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Reduced Heat Kernels on Nilpotent Lie Groups

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Abstract: Let U be a basis representation of an irreducible unitary representation of a nilpotent Lie group G in $L_2(\mathbf{R}^k)$ and let dU denote the representation of the Lie algebra $\mathfrak{g}$ obtained by differentiation. If $b_1, \ldots, b_d$ is a basis of $\mathfrak{g}$ and $B_i = dU(b_i)$ we consider the operators

$$H = -\sum_{i,j=1}^{d} c_{ij} B_i B_j + \sum_{i=1}^{d} c_i B_i ,$$

where $C = (c_{ij})$ is a real symmetric strictly positive matrix and $c_i \in \mathbf{C}$. Then H generates a continuous semigroup S, holomorphic in the open right half-plane, with a reduced kernel κ defined by

$$(S_z \varphi)(x) = \int_{\mathbf{R}^k} dy\, \kappa_z(x; y)\, \varphi(y) .$$

We prove Gaussian off-diagonal bounds and "exponential" on-diagonal bounds for κ. For example, if $c_i = 0$ we establish that

$$|\kappa_t(x; y)| \leqq a(1 \wedge \varepsilon\mu t)^{-k/2} e^{-\lambda_1 t} e^{-d(x;y)^2 (4(1+\varepsilon)t)^{-1}}$$

for all $t > 0$ and $\varepsilon \in \langle 0, 1]$, where μ is the smallest eigenvalue of C, λ_1 is the smallest eigenvalue of H and d is a natural distance associated with the coefficients C and the representation U. Bounds are also obtained for $c_i \neq 0$ and complex t. Alternatively, if H is self-adjoint then

$$|\kappa_z(x; y)| \leqq a e^{-\lambda_1 \operatorname{Re} z} e^{-b(|x|^\alpha + |y|^\alpha)}$$

for all $z \in \mathbf{C}$ with $\operatorname{Re} z \geqq 1$, for some $\alpha \in \langle 0, 2]$.

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1. Introduction

The theory of strongly elliptic and subelliptic operators extends naturally from the Euclidean space $\mathbf{R}^d$ to a general Lie group G (see, for example, [Rob, VSC]). In particular every strongly elliptic operator has a representative affiliated with each continuous Banach space representation U of the group. This representative is a closable operator whose closure generates a continuous, holomorphic, semigroup S with an action determined by an integral kernel K,

$$S_t = \int_G dg\, K_t(g)\, U(g)\,,$$

where dg denotes left-invariant Haar measure. The kernel K is a universal, representation-independent, function whose smoothness and boundedness properties have been examined in detail. The kernel satisfies Gaussian upper bounds and for second-order operators with real coefficients it is positive and satisfies complementary Gaussian lower bounds. The derivation of good asymptotic estimates is, however, a more difficult and more specialized problem. The most detailed results have been derived for Laplacians and sublaplacians on unimodular Lie groups whose volume grows polynomially. In particular this includes all the nilpotent Lie groups. But in this latter context there are many new, interesting, representation-dependent, questions concerning the kernel.

The irreducible unitary representations of a d-dimensional, connected, simply connected, nilpotent Lie group G are described by Kirillov theory [Kir]. If $l \in \mathfrak{g}^*$, the dual of the Lie algebra $\mathfrak{g}$ of G, and if $\mathfrak{m} \subseteq \mathfrak{g}$ is a polarizing subalgebra of l then $\chi(\exp a) = \exp(2\pi i l(a))$ defines a one-dimensional representation of $M = \exp \mathfrak{m}$ from which one can induce a unitary representation of G (see, for example, [CoG]). Moreover, there is a one-to-one correspondence between the orbits in $\mathfrak{g}^*$ under the coadjoint action of the group and the unitary dual of G. The induced representations corresponding to the pair l and $\mathfrak{m}$ can be explicitly constructed on the space $L_2(\mathbf{R}^k)$, where k is the codimension of $\mathfrak{m}$ in $\mathfrak{g}$, and other elements of $\mathfrak{g}^*$ on the orbit of l and other polarizing subalgebras of l induce unitarily equivalent representations of the group on $L_2(\mathbf{R}^k)$. We assume throughout that $k \geqq 1$ since the one-dimensional representations corresponding to the case $k = 0$ offer no problem.

Now if S is the semigroup generated by the closure of a strongly elliptic or subelliptic operator in a unitary representation corresponding to l and $\mathfrak{m}$ then the action of S is given by an integral kernel κ on $\mathbf{R}^k \times \mathbf{R}^k$,

$$(S_t\varphi)(x) = \int_{\mathbf{R}^k} dy\, \kappa_t(x;y)\, \varphi(y)$$

for all $\varphi \in L_2(\mathbf{R}^k)$. We refer to κ as the reduced kernel. It is the central object of study in the sequel. The description reduced kernel is used because κ is obtained from the universal kernel K by first identifying it with a function over $\mathbf{R}^d \times \mathbf{R}^d$ by use of the exponential map and then "integrating out" the surplus variables (see [CoG] pp. 134–135). A key feature of this reduction process is that K is multiplied by a complex-valued function prior to the integration. Therefore the reality and positivity properties of K and κ can be quite distinct. As an illustration let us consider the connected simply connected three-dimensional Heisenberg group.

Let a_1, a_2, a_3 be a basis of the Lie algebra $\mathfrak{g}$ of the Heisenberg group G satisfying $[a_1, a_2] = a_3$ with the other commutators zero. Then the standard irreducible representation U of G on $L_2(\mathbf{R})$ is determined by exponentiation of the representation $dU(a_1) = -iP$, $dU(a_2) = iQ$, $dU(a_3) = iI$ of the Lie algebra $\mathfrak{g}$, where $(Pf)(x) = if'(x)$ and $(Qf)(x) = xf(x)$ for all $f \in C_c^\infty(\mathbf{R})$ and $x \in \mathbf{R}$. The Laplacian corresponding to the standard basis a_1, a_2, a_3 is represented by

$$H = -\sum_{i=1}^{3} dU(a_i)^2 = P^2 + Q^2 + I = -\frac{d^2}{dx^2} + x^2 + I \, .$$

It is a positive self-adjoint operator and in addition is real, i.e., it leaves the real subspace of $L_2(\mathbf{R})$ invariant. If, however, one considers the Laplacians corresponding to the one-parameter family of bases $b_1 = a_1 + \nu a_2$, $b_2 = a_2$, $b_3 = a_3$, with $\nu \in \mathbf{R}$, then

$$H_\nu = -\sum_{i=1}^{3} dU(b_i)^2 = (P - \nu Q)^2 + Q^2 + I = -\left(\frac{d}{dx} + i\nu x\right)^2 + x^2 + I$$

and $H_\nu, \nu \neq 0$, is not real although it is still positive and $H_0 = H$. In fact one has

$$H_\nu = e^{-i\nu Q^2/2} H e^{i\nu Q^2/2} \, .$$

Now the reduced kernel κ corresponding to H is pointwise positive and is given by Mehler's formula;

$$\kappa_t(x; y) = (\pi(1 - e^{-4t}))^{-1/2} e^{-(x+y)^2(\tanh t)/4} e^{-(x-y)^2(\coth t)/4} e^{-2t}$$

for all $t > 0$ and $x, y \in \mathbf{R}$ (see [Dav 1] Theorem 7.13). But then the kernel κ^ν corresponding to H_ν is given by

$$\kappa_t^\nu(x; y) = e^{-i\nu(x^2 - y^2)/2} \kappa_t(x; y) \, ,$$

and for $\nu \neq 0$ this is complex-valued. This is somewhat surprising as the H_ν are all Laplacians, albeit defined with different bases, and hence the corresponding universal kernels K^ν are strictly positive and satisfy Gaussian lower bounds (see, for example, [Rob] Sect. III.5). These observations clearly indicate that the analysis of the reduced kernels is quite different from that of the universal kernels.

