ASYMPTOTICS OF SEMIGROUP KERNELS

A.F.M. TER ELST AND DEREK W. ROBINSON

Dedicated to Alan McIntosh on occasion of his 60-th birthday

Abstract. We review the large time behaviour of the semigroup kernel associated with a homogeneous operator on a Lie group with polynomial growth. We consider complex second-order operators and two classes of higher order operators.

1. Introduction

There is a vast literature on second-order elliptic operators on Lie groups with real symmetric coefficients. (See [Rob], [VSC], and references cited therein.) The closure of such an operator generates a semigroup which is holomorphic in a sector, the semigroup has a smooth kernel and the kernel, together with all its derivatives, satisfies the canonical Gaussian upper bounds for small time. These results have been extended to various other classes of complex subelliptic operators of any order on a Lie group and in particular one has again the Gaussian upper bounds for small time. If the operator is a real symmetric pure second-order operator and the Lie group has polynomial growth then the kernel satisfies the Gaussian upper bounds for all time. The aim of this note is to indicate the difficulties that one can expect for the large time canonical Gaussian upper bounds associated to other classes of operators on Lie groups with polynomial growth. In particular we discuss the class of pure second-order operators with complex constant coefficients and two classes of higher order homogeneous operators.

Let G be a connected Lie group with Lie algebra $\mathfrak{g}$. Let $a_1, \ldots, a_{d'}$ be an algebraic basis for $\mathfrak{g}$, i.e., independent elements which together with their multi-commutators up to order s span $\mathfrak{g}$. The smallest number s for which this is valid is called the **rank** of the algebraic basis. Let dg be a (left) Haar measure on G. For all $p \in [1, \infty]$ let L denote the left regular representation in $L_p(G) = L_p(G\,; dg)$. For all $i \in \{1, \ldots, d'\}$ let A_i be the infinitesimal generator of the one parameter group $t \mapsto L(\exp(-ta_i))$. We also need multi-index notation since the A_i do not commute in general. Set $J(d') = \bigcup_{n=0}^{\infty} \{1, \ldots, d'\}^n$ and

1991 *Mathematics Subject Classification.* 22E25, 35B40, 35J30.

if $\alpha = (i_1, \ldots, i_n) \in J(d')$ set $A^\alpha = A_{i_1} \ldots A_{i_n}$ and $|\alpha| = n$. Associated to the algebraic basis there is a modulus on G, i.e., the distance to the identity element e of G. Introduce D as the set of functions

$$W = \{\psi \in C_c^\infty(G) : \psi \text{ is real and } \sup_{g \in G} \sum_{k=1}^{d'} |(A_k\psi)(g)|^2 \leq 1\} \quad .$$

For all $g \in G$ define

$$|g|' = \sup_{\psi \in W} |\psi(g) - \psi(e)| \quad .$$

Finally, for all $\rho > 0$ let the **volume** $V'(\rho)$ be the Haar measure of the ball $\{g \in G : |g|' < \rho\}$.

The Lie algebra $\mathfrak{g}$ is called **nilpotent** if there exists an $n \in \mathbf{N}$ such that

$$[b_1, [b_2, \ldots, [b_{n-1}, b_n] \ldots]] = 0$$

for all $b_1, \ldots, b_n \in \mathfrak{g}$. If $\mathfrak{g}$ is nilpotent then define the **rank** r of $\mathfrak{g}$ by

$$r = \max\{n \in \mathbf{N} : \exists_{b_1, \ldots, b_n \in \mathfrak{g}} [b_1, [b_2, \ldots, [b_{n-1}, b_n] \ldots]] \neq 0\} \quad .$$

Let $\tilde{\mathfrak{g}}(d', r)$ be the nilpotent Lie algebra with maximal dimension, d' generators and rank r. We denote the generators by $\tilde{a}_1, \ldots, \tilde{a}_{d'}$ and the associated infinitesimal generators by $\widetilde{A}_1, \ldots, \widetilde{A}_{d'}$. Let $\widetilde{G}(d', r)$ be the connected simply connected Lie group with Lie algebra $\tilde{\mathfrak{g}}(d', r)$.

Now we are able to introduce the operators we want to consider. Let $m \in 2\mathbf{N}$. On a general Lie group G the operator

$$H = \sum_{|\alpha| \leq m} c_\alpha A^\alpha$$

with $c_\alpha \in \mathbf{C}$ and domain $D(H) = \bigcap_{|\alpha| \leq m} D(A^\alpha)$ is called **subcoercive of step** r if the comparable operator

$$\widetilde{H} = \sum_{|\alpha| = m} c_\alpha \widetilde{A}^\alpha$$

on $L_2(\widetilde{G}(d', r))$ satisfies a Gårding inequality, i.e.,

$$\mathrm{Re}(\tilde{\varphi}, \widetilde{H}\tilde{\varphi}) \geq \tilde{\mu} \sum_{|\alpha| = m/2} \|\widetilde{A}^\alpha \tilde{\varphi}\|_2^2$$

for all $\tilde{\varphi} \in C_c^\infty(\widetilde{G}(d', r))$, for some $\tilde{\mu} > 0$. Note that the condition is on the principal part of the operator and is independent of the lower order terms. If H is subcoercive of step r then H is also subcoercive of step $r - 1$ (see [ElR1], Corollary 3.6).

