On anomalous asymptotics of heat kernels

EINDHOVEN UNIVERSITY OF TECHNOLOGY
Department of Mathematics and Computing Science

RANA 99-26
September 1999

On anomalous asymptotics of heat kernels

by

A.F.M. ter Elst and D.W. Robinson

Reports on Applied and Numerical Analysis
Department of Mathematics and Computing Science
Eindhoven University of Technology
P.O. Box 513
5600 MB Eindhoven, The Netherlands
ISSN: 0926-4507

On anomalous asymptotics of heat kernels

A.F.M. ter Elst[1] and Derek W. Robinson[2]

Abstract

Let A_1, A_2, A_3 denote a vector space basis, formed by right invariant vector fields, of the Lie algebra $\mathfrak{g}$ of the three-dimensional Lie group G of Euclidean motions of the plane. We demonstrate that for $m \geq 4$ the semigroup kernel K_t associated with the strongly elliptic operator $H = (-1)^{m/2} \sum_{i=1}^{3} A_i^m$ satisfies m-th order Gaussian bounds for all $t \geq 1$ if, and only if, two of the A_i span the nilradical of $\mathfrak{g}$. If this condition is not satisfied the kernel has an anomalous asymptotics. It behaves like an m-th order kernel in one direction and like a second-order kernel in the other two directions. No such anomaly occurs for the kernels associated with the operators $H = (-\sum_{i=1}^{3} A_i^2)^{m/2}$.

September 1999

AMS Subject Classification: 22E25, 35B40, 35B27.

Home institutions:

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

2. Centre for Mathematics and its Applications
School of Mathematical Sciences
Australian National University
Canberra, ACT 0200
Australia

1 Introduction

The rate of dissipation of heat on a manifold is determined by the available volume. This geometric principle is illustrated by the behaviour of the heat kernel K associated with a right invariant sublaplacian on a Lie group G of polynomial growth. Then one has bounds

$$c^{-1}\,V(t)^{-1/2} \leq \|K_t\|_\infty \leq c\,V(t)^{-1/2} \tag{1}$$

for all $t > 0$ where $V(t)$ denotes the volume of the ball of radius t measured with respect to the subelliptic distance (see [Rob], Theorems IV.4.16 and IV.4.21, or [VSC], Theorem VIII.2.9). The asymptotic properties of the kernels associated with higher-order operators is less clear.

Let $\mathfrak{g}$ denote the Lie algebra of G and $A_1, \ldots, A_d$ a vector space basis of $\mathfrak{g}$ formed by right-invariant vector fields. First, let K denote the semigroup kernel corresponding to a power of the Laplacian $H = (-\sum_{i=1}^d A_i^2)^{m/2}$. Then one has the m-th order analogue

$$c^{-1}\,V(t)^{-1/m} \leq \|K_t\|_\infty \leq c\,V(t)^{-1/m} \tag{2}$$

of the bounds (1) for all $t > 0$ The upper bounds are a consequence of the Gaussian bounds established in Theorem 3.1 below and then the lower bounds follow from [ElR4], Corollary 2.4. Secondly, consider the kernel corresponding to the operator $H = (-1)^{m/2}\sum_{i=1}^d A_i^m$. Then the situation is more complex. If G is nilpotent the bounds (2) are again valid for all $t > 0$ because the Gaussian upper bounds on K follow from [ERS1], Theorem 3.5. More generally, if G is the local direct product $C \times_l N$ of a compact Lie group C and a nilpotent Lie group N then the bounds (2) are valid. The key upper bounds (2) are a consequence of Theorem 4.3 of [DER], with $m = \underline{m}$. The special form of H allows one to verify that Condition I_1 of [DER], Theorem 4.1, holds and hence all the equivalent conditions of Theorems 4.1 and 4.3 are valid. In particular H satisfies the strong Gårding inequality

$$(\varphi, H\varphi) \geq \mu \sup_{|\alpha|=m/2} \|A^\alpha \varphi\|_2^2 \tag{3}$$

for some $\mu > 0$ and all $\varphi \in D(H)$ where we have used the standard multi-index notation. Conversely, Dungey [Dun], Theorem 1.1, has shown that if H satisfies (3) and K satisfies Gaussian bounds for all $t > 0$ then G is the local direct product $C \times_l N$ of a compact Lie group C and a nilpotent Lie group N. Therefore it is of interest to examine possible upper bounds and the possible asymptotic behaviour of K for groups which are not of the special form $C \times_l N$. The purpose of this note is to investigate this problem for the simplest such group, the three-dimensional group of Euclidean motions in the plane. Our analysis establishes that for large t the bounds (2) are the exception rather than the rule. Indeed many m-th order operators have the large time characteristics of second-order operators in some directions.

Let G denote the three-dimensional, connected, simply-connected Lie group of Euclidean motions, $\mathfrak{g}$ its (solvable) Lie algebra and $\mathfrak{n}$ the (two-dimensional) nilradical of $\mathfrak{g}$. Further let $|\cdot|$ be the modulus associated to a fixed basis of $\mathfrak{g}$ and note that different bases give equivalent moduli. Fix a basis a_1, a_2, a_3 of $\mathfrak{g}$. Next let A_1, A_2, A_3 denote the infinitesimal generators of the one-parameter groups $t \mapsto L(\exp(-ta_i))$ where L is the left regular representation of G in $L_2(G)$. All the operators H we consider are m-th order polynomials in the A_i with the common feature that the corresponding semigroup kernels K are smooth functions satisfying Gaussian bounds

$$|K_t(g)| \le c\,t^{-3/m} e^{\omega t} e^{-b(|g|^m t^{-1})^{1/(m-1)}} \quad ,$$

with $b, c > 0$ and $\omega \ge 0$, uniformly for all $g \in G$ and $t > 0$ (for details see [Rob], Chapters I and III, or for a short proof, [ElR3]). Our interest is to derive bounds of this nature with the optimal behaviour as $t \to \infty$.

Theorem 1.1 *Let $H = (-1)^{m/2} \sum_{i=1}^3 A_i^m$ with $m \ge 4$ even. The following conditions are equivalent.*

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

$$|K_t(g)| \le c\,t^{-3/m} e^{-b(|g|^m t^{-1})^{1/(m-1)}} \tag{4}$$

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

II. *There exists a $c > 0$ such that $c\,t^{-3/m} \le \|K_t\|_\infty$ for all $t \ge 1$.*

III. $\lim_{t\to\infty} t^{3/m} K_t(e)$ *exists and is not* 0.

IV. *The nilradical $\mathfrak{n}$ is spanned by two of the basis elements a_1, a_2, a_3.*

The theorem implies that the geometric bounds (2) and the good Gaussian bounds (4) are only valid for large t for very special bases. This contrasts starkly with the situation for powers of the Laplacian, Theorem 3.1 below, for which the Gaussian bounds are satisfied independently of the choice of basis a_1, a_2, a_3. Note that Theorem 1.1 gives examples for which K satisfies the Gaussian bounds (4) but H does not satisfy the strong Gårding inequality (3). Indeed (4) together with (3) would imply that G is of the form $C \times_l N$, by [Dun], Theorem 1.1, which is a contradiction.

The next result gives detailed bounds on the kernels of Theorem 1.1 for general bases. To state it we need an explicit description of G.

First, there is a basis b_1, b_2, b_3 of $\mathfrak{g}$ satisfying $[b_1, b_2] = b_3$, $[b_1, b_3] = -b_2$ and $[b_2, b_3] = 0$. Then $\mathfrak{n} = \operatorname{span}\{b_2, b_3\}$. Secondly, define the homeomorphism $\Phi: \mathbf{R}^3 \to G$ 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 there is a $c > 0$ such that $c^{-1}|x| \le |\Phi(x)| \le c|x|$ for all $x \in \mathbf{R}^3$. (Actually, if the modulus $|\cdot|$ is defined with respect to the basis b_1, b_2, b_3 then $|\Phi(x)| = |x|$ for all $x \in \mathbf{R}^3$.) Thirdly, for $b, t > 0$ and $n \ge 2$ even introduce the Gaussians $G_{b,t}^{(n)}: \mathbf{R}^2 \to \mathbf{R}$ by

$$G_{b,t}^{(n)}(x_2, x_3) = t^{-2/n} e^{-b((x_2^2 + x_3^2)^{n/2} t^{-1})^{1/(n-1)}}$$

on the commutative group $\mathbf{R}^2$.