The Heisenberg group also indicates the possible asymptotic properties of reduced kernels. For example,

$$|\kappa_t^\nu(x; x)| \sim (4\pi t)^{-1/2} e^{-tx^2}$$

for all small $t > 0$ but

$$|\kappa_t^\nu(x; x)| \sim \pi^{-1/2} e^{-x^2} e^{-2t}$$

for large t. Thus the kernel is fast decreasing on the diagonal and for large t the decrease is of the form $\exp(-\lambda_1 t)$, where $\lambda_1 = 2$ is the smallest eigenvalue of H_ν. Alternatively,

$$|\kappa_t^\nu(x + y/2; x - y/2)| \sim (4\pi t)^{-1/2} e^{-y^2/(4t)} e^{-tx^2}$$

for all small $t > 0$ but

$$|\kappa_t^\nu(x + y/2; x - y/2)| \sim \pi^{-1/2} e^{-y^2/4} e^{-2t} e^{-x^2}$$

for large t. Note that the Gaussian which dictates the off-diagonal decay for small t has an exponent 1/4 which is identical to that of the universal kernel (see [KuS]).

Our aim is to establish broadly similar asymptotic estimates for reduced kernels for a general nilpotent group. The most precise results are for pure second-order strongly elliptic operators with real symmetric coefficients but we also obtain estimates for more general second-order operators and higher-order operators with complex coefficients. There are two types of result which follow from two different approaches.

The first approach concentrates on the small t behaviour and the off-diagonal decay of the reduced kernel. It consists of extending the Nash inequality methods of [Rob] and this involves tailoring the Nash inequalities to particular unitary representations. This enables us to establish that the kernels of m^{th} order strongly elliptic operators have the expected singularity $t^{-k/m}$ for small $t > 0$. Moreover, in the case of second-order operators H with real principal coefficients one obtains Gaussian bounds $a_\varepsilon t^{-k/2} \exp(-d(x;y)^2(4(1+\varepsilon)t)^{-1})$ for all $\varepsilon, t \in \langle 0,1]$. (The distance d appearing in the estimates is the natural distance in $\mathbf{R}^k$ determined by the operator H in the particular representation.) If the operator also has real first-order coefficients these estimates can be extended to all $t > 0$ and one has an additional factor $\exp(-\lambda_1 t)$, where λ_1 is the smallest eigenvalue of H. Thus one obtains bounds which closely approximate the optimal off-diagonal decay and incorporate the optimal large t behaviour. Nevertheless, this approach gives no information about the on-diagonal decrease properties of the kernel.

The second approach concentrates on the large t behaviour and the on-diagonal properties. It consists of a blend of spectral theory and Sobolev inequalities and applies to self-adjoint strongly elliptic or subelliptic operators of all orders. One derives bounds on the reduced kernel with the optimal decay $\exp(-\lambda_1 t)$ for large t which are "exponentially" decreasing along the diagonal. Estimates of this type have been previously obtained for Markov semigroups (see, for example, [Dav 2], Chapter 4) but the proofs depend heavily upon positivity arguments and hence are not applicable in the current context.

2. Preliminaries

As a preliminary to the estimation of semigroup kernels we first recall some further elements of Kirillov's theory of unitary representations and derive some useful results on particular representations and equivalences. Secondly, we give a precise definition of the reduced kernels and derive some of their simplest properties. Thirdly, we recall the definition of strongly elliptic operators and the associated semigroup kernels. For the Kirillov theory we mostly adopt the notation and terminology of Corwin and Greenleaf [CoG].

Let G be a connected, simply connected, d-dimensional, nilpotent Lie group with Lie algebra $\mathfrak{g}$ and fix $l \in \mathfrak{g}^*$. Let $\mathfrak{m}$ denote a polarizing subalgebra for l of dimension $d_\mathfrak{m}$ and let $M = \exp(\mathfrak{m})$ denote the corresponding subgroup of G. Further let $a_1, \ldots, a_{d_\mathfrak{m}}, \ldots, a_{d_\mathfrak{m}+k}$ be a weak Malcev basis of $\mathfrak{g}$ passing through $\mathfrak{m}$, i.e., $\operatorname{span}\{a_1, \ldots, a_j\}$ is a subalgebra of $\mathfrak{g}$ for all $j \leqq d = d_\mathfrak{m} + k$ and $\mathfrak{m} = \operatorname{span}\{a_1, \ldots, a_{d_\mathfrak{m}}\}$. One can then define a one-dimensional representation of the subgroup M by setting $\chi(\exp a) = \exp(2\pi i l(a))$ for each $a \in \mathfrak{m}$ and this representation induces an irreducible unitary representation $\pi = \operatorname{ind}(M \uparrow G, \chi)$ on the Hilbert space $\mathcal{H}_\pi$ (see [CoG], Chapter 2). Explicitly, introduce a map $\gamma : \mathbf{R}^k \to G$ by

$$\gamma(x) = \gamma(x_1, \ldots, x_k) = \exp(x_1 a_{d_\mathfrak{m}+1}) \cdots \exp(x_k a_{d_\mathfrak{m}+k}) .$$

The homogeneous space $M\backslash G$ of right cosets of the subgroup M has a unique, up to a positive constant, right invariant measure $d\dot{g}$ given by the image of the Lebesgue measure of $\mathbf{R}^k$ under the analytic diffeomorphism $x \mapsto M\gamma(x)$. Next, let $\mathscr{H}_\pi$ be the Hilbert space of (equivalence classes) of Borel measurable functions $\varphi : G \to \mathbf{C}$ such that

$$\varphi(mg) = \chi(m)\,\varphi(g)$$

for all $m \in M$ and $g \in G$ and

$$\int_{M\backslash G} d\dot{g}\,|\,\varphi(g)|^2 < \infty\,.$$

Then $(\pi(g)\varphi)(h) = \varphi(hg)$ defines a unitary representation of G in $\mathscr{H}_\pi$, which is irreducible.

The map $(m,x) \mapsto m \cdot \gamma(x)$ is a diffeomorphism from $M \times \mathbf{R}^k$ onto G and allows one to define a unitary map $J : L_2(\mathbf{R}^k) \to \mathscr{H}_\pi$ by

$$(J\varphi)(m\gamma(x)) = \chi(m)\,\varphi(x)$$

for all $m \in M$ and $x \in \mathbf{R}^k$. One can then transfer the action π of G on $\mathscr{H}_\pi$ to a unitary action U on $L_2(\mathbf{R}^k)$ by use of J. This is the basis realization of π in [CoG], p. 125. The resulting representation depends on the choice of Malcev basis but each choice leads to a unitarily equivalent representation. An explicit description of the representation U is as follows. Let $E = (E_1, E_2) : G \to M \times \mathbf{R}^k$ be the inverse of the map $(m, x) \mapsto m \cdot \gamma(x)$. Then

$$(U(g)\varphi)(x) = \chi(E_1(\gamma(x)g))\,\varphi(E_2(\gamma(x)g)) \tag{1}$$

for all $g \in G$, $\varphi \in L_2(\mathbf{R}^k)$ and almost all $x \in \mathbf{R}^k$. Moreover, E_1 and E_2 are polynomial maps. Note that U depends on the weak Malcev basis only through $\operatorname{span}\{a_1, \ldots, a_{d_{\mathrm{m}}}\}$ and $a_{d_{\mathrm{m}}+1}, \ldots, a_{d_{\mathrm{m}}+k}$.