Example 1.1. Let $c_{ij} \in \mathbf{C}$ and suppose there exists a $\mu > 0$ such that

$$\operatorname{Re} \sum_{i,j=1}^{d'} c_{ij}\, \overline{\xi_i}\, \xi_j \geq \mu\, |\xi|^2 \tag{1}$$

for all $\xi \in \mathbf{C}^{d'}$. Then the operator $-\sum_{i,j=1}^{d'} c_{ij}\, A_i\, A_j$ is a subcoercive operator of step r for all $r \in \mathbf{N}$. This is easy to verify. Conversely, if $-\sum_{i,j=1}^{d'} c_{ij}\, A_i\, A_j$ is a subcoercive operator of step r for some $r \geq 2$ then (1) is valid. (See [ElR1], Proposition 3.7.)

For all $m \in 2\mathbf{N}$ the operators $\Big(-\sum_{i=1}^{d'} A_i 2\Big)^{m/2}$ and $(-1)^{m/2} \sum_{i=1}^{d'} A_i^m$ are also subcoercive operators of step r for all $r \in \mathbf{N}$, but the proof is not trivial. (See [ElR2], Example 4.4.)

The group $\widetilde{G}(2,2)$ is the Heisenberg group and the operator $-\widetilde{A}_1 2 - \widetilde{A}_2 2 - 10i[\widetilde{A}_1, \widetilde{A}_2]$ is subcoercive of step 1, but not subcoercive of order r for any $r \geq 2$.

The small time theory is well developed. Set

$$G^{(m)}_{b,t}(g) = V'(t)^{-1/m}\, e^{-b((|g|')^m t^{-1})^{1/(m-1)}}$$

for all $b > 0$, $t > 0$ and $g \in G$.

Theorem 1.2. *Let $a_1, \ldots, a_{d'}$ be an algebraic basis of rank r for the Lie algebra of a Lie group G. Let $m \in 2\mathbf{N}$ and H an m-th order subcoercive operator of step s with $s \geq r$. Then one has the following.*

I. *The closure of H generates a semigroup S on L_p for all $p \in [1, \infty]$.*

II. *The semigroup S is holomorphic.*

III. *The semigroup has a smooth rapidly decreasing p-independent kernel K, i.e., $S_t\varphi = K_t * \varphi$ for all $\varphi \in L_p$ and $t > 0$.*

IV. *For all $\alpha \in J(d')$ there exist $b, c > 0$ and $\omega \geq 0$ such that*

$$|A^\alpha K_t| \leq c\, t^{-|\alpha|/m}\, e^{\omega t}\, G^{(m)}_{b,t} \tag{2}$$

for all $t > 0$.

V. *If $p \in \langle 1, \infty\rangle$ then H is closed on L_p. Moreover, if the semigroup S is uniformly bounded on L_p then for all $N \in \mathbf{N}$ one has $D(H^{N/m}) = \bigcap_{|\alpha|=N} D(A^\alpha)$.*

Proof. See [ElR1], Theorems 2.5 and 4.1, and for Statement V see [BER]. $\square$

The bounds (2) are optimal for $t \in \langle 0, 1]$ and describe the Gaussian decay. For large t the factor $e^{\omega t}$ reflects the semigroup property and the contribution of the lower order terms in H. Each derivative of K

gives a $t^{-1/m}$-singularity. We say that $A^\alpha K$ has the **canonical** (large time) Gaussian upper bounds if the bounds (2) are valid for all $t > 0$ with $\omega = 0$. On a subclass of Lie groups these bounds are valid for particular operators.

2. Second-order operators

A Lie group is said to have **polynomial growth** if there exist $c > 0$ and $D \in \mathbf{N}_0$ such that the volume $V'(\rho) \leq c\,\rho^D$ for all $\rho \geq 1$ ([Gui] and [Jen]). It turns out that this definition is independent of the choice of the algebraic basis.

Theorem 2.1. *If G has polynomial growth and H is a pure second-order real symmetric subcoercive operator of step 2 then there exist $b, c > 0$ such that*

$$|K_t| \leq c\,G^{(2)}_{b,t} \quad \textit{and} \quad |A_i K_t| \leq c\,t^{-1/2}\,G^{(2)}_{b,t}$$

for all $t > 0$ and $i \in \{1, \ldots, d'\}$.

Proof. See [SC]. □

In the situation of Theorem 2.1 the reality of the coefficients implies that the kernel K is positive and by the Beurling-Deny criterium the semigroup S is a contraction semigroup on L_∞. Therefore K is integrable and $\int K_t = 1$ for all $t > 0$. By duality the semigroup is also a contraction semigroup on L_1 and then a Nash inequality provides L_∞-bounds on K_t. Finally by a Davies perturbation the L_∞-bounds for K can be strengthened to the Gaussian bounds of Theorem 2.1.