Theorem 1.2 *Let $H = (-1)^{m/2} \sum_{i=1}^3 A_i^m$ with $m \ge 4$ even and assume the nilradical $\mathfrak{n}$ is not spanned by any pair of the basis elements a_1, a_2, a_3. Then the following is valid.*

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

$$|K_t(\Phi(x_1,x_2,x_3))| \leq c\,t^{-1/m} e^{-b(|x_1|^m t^{-1})^{1/(m-1)}} \Big(G^{(m)}_{b,t} * G^{(2)}_{b',t}\Big)(x_2,x_3)$$

for all $t > 0$ and $(x_1,x_2,x_3) \in \mathbf{R}^3$ where $*$ denotes convolution on $\mathbf{R}^2$. In particular there are $b, b', c > 0$ such that

$$|K_t(\Phi(x_1,x_2,x_3))| \leq \begin{cases} c\,t^{-3/m} e^{-b(|x_1|^m t^{-1})^{1/(m-1)}} e^{-b((x_2^2+x_3^2)^{m/2} t^{-1})^{1/(m-1)}} & \textit{if } t \leq 1 \\ c\,t^{-(m+1)/m} e^{-b(|x_1|^m t^{-1})^{1/(m-1)}} \Big(e^{-b((x_2^2+x_3^2)^{m/2} t^{-1})^{1/(m-1)}} \vee e^{-b'(x_2^2+x_3^2)t^{-1}}\Big) & \\ & \textit{if } t \geq 1 \end{cases}$$

for all $t > 0$ and $(x_1,x_2,x_3) \in \mathbf{R}^3$

II. $\lim_{t\to\infty} t^{(m+1)/m} K_t(e)$ *exists and is not zero.*

The asymptotic behaviour of the kernels K associated with the homogeneous operators $H = (-1)^{m/2} \sum_{i=1}^3 A_i^m$ can be described in much greater detail. We will demonstrate that the kernel is accurately approximated for large t by the kernel of an m-th order, weighted strongly elliptic operator with constant coefficients on $\mathbf{R}^3$.

The above results extend to subelliptic operators $H = (-1)^{m/2} \sum_{i=1}^2 A_i^m$ with a_1, a_2 an algebraic basis of $\mathfrak{g}$. The subelliptic geometry changes the detail of the small t estimates but not the large t estimates. One has normal Gaussian behaviour if $\mathfrak{n}$ contains one of the a_i and anomalous behaviour if this is not the case.

2 Proof of Theorems 1.1 and 1.2

We begin by establishing crude upper bounds on the kernel K by standard arguments based on Sobolev inequalities and perturbation theory. The bounds are established on $L_2(\mathbf{R}^3)$.

Let B_1, B_2, B_3 denote the representatives of b_1, b_2, b_3 in the left regular representation of G on $L_2(G)$. Then B_1, B_2, B_3 transfer to operators $\widetilde{B}_1, \widetilde{B}_2, \widetilde{B}_3$ on $L_2(\mathbf{R}^3)$ by use of the homeomorphism Φ. Explicitly, if $\varphi \in C_c^\infty(\mathbf{R}^3)$ then

$$(\widetilde{B}_1\varphi)(x) = \Big(B_1(\varphi\circ\Phi^{-1})\Big)(\Phi(x)) = -(\partial_1\varphi)(x) \quad ,$$

$$(\widetilde{B}_2\varphi)(x) = \Big(B_2(\varphi\circ\Phi^{-1})\Big)(\Phi(x)) = -\cos x_1\,(\partial_2\varphi)(x) + \sin x_1\,(\partial_3\varphi)(x) \quad ,$$

$$(\widetilde{B}_3\varphi)(x) = \Big(B_3(\varphi\circ\Phi^{-1})\Big)(\Phi(x)) = -\sin x_1\,(\partial_2\varphi)(x) - \cos x_1\,(\partial_3\varphi)(x)$$

for all $x = (x_1,x_2,x_3) \in \mathbf{R}^3$ where $\partial_k = \partial/\partial x_k$. Since b_1, b_2, b_3 is a basis of $\mathfrak{g}$ there is a non-singular, real-valued, matrix (ν_{kl}) such that $a_k = \sum_{l=1}^3 \nu_{kl} b_l$. Then A_1, A_2, A_3 transfer to operators $\widetilde{A}_k = \sum_{l=1}^3 \nu_{kl}\widetilde{B}_l$ on $L_2(\mathbf{R}^3)$ for all $k \in \{1,2,3\}$. Hence the operator H is represented on $L_2(\mathbf{R}^3)$ by

$$\widetilde{H}\varphi = \Big(H(\varphi\circ\Phi^{-1})\Big)\circ\Phi = (-1)^{m/2}\sum_{k=1}^3 \widetilde{A}_k^m\varphi$$

for all $\varphi \in C_c^\infty(\mathbf{R}^3)$.

Next for all $\rho \in \mathbf{R}^3$ introduce the multiplication operator U_ρ by $(U_\rho\varphi)(x) = e^{\rho.x}\varphi(x)$ and set $\widetilde{H}_\rho = U_\rho \widetilde{H} U_\rho^{-1}$. Further let $\tilde{h}$ and $\tilde{h}_\rho$ denote the forms associated with $\widetilde{H}$ and $\widetilde{H}_\rho$ on $L_2(\mathbf{R}^3)$.

Lemma 2.1 *There is a $\gamma \geq 0$ and for each $\varepsilon > 0$ a $c_\varepsilon > 0$ such that*

$$|\tilde{h}_\rho(\varphi) - \tilde{h}(\varphi)| \leq \varepsilon \tilde{h}(\varphi) + c_\varepsilon \omega_\gamma(\rho) \|\varphi\|_2^2$$

for all $\varphi \in D(\tilde{h})$ where $\omega_\gamma(\rho) = \rho_1^m + \rho_2^m + \rho_3^m + \gamma(\rho_2^2 + \rho_3^2)$. Moreover, if $a_1 = \nu_{11} b_1$ with $\nu_{11} \in \mathbf{R}$ and a_2, a_3 span $\mathfrak{n}$ then one may choose $\gamma = 0$.

Proof One has $U_\rho \widetilde{A}_k U_\rho^{-1} = \widetilde{A}_k + L_k(\rho)$ with

$$L_k(\rho) = \nu_{k1}\rho_1 + \nu_{k2}(\rho_2 c_1 - \rho_3 s_1) + \nu_{k3}(\rho_2 s_1 + \rho_3 c_1)$$

where $c_1(x) = \cos x_1$ and $s_1(x) = \sin x_1$. We consider $L_k(\rho)$ both as a multiplication operator on $L_2(\mathbf{R}^3)$ as as a function on $\mathbf{R}^3$. Moreover,

$$\tilde{h}_\rho(\varphi) - \tilde{h}(\varphi) = \sum_{k=1}^{3} \Big(((\widetilde{A}_k - L_k(\rho))^n \varphi, (\widetilde{A}_k + L_k(\rho))^n \varphi) - (\widetilde{A}_k^n \varphi, \widetilde{A}_k^n \varphi) \Big) \tag{5}$$

with $n = m/2$. But

$$(\widetilde{A}_k + L_k(\rho))^n \varphi = \widetilde{A}_k^n \varphi + \sum_{l=0}^{n-1} c_{n;l}^{(k)}(\rho)\, \widetilde{A}_k^l \varphi$$

where the coefficients have the form

$$c_{n;l}^{(k)}(\rho) = \sum c_{l,j_1,\ldots,j_p}^{(k)} \prod_{i=1}^{p} (\widetilde{A}_k^{j_i} L_k(\rho)) \quad .$$