We begin by observing that the basis realization gives a simple result for the action of the representation on the L_p-spaces associated with the representation space.

Lemma 2.1. *Let U be a basis realization on $L_2(\mathbf{R}^k)$ of the induced representation π. Then U extends to a continuous isometric representation on each of the spaces $L_p(\mathbf{R}^k)$, $p \in [1, \infty]$.*

Proof. For each $g \in G$ there is a polynomial $\sigma_g : \mathbf{R}^k \to \mathbf{R}$ and a polynomial diffeomorphism $\theta_g : \mathbf{R}^k \to \mathbf{R}^k$ such that

$$(U(g)\varphi)(x) = e^{i\sigma_g(x)}\varphi(\theta_g(x)) \tag{2}$$

for all $\varphi \in L_2(\mathbf{R}^k)$. This is just a restatement of (1). It is important that the Jacobian of the transformation θ_g has modulus one, since U is unitary. Therefore

$$\|U(g)\varphi\|_1 = \int_{\mathbf{R}^k} dx\,|\varphi(\theta_g(x))| = \int_{\mathbf{R}^k} dx\,|\varphi(x)| = \|\varphi\|_1$$

for all $\varphi \in L_1(\mathbf{R}^k) \cap L_2(\mathbf{R}^k)$. Similarly, $\|U(g)\varphi\|_\infty = \|\varphi\|_\infty$ for all $\varphi \in L_2(\mathbf{R}^k) \cap L_\infty(\mathbf{R}^k)$. Hence U extends to a group of isometries on each of the L_p-spaces. Now continuity follows for $\varphi \in C_c^\infty(G)$ because

$$\|U(g)\varphi - \varphi\|_p \leqq \Bigg(\int_{\mathbf{R}^k} dx\, |\varphi(\theta_g(x)) - \varphi(x)|^p \Bigg)^{1/p} + \Bigg(\int_{\mathbf{R}^k} dx\, |e^{i\sigma_g(x)} - 1|^p |\varphi(x)|^p \Bigg)^{1/p} .$$

The continuity is verified using the properties of σ and θ together with the Lebesgue dominated convergence theorem. Strong continuity on $L_p(\mathbf{R}^k)$, $p \in [1, \infty\rangle$, follows by a density argument and weak* continuity on $L_\infty(\mathbf{R}^k)$ follows by duality. □

In the subsequent proofs of kernel bounds some weak Malcev bases are more suitable than others in the basis realizations. We initially establish Nash inequalities for a basis realization of the representation associated with a weak Malcev basis with the following ideal property:

$$[a, a_{d_{\mathfrak{m}}+j}] \in \operatorname{span}\{a_1, \ldots, a_{d_{\mathfrak{m}}+j-1}\} \quad \text{for all} \quad a \in \mathfrak{g} \quad \text{and} \quad j \in \{1, \ldots, k\} . \tag{3}$$

These inequalities are then instrumental in the derivation of bounds on the reduced kernel in this particular realization of the unitary representation. Separate arguments are necessary to extend the bounds to other realizations.

Lemma 2.2. *There exists a weak Malcev basis passing through the polarizing subalgebra* $\mathfrak{m}$ *with the ideal property* (3).

Proof. One can easily construct a weak Malcev basis of $\mathfrak{m}$ (see [CoG], Theorem 1.1.13(a)) and one has to extend this basis to a basis of $\mathfrak{g}$ with the property (3).

Therefore, given a proper subalgebra $\mathfrak{h}$ of $\mathfrak{g}$, one has to construct an element $a \in \mathfrak{g}\backslash\mathfrak{h}$ such that $[\mathfrak{g}, a] \subseteq \mathfrak{h}$. Then $\mathfrak{h}_1 = \operatorname{span}(\mathfrak{h}, a)$ is a subalgebra of $\mathfrak{g}$ with $\dim \mathfrak{h}_1 = 1 + \dim \mathfrak{h}$ and the lemma follows by induction. Let $\mathfrak{g}^{(n)}, n \in \mathbf{N}$, be the decreasing central series of $\mathfrak{g}$, i.e., $\mathfrak{g}^{(1)} = \mathfrak{g}$ and $\mathfrak{g}^{(n+1)} = [\mathfrak{g}, \mathfrak{g}^{(n)}]$. There exists $n \in \mathbf{N}$ such that $\mathfrak{g}^{(n+1)} \subseteq \mathfrak{h}$ but $\mathfrak{g}^{(n)} \not\subseteq \mathfrak{h}$. Let $a \in \mathfrak{g}^{(n)}\backslash\mathfrak{h}$. Then $[\mathfrak{g}, a] \subseteq [\mathfrak{g}, \mathfrak{g}^{(n)}] = \mathfrak{g}^{(n+1)} \subseteq \mathfrak{h}$. □

Thus for the given polarizing subalgebra $\mathfrak{m}$ one can always find a weak Malcev basis passing through $\mathfrak{m}$ which has the ideal property (3). We next examine the equivalence of two basis realizations corresponding to two weak Malcev bases passing through the same polarizing subalgebra.

Lemma 2.3. *Let* $a_1, \ldots, a_{d_{\mathfrak{m}}}, \ldots, a_d$ *and* $\tilde{a}_1, \ldots, \tilde{a}_{d_{\mathfrak{m}}}, \ldots, \tilde{a}_d$ *be two weak Malcev bases passing through* $\mathfrak{m}$ *and* U, $\tilde{U}$, *the corresponding basis realizations of the induced representation in* $L_2(\mathbf{R}^k)$. *Then there exist a polynomial* $\sigma : \mathbf{R}^k \to \mathbf{R}$, *a polynomial diffeomorphism* $\theta : \mathbf{R}^k \to \mathbf{R}^k$ *and a constant* $c > 0$ *such that the modulus of the Jacobian satisfies* $|\det \theta'(x)| = c^2$ *for all* $x \in \mathbf{R}^k$ *and*

$$U = V \tilde{U} V^* ,$$

where V *is the unitary map on* $L_2(\mathbf{R}^k)$ *defined by*

$$(V\varphi)(x) = c e^{i\sigma(x)} \varphi(\theta(x)) .$$

Proof. Define the maps $\gamma : \mathbf{R}^k \to G$, $E_1 : G \to M$, $E_2 : G \to \mathbf{R}^k$ and $J : L_2(\mathbf{R}^k) \to \mathscr{H}_\pi$ as above with respect to the basis $a_1, \ldots, a_d$ and the analogous maps $\tilde{\gamma}, \tilde{E}_1$ and $\tilde{E}_2$ with respect to the basis $\tilde{a}_1, \ldots, \tilde{a}_d$. For the definition of $\tilde{J}$ one has to be careful since one can fix only once the measure on $M\backslash G$. This we did via the bijection $x \mapsto M\gamma(x)$. Therefore the image of Lebesgue measure under the map $x \mapsto M\tilde{\gamma}(x)$ equals a positive constant times the measure $d\dot{g}$ on $M\backslash G$. Hence there exists a $c > 0$ such that

$$(\tilde{J}\varphi)(m\tilde{\gamma}(x)) = c\chi(m)\varphi(x)$$

defines a unitary map from $L_2(\mathbf{R}^k)$ onto $\mathscr{H}_\pi$.