If the coefficients are complex then K is not positive and there is no version of the Beurling-Deny criterium for complex operators [ABBO]. It is a recent result that the reality of the coefficients in Theorem 2.1 is superfluous.

Theorem 2.2. *If G has polynomial growth and H is a pure second-order (complex) subcoercive operator of step 2 then there exist $b, c > 0$ such that*

$$|K_t| \leq c\,G^{(2)}_{b,t} \quad \textit{and} \quad |A_i K_t| \leq c\,t^{-1/2}\,G^{(2)}_{b,t}$$

for all $t > 0$ and $i \in \{1, \ldots, d'\}$.

Proof. See [DER2]. □

Although the first-order derivatives of the kernel satisfy the canonical large time Gaussian upper bounds, in general higher order derivatives fail to have the canonical large time Gaussian upper bounds.

Theorem 2.3. *Suppose G has polynomial growth and let H be a pure second-order (complex) subcoercive operator of step 2. The following are equivalent.*

I. *There exist $b, c > 0$ such that*
$$|A_i A_j K_t| \leq c\, t^{-1}\, G^{(2)}_{b,t}$$
for all $t > 0$ and $i, j \in \{1, \ldots, d'\}$.

II. *There exists a $c > 0$ such that $\|A_i A_j S_t\|_{2\to 2} \leq c\, t^{-1}$ for all $t > 0$ and $i, j \in \{1, \ldots, d'\}$.*

III. *For all $p \in \langle 1, \infty\rangle$ there exists a $c > 0$ such that $\|A_i A_j \varphi\|_p \leq c\, \|H\varphi\|_p$ for all $\varphi \in D(H)$ and $i, j \in \{1, \ldots, d'\}$.*

IV. *There exist $\sigma \in \langle 0, 1\rangle$, $c > 0$ and for all $R \in \langle 0, \infty\rangle$ a function $\eta_R \in C^\infty(G)$ such that $0 \leq \eta_R \leq 1$, $\eta_R(g) = 1$ for all $g \in G$ with $|g|' \leq \sigma R$, $\eta_R(g) = 0$ for all $g \in G$ with $|g|' \geq R$ and $\|A^\alpha \eta_R\|_\infty \leq c\, R^{-|\alpha|}$ for all $\alpha \in J(d')$ with $|\alpha| = 2$.*

V. *The Lie algebra of G is the direct product of the Lie algebra of a compact group and a nilpotent Lie algebra.*

Proof. For real symmetric operators this theorem has been proved in [ERS2]. The general case is again in [DER2]. □

In [Ale] Alexopoulos gave an example of a sublaplacian H on the covering group of the Euclidean motion group for which Condition III of Theorem 2.3 fails.

A similar theorem is valid for n derivatives instead of only two derivatives, with $n \geq 3$. In particular, on a nilpotent Lie group all higher order derivatives of the kernel associated to a complex second-order operator of step r, with $r \geq 2$, satisfy the canonical Gaussian upper bounds for large time. That is a special case of the following theorem.

Theorem 2.4. *Let G be a nilpotent Lie group and let r be the rank of its Lie algebra. Let $m \in 2\mathbf{N}$ and let H be a pure m-th order operator which is subcoercive of step r. Then for all $\alpha \in J(d')$ there exist $b, c > 0$ such that*
$$|A^\alpha K_t| \leq c\, t^{-|\alpha|/m}\, G^{(m)}_{b,t}$$
for all $t > 0$.

Moreover, for all $N \in \mathbf{N}$ and $p \in \langle 1, \infty\rangle$ there exists a $c > 0$ such that

(3)
$$c^{-1} \max_{|\alpha|=N} \|A^\alpha \varphi\|_p \leq \|H^{N/m}\varphi\|_p \leq c \max_{|\alpha|=N} \|A^\alpha \varphi\|_p$$

for all $\varphi \in D(H^{N/m}) = \bigcap_{|\alpha|\leq N} D(A^\alpha)$.

Proof. See [NRS] or [ERS1]. □

3. Sums of subcoercive operators

Before we describe a more general theorem we first consider an example on $\mathbf{R}^d$.

Example 3.1. Let $\Delta = -\sum_{i=1}^d \partial_i 2$ be the Laplacian on $\mathbf{R}^d$ and $n, m \in 2\mathbf{N}$ such that $n \leq m$. Set

$$H = \Delta^{n/2} + \Delta^{m/2} \quad .$$

Let K, $K^{(n)}$ and $K^{(m)}$ denote the kernels of the semigroups generated by H, $\Delta^{n/2}$ and $\Delta^{m/2}$. Then

$$K_t * \varphi = S_t\varphi = e^{-tH}\varphi = e^{-t\Delta^{n/2}}e^{-t\Delta^{m/2}}\varphi = K_t^{(n)} * K_t^{(m)} * \varphi$$

for all $\varphi \in L_2(\mathbf{R}^d)$ since $\Delta^{n/2}$ and $\Delta^{m/2}$ commute. So $K_t = K_t^{(n)} * K_t^{(m)}$ for all $t > 0$. Hence there exist $b, c > 0$ such that

$$|K_t| \leq c\,(G_{b,t}^{(n)} * G_{b,t}^{(m)})$$

for all $t > 0$ and $x \in \mathbf{R}^d$. These bounds can be reexpressed as follows. Set

$$E_{b,t}^{(m,n)}(x) = (t^{-d/n} \wedge t^{-d/m})(e^{-b(|x|^n t^{-1})^{n/(n-1)}} \vee e^{-b(|x|^m t^{-1})^{m/(m-1)}}) \quad .$$