The sum is over all $p \in \{1, \ldots, n\}$ and $j_1, \ldots, j_p \geq 0$ such that $j_1 + \ldots + j_p + p + l = n$ and the $c_{l,j_1,\ldots,j_p}^{(k)}$ are numerical constants. Now one immediately obtains bounds $\|L_k(\rho)\|_\infty \leq c_0(\rho_1^2 + \rho_2^2 + \rho_3^2)^{1/2}$ and $\|\widetilde{A}_k^j L_k(\rho)\|_\infty \leq c_j(\rho_2^2 + \rho_3^2)^{1/2}$ if $j \geq 1$. Therefore, fixing $\gamma > 0$ one has bounds

$$\|c_{n;l}^{(k)}(\rho)\|_\infty^2 \leq c_0'\,(\rho_1^2 + \rho_2^2 + \rho_3^2)^{n-l} + c_1'\,\gamma\,(\rho_2^2 + \rho_3^2) \leq c\,\omega_\gamma(\rho)^{(n-l)/n} \quad . \tag{6}$$

Next it follows from (5) that

$$|\tilde{h}_\rho(\varphi) - \tilde{h}(\varphi)| \leq 2 \sum_{k=1}^{3} \|\widetilde{A}_k^n \varphi\|_2 \sum_{l=0}^{n-1} \|c_{n;l}^{(k)}(\rho)\|_\infty \|\widetilde{A}_k^l \varphi\|_2 + \sum_{k=1}^{3} \Big(\sum_{l=0}^{n-1} \|c_{n;l}^{(k)}(\rho)\|_\infty \|\widetilde{A}_k^l \varphi\|_2 \Big)^2 . \tag{7}$$

Then the leading term in (7) is bounded by

$$2 \sum_{k=1}^{3} \|\widetilde{A}_k^n \varphi\|_2 \sum_{l=0}^{n-1} \|c_{n;l}^{(k)}(\rho)\|_\infty \|\widetilde{A}_k^l \varphi\|_2 \leq \varepsilon\, \tilde{h}(\varphi) + \varepsilon^{-1} \sum_{k=1}^{3} \Big(\sum_{l=0}^{n-1} \|c_{n;l}^{(k)}(\rho)\|_\infty \|\widetilde{A}_k^l \varphi\|_2 \Big)^2$$

for all $\varepsilon > 0$. But

$$\begin{aligned} \|c_{n;l}^{(k)}(\rho)\|_\infty \|\widetilde{A}_k^l \varphi\|_2 &\leq \delta\, \tilde{h}(\varphi)^{1/2} + \delta^{-l/(n-l)}\, \|c_{n;l}^{(k)}(\rho)\|_\infty^{n/(n-l)} \|\varphi\|_2 \\ &\leq \delta\, \tilde{h}(\varphi)^{1/2} + \delta^{-l/(n-l)}\, c^{n/(2(n-l))}\, \omega_\gamma(\rho)^{1/2}\, \|\varphi\|_2 \end{aligned}$$

for all $\delta > 0$, $l \in \{0, \ldots, n-1\}$ and $k \in \{1,2,3\}$, by (6). Then the first statement of the lemma follows by adding the contributions and choosing δ appropriately.

Finally, if $a_1 = \nu_{11} b_1$ then $\nu_{12} = 0 = \nu_{13}$ and if a_2, a_3 span $\mathfrak{n}$ then $\nu_{21} = 0 = \nu_{31}$. Hence $(\widetilde{A}_k^j L_k(\rho)) = 0$ for all $j \geq 1$ and $k \in \{1,2,3\}$ and the bounds (6) are valid with $\gamma = 0$. Then the subsequent arguments are also valid with $\gamma = 0$. □

Since $m \geq 4$ and G is three-dimensional one has a Sobolev inequality

$$\|\varphi\|_\infty^2 \leq c\,(h(\varphi) + \|\varphi\|_2^2)$$

for all $\varphi \in D(h)$. Therefore using the estimate of Lemma 2.1 one deduces that there are $b, c > 0$ such that

$$\|\varphi\|_\infty^2 \leq c\,(t h_\rho(\varphi) + e^{tb\omega_\gamma(\rho)} \|\varphi\|_2^2)$$

for all $\varphi \in D(h)$ and all $t \geq 1$. But standard estimates give bounds $\|S_t^\rho \varphi\|_2^2 \leq M e^{tb'\omega_\gamma(\rho)} \|\varphi\|_2^2$ and $|h_\rho(S_t^\rho \varphi)| \leq M t^{-1} e^{tb'\omega_\gamma(\rho)} \|\varphi\|_2^2$ for all $\varphi \in L_2(\mathbf{R}^3)$ and all $t > 0$ where S^ρ is the semigroup generated by $\widetilde{H}_\rho$. Hence one obtains bounds $\|S_t^\rho\|_{2\to\infty} \leq c\, e^{tb\omega_\gamma(\rho)}$ for all $t \geq 1$. Since the corresponding kernel K^ρ satisfies $\|K_t^\rho\|_\infty \leq \|S_{t/2}^\rho\|_{2\to\infty} \|S_{t/2}^{-\rho}\|_{2\to\infty}$ one immediately obtains crude bounds on the kernel K.

Lemma 2.2 *There are $b, c > 0$ and $\gamma \geq 0$ such that*

$$|K_t(\Phi(x))| \leq c\,(1 \wedge t)^{-3/m} \inf_{\rho \in \mathbf{R}^3} e^{tb\omega_\gamma(\rho)} e^{-\rho . x}$$

for all $x \in \mathbf{R}^3$ and $t > 0$. Moreover, if $a_1 = \nu_{11} b_1$ with $\nu_{11} \in \mathbf{R}$ and a_2, a_3 span $\mathfrak{n}$ then one may choose $\gamma = 0$.

Proof The bounds for $t \in \langle 0, 1]$ follow from the standard small time Gaussian bounds. The bounds for $t \geq 1$ are a consequence of the previous reasoning. □

If $\gamma = 0$ then the bounds of the lemma can be reexpressed as

$$|K_t(\Phi(x))| \leq c\,(1 \wedge t)^{-3/m} e^{-b(|x|^m t^{-1})^{1/(m-1)}}$$

uniformly for all $t > 0$, i.e., one has Gaussian bounds with an additional polynomial growth factor $(1+t)^{3/m}$. If, however, $\gamma > 0$ one has bounds

$$|K_t(\Phi(x))| \leq c\,(1+t)^{(m+1)/m}\, t^{-1/m} e^{-b(|x_1|^m t^{-1})^{1/(m-1)}} \Big(G_{b,t}^{(m)} * G_{b',t}^{(2)}\Big)(x_2, x_3) \qquad (8)$$

uniformly for all $t > 0$ and $x = (x_1, x_2, x_3) \in \mathbf{R}^3$ and these are of the type given in Theorem 1.2 but again with the additional growth factor (see [DER] Proposition 2.10.I). Next we use arguments based on periodicity to remove this factor.

The operator $\widetilde{H}$ on $L_2(\mathbf{R}^3)$ is strongly elliptic with periodic coefficients. Therefore one can analyze it with the Bloch decomposition as in [ERS3]. Let H_θ be the operator on $L_2([-\pi,\pi]^3)$ obtained by replacing each ∂_k in $\widetilde{H}$ by $\partial_k - i\theta_k$, where $\theta \in \mathbf{C}^3$ and the ∂_k on $L_2([-\pi,\pi]^3)$ have periodic boundary conditions. Then H_0 has a compact resolvent with a simple eigenvalue 0 and eigenfunction $\varphi_0 = \mathbb{1}$, the constant function with value 1. Therefore by holomorphic perturbation theory there exist $\delta, \varepsilon > 0$ and holomorphic functions $\lambda_0 \colon \Omega \to \mathbf{C}$ and $\theta \mapsto \varphi_\theta$ from Ω into $L_2([-\pi,\pi]^3)$ such that $H_\theta \varphi_\theta = \lambda_0(\theta)\, \varphi_\theta$ and $\lambda_0(\theta)$ is the unique eigenvalue of H_θ with $|\lambda_0(\theta)| < \varepsilon$ for all $\theta \in \Omega$, where $\Omega = \{\theta \in \mathbf{C}^3 : |\theta| < \delta\}$. (Cf. [ERS3], Proposition 2.7.)