One now easily verifies that $V = J^{-1}\tilde{J}$ intertwines the representations U and $\tilde{U}$ and V is unitary. Moreover,

$$(V\varphi)(x) = (\tilde{J}\varphi)(\gamma(x)) = c\chi(\tilde{E}_1\gamma(x))\,\varphi(\tilde{E}_2\gamma(x)) = ce^{i\sigma(x)}\varphi(\theta(x))\,,$$

where $\theta = \tilde{E}_2 \circ \gamma$ is a ploynomial from $\mathbf{R}^k$ into $\mathbf{R}^k$ and $\sigma(x) = 2\pi l(\exp^{-1}\tilde{E}_1\gamma(x))$ is a second ploynomial. It remains to show that θ is a polynomial diffeomorphism with a Jacobian whose modulus is equal to c^2.

Define $\tilde{\theta} : \mathbf{R}^k \to \mathbf{R}^k$ by $\tilde{\theta} = E_2 \circ \tilde{\gamma}$. Then for all $x \in \mathbf{R}^k$ one has

$$\theta(\tilde{\theta}(x)) = \tilde{E}_2\gamma E_2\tilde{\gamma}(x) = \tilde{E}_2((E_1(\tilde{\gamma}(x)))^{-1}\,\tilde{\gamma}(x)) = \tilde{E}_2(\tilde{\gamma}(x)) = x$$

and similarly $\tilde{\theta}\theta(x) = x$, so θ is a polynomial diffeomorphism. Then $x \to \det\theta'(x)$ and $x \mapsto \det\tilde{\theta}'(\theta(x))$ are polynomials and $\det\tilde{\theta}'(\theta(x)) \cdot \det\theta'(x) = \det(\tilde{\theta}\theta)'(x) = 1$. So $\det\theta'$ is constant and non-zero. Since V is unitary the absolute value of this constant must be equal to c^2. □

Next we give a more precise definition of the reduced kernels. Let $\pi = \operatorname{ind}(M \uparrow G, \chi)$ be the induced irreducible unitary representation on $\mathscr{H}_\pi$ described above. If $\tau \in \mathscr{S}(G)$ then the operator

$$\pi(\tau) = \int_G dg\,\tau(g)\,\pi(g)$$

is of trace class on $\mathscr{H}_\pi$ (see [CoG], Sect. 4.2). Moreover, in the basis realization U of π on $L_2(\mathbf{R}^k)$ corresponding to $l, \mathfrak{m}$ and a weak Malcev basis $a_1, \ldots, a_d$ passing through $\mathfrak{m}$, the action of $U(\tau)$ is determined by an integral kernel κ_τ,

$$(U(\tau)\varphi)(x) = \int_{\mathbf{R}^k} dy\,\kappa_\tau(x; y)\,\varphi(y)\,,$$

where $\kappa_\tau \in \mathscr{S}(\mathbf{R}^k \times \mathbf{R}^k)$. Finally, κ_τ is given in terms of τ by the reduction formula

$$\kappa_\tau(x; y) = \int_M dm\,\chi(m)\,\tau(\gamma(x)^{-1}m\gamma(y))\,, \qquad (4)$$

where χ and γ are the maps introduced earlier. This relation is of fundamental importance in the sequel.

There are some simple relationships between the kernels corresponding to unitarily equivalent representations. First we consider the relationship for kernels corresponding to different basis realizations.

Lemma 2.4. *Let U and $\tilde{U}$ be two basis realizations on $L_2(\mathbf{R}^k)$ of the induced representation π, as in Lemma* 2.3, *and κ_τ and $\tilde{\kappa}_\tau$ the kernels corresponding to* *the two representations and* $\tau \in \mathcal{S}(G)$. *Then*

$$\kappa_\tau(x; y) = c^2 e^{i(\sigma(x)-\sigma(y))} \tilde{\kappa}_\tau(\theta(x); \theta(y))$$

for all $x, y \in \mathbf{R}^k$, *where* σ, θ, c *are defined by Lemma* 2.3.

Proof. One has

$$\int_{\mathbf{R}^k} dx \int_{\mathbf{R}^k} dy\, \overline{\xi(x)}\, \kappa_\tau(x; y)\, \psi(y) = (\xi, U(\tau)\psi) = (V^*\xi, \tilde{U}(\tau)V^*\psi)$$

$$= \int_{\mathbf{R}^k} dx \int_{\mathbf{R}^k} dy\, \overline{(V^*\xi)(x)}\, \tilde{\kappa}_\tau(x; y)\, (V^*\psi)(y)$$

for all $\xi, \psi \in L_2(\mathbf{R}^k)$, where

$$(V^*\xi)(x) = c^{-1} e^{-i\sigma(\theta^{-1}(x))} \xi(\theta^{-1}(x)) .$$

Therefore, since c^2 is the absolute value of the Jacobian of the transformation $x \mapsto \theta(x)$ one immediately finds the desired relation between the two kernels. □

Secondly, we compare the kernels corresponding to shifts under the group. If π is a unitary representation of G on $\mathcal{H}_\pi$ then for each $h \in G$ one has a unitarily equivalent representation π_h given by $\pi_h(g) = \pi(hgh^{-1}) = \pi(h)\pi(g)\pi(h^{-1})$. Moreover, if π is the induced representation corresponding to l and $\mathfrak{m}$ then π_h is the induced representation corresponding to the images l_h and $\mathfrak{m}_h$ of l and $\mathfrak{m}$ under the coadjoint and adjoint action of the group, respectively. Furthermore, if U denotes the basis realization of π on $L_2(\mathbf{R}^k)$ corresponding to a weak Malcev basis passing through $\mathfrak{m}$ then there is a realization U_h corresponding to the images of l, $\mathfrak{m}$ and the basis. But for each $h \in G$ there is a polynomial $\sigma_h : \mathbf{R}^k \to \mathbf{R}$ and a polynomial diffeomorphism $\theta_h : \mathbf{R}^k \to \mathbf{R}^k$ such that

$$(U(h)\varphi)(x) = e^{i\sigma_h(x)} \varphi(\theta_h(x))$$

for all $\varphi \in L_2(\mathbf{R}^k)$. This is again a rephrasing of (1) and again the Jacobian of the transformation θ_h has modulus one. Therefore, if κ_τ and κ_τ^h are the kernels corresponding to U and U_h and $\tau \in \mathcal{S}(G)$ then

$$\kappa_\tau^h(x; y) = e^{i(\sigma_h(x)-\sigma_h(y))} \kappa_\tau(\theta_h(x); \theta_h(y)) \tag{5}$$

for all $x, y \in \mathbf{R}^k$. This is the direct analogue of the conclusion of Lemma 2.4 for the kernels corresponding to representations arising from different Malcev bases passing through the same polarizing subalgebra. Nevertheless, unitary equivalence of representations does not always imply that the kernels are related in the manner of (5). There is a third form of unitary equivalence of induced representations for which the relationship between the kernels is quite different.