Then for all $b > 0$ there exist $b', c > 0$ such that

$$G_{b,t}^{(n)} * G_{b,t}^{(m)} \leq c\,E_{b',t}^{(m,n)}$$

and

$$E_{b,t}^{(m,n)} \leq c\,(G_{b',t}^{(n)} * G_{b',t}^{(m)})$$

for all $t > 0$. Thus there are $b, c > 0$ such that $|K_t| \leq c\,E_{b,t}^{(m,n)}$ for all $t > 0$.

Using Fourier analysis it is not hard to show that there exists a $c > 0$ such that

$$c^{-1}\,t^{-\nu}t^{-d/n} \leq \|K_t - K_t^{(n)}\|_\infty \leq c\,t^{-\nu}t^{-d/n}$$

uniformly for all $t \geq 1$, where $\nu = (m-n)/n$. So for large t the kernel $K^{(n)}$ is a first approximation of K. One might hope that one has bounds $|K_t| \leq c\,G_{b,t}^{(n)}$ for suitable $b, c > 0$, uniformly for all $t \geq 1$, but these are not valid by the following argument. If $y \in \mathbf{R}^d$ then the Lebesgue dominated convergence theorem implies that

$$\lim_{t\to\infty} t^{d/m} K_t(t^{1/m}y) = (2\pi)^{-d}\int dp\, e^{-ip\cdot y}e^{-|p|^m}$$

and the integral is not zero for all $y \in \mathbf{R}^d$. But

$$\lim_{t\to\infty} t^{d/m} G_{b,t}^{(n)}(t^{1/m}y) = 0$$

for all $b > 0$ and $y \in \mathbf{R}^d$. Therefore there are no $b, c > 0$ such that $|K_t| \leq c\, G^{(n)}_{b,t}$ uniformly for all $t \geq 1$.

The general case on a nilpotent Lie group is as follows.

Theorem 3.2. *Let G be a nilpotent Lie group and let r be the rank of its Lie algebra. Let $k \in \mathbf{N}\backslash\{1\}$ and $m_1, \ldots, m_k \in 2\mathbf{N}$ with $m_1 > m_2 > \ldots > m_k$. For all $j \in \{1, \ldots, k\}$ let H_{m_j} be a pure m_j-th order subcoercive operator of step r. Set $H = \sum_{j=1}^k H_{m_j}$ and let K be the kernel of the semigroup generated by H. Then one has the following.*

I. *For all α there are $b, c > 0$ such that*

$$|A^\alpha K_t| \leq c\,(t^{-|\alpha|/m} \wedge t^{-|\alpha|/\underline{m}})\,(G^{(m)}_{b,t} * G^{(\underline{m})}_{b,t})$$

for all $t > 0$ where $m = m_1$ and $\underline{m} = m_k$.

II. *For all $\alpha \in J(d')$ and $p \in \langle 1, \infty\rangle$ there exists a $c > 0$ such that*

$$\|A^\alpha \varphi\|_p \leq c \|H^{|\alpha|/m_j} \varphi\|_p$$

for all $j \in \{1, \ldots, k\}$ and $\varphi \in D(H^{|\alpha|/m_j})$.

III. *For all $\alpha \in J(d')$ there exist $b, c > 0$ such that*

$$|A^\alpha K_t - A^\alpha K^{(\underline{m})}_t| \leq c\,t^{-\nu} t^{-|\alpha|/\underline{m}}\ (G^{(m)}_{b,t} * G^{(\underline{m})}_{b,t})$$

for all $t \geq 1$, where $K^{(\underline{m})}$ denotes the kernel of $H_{\underline{m}}$ and $\nu = (m_{k-1} - m_k)/m_k$.

Proof. See [DER1], Theorems 2.1 and 2.12. □

Again Statement III of Theorem 3.2 indicates that $K^{(\underline{m})}$ is the first order approximation of the kernel K for large t. Thus the large time behaviour is determined by the lowest order terms in H. The kernel K can be bounded by a Gaussian only in a very special case.