The behaviour of the λ_0 depends on whether Condition IV of Theorem 1.1 is valid or not. If it is we again make a technical restriction which we later remove.

Lemma 2.3

I. *If $\mathfrak{n}$ is not spanned by any pair of a_1, a_2, a_3 then there exist $c \geq 1$ and $c_1, c_2 > 0$ such that*

$$|\lambda_0(\theta) - \hat{\lambda}_0(\theta)| \leq c\,(\theta_1^m + \theta_2^2 + \theta_3^2)^{(m+1)/m}$$

for all $\theta \in \Omega$, where $\hat{\lambda}_0(\theta) = c_1\theta_1^m + c_2(\theta_2^2 + \theta_3^2)$.

II. *If $a_1 = \nu_{11}b_1$ with $\nu_{11} \in \mathbf{R}$ and a_2, a_3 span $\mathfrak{n}$ then there exist $c \geq 1$, $\mu > 0$ and a homogeneous m-th order polynomial $\hat{\lambda}_0 \colon \mathbf{R}^3 \to \mathbf{R}$ such that*

$$|\lambda_0(\theta) - \hat{\lambda}_0(\theta)| \leq c\,|\theta|^{(m+1)/m}$$

for all $\theta \in \Omega$. Moreover, the coefficients of $\hat{\lambda}_0(\theta)$ are real and $\hat{\lambda}_0(\theta) \geq \mu\,|\theta|^m$ for all $\theta \in \mathbf{R}^3$.

Proof For all $k \in \{1,2,3\}$ and $\theta \in \mathbf{R}^3$ set

$$L_\theta^{(k)} = i\Big(\nu_{k1}\theta_1 + \nu_{k2}(c_1\,\theta_2 - s_1\,\theta_3) + \nu_{k3}(s_1\,\theta_2 + c_1\theta_3)\Big)$$

and

$$L_\partial^{(k)} = -\nu_{k1}\partial_1 - \nu_{k2}(c_1\,\partial_2 - s_1\,\partial_3) - \nu_{k3}(s_1\,\partial_2 + c_1\partial_3) \quad .$$

In particular $L_\theta^{(k)} = L_k(i\theta)$. We consider $L_\theta^{(k)}$ as a multiplication operator and $L_\partial^{(k)}$ as a partial differential operator on $L_2([-\pi,\pi]^3)$. Then $H_\theta = (-1)^{m/2}\sum_{k=1}^3 (L_\theta^{(k)} + L_\partial^{(k)})^m$. Note that if ψ is a linear combination of c_1 and s_1 then $H_0\psi = \nu\,\psi$, where $\nu = \sum_{k=1}^3 \nu_{k1}^m$. Since λ_0 and $\theta \mapsto \varphi_\theta$ are holomorphic and $\theta \mapsto H_\theta$ is a polynomial one can write

$$\lambda_0(\theta) = \sum_{n=0}^\infty \lambda^{(n)}(\theta) \quad , \quad \varphi_\theta = \sum_{n=0}^\infty \varphi^{(n)}(\theta) \quad \text{and} \quad H_\theta = \sum_{n=0}^m H^{(n)}(\theta)$$

for all $\theta \in \Omega$, where each $\lambda^{(n)}(\theta)$, $\varphi^{(n)}(\theta)$ and $H^{(n)}(\theta)$ is homogeneous of degree n in θ, if δ is sufficiently small. Then $\lambda^{(0)}(\theta) = 0$, $\varphi^{(0)}(\theta) = \mathbb{1}$ and $H^{(0)}(\theta) = H_0$. So

$$\sum_{n=0}^m H^{(n)}(\theta) \sum_{n=0}^\infty \varphi^{(n)}(\theta) = H_\theta\,\varphi_\theta = \lambda_0(\theta)\,\varphi_\theta = \sum_{n=1}^\infty \lambda^{(n)}(\theta) \sum_{n=0}^\infty \varphi^{(n)}(\theta) \tag{9}$$

for all $\theta \in \mathbf{R}^3$ with $|\theta| < \delta$.

Comparing the linear terms gives $H_0\,\varphi^{(1)}(\theta) + H^{(1)}(\theta)\,\mathbb{1} = \lambda^{(1)}(\theta)\,\mathbb{1}$ and

$$(2\pi)^3\,\lambda^{(1)}(\theta) = (\mathbb{1}, H_0\,\varphi^{(1)}(\theta)) + (\mathbb{1}, H^{(1)}(\theta)\,\mathbb{1}) = 0 \quad .$$

Then $H_0\,\varphi^{(1)}(\theta) = -H^{(1)}(\theta)\,\mathbb{1}$ is a linear combination of c_1 and s_1. Since $\varphi^{(1)}(\theta)$ is linear this implies that there is a linear function $\tau_1 \colon \mathbf{R}^3 \to \mathbf{C}$ such that $\varphi^{(1)}(\theta) = \tau_1(\theta)\,\mathbb{1} - \nu^{-1}H^{(1)}(\theta)\,\mathbb{1}$ for all $\theta \in \mathbf{R}^3$ with $|\theta| < \delta$.

Comparing the second order terms in (9) gives

$$(2\pi)^3\,\lambda^{(2)}(\theta) = (\mathbb{1}, H^{(2)}(\theta)\,\mathbb{1}) - \nu^{-1}(\mathbb{1}, H^{(1)}(\theta)\,H^{(1)}(\theta)\,\mathbb{1})$$
$$= (\mathbb{1}, H^{(2)}(\theta)\,\mathbb{1}) - \nu^{-1}\|H^{(1)}(\theta)\,\mathbb{1}\|_2^2 \quad .$$

We calculate both terms. One has

$$H^{(1)}(\theta)\,\mathbb{1} = (-1)^{m/2}\sum_{k=1}^{3}(L_\partial^{(k)})^{m-1}L_\theta^{(k)}\mathbb{1}$$
$$= \sum_{k=1}^{3}\nu_{k1}^{m-1}\partial_1 L_\theta^{(k)}\,\mathbb{1} = -i\sum_{k=1}^{3}\nu_{k1}^{m-1}\Big((\nu_{k2}\,\theta_3 - \nu_{k3}\,\theta_2)c_1 + (\nu_{k2}\,\theta_2 + \nu_{k3}\,\theta_3)s_1\Big)\ . \quad (10)$$

Then

$$\|H^{(1)}(\theta)\,\mathbb{1}\|_2^2 = 2^{-1}(2\pi)^3\sum_{k,l=1}^{3}\nu_{k1}^{m-1}\nu_{l1}^{m-1}\Big((\nu_{k2}\,\theta_3 - \nu_{k3}\,\theta_2)(\nu_{l2}\,\theta_3 - \nu_{l3}\,\theta_2)$$
$$+ (\nu_{k2}\,\theta_2 + \nu_{k3}\,\theta_3)(\nu_{l2}\,\theta_2 + \nu_{l3}\,\theta_3)\Big)$$
$$= 2^{-1}(2\pi)^3(\theta_2^2+\theta_3^2)\left(\Big(\sum_{k=1}^{3}\nu_{k1}^{m-1}\nu_{k2}\Big)^2 + \Big(\sum_{k=1}^{3}\nu_{k1}^{m-1}\nu_{k3}\Big)^2\right)$$

for all $\theta \in \mathbf{R}^3$ with $|\theta| < \delta$. Similarly,

$$(\mathbb{1}, H^{(2)}(\theta)\,\mathbb{1}) = \sum_{k=1}^{3}((L_\partial^{(k)})^{m/2-1}L_\theta^{(k)}\,\mathbb{1}, (L_\partial^{(k)})^{m/2-1}L_\theta^{(k)}\,\mathbb{1})$$
$$= 2^{-1}(2\pi)^3(\theta_2^2+\theta_3^2)\Big(\sum_{k=1}^{3}\nu_{k1}^{m-2}(\nu_{k2}^2+\nu_{k3}^2)\Big) \quad .$$

