 17. *Suppose the operator $H = -\Delta + V$ on $L^2(\mathbb{R}^N, dx)$ has ground state $\varphi = e^{-W}$, where ∇W and ΔW are bounded functions on $\mathbb{R}^N$. Then $e^{-\hat{H}t}$ is a norm analytic operator-valued function on $L^1(\mathbb{R}^N, dx)$ for $0 < t < \infty$.*

Proof. A direct computation shows that

$$\hat{H}f = -\Delta f - 2(\Delta W)f - 2\nabla W \cdot \nabla f$$

on $C_0^\infty(\mathbb{R}^N)$. We may rewrite this as

$$\hat{H} = -\Delta + A$$

where A is a perturbation $-\Delta$ with relative bound zero. Since Δ is the generator of a bounded holomorphic semigroup on $L^1(\mathbb{R}^N, dx)$, the result follows by [6, Theorem 10.54]. ∎

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