Proposition 3.3. *Let $n \in \mathbf{N}\backslash\{1\}$ and adopt the notation of Theorem 3.2. The following are equivalent.*

I. *There exist $b, c > 0$ such that $|K_t| \leq c\, G^{(n)}_{b,t}$ for all $t > 0$.*

II. *$n = m = \underline{m}$ or G is compact and $n \geq m$.*

Proof. See [DER1], Proposition 2.15. □

4. Higher order operators

It follows from Theorem 2.4 and Example 1.1 that for all $m \in 2\mathbf{N}$ the kernel of the semigroup generated by the operator $\Big(-\sum_{i=1}^{d'} A_i 2\Big)^{m/2}$ satisfies canonical Gaussian upper bounds for all time if G is nilpotent. The condition that G is nilpotent can be relaxed.

Theorem 4.1. *Let $a_1, \ldots, a_{d'}$ be an algebraic basis of rank r for the Lie algebra of a Lie group G with polynomial growth. Let $m \in 2\mathbf{N}$ and let K be the kernel of the semigroup generated by the operator $\Big(- \sum_{i=1}^{d'} A_i 2\Big)^{m/2}$. Then there exist $b, c > 0$ such that $|K_t| \leq c\, G_{b,t}^{(m)}$ for all $t > 0$.*

Proof. See [ElR3], Theorem 3.1. □

It also follows from Theorem 2.4 and Example 1.1 that for all $m \in 2\mathbf{N}$ the kernel of the semigroup generated by the operator $(-1)^{m/2} \sum_{i=1}^{d'} A_i^m$ satisfies canonical Gaussian upper bounds for all time if G is nilpotent. Nevertheless in contrast to Theorem 4.1, this result does not extend to Lie groups with polynomial growth, in general. We next describe a counter example.

5. The Euclidean motion group

The Lie algebra $\mathfrak{g}$ of the Euclidean motion group is the three dimensional Lie algebra with basis b_1, b_2, b_3 and commutation relations

$$[b_1, b_2] = b_3 \quad , \quad [b_1, b_3] = -b_2 \quad , \quad [b_2, b_3] = 0 \quad .$$

Then $\mathfrak{g}$ is solvable, but not nilpotent. The maximal nilpotent ideal of $\mathfrak{g}$, the nilradical, equals $\mathfrak{n} = \operatorname{span}(b_2, b_3)$. Let G be the connected simply connected Lie group with Lie algebra $\mathfrak{g}$. Then G is the covering group of the Euclidean motion group. Let a_1, a_2 be an algebraic basis for $\mathfrak{g}$, let $m \in 2\mathbf{N}\backslash\{2\}$ and set

$$H = (-1)^{m/2}(A_1^m + A_2^m) \quad . \tag{4}$$

Let K be the kernel of the semigroup generated by H. One has $V'(\rho) \asymp \rho 3$ for $\rho \geq 1$, so G has polynomial growth.

Theorem 5.1. *The following are equivalent.*

I. *There exist $b, c > 0$ such that*

$$|K_t| \leq c\, G_{b,t}^{(m)}$$

uniformly for all $t > 0$.

II. *There exists a $c \geq 1$ such that*

$$c^{-1}\, V(t)^{-1/m} \leq \|K_t\|_\infty \leq c\, V(t)^{-1/m}$$

uniformly for all $t > 0$.

III. *$a_1 \in \mathfrak{n}$ or $a_2 \in \mathfrak{n}$.*

Proof. See [ElR3] Theorem 1.1 and Remark 2.5. □

A sketch of the beginning of the proof is as follows. Define $\Phi\colon \mathbf{R}3 \to G$ by

$$\Phi(x_1, x_2, x_3) = \exp(x_1 b_1) \exp(x_2 b_2) \exp(x_3 b_3) \quad .$$

Then Φ is a diffeomorphism. Set $B_i = dL(b_i)$ and $\check{B}_i = (\Phi^{-1})_* B_i$. Then

$$\begin{aligned} \check{B}_1 &= -\partial_1, \\ \check{B}_2 &= -\cos x_1\, \partial_2 + \sin x_1\, \partial_3, \\ \check{B}_3 &= -\sin x_1\, \partial_2 - \cos x_1\, \partial_3 \quad , \end{aligned}$$

where the ∂_i are the partial derivatives on $\mathbf{R}3$. Set $\check{H} = (\Phi^{-1})_* H$. Note that

$$(\varphi, \check{H}\varphi) = \sum_{i=1}^{2} (\check{A}_i^{m/2}\varphi, \check{A}_i^{m/2}\varphi) \tag{5}$$

for all $\varphi \in D(\check{H})$. Then the quadratic form on the right hand side of (5) can be written in the form

$$(\varphi, \check{H}\varphi) = \sum_{\substack{\alpha,\beta \in J(3) \\ 1 \le |\alpha|, |\beta| \le m/2}} (\partial^\alpha \varphi, c_{\alpha,\beta}\, \partial^\beta \varphi)$$

with the $c_{\alpha,\beta}$ a function which is a polynomial of functions $x \mapsto \sin x_1$ and $x \mapsto \cos x_1$. Hence the quadratic form associated to $\check{H}$ might contain second-order terms. The large time behaviour of the kernel can be obtained using a Bloch–Zak decomposition or by using homogenization theory.

Example 5.2. If $H = B_1 4 + B_2 4$ then K satisfies the canonical Gaussian upper bounds.