So $\lambda^{(2)}(\theta) = 2^{-1}c_2(\theta_2^2+\theta_3^2)$ where

$$c_2 = \sum_{k=1}^{3}\nu_{k1}^{m-2}(\nu_{k2}^2+\nu_{k3}^2) - \nu^{-1}\Big(\sum_{k=1}^{3}\nu_{k1}^{m-1}\nu_{k2}\Big)^2 - \nu^{-1}\Big(\sum_{k=1}^{3}\nu_{k1}^{m-1}\nu_{k3}\Big)^2 \quad .$$

But it follows from the Cauchy–Schwarz inequality that

$$\Big(\sum_{k=1}^{3}\nu_{k1}^{m-1}\nu_{kl}\Big)^2 \le \sum_{k=1}^{3}\nu_{k1}^{m}\sum_{k=1}^{3}\nu_{k1}^{m-2}\nu_{kl}^2 = \nu\sum_{k=1}^{3}\nu_{k1}^{m-2}\nu_{kl}^2$$

for all $l \in \{2,3\}$. So $c_2 \ge 0$. Moreover, since $(\nu_{11}^{m/2}, \nu_{21}^{m/2}, \nu_{31}^{m/2}) \neq (0,0,0)$ the Cauchy–Schwarz inequality implies that $c_2 = 0$ if, and only if, there are $\rho_2, \rho_3 \in \mathbf{R}$ such that $\nu_{k1}^{m/2-1}\nu_{kl} = \rho_l\nu_{k1}^{m/2}$ for all $k \in \{1,2,3\}$ and $l \in \{2,3\}$. If, however, $\mathfrak{n}$ is not spanned by any pair of a_1, a_2, a_3 then there are $k_1, k_2 \in \{1,2,3\}$ with $k_1 \neq k_2$ such that $\nu_{k_1 1} \neq 0 \neq \nu_{k_2 1}$. So if, in addition, $c_2 = 0$ then there are $\rho_2, \rho_3 \in \mathbf{R}$ such that $\nu_{k_i l} = \rho_l\nu_{k_i 1}$ for all $l \in \{2,3\}$ and $i \in \{1,2\}$. Then $a_{k_i} = \nu_{k_i 1}(b_1 + \rho_2\,b_2 + \rho_3\,b_3)$ for all $i \in \{1,2\}$ and a_{k_1} and a_{k_2} are linearly dependent. Therefore $c_2 > 0$. Conversely, if $\mathfrak{n}$ is spanned by a pair of a_1, a_2, a_3 then it is easy to show that $c_2 = 0$.

Note that the coefficients of θ_1^n in $\varphi^{(n)}(\theta)$ and $\lambda^{(n)}(\theta)$ equal $\varphi^{(n)}(\theta_0)$ and $\lambda^{(n)}(\theta_0)$, where for simplicity we assume that $\theta_0 = (1,0,0) \in \Omega$. Then $\varphi^{(1)}(\theta_0) = \tau_1(\theta_0)\,\mathbb{1} - \nu^{-1}H^{(1)}(\theta_0)\,\mathbb{1} = \tau_1(\theta_0)\,\mathbb{1}$ by (10). Let $n \in \{2,\ldots,m\}$ and suppose there are constants $\rho_1,\ldots,\rho_{n-1} \in \mathbf{C}$ such that $\lambda^{(j)}(\theta_0) = 0$ and $\varphi^{(j)}(\theta_0) = \rho_j\,\mathbb{1}$ for all $j \in \{1,\ldots,n-1\}$. Comparing the n-th order terms in (9) at θ_0 gives

$$\lambda^{(n)}(\theta_0)\,\mathbb{1} = H^{(n)}(\theta_0)\,\mathbb{1} + \sum_{j=1}^{n-1} \rho_j H^{(n-j)}(\theta_0)\,\mathbb{1} + H_0\,\varphi^{(n)}(\theta_0) \quad .$$

Since $L_{\theta_0}^{(k)}$ is an operator of multiplication with a constant it follows that $H^{(j)}(\theta_0)\,\mathbb{1} = 0$ for all $j \in \{1,\ldots,m-1\}$. So if $n < m$ then $(2\pi)^3\,\lambda^{(n)}(\theta_0) = (\mathbb{1}, H_0\,\varphi^{(n)}(\theta_0)) = 0$ and $H_0\,\varphi^{(n)}(\theta_0) = 0$, which implies that $\varphi^{(n)}(\theta_0) = \rho_n\,\mathbb{1}$ for some $\rho_n \in \mathbf{C}$. Alternatively, if $n = m$ then $(2\pi)^3\,\lambda^{(m)}(\theta_0) = (\mathbb{1}, H^{(m)}(\theta_0)\,\mathbb{1}) = (-1)^{m/2}\sum_{k=1}^3(\mathbb{1}, (L_{\theta_0}^{(k)})^m\,\mathbb{1}) = (2\pi)^3\,\nu$. So if $\mathfrak{n}$ is not spanned by any pair of a_1, a_2, a_3 then $c_1 = \nu$ and one sets $\hat\lambda_0(\theta) = c_1\,\theta_1^m + 2^{-1}c_2(\theta_2^2+\theta_3^2)$. This establishes Statement I of the lemma.

Finally, if $a_1 = \nu_{11}b_1$ and a_2, a_3 span $\mathfrak{n}$ then for each $k \in \{1,2,3\}$ the operators $L_\theta^{(k)}$ and $L_\partial^{(k)}$ commute. Hence it follows as in the last part of the proof of Statement I that $\lambda^{(n)}(\theta) = 0$ for all $n \in \{1,\ldots,m-1\}$ and $(2\pi)^3\,\lambda^{(m)}(\theta) = (-1)^{m/2}\sum_{k=1}^3(\mathbb{1}, (L_\theta^{(k)})^m\mathbb{1})$ for all $\theta \in \mathbf{R}^3$ with $|\theta| < \delta$. Obviously $\lambda^{(m)}(\theta)$ extends to a real homogeneous polynomial of degree m. It remains to show that $\lambda^{(m)}(\theta) \neq 0$ for all $\theta \in \mathbf{R}^3$ with $0 < |\theta| < \delta$. Let $\theta \in \mathbf{R}^3$ with $|\theta| < \delta$ and suppose that $\lambda^{(m)}(\theta) = 0$. Then $\sum_{k=1}^3 \|(L_\theta^{(k)})^{m/2}\mathbb{1}\|_2^2 = (2\pi)^3\,\lambda^{(m)}(\theta) = 0$. So $(L_\theta^{(k)})^{m/2}\mathbb{1} = 0$, for each k, almost everywhere. Since $(L_\theta^{(k)})^{m/2}\mathbb{1}$ is continuous one deduces that $(L_\theta^{(k)}\mathbb{1})(x) = 0$ pointwise. Setting $x = 0$ gives $\sum_{l=1}^3 \nu_{kl}\theta_l = 0$ for each k. But the matrix (ν_{kl}) is not singular and hence $\theta = 0$. This completes the proof of the lemma.□