If $l \in \mathfrak{g}^*$ and $\mathfrak{m}_1, \mathfrak{m}_2$ are two different polarizing subalgebras then the induced representations π_1 and π_2 corresponding to $(l, \mathfrak{m}_1)$ and $(l, \mathfrak{m}_2)$ are unitarily equivalent. But the connection between the reduced kernels $\kappa_\tau^{(1)}$ and $\kappa_\tau^{(2)}$ associated with a $\tau \in \mathcal{S}(G)$ and two weak Malcev bases is not generally of the above form. For example, consider the case that $\mathfrak{m}_1$ and $\mathfrak{m}_2$ have codimension one in $\mathfrak{g}$ but $\mathfrak{m}_1 \cap \mathfrak{m}_2$ has codimension two. Then one can choose elements $a_1, \ldots, a_d \in \mathfrak{g}$ such that $a_1, \ldots, a_{d-2}, a_{d-1}, a_d$ is a weak Malcev basis passing through $\mathfrak{m}_1$, $a_1, \ldots, a_{d-2}$, a_d, a_{d-1} is a weak Malcev basis passing through $\mathfrak{m}_2$, and $l([a_{d-1}, a_d]) = 1$. The corresponding unitarily equivalent representations U_1 and U_2 on $L_2(\mathbf{R})$ can then be expressed as

$$dU_1(a_d) = \frac{\partial}{\partial x} + 2\pi i l(a_d), \quad dU_1(a_{d-1}) = -2\pi i x + 2\pi i l(a_{d-1}),$$

$$dU_2(a_d) = 2\pi i x + 2\pi i l(a_d), \quad dU_2(a_{d-1}) = \frac{\partial}{\partial x} + 2\pi i l(a_{d-1}),$$

and

$$dU_1(a) = dU_2(a) = 2\pi i l(a)$$

for all $a \in \operatorname{span}\{a_1, \ldots, a_{d-2}\}$. Now, however, the unitary equivalence of the representations is given by Fourier transformation and the kernels are linked by the relation

$$\kappa_\tau^{(1)}(x; y) = (\mathscr{F}\kappa_\tau^{(2)})(-x; y),$$

where $\mathscr{F}$ denotes the Fourier transform with respect to both variables.

Next we recall some basic properties of strongly elliptic operators on Lie groups and the corresponding semigroups. We mostly follow the notation and terminology of [Rob].

Each strongly elliptic operator on the d-dimensional Lie group G is defined in terms of a basis $b_1, \ldots, b_d$ of the Lie algebra $\mathfrak{g}$ and a form C, i.e., a family $c_\alpha \in \mathbf{C}$ of complex-valued coefficients indexed by a multi-index $\alpha = (\alpha_1, \ldots, \alpha_d)$ with $\alpha_i \in \mathbf{N}_0$ and $|\alpha| = \alpha_1 + \cdots + \alpha_d$. The form C is called an m^{th} order strongly elliptic form if $c_\alpha = 0$ for $|\alpha| > m$ and the ellipticity constant

$$\mu_C = \inf\left\{\operatorname{Re} \sum_{\alpha:|\alpha|=m} c_\alpha (i\xi)^\alpha : \xi \in \mathbf{R}^d, |\xi| = 1\right\}$$

is strictly positive. Given the basis and the strongly elliptic form one can define a strongly elliptic element of the complex universal enveloping algebra $\mathfrak{G}$ of $\mathfrak{g}$ by

$$h_m = \sum_{\alpha:|\alpha|\leqq m} c_\alpha b^\alpha,$$

where $b^\alpha = b_1^{\alpha_1} \cdots b_d^{\alpha_d}$. There is a unique anti-automorphism $a \mapsto a^\dagger$ on $\mathfrak{G}$ such that $x^\dagger = -x$ for all $x \in \mathfrak{g}$ and the image $h_m^\dagger$ of h_m under this mapping is called the formal adjoint of h_m. It is a strongly elliptic element,

$$h_m^\dagger = \sum_{\alpha:|\alpha|\leqq m} c_\alpha^\dagger b^\alpha,$$

with coefficients $c_\alpha^\dagger$ uniquely determined by the c_α and with $c_\alpha^\dagger = \overline{c_\alpha}$ if $|\alpha| = m$.

Next let $(\mathscr{X}, U, G)$ be a continuous representation of G on the Banach space $\mathscr{X}$ and let $B_i = dU(b_i)$ denote the generator of the one-parameter subgroup $t \mapsto U(\exp(-tb_i))$. Then there is a densely defined, closable, operator H_m on χ

such that

$$H_m = dU(C) = \sum_{\alpha:|\alpha|\leqq m} c_\alpha B^\alpha$$

with $B^\alpha = B_1^{\alpha_1} \cdots B_d^{\alpha_d}$ and $D(H_m)$ is the common domain $\mathscr{X}_m$ of all the B^α with $|\alpha| = m$. The formal adjoint $H_m^\dagger$ of H_m is defined in an analogous manner from $h_m^\dagger$. These operators are called m^{th} order strongly elliptic operators and the coefficients c_α with $|\alpha| = m$ are called the principal coefficients.

Second-order operators can be reexpressed in the form

$$H_2 = -\sum_{i,j=1}^{d} c_{ij} A_i A_j + \sum_{i=1}^{d} c_i A_i + c_0 I\ ,$$

where the matrix $C = (c_{ij})$ of principal coefficients is strictly positive and symmetric. The ellipticity constant is then identified as the smallest eigenvalue of C. In the sequel we will consider second-order operators for which the principal coefficients c_{ij} are real.

The basic results we need are the following.

The closure $\overline{H_m}$ of the strongly elliptic operator H_m generates a continuous semigroup S on $\mathscr{X}$ with a universal kernel $K_t \in \mathscr{S}(G)$ which depends only on the basis $b_1, \ldots, b_d$ and the form C, i.e., $S_t = U(K_t)$ with K_t independent of the particular representation. The kernel satisfies Gaussian bounds of order m,

$$|K_t(g)| \leqq a t^{-d/m} e^{\omega t} e^{-b(|g|^m t^{-1})^{1/(m-1)}}\ ,$$

where $a, b > 0$, $\omega \geqq 0$ and $g \mapsto |g|$ is a modulus on the group. The kernel is positive if and only if the operator is of second-order with real coefficients. Finally, the kernel $K^\dagger$ corresponding to the formal adjoint satisfies

$$K_t^\dagger(g) = \Delta(g)^{-1}\overline{K_t(g^{-1})}\ ,$$

where Δ is the modular function on G.

In fact there exists $\theta \in \langle 0, \pi/2]$ such that for any $g \in G$ the function $t \mapsto K_t(g)$ extends to a function which is holomorphic in the subsector $\{z \in \mathbf{C} : |\arg z| < \theta\}$ of the right half plane and $S_t = U(K_t)$ extends to a holomorphic semigroup on the sector $\{z \in \mathbf{C} : |\arg z| < \theta\}$. Note that this subsector is representation independent. Moreover, $\theta = \pi/2$ if the principal coefficients are real. The Gaussian bounds extend to this universal subsector but the relation with the formal adjoint becomes

$$K_z^\dagger(g) = \Delta(g)^{-1}\overline{K_{\bar{z}}(g^{-1})}\ .$$

If the Lie group G is nilpotent then there are a number of properties of the semigroup generated by the strongly elliptic operator in the irreducible representations which follow from the general theory.