If $H = B_1 4 + (B_1 + B_2)4$ then K does not satisfy the canonical Gaussian upper bounds for large time. If one expands $(\check{B}_1 + \check{B}_2)2\varphi$ as in (5) then one obtains on both side of the inner product a term $\check{B}_3\varphi$, so

$$(\varphi, \check{H}\varphi) = (\check{B}_3\varphi, \check{B}_3\varphi) + \text{higher order derivatives} \quad .$$

Similarly to the situation in Theorem 3.2 for sums of subcoercive operators on nilpotent Lie groups one has a contribution of a second-order operator and K does not satisfy the m-th order canonical Gaussian upper bounds for large time.

However, if $H = (B_1 + B_2)4 + B_3 4$ then K does have the canonical Gaussian upper bounds for large time, since Condition III of Theorem 5.1 is valid. This is surprising since the quadratic form has a second-order term contribution as in the second example. But homogenization is a non-linear process and for the homogenized operator in this case the coefficients of the second-order terms cancel. It turns out that the homogenization of $\check{H}$ is again a fourth-order operator and K satisfies the canonical fourth-order Gaussian upper bounds.

Next we describe the behaviour of the kernel in case the equivalent conditions of Theorem 5.1 are not valid.

Theorem 5.3. *Let H be as in* (4)*. Suppose $a_1 \notin \mathfrak{n}$ and $a_2 \notin \mathfrak{n}$. Then one has the following.*

I. *There exist $b, c > 0$ such that*

$$|K_t(g)| \le c \int_N dh\, G^{(m)}_{b,t}(gh^{-1})\, G^{[2]}_{b,t}(h)$$

uniformly for all $g \in G$ and $t \ge 1$, where $N = \exp \mathfrak{n}$ and

$$G^{[2]}_{b,t}(\Phi(0, x_2, x_3)) = t^{-1} e^{-b(x_2 2 + x_3 2)t^{-1}}$$

is the second-order Gaussian on N.

II. *There exists a $c > 0$ such that*

$$c^{-1}\, t^{-(m+1)/m} \le \|K_t\|_\infty \le c\, t^{-(m+1)/m}$$

uniformly for all $t \ge 1$.

III. *There exist $c, c', c_1 > 0$ such that*

$$\|\check{K}_t - \widehat{K}_t\|_\infty \le c\, t^{-(m+1)/m}\, t^{-1/m}$$

uniformly for all $t \ge 1$, where $\check{K}$ is the kernel of the semigroup generated by $\check{H} = (\Phi^{-1})_* H$ and $\widehat{K}$ is the kernel of the semigroup generated by

$$(-1)^{m/2} c_1\, \partial_1^m - c'(\partial_2 2 + \partial_3 2) \quad .$$

Proof. See [ElR3]. □

If $H = (-1)^{m/2} \sum_{|\alpha|=|\beta|=m/2} \partial^\alpha\, c_{\alpha,\beta}\, \partial^\beta$ is a pure m-th order strongly elliptic operator on $\mathbf{R}^d$ with complex measurable coefficients then the solution of the Kato problem solved by Auscher, Hofmann, McIntosh and Tchamitchian states that $D(H^{1/2}) = W^{m/2,2}$ and there exists a $c > 0$ such that

$$c^{-1} \max_{|\alpha|=m/2} \|\partial^\alpha \varphi\|_2 \le \|H^{1/2}\varphi\|_2 \le c \max_{|\alpha|=m/2} \|\partial^\alpha \varphi\|_2 \tag{6}$$

for all $\varphi \in D(H^{1/2})$ (see [AHMT], Theorem 1.5). In [AHMT] the identity $D(H^{1/2}) = W^{m/2,2}$ and the homogeneous estimates (6) were proved first under the additional assumption that the kernel of the semigroup generated by H has the canonical Gaussian upper bounds.

A similar result is valid for subcoercive operators with constant coefficients on nilpotent groups by (3) in Theorem 2.4. If the group is simply connected then an operator as in Theorem 2.4 is unitarily equivalent to an operator on $\mathbf{R}^d$ with polynomial coefficients. If G is a general Lie group and H is a pure m-th order operator which generates a bounded semigroup on L_2 then it follows from Theorem 1.2.V that there exists a $c > 0$ such that

$$\begin{aligned} c^{-1}\big(\max_{|\alpha|=m/2} \|A^\alpha\varphi\|_2 + \|\varphi\|_2\big) &\leq \|H^{1/2}\varphi\|_2 + \|\varphi\|_2 \\ &\leq c\,\big(\max_{|\alpha|=m/2} \|A^\alpha\varphi\|_2 + \|\varphi\|_2\big) \end{aligned} \tag{7}$$

for all $\varphi \in D(H^{1/2})$. But if the group is not homogeneous then one cannot easily scale the L_2-norm $\|\varphi\|_2$ of φ away in (7). Nevertheless the homogeneous estimates (3) are valid on nilpotent Lie groups, even if the nilpotent group is not homogeneous.