Proof of Theorem 1.2 Suppose that $\mathfrak{n}$ is not spanned by any pair of a_1, a_2, a_3. Let $\hat\lambda_0$, c_1, c_2 and c be as in Lemma 2.3.I. Then there is a $c_3 \in \langle 0, c_1 \wedge c_2\rangle$ such that $\operatorname{Re}\lambda_0(\theta) \geq c_3(\theta_1^m + \theta_2^2 + \theta_3^2)$ for all $\theta \in \Omega$, if δ is small enough. Set $\widehat{H} = (-1)^{m/2}c_1\,\partial_1^m - c_2(\partial_2^2+\partial_3^2)$. Then $\widehat{H}$ is a weighted strongly elliptic operator on $\mathbf{R}^3$ (see [ElR2]). Using the crude Gaussian estimates (8) one can argue as in the proof of Theorem 3.5 in [ERS3] to deduce that there are $c', \mu > 0$ such that

$$\|K_t \circ \Phi - \widehat{K}_t\|_\infty \leq c'\,e^{-\mu t} + c' \int_{\{\theta \in \mathbf{R}^3 : |\theta| < \delta\}} d\theta\; e^{-c_3(\theta_1^m+\theta_2^2+\theta_3^2)t}\Big(|\theta| + t(\theta_1^m + \theta_2^2 + \theta_3^2)^{(m+1)/m}\Big)$$

for all $t \geq 1$, where $\widehat{K}$ is the kernel of the semigroup generated by $\widehat{H}$. Hence there is a $c'' > 0$ such that

$$\|K_t \circ \Phi - \widehat{K}_t\|_\infty \leq c''\,t^{-(m+2)/m} \tag{11}$$

for all $t \geq 1$. Since $(-1)^{m/2}\partial_1^m$ and $-(\partial_2^2 + \partial_3^2)$ commute the kernel $\widehat{K}$ has Gaussian bounds

$$\begin{aligned} |\widehat{K}_t(x_1,x_2,x_3)| &\leq c\,t^{-(m+1)/m} e^{-b(|x_1|^m t^{-1})^{1/(m-1)}} e^{-b(x_2^2+x_3^2)t^{-1}} \\ &\leq c'\,t^{-1/m} e^{-b(|x_1|^m t^{-1})^{1/(m-1)}} \Big(G_{b',t}^{(m)} * G_{b',t}^{(2)}\Big)(x_2,x_3) \end{aligned} \tag{12}$$

for all $t \geq 1$ (see [DER], Proposition 2.10.III). Then one can combine (11) and (12) and interpolate with the bounds (8) as in the proof of Corollary 3.6 of [ERS3]. It follows that for all $\varepsilon > 0$ there are $b, b', c > 0$ such that

$$|K_t \circ \Phi(x) - \widehat{K}_t(x)| \leq c\,t^{-(1-\varepsilon)/m}\,t^{-1/m} e^{-b(|x_1|^m t^{-1})^{1/(m-1)}} \Big(G_{b,t}^{(m)} * G_{b',t}^{(2)}\Big)(x_2,x_3) \tag{13}$$

for all $t \geq 1$ and $x = (x_1, x_2, x_3) \in \mathbf{R}^3$. The bounds (12) and (13) imply the first bounds of Theorem 1.2.I in case $t \geq 1$. The bounds for $t \leq 1$ follow from the local Gaussian bounds and Propositions 2.10.I and 2.10.II of [DER].

Finally it follows from (11) and Fourier theory that

$$\lim_{t\to\infty} t^{(m+1)/m} K_t(e) = \lim_{t\to\infty} t^{(m+1)/m} \widehat{K}_t(0)$$
$$= \int_{\mathbf{R}^3} dp\, e^{-(c_1 p_1^m + c_2(p_2^2+p_3^2))} = 2\pi\, \Gamma(m^{-1})\, c_1^{-1/m} (c_2 m)^{-1}$$

and the proof of Theorem 1.2 is complete. □

Remark 2.4 Note that actually $\lim_{t\to\infty} t^{(m+1)/m} K_t(g) = 2\pi\,\Gamma(m^{-1})\, c_1^{-1/m}(c_2 m)^{-1}$ for all $g \in G$, by the same argument.

Proof of Theorem 1.1 "I⇒II". Since H is self-adjoint it follows from Corollary 2.4 of [ElR4] that $K_t(e) \geq c\,t^{-3/m}$ for some $c > 0$ and all $t > 0$. This implies Condition II.

"II⇒IV". If Condition IV is not valid then Theorem 1.2.I implies that there is a $c > 0$ such that $\|K_t\|_\infty \leq c\,t^{-(m+1)/m}$ for all $t \geq 1$. This contradicts Condition II.

Obviously Condition III implies Condition II, so it suffices to show the implications IV⇒I and IV⇒III. We first prove these implications if $a_1 = \nu_{11}\, b_1$ and $a_2, a_3 \in \mathfrak{n}$.

Let $\mu > 0$ and $\hat{\lambda}_0(\theta)$ be as in Lemma 2.3.II. There exist $c_\alpha \in \mathbf{R}$ such that $\hat{\lambda}_0(\theta) = \sum_{|\alpha|=m} c_\alpha\, \theta^\alpha$ for all $\theta \in \mathbf{R}^3$. Set $\widehat{H} = (-1)^{m/2} \sum_{|\alpha|=m} c_\alpha\, \partial^\alpha$. Since $\hat{\lambda}_0(\theta) \geq \mu\, |\theta|^m$ for all $\theta \in \mathbf{R}^3$ it follows that $\widehat{H}$ is a strongly elliptic operator on $\mathbf{R}^3$. If $\widehat{K}$ is the kernel of the semigroup generated by $\widehat{H}$ then it follows as in [ERS3] that there is a $c > 0$ such that $\|K_t \circ \Phi - \widehat{K}_t\|_\infty \leq c\,t^{-3/m}\, t^{-1/m}$ for all $t \geq 1$. Arguing as in the proof of Theorem 1.2 the Gaussian upper bounds of Condition I follow. Moreover,

$$\lim_{t\to\infty} t^{3/m} K_t(e) = \lim_{t\to\infty} t^{3/m} \widehat{K}_t(0) = \int_{\mathbf{R}^3} d\theta\, e^{-\hat{\lambda}_0(\theta)} \neq 0 \quad ,$$

which is Condition III.

Finally suppose that Condition IV is valid. We may assume that $a_2, a_3 \in \mathfrak{n}$. Then $\nu_{11} \neq 0$. Set $a = \nu_{11}^{-1}(\nu_{13}\, b_2 - \nu_{12}\, b_3) \in \mathfrak{n}$. Let Ψ be the inner automorphism of G induced by $\exp a$, so $\Psi(g) = (\exp a)\, g \exp(-a)$. Then $\Psi(\exp a_k) = \exp \breve{a}_k$ for all $k \in \{1,2,3\}$, where $\breve{a}_1 = \nu_{11}\, b_1$, $\breve{a}_2 = a_2$ and $\breve{a}_3 = a_3$. Let U be the unitary map from $L_2(G)$ onto $L_2(G)$ defined by $U\varphi = \varphi \circ \Psi^{-1}$. Then $UHU^{-1} = (-1)^{m/2} \sum_{k=1}^3 \breve{A}_k^m$, where $\breve{A}_k$ is the generator in the direction $\breve{a}_k$. So the kernel $\breve{K}$ of the semigroup generated by the operator UHU^{-1} has Gaussian bounds and $\lim_{t\to\infty} t^{3/m}\, \breve{K}_t(e)$ exists and is not zero by the foregoing arguments. But $K_t = \breve{K}_t \circ \Psi$. Since Ψ is an automorphism of G the Conditions I and III for K follow from those for $\breve{K}$. □

Also here Condition III can be strengthened (or weakened) to $\lim_{t\to\infty} t^{3/m} K_t(g) = c$ for all $g \in G$ with $c \neq 0$ a constant independent of g.

Remark 2.5 The foregoing arguments apply with very little alteration to subelliptic operators $H = (-1)^{m/2} \sum_{i=1}^2 A_i^m$ with a_1, a_2 an algebraic basis of $\mathfrak{g}$. The subelliptic geometry changes the local singularity of K_t from $t^{-3/m}$ to $t^{-4/m}$ but the behaviour for large t remains unchanged. Examination of the proof of Lemma 2.3 shows that the previous condition for normal Gaussian behaviour for large t is replaced by the requirement that $\mathfrak{n}$ contains one of the a_i. If this condition is not fulfilled one has the anomalous second-order asymptotics.