Let U be a basis realization on $L_2(\mathbf{R}^k)$ of the induced representation π of the nilpotent group and K_t the kernel corresponding to the strongly elliptic element h_m of $\mathfrak{G}$. Since $K_t \in \mathscr{S}(G)$ there is a reduced kernel $\kappa_t \in \mathscr{S}(\mathbf{R}^k \times \mathbf{R}^k)$ defined by the analogue of (4),

$$\kappa_t(x; y) = \int_M dm\, \chi(m) K_t(\gamma(x)^{-1} m \gamma(y))\ . \tag{6}$$

Then the semigroup S corresponding to h_m in the representation U on $L_2(\mathbf{R}^k)$ is given by

$$(S_t\varphi)(x) = (U(K_t)\varphi)(x) = \int_{\mathbf{R}^k} dy\, \kappa_t(x;y)\,\varphi(y)\,.$$

Note that as a consequence of Lemma 2.1 and the general theory of strongly elliptic operators the semigroup S extends from $L_2(\mathbf{R}^k)$ to a continuous semigroup on each of the spaces $L_p(\mathbf{R}^k)$, $p \in [1, \infty]$. Moreover,

$$\|S_t\|_{1\to 1} \leqq \|K_t\|_1, \qquad \|S_t\|_{\infty\to\infty} \leqq \|K_t^\dagger\|_1 = \|K_t\|_1$$

and, by interpolation,

$$\|S_t\|_{p\to p} \leqq \|K_t\|_1\,.$$

Since K is universal these bounds are representation independent.

Similar properties are true for complex t in the universal sector of holomorphy. The reduced kernel is defined by (6),

$$\kappa_z(x;y) = \int_M dm\,\chi(m) K_z(\gamma(x)^{-1} m\gamma(y))\,,$$

and $z \mapsto \kappa_z(x;y)$ remains holomorphic in the subsector. This follows from the Gaussian bounds on K and the estimates of Lemma 4.2.3 in [CoG]. Combination of these estimates with the Gaussian bounds guarantees that the integral relating K and κ is convergent uniformly on compact subsets of $\mathbf{R}^k \times \mathbf{R}^k$. The action of S_z is determined by κ_z within the universal subsector of holomorphy as a consequence of the general theory. Now, however, one has

$$\|S_z\|_{1\to 1} \leqq \|K_z\|_1, \qquad \|S_z\|_{\infty\to\infty} \leqq \|K_z^\dagger\|_1 = \|K_{\bar z}\|_1$$

and interpolation gives

$$\|S_z\|_{p\to p} \leqq \|K_z\|_1^{1/p}\|K_{\bar z}\|_1^{1-1/p}\,.$$

Again these bounds are representation independent.

We next establish that the S_t, $t > 0$, are compact operators on the L_p-spaces and the semigroup generator has a compact resolvent on each of these spaces.

Theorem 2.5. *Let $l \in \mathfrak{g}^*$, $a_1, \ldots, a_{d_m}, \ldots, a_{d_m+k}$ a weak Malcev basis passing through a polarizing subalgebra $\mathfrak{m}$ of l and U the corresponding basis realization on $L_2(\mathbf{R}^k)$. Next, let C be a strongly elliptic form of order $m, p \in [1,\infty]$ and $H_m = dU(C)$ the corresponding strongly elliptic operator on $L_p(\mathbf{R}^k)$. Then the spectrum of the closure of H_m is a countable discrete set with accumulation point at infinity and each point in the spectrum corresponds to an eigenvalue of finite multiplicity. Moreover, the spectrum and the eigenspaces are independent of p.*

Proof. If $t > 0$ and $p, q \in [1,\infty]$, then S_t is a continuous operator from $L_p(\mathbf{R}^k)$ into $L_q(\mathbf{R}^k)$ since $\kappa_t \in \mathscr{S}(\mathbf{R}^k \times \mathbf{R}^k)$. So for all $p \in [1,\infty]$ the operator $S_t = S_{t/3} \circ S_{t/3} \circ S_{t/3} : L_p \to L_2 \to L_2 \to L_p$ is compact since $S_{t/3} = U(K_{t/3}) : L_2 \to L_2$ is compact (see [CoG], Theorem 4.2.1).

Next, if $p \in [1,\infty\rangle$ and $\lambda > 0$ is large enough then the integral

$$(\lambda I + \overline{H_m})^{-1} = \int_0^\infty dt\, e^{-\lambda t} S_t$$

is norm convergent in $\mathscr{L}(L_p)$, so $(\lambda I + \overline{H_m})^{-1}$ is compact from L_p into L_p. By duality, the resolvent operator $(\lambda I + \overline{H_m})^{-1} = ((\lambda I + \overline{H_m^\dagger})^{-1})^*$ is also compact from L_∞ into L_∞. The spectrum of $\overline{H_m}$ must have an accumulation point at infinity since the representation space is infinite dimensional.

Finally, let $\varphi \in L_p$ be an eigenvector for the operator $\overline{H_m}$ on L_p with eigenvalue λ. Then $\varphi \in D^\infty(\overline{H_m}) = \mathscr{S}(\mathbf{R}^k)$, by [CoG] Theorem 4.1.1(i) and the Sobolev embedding theorem. Hence $\varphi \in L_q$, for all $q \in [1,\infty]$ and $H\varphi = \lambda\varphi$ in L_q. Thus the spectra and eigenspaces are independent of p. □

In Sect. 5 we will derive some crude estimates on the growth behaviour of the eigenvalues in order to establish bounds on the reduced kernel for large time.

3. Young and Nash Inequalities

Our aim is to derive bounds on the reduced semigroup kernel κ_t defined by (6) in an arbitrary irreducible unitary representation of the group. We accomplish this in two steps. First, we derive bounds with the correct singular structure for small values of t. Secondly, by a separate argument, we establish bounds with the correct asymptotic decrease for large t. The derivation of small t bounds on the universal kernel K in [Rob], Chapter IV, via Nash inequalities extends to give the small t bounds, but this extension requires a form of the Nash inequalities tailored to the particular unitary representation. We begin by considering a particular basis realization of the representation.

Let U be the basis realization of the nilpotent Lie group G corresponding to a weak Malcev basis $a_1, \ldots, a_{d_m}, \ldots, a_{d_m+k}$ passing through a polarizing subalgebra $\mathfrak{m}$ for an $l \in \mathfrak{g}^*$. If $\varphi \in L_2(\mathbf{R}^k)$ and $\psi \in L_1(G; dg)$ one can define a convolution product $\psi *_U \varphi$ by introducing

$$U(\psi) = \int_G dg\, \psi(g) U(g),$$

and then setting

$$\psi *_U \varphi = U(\psi)\varphi .$$

The aim of this section is to establish a version of Young's inequality for this product whenever the weak Malcev basis has the ideal property (3). Therefore we introduce the space $\mathscr{L}_q$ with $q \in [1,\infty]$ as the set of (equivalence classes of) measurable functions ψ over $\mathbf{R}^{d_m} \times \mathbf{R}^k$ for which the norm $|||\psi|||_q$ is finite where

$$|||\psi|||_q = \int_{\mathbf{R}^{d_m}} dw \left(\int_{\mathbf{R}^k} dx |\psi(\beta(w)\gamma(x))|^q \right)^{1/q}$$

for $q \in [1,\infty\rangle$,

$$|||\psi|||_\infty = \int_{\mathbf{R}^{d_m}} dw \operatorname*{ess\,sup}_{x \in \mathbf{R}^k} |\psi(\beta(w)\gamma(x))| ,$$

and $\beta : \mathbf{R}^{d_m} \to M$ is the map

$$\beta(w_1, \ldots, w_{d_m}) = \exp(w_1 a_1) \cdots \exp(w_{d_m} a_{d_m}) .$$

Note that the product $*_U$ and the spaces $\mathscr{L}_q$, $q \neq 1$ all depend on the choice of basis. Only the space $\mathscr{L}_1$ is independent of the basis since $\mathscr{L}_1 = L_1(G)$.