If G is the covering group of the Euclidean motion group and $H = B_1 4 + B_2 4$, with the notation as in the beginning of this section, then it follows from Theorem 5.1 that the kernel of the semigroup S generated by H has the canonical Gaussian upper bounds. Moreover, S is bounded on L_2 and $D(H^{1/2}) = \bigcap_{|\alpha|=2} D(A^\alpha)$ on L_2. Nevertheless the analogue of the homogeneous estimates (6) and (3) are not valid.

Proposition 5.4. *Let G be the covering group of the Euclidean motion group and adopt the notation as in the beginning of this section. Let a_1, a_2 be an algebraic basis for $\mathfrak{g}$ such that $a_1 \in \mathfrak{n}$ or $a_2 \in \mathfrak{n}$. Let $m \in 2\mathbf{N}\backslash\{2\}$ and set $H = (-1)^{m/2}(A_1^m + A_2^m)$. Then there does* **not** *exist a $c > 0$ such that*

$$\max_{|\alpha|=m/2} \|A^\alpha\varphi\|_2 \leq c\,\|H^{1/2}\varphi\|_2$$

for all $\varphi \in D(H^{1/2})$.

Proof. Suppose there exists a $c > 0$ such that $\max_{|\alpha|=m/2} \|A^\alpha\varphi\|_2 \leq c\,\|H^{1/2}\varphi\|_2$ for all $\varphi \in D(H^{1/2})$. We will show that Condition IV of Theorem 2.3 is valid.

Let K be the kernel of the semigroup S generated by H. Then

$$\max_{|\alpha|=m/2} \|A^\alpha S_t\varphi\|_2 \leq c\,\|H^{1/2}S_t\varphi\|_2 \leq (2e)^{-1/2}t^{-1/2}\|\varphi\|_2$$

for all $t > 0$ by spectral theory. By Theorem 5.1 the kernel K satisfies the canonical Gaussian upper bounds. Hence by a quadrature estimate it follows that there exists a $c_1 > 0$ such that

$$\|S_t\|_{1\to 2} \leq c_1 V'(t)^{-1/(2m)} \quad \text{and} \quad \|K_t\|_2 \leq c_1 V'(t)^{-1/(2m)}$$

for all $t > 0$. Therefore one has

$$\begin{aligned}\|A^\alpha K_t\|_\infty &\leq \|A^\alpha S_{3t}\|_{1\to\infty} \leq \|A^\alpha S_{2t}\|_{2\to\infty}\|S_t\|_{1\to 2} = \|A^\alpha K_{2t}\|_2\|S_t\|_{1\to 2} \\ &\leq \|A^\alpha S_t\|_{2\to 2}\|K_t\|_2\|S_t\|_{1\to 2} \leq (2e)^{-1/2} c\, c_1 2\, t^{-1/2} V'(t)^{-1/m}\end{aligned}$$

for all $t > 0$ and $\alpha \in J(d')$ with $|\alpha| = m/2$. Hence there exists a $c_2 > 0$ such that

$$\max_{|\alpha|=m/2} \|A^\alpha K_t\|_\infty \leq c_2\, t^{-1/2} V'(t)^{-1/m} \tag{8}$$

for all $t > 0$.

Since H does not have a constant term one has $H\mathbb{1} = 0$ on L_∞, where $\mathbb{1}$ is the constant function with value one. Hence $S_t\mathbb{1} = \mathbb{1}$ and $\int K_t = 1$ for all $t > 0$. Moreover, since H is self-adjoint one deduces that $\overline{K_t(g^{-1})} = K_t(g)$ for all $g \in G$ and $t > 0$. Hence

$$\begin{aligned}\operatorname{Re} K_{2t}(g) &= \operatorname{Re} \int dh\, K_t(h)\, K_t(h^{-1}g) \\ &\leq \int dh\, |K_t(h)|^2 = \int dh K_t(h)\, K_t(h^{-1}) = K_{2t}(e)\end{aligned}$$

for all $t > 0$ and $g \in G$ by the Schwartz inequality. By Theorem 5.1 there exist $b, c_3 > 0$ such that $|K_t| \leq c_3\, G^{(m)}_{b,t}$ for all $t > 0$. Then for all $\kappa > 0$ one has

$$\begin{aligned}K_t(e) &\geq V'(\kappa t^{1/m})^{-1} \int_{\{g\in G:|g|'\leq\kappa t^{1/m}\}} dg\ \operatorname{Re} K_t(g) \\ &= V'(\kappa t^{1/m})^{-1}\Big(1 - \int_{\{g\in G:|g|'>\kappa t^{1/m}\}} dg\ \operatorname{Re} K_t(g)\Big) \\ &\geq V'(\kappa t^{1/m})^{-1}\Big(1 - \int_{\{g\in G:|g|'>\kappa t^{1/m}\}} dg\, c_3\, G^{(m)}_{b,t}(g)\Big)\end{aligned}$$

for all $t > 0$. But the last integral tends to zero as $\kappa \to \infty$. Hence there exists a $\kappa > 0$ such that $K_t(e) \geq 2^{-1} V'(\kappa t^{1/m})^{-1}$ for all $t > 0$. But since G has polynomial growth there then exists a $c_4 > 0$ such that $K_t(e) \geq c_4\, V'(t)^{-1/m}$ for all $t > 0$.