3 Powers of the Laplacian

The next theorem shows that the anomalous behaviour exhibited by Theorem 1.1 cannot occur if H is replaced by a power of the Laplacian. Note that the following argument is independent of the group structure and applies equally well to powers of operators on a space of polynomial growth.

Theorem 3.1 *Let G be a Lie group with polynomial growth, $a_1, \ldots, a_{d'}$ an algebraic basis of the corresponding Lie algebra $\mathfrak{g}$ and $A_1, \ldots, A_{d'}$ the representatives in the left regular representation on $L_2(G)$. Further let $|\cdot|'$ and V denote the associated subelliptic distance and volume. Finally let $H = (-\sum_{i=1}^{d'} A_i^2)^{m/2}$, with $m \geq 2$ even, and K the corresponding semigroup kernel. Then there exist $b, c > 0$ such that*

$$|K_t(g)| \leq c\, V(t)^{-1/m} e^{-b((|g|')^m t^{-1})^{1/(m-1)}}$$

and

$$\sup_{1 \leq i \leq d'} |(A_i K_t)(g)| \leq c\, t^{-1/m} V(t)^{-1/m} e^{-b((|g|')^m t^{-1})^{1/(m-1)}}$$

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

Proof The bounds are well known for $m = 2$ and the general bounds follows from this special case in three steps. The first step reduces the proof to the case $D' = D \geq 4$, where D' and D are the local and global dimension of G corresponding to the algebraic basis.

If $D' > D$ define $G_2 = H^{D'-D} \times \mathbf{R}^3$ where H is the three-dimensional Heisenberg group, if $D' < D$ define $G_2 = \mathbf{T}^{D-D'} \times \mathbf{R}^3$ and if $D' = D$ define $G_2 = \mathbf{R}^3$. Then consider the group $\widetilde{G} = G \times G_2$. Choose a full basis of the Lie algebra $\mathfrak{g}_2$ of the group G_2 and consider the algebraic basis of $\widetilde{G}$ obtained by the union of the algebraic basis of G and the full basis of G_2. Let $\widetilde{D}'$ denote the local dimension of $\widetilde{G}$ with respect to the corresponding basis and $\widetilde{D}$ the dimension at infinity. It follows that $\widetilde{D}' = \widetilde{D} \geq 4$. Next let Δ_2 denote the Laplacian corresponding to the full basis of $\mathfrak{g}_2$ and $\widetilde{H}_2 = H_2 \otimes I + I \otimes \Delta_2$, where $H_2 = -\sum_{i=1}^{d'} A_i^2$. Note that there is a $c > 0$ such that $\widetilde{V}(t) \geq c\, V(t)\, V_2(t)$ for all $t > 0$ where $\widetilde{V}$ and V_2 are the volumes on $\widetilde{G}$ and G_2 corresponding to the appropriate bases. Now suppose the estimates of the proposition are valid for the kernel $\widetilde{K}$ associated with $(\widetilde{H}_2)^{m/2}$. But with $\tilde{g} = (g, g_2) \in \widetilde{G}$ one has

$$K_t(g) = \int_{G_2} dg_2\, \widetilde{K}_t((g, g_2))$$

for all $g \in G$. Hence

$$\begin{aligned} |K_t(g)| &\leq \tilde{c}\, V(t)^{-1/m} e^{-\tilde{b}((|g|')^m t^{-1})^{1/(m-1)}} V_2(t)^{-1/m} \int_{G_2} dg_2\, e^{-\tilde{b}(|g_2|^m t^{-1})^{1/(m-1)}} \\ &\leq c\, V(t)^{-1/m} e^{-\tilde{b}((|g|')^m t^{-1})^{1/(m-1)}} \quad . \end{aligned}$$

Thus the estimates on G follow from those on the larger group $\widetilde{G}$. Therefore we now assume $D' = D \geq 4$. Then $V(t)$ behaves like t^D for all $t > 0$.

The second step consists of deriving the Gaussian bounds on the ball $\{g : |g|' \leq t^{1/m}\}$. First, let $S^{(2)}$ denote the semigroup generated by the (sub)Laplacian H_2. Then there is a $c > 0$ such that $\|S_t^{(2)}\|_{2\to\infty} \leq c\, t^{-D/4}$ for all $t > 0$. Secondly, if $n > D/4$ then

$$\|(\lambda I + H_2)^{-n}\|_{2\to\infty} \leq c\, (n!)^{-1}\, \Gamma(n - D/4)\, \lambda^{-n+D/4} = c_n\, \lambda^{-n+D/4}$$

for all $\lambda > 0$ by Laplace transformation. Hence if S is the semigroup generated by H then

$$\|S_t\|_{2\to\infty} \leq c_n\, \lambda^{-n+D/4} \|(\lambda I + H_2)^n S_t\|_{2\to 2} \leq c'_n\, \lambda^{-n+D/4}(\lambda^n + t^{-2n/m})$$

for all $\lambda, t > 0$ with a suitable $c'_n > 0$, where the last bound follows from spectral theory. Thirdly, setting $\lambda = t^{-2/m}$ gives bounds $\|S_t\|_{2\to\infty} \leq 2c'_n\, t^{-D/(2m)}$. Hence

$$\|K_t\|_\infty \leq \|S_{t/2}\|^2_{2\to\infty} \leq c'\, t^{-D/m}$$

and consequently

$$|K_t(g)| \leq c' e^b\, t^{-D/m} e^{-b((|g|')^m t^{-1})^{1/(m-1)}}$$

for all $b > 0$, $g \in G$ and $t > 0$ with $|g|' \leq t^{1/m}$.

The final step of the proof is to derive the bounds on $\{g : |g|' \geq t^{1/m}\}$. The starting point is the Cauchy integral representation

$$S_t = \frac{1}{2\pi i} \int_\Gamma d\lambda\, e^{\lambda t} (\lambda I + H_2^n)^{-1}$$

where $n = m/2$ and Γ is a curve running from infinity with $\arg \lambda = -\pi + \varepsilon$ around the origin in the sector $\Lambda(\pi - \varepsilon)$ to infinity with $\arg \lambda = \pi - \varepsilon$ for some fixed $\varepsilon \in \langle 0, \pi/2\rangle$ with $\Lambda(\theta) = \{z \in \mathbf{C}\backslash\{0\} : |\arg z| \leq \theta\}$. If $\lambda \in \mathbf{C}\backslash\langle -\infty, 0]$ and $\alpha \in \langle 0, 1\rangle$ define $\lambda^\alpha = |\lambda|^\alpha e^{i\alpha \arg \lambda}$. Set $\omega = e^{2\pi i/n}$ and

$$c_k = -e^{-\pi i/n} \prod_{l=1, l\neq k} (\omega^k - \omega^l)^{-1}$$

for all $k \in \{1, \ldots, n\}$. Then, by partial fractions,

$$(\lambda I + H_2^n)^{-1} = \sum_{k=1}^n c_k\, (\lambda^{1/n})^{1-n}\, (\lambda_k\, I + H_2)^{-1}$$

for all $\lambda \in \mathbf{C}\backslash\langle -\infty, 0]$, where $\lambda_k = -e^{-\pi i/n}\, \lambda^{1/n}\, \omega^k$. Therefore

$$|K_t(g)| \leq \sum_{k=1}^n (2\pi)^{-1}\, |c_k| \int_\Gamma d|\lambda|\, |e^{\lambda t}|\, |\lambda|^{-1+1/n} |R_{\lambda_k}(g)| \tag{14}$$

where R_μ denotes the kernel of the operator $(\mu\, I + H_2)^{-1}$. Note that $|\arg \lambda_k| \leq \pi - \varepsilon/n$ for all $\lambda \in \Lambda(\pi - \varepsilon)$ and $k \in \{1, \ldots, n\}$. Moreover, there exist $b, c > 0$ such that

$$|R_\mu(g)| \leq c\,(|g|')^{-(D-2)} e^{-b|\mu|^{1/2}|g|'} \tag{15}$$

uniformly for all $\mu \in \Lambda(\pi - \varepsilon/n)$ and $g \in G\backslash\{e\}$ (see, for example, the appendix of [ElR1]).