Proposition 3.1. *Let $a_1, \ldots, a_{d_m}, \ldots, a_{d_m+k}$ be a weak Malcev basis passing through $\mathfrak{m}$ which has the ideal property (3). If $p, q, r \in [1, \infty]$ and $1 + 1/r = 1/p + 1/q$ then $\psi *_U \varphi \in L_r(\mathbf{R}^k)$ and*

$$\|\psi *_U \varphi\|_r \leqq \|\varphi\|_p \, |||\psi|||_q$$

for all $\varphi \in L_p(\mathbf{R}^k) \cap L_2(\mathbf{R}^k)$ and $\psi \in \mathscr{L}_q \cap L_1(G)$. Hence the map $(\psi, \varphi) \mapsto \psi *_U \varphi$ from $(\mathscr{L}_q \cap \mathscr{L}_1) \times (L_p(\mathbf{R}^k) \cap L_2(\mathbf{R}^k))$ into $L_r(\mathbf{R}^k)$ can be extended to a map from $\mathscr{L}_q \times L_p(\mathbf{R}^k)$ into $L_r(\mathbf{R}^k)$, which we will still denote by $*_U$, and

$$\|\psi *_U \varphi\|_r \leqq \|\varphi\|_p \, |||\psi|||_q$$

for all $\varphi \in L_p(\mathbf{R}^k)$ and $\psi \in \mathscr{L}_q$.

Remark 3.2. The inequalities of the proposition correspond to the classical Young inequalities when $G = \mathbf{R}^k$ and U is the action by translation.

The proof of the proposition relies on a combinatorial result for products of exponentials, an interpolation property of the spaces $\mathscr{L}_q$ and adaptation of the interpolation proof of the classical Young inequalities.

Lemma 3.3. *Let $a_1, \ldots, a_{d_m}, \ldots, a_{d_m+k}$ be a weak Malcev basis passing through $\mathfrak{m}$ which has the ideal property (3). If $w \in \mathbf{R}^{d_m}$ and $x, y \in \mathbf{R}^k$ then there exist an $m (= m_{w,x,y}) \in M$ and a $z (= z_{w,x,y}) \in \mathbf{R}^k$ such that*

$$\gamma(x)\, \beta(w)\, \gamma(y) = m \gamma(z) .$$

Moreover, there exist polynomials $p_1, \ldots, p_{k-1}$ such that

$$\begin{aligned}
z_k &= y_k + x_k , \\
z_{k-1} &= y_{k-1} + x_{k-1} + p_{k-1}(w, y_k, x_k) , \\
z_{k-2} &= y_{k-2} + x_{k-2} + p_{k-2}(w, y_k, x_k, y_{k-1}, x_{k-1}) , \\
&\vdots \\
z_1 &= y_1 + x_1 + p_1(w, y_k, x_k, \ldots, y_2, x_2) ,
\end{aligned}$$

where the p_j only depend on the indicated variables.

Proof. By using the Baker–Campbell–Hausdorff formula one can reexpress the product $\gamma(x)\, \beta(w)\, \gamma(y)$ as a single exponential and then separate the terms starting with $z_k, z_{k-1}, \ldots$. It follows from this process and the ideal property (3) of the Malcev basis that the product can be expressed in the desired form. □

The most important implication of the lemma for the subsequent calculations is summarized in the following corollary.

Corollary 3.4. *If $z_{w,x,y}$ is defined by Lemma 3.3, then the maps $x \mapsto z_{w,x,y}$ and $y \mapsto z_{w,x,y}$ from $\mathbf{R}^k$ into $\mathbf{R}^k$ are bijections and have Jacobian one.*

Proof. The Jacobi matrices are triangular and the diagonal elements are all equal to one. Therefore the determinants have value one. □

Lemma 3.5. *Let $p_1, p_2, q_1, q_2 \in [1, \infty]$. If T is a linear operator from the space $\mathscr{L}_{p_1} \cap \mathscr{L}_{p_2}$ to the space $L_{q_1}(\mathbf{R}^k) \cap L_{q_2}(\mathbf{R}^k)$ and*

$$\|T\psi\|_{q_1} \leqq M_1 |||\psi|||_{p_1}\,, \qquad \|T\psi\|_{q_2} \leqq M_2 |||\psi|||_{p_2}\,,$$

then T extends to a bounded linear operator from $\mathscr{L}_{p_\gamma}$ to $L_{q_\gamma}(\mathbf{R}^k)$ with norm less than or equal to $M_1^{1-\gamma} M_2^{\gamma}$, where

$$p_\gamma^{-1} = (1-\gamma) p_1^{-1} + \gamma p_2^{-1}, \qquad q_\gamma^{-1} = (1-\gamma) q_1^{-1} + \gamma q_2^{-1}$$

and $\gamma \in [0, 1]$.

This is just a variant of the Riesz–Thorin interpolation theorem which is established by a slight modification of the arguments used to prove the classical version.

Now we are prepared to prove the proposition.

Proof of Proposition 3.1. First, consider the case $p = q = r = 1$. Let $\varphi \in L_1(\mathbf{R}^k) \cap L_2(\mathbf{R}^k)$ and $\psi \in L_1(G)$. Since U extends to an isometric continuous representation on $L_1(\mathbf{R}^k)$ one has

$$\|\psi *_U \varphi\|_1 = \|U(\psi)\varphi\|_1 \leqq \|\psi\|_1 \|\varphi\|_1\,. \tag{7}$$

Since $\mathscr{L}_1 = L_1(G)$ and $|||\psi|||_1 = \|\psi\|_1$ this establishes the special case of the desired result.