It follows from a subelliptic variation of Lemma III.3.3 of [Rob] that there exists a $c_5 > 0$ such that

$$\max_{|\alpha|=n} \|A^\alpha\varphi\|_\infty \leq \varepsilon^{m/2-n} \max_{|\alpha|=m/2} \|A^\alpha\varphi\|_\infty + c_5\, \varepsilon^{-n}\|\varphi\|_\infty$$

for all $n \in \{1, \ldots, m/2-1\}$ and $\varphi \in \bigcap_{|\alpha|=m/2} D(A^\alpha)$ in the L_∞-sense. Hence by (8), using the Gaussian upper bounds for K and choosing

$\varepsilon = t^{-n/m}$ one deduces that

$$\max_{|\alpha|=n} \|A^\alpha K_t\|_\infty \leq (c_2 + c_3 c_5)\, t^{-n/m}\, V'(t)^{-1/m}$$

for all $t > 0$ and $n \in \{1, \ldots, m/2\}$. Then

$$|K_t(g) - K_t(e)| \leq |g|' \Big(\sum_{i=1}^{d'} \|A_i K_t\|_\infty 2 \Big)^{1/2} \leq c_6\, |g|'\, t^{-1/m}\, V'(t)^{-1/m}$$

for all $g \in G$ and $t > 0$, where $c_6 = (d')^{1/2}(c_2 + c_3 c_5)$. It follows that

$$\begin{aligned} c_3 c_4^{-1}\, e^{-b((|g|')^m t^{-1})^{1/(m-1)}} \geq \left| \frac{K_t(g)}{K_t(e)} \right| &\geq 1 - \frac{|K_t(g) - K_t(e)|}{K_t(e)} \\ &\geq 1 - c_6 c_4^{-1}\, |g|'\, t^{-1/m} \end{aligned} \tag{9}$$

for all $g \in G$ and $t > 0$. Next let $\tau \colon \mathbf{C} \to \mathbf{R}$ be a C^∞-function such that $0 \leq \tau \leq 1$, $\tau(z) = 0$ for all $|z| \geq c_3 c_4^{-1} e^{-b}$ and $\tau(z) = 1$ for all $|z| \leq 2^{-1} c_3 c_4^{-1} e^{-b}$. For all $R > 0$ define $\eta_R \in C^\infty(G)$ by

$$\eta_R(g) = \tau\Big(\frac{K_{R^m}(g)}{K_{R^m}(e)} \Big) \quad .$$

Then it follows from (9) that $\eta_R(g) = 0$ if $|g|' \geq R$ and $\eta_R(g) = 1$ if $|g|' \leq \sigma R$ where $\sigma = c_4 c_6^{-1}(1 - 2^{-1} c_3 c_4^{-1} e^{-b})$.

Next we show that the derivatives have the right decay. Let $\alpha \in J(d')$ with $|\alpha| = m/2$. Then

$$(A^\alpha \eta_R)(g) = \sum \tau^{(l)} \Big(\frac{K_{R^m}(g)}{K_{R^m}(e)} \Big) \prod_{p=1}^{l} \frac{(A^{\beta_p} K_{R^m})(g)}{K_{R^m}(e)} \tag{10}$$

uniformly for all $g \in G$ and $R > 0$, where the sum is finite and over a subset of all $l \in \{1, \ldots, n\}$ and $\beta_1, \ldots, \beta_l \in J(d')$ with $|\beta_p| \geq 1$ for all $p \in \{1, \ldots, l\}$ and $|\beta_1| + \ldots + |\beta_l| = n$. Then

$$\Big| \prod_{p=1}^{l} \frac{(A^{\beta_p} K_{R2})(g)}{K_{R2}(e)} \Big| \leq \prod_{p=1}^{l} (c_2 + c_3 c_5) c_4^{-1} R^{-|\beta_p|} = (c_2 + c_3 c_5)^l c_4^{-l} R^{-n}$$

uniformly for $g \in G$ and $R > 0$. Hence Condition IV of Theorem 2.3 is valid. Therefore by Theorem 2.3 $\mathfrak{g}$ is the direct product of the Lie algebra of a compact group and a nilpotent Lie algebra. This is a contradiction and the proof of the proposition is complete. $\square$

Acknowledgements

This paper has been written whilst the first named author was on sabbatical leave visiting the Centre for Mathematics and its Applications at the ANU. He wishes to thank the CMA for its hospitality and the support from a grant of the Australian Research Council.

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Department of Mathematics and Computing Science, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

E-mail address: terelst@win.tue.nl

Centre for Mathematics and its Applications, Mathematical Sciences Insitute, Australian National University, Canberra, ACT 0200, Australia

E-mail address: Derek.Robinson@maths.anu.edu.au