Let $t > 0$ and $g \in G$ with $|g|' \geq t^{1/m}$. Choose Γ to be the contour in the complex plane formed by connecting the two line segments $L_{R,\pm} = \{\lambda \in \mathbf{C} : \arg \lambda = \pm(\pi - \varepsilon), |\lambda| \geq R\}$ and the arc $A_R = \{\lambda \in \mathbf{C} : \arg \lambda \in [-\pi + \varepsilon, \pi - \varepsilon], |\lambda| = R\}$, where $R = (b\, m^{-1}\, |g|'\, t^{-1})^{m/(m-1)}$ is chosen such that the function $x \mapsto x\, t - b\, x^{1/m} |g|'$ on $[0, \infty\rangle$ attains its minimum at R.

One then estimates for each $k \in \{1, \ldots, n\}$ that

$$\begin{aligned}\int_{A_R} d|\lambda|\, |e^{\lambda t}|\, |\lambda|^{-1+1/n} |R_{\lambda_k}(g)| &\leq c'\, t^{-2/(m-1)} (|g|')^{-D+2m/(m-1)} e^{-\omega((|g|')^m t^{-1})^{1/(m-1)}} \\ &\leq c'\, t^{-D/m} e^{-\omega((|g|')^m t^{-1})^{1/(m-1)}}\end{aligned}$$

since $|g|' \geq t^{1/m}$ and $D \geq 4 \geq 2m/(m-1)$, with $\omega = (bm^{-1})^{m/(m-1)}(m-1)$. Moreover,

$$\int_{L_{R,\pm}} d|\lambda|\, |e^{\lambda t}|\, |\lambda|^{-1+1/n} |R_{\lambda_k}(g)| \leq 2c\, e^{-2^{-1}Rt\cos\varepsilon}(|g|')^{-D+2} t^{-1/n} \int_0^\infty d\nu\, \nu^{-1+1/n} e^{-2^{-1}\nu\cos\varepsilon}$$

$$\leq c'\, t^{-D/m} e^{-\omega'((|g|')^m t^{-1})^{1/(m-1)}}$$

since $D > 2$, with $\omega' = 2^{-1}(bm^{-1})^{m/(m-1)}\cos\varepsilon$. A combination of the last two estimates and equation (14) gives the required Gaussian bounds for the kernel.

The bounds on the derivatives follow by a similar argument. First, one estimates $\|A_i S_t\|_{2\to\infty}$ as before but using the bounds $\|A_i S_t^{(2)}\|_{2\to\infty} \leq c\, t^{-D/4} t^{-1/2}$. Then one has the resolvent bound $\|A_i(\lambda I + H_2)^{-n}\|_{2\to\infty} \leq c\, \lambda^{-n+D/4+1/2}$. Consequently one obtains $\|A_i K_t\|_\infty \leq a\, t^{-(D+1)/m}$. Secondly, on the set $\{g : |g|' \geq t^{1/m}\}$ one has

$$|(A_i K_t)(g)| \leq \sum_{k=1}^n (2\pi)^{-1} |c_k| \int_\Gamma d|\lambda|\, |e^{\lambda t}|\, |\lambda|^{-1+1/n} |(A_i R_{\lambda_k})(g)|$$

in place of (14) and

$$|(A_i R_\mu)(g)| \leq a\, (|g|')^{-(D-1)} e^{-b|\mu|^{1/2}|g|'}$$

in place of (15). The latter estimate again follows from the appendix of [ElR1]. The only difference is the introduction of an extra factor $(|g|')^{-1}$, which is bounded by $t^{-1/m}$. □

Remark 3.2 The situation is quite different for higher derivatives. If $n \geq 2$ one has bounds $\|A^\alpha K_t\|_\infty \leq c\, t^{-|\alpha|/m}\, V(t)^{-1/m}$ for all $t > 0$ and α with $|\alpha| = n$ if, and only if, $G = C \times_l N$ is the local direct product of a connected compact Lie group C and a connected nilpotent Lie group N. If $m = 2$ this result is contained in [ERS2], Theorem 1.1. The general case can be deduced from the special case.

Remark 3.3 It also follows that the powers $H = \Delta^{m/2}$ of the sublaplacian $\Delta = -\sum_{i=1}^{d'} A_i^2$, with $m \geq 4$, satisfy the strong Gårding inequality (3) if, and only if, $G = C \times_l N$. The inequality (3) for H is equivalent to $\|A^\alpha \Delta^{-m/4}\|_{2\to 2} \leq \infty$ for all α with $|\alpha| = m/2$. But then by [ERS2], Theorem 4.4, this is equivalent to $G = C \times_l N$.

Remark 3.4 The foregoing arguments also apply to powers of n-th order operators. If H generates a holomorphic semigroup with a kernel satisfying n-order Gaussian bounds and if H^m also generates a holomorphic semigroup then the latter semigroup has a kernel which satisfies Gaussian bounds of order nm.

We conclude with a specific illustration of the power of these results.

Example 3.5 Let B_1, B_2, B_3 denote the representatives of the standard basis b_1, b_2, b_3 of the Lie algebra of the Euclidean motion group. Then the kernel of $H = (B_1+B_2)^4 + B_2^4 + B_3^4$ satisfies fourth-order Gaussian bounds by Theorem 1.1. Hence the kernel of the operator $((B_1 + B_2)^4 + B_2^4 + B_3^4)^2$ satisfies eighth-order Gaussian bounds by Theorem 3.1.

Acknowledgements

This work started whilst the second named author was visiting the Eindhoven University of Technology in 1998 and was completed during a second visit in 1999. These visits were made possible by financial support of the EUT and travel funds from the CMA.

References

[Dun] DUNGEY, N., Higher order operators and Gaussian bounds on Lie groups of polynomial growth. Research Report MRR 053-98, The Australian National University, Canberra, Australia, 1998.

[DER] DUNGEY, N., ELST, A.F.M. TER and ROBINSON, D.W., Asymptotics of sums of subcoercive operators. *Colloq. Math.* (2000). To appear.

[ElR1] ELST, A.F.M. TER and ROBINSON, D.W., Functional analysis of subelliptic operators on Lie groups. *J. Operator Theory* **31** (1994), 277–301.

[ElR2] ——, Weighted strongly elliptic operators on Lie groups. *J. Funct. Anal.* **125** (1994), 548–603.

[ElR3] ——, Elliptic operators on Lie groups. *Acta Appl. Math.* **44** (1996), 133–150.

[ElR4] ——, Local lower bounds on heat kernels. *Positivity* **2** (1998), 123–151.

[ERS1] ELST, A.F.M. TER, ROBINSON, D.W. and SIKORA, A., Heat kernels and Riesz transforms on nilpotent Lie groups. *Coll. Math.* **74** (1997), 191–218.

[ERS2] ——, Riesz transforms and Lie groups of polynomial growth. *J. Funct. Anal.* **162** (1999), 14–51.

[ERS3] ——, On second-order periodic elliptic operators in divergence form. Research Report MRR99-016, The Australian National University, Canberra, Australia, 1999.

[Rob] ROBINSON, D.W., *Elliptic operators and Lie groups.* Oxford Mathematical Monographs. Oxford University Press, Oxford etc., 1991.

[VSC] VAROPOULOS, N.T., SALOFF-COSTE, L. and COULHON, T., *Analysis and geometry on groups.* Cambridge Tracts in Mathematics 100. Cambridge University Press, Cambridge, 1992.