Secondly, we consider the case $p = 1$ and $q = r = \infty$. Let $\varphi \in L_1(\mathbf{R}^k) \cap L_2(\mathbf{R}^k)$ and $\psi \in \mathscr{L}_1 \cap \mathscr{L}_\infty$. Then it follows from (1) that

$$\begin{aligned}(U(\psi)\varphi)(x) &= \int_{\mathbf{R}^{dm}} dw \int_{\mathbf{R}^k} dy\, \psi(\beta(w)\gamma(y))\,(U(\beta(w)\gamma(y))\varphi)(x) \\ &= \int_{\mathbf{R}^{dm}} dw \int_{\mathbf{R}^k} dy\, \psi(\beta(w)\gamma(y))\,\chi(m_{w,x,y})\,\varphi(z_{w,x,y})\,,\end{aligned}$$

where we have used the notation of Lemma 3.3 in the last step. Therefore

$$(\psi *_U \varphi)(x) = \int_{\mathbf{R}^{dm}} dw \int_{\mathbf{R}^k} dy\, \psi(\beta(w)\gamma(y))\,\chi(m_{w,x,y})\,\varphi(z_{w,x,y})\,,$$

and hence

$$|(\psi *_U \varphi)(x)| \leqq \int_{\mathbf{R}^{dm}} dw \int_{\mathbf{R}^k} dy\, |\psi(\beta(w)\gamma(y))| \cdot |\varphi(z_{w,x,y})|\,. \tag{8}$$

Therefore

$$
\begin{aligned}
\|\psi *_U \varphi\|_\infty &\leqq \sup_{x\in\mathbf{R}^k} \int_{\mathbf{R}^{dm}} dw \int_{\mathbf{R}^k} dy |\psi(\beta(w)\gamma(y))| \cdot |\varphi(z_{w,x,y})| \\
&\leqq \sup_{x\in\mathbf{R}^k} \int_{\mathbf{R}^{dm}} dw \int_{\mathbf{R}^k} dy \sup_{y'\in\mathbf{R}^k} |\psi(\beta(w)\gamma(y'))| \cdot |\varphi(z_{w,x,y})| \\
&= \int_{\mathbf{R}^{dm}} dw \int_{\mathbf{R}^k} dz \sup_{y'\in\mathbf{R}^k} |\psi(\beta(w)\gamma(y'))| \cdot |\varphi(z)| \\
&= |||\psi|||_\infty \|\varphi\|_1 ,
\end{aligned}
\tag{9}
$$

where the third step uses a change of variables $y \mapsto z_{w,x,y}$ and Corollary 3.4.

Thirdly, we interpolate between the estimates (7) and (9).

The estimate (7) states that for $\varphi \in L_1(\mathbf{R}^k) \cap L_2(\mathbf{R}^k)$ the linear operator T_φ defined by

$$T_\varphi \psi = \psi *_U \varphi$$

is bounded from $\mathscr{L}_1$ to $L_1(\mathbf{R}^k)$ and

$$\|T_\varphi \psi\|_1 \leqq \|\varphi\|_1 \, |||\psi|||_1 \, .$$

Similarly, (9) states that the operator T_φ is bounded from $\mathscr{L}_1 \cap \mathscr{L}_\infty$ to $L_\infty(\mathbf{R}^k)$ and

$$\|T_\varphi \psi\|_\infty \leqq \|\varphi\|_1 \, |||\psi|||_\infty \, .$$

Therefore it follows from Lemma 3.5 that T_φ extends to a bounded operator from $\mathscr{L}_q$ to $L_q(\mathbf{R}^k)$ for each $q \in [1, \infty]$ and

$$\|\psi *_U \varphi\|_q = \|T_\varphi \psi\|_q \leqq \|\varphi\|_1 \, |||\psi|||_q \, . \tag{10}$$

Fourthly, the Hölder inequality gives

$$
\begin{aligned}
\|\psi *_U \varphi\|_\infty &\leqq \sup_{x\in\mathbf{R}^k} \int_{\mathbf{R}^{dm}} dw \int_{\mathbf{R}^k} dy |\psi(\beta(w)\gamma(y))| \cdot |\varphi(z_{w,x,y})| \\
&\leqq \sup_{x\in\mathbf{R}^k} \int_{\mathbf{R}^{dm}} dw \left(\int_{\mathbf{R}^k} dy |\psi(\beta(w)\gamma(y))|^q \right)^{1/q} \left(\int_{\mathbf{R}^k} dy |\varphi(z_{w,x,y})|^r \right)^{1/r}
\end{aligned}
$$

for all $\varphi \in L_r(\mathbf{R}^k) \cap L_2(\mathbf{R}^k)$ and $\psi \in \mathscr{L}_q \cap L_1$ whenever $1/q + 1/r = 1$. Then by a change of variables one obtains the bounds

$$\|\psi *_U \varphi\|_\infty \leqq \|\varphi\|_r \, |||\psi|||_q \, . \tag{11}$$

Therefore if U_ψ is defined as an operator from $L_r(\mathbf{R}^k) \cap L_2(\mathbf{R}^k)$ to $L_\infty(\mathbf{R}^k)$ by

$$U_\psi \varphi = \psi *_U \varphi$$

for $\psi \in \mathscr{L}_q$ then (10), together with (11), gives bounds

$$\|U_\psi \varphi\|_q \leqq |||\psi|||_q \|\varphi\|_1 \, , \qquad \|U_\psi \varphi\|_\infty \leqq |||\psi|||_q \|\varphi\|_r \, .$$

Hence U_ψ extends to a bounded linear operator from $L_{p_\gamma}(\mathbf{R}^k)$ to $L_{q_\gamma}(\mathbf{R}^k)$ where $p_\gamma^{-1} = \gamma r^{-1} + (1-\gamma)$, $q_\gamma^{-1} = (1-\gamma)q^{-1}$ and $\gamma \in [0,1]$. Moreover,

$$\|\psi *_U \varphi\|_{q_\gamma} = \|U_\psi \varphi\|_{q_\gamma} \leqq |||\psi|||_q \|\varphi\|_{p_\gamma}$$

by the usual Riesz–Thorin theorem. But $1 + q_\gamma^{-1} = q^{-1} + p_\gamma^{-1}$ and hence one obtains the desired result. □

The version of Young's inequalities given in Proposition 3.1 can be used to derive Nash inequalities by the arguments of [Rob], Chapter III, Sect. 3.

Let $b_1, \ldots, b_{d'}$ be an algebraic basis of $\mathfrak{g}$, $B_i = dU(b_i)$ the representatives on $L_2(\mathbf{R}^k)$ and $L'_{2;n}(\mathbf{R}^k)$ the corresponding C^n-subspaces (see [Rob], Sect. IV.4). So

$$L'_{2;n}(\mathbf{R}^k) = \bigcap_{i_1,\ldots,i_n \in \{1,\ldots,d'\}} D(B_{i_1} \cdots B_{i_n}) \,.$$

Next let ρ denote the subelliptic distance associated with the basis and $|\cdot|'$ the corresponding modulus, i.e., $|g|' = \rho(g;e)$ (see [Rob], Sect. IV.4). If $\alpha : [0,1] \to G$ is an absolutely continuous path from the identity e to g with tangents in the space spanned by $b_1, \ldots, b_{d'}$ then there are $\alpha_i \in L_\infty([0,1])$ such that

$$\frac{d\psi(\alpha(t))}{dt} = \sum_{i=1}^{d'} \alpha_i(t)\,(\tilde{B}_i \psi)(\alpha(t))$$

for all $\psi \in C^\infty(G)$, where $\tilde{B}_i$ is the left invariant vector field on G corresponding to the direction b_i. We define

$$|g|' = \inf_\alpha \int_0^1 dt \left(\sum_{i=1}^{d'} \alpha_i(t)^2 \right)^{1/2} ,$$

where the infimum is over all possible paths. Therefore

$$((I - U(g)\varphi)(x) = \int_0^1 dt \sum_{i=1}^{d'} \alpha_i(t)\,(U(\alpha(t))B_i\varphi)(x)$$

for all $\varphi \in C_c^\infty(\mathbf{R}^k)$ and consequently

$$\|(I - U(g))\varphi\|_2 \leqq \int_0^1 dt \left(\sum_{i=1}^{d'} \alpha_i(t)^2 \right)^{1/2} \left(\sum_{i=1}^{d'} \|B_i \varphi\|_2^2 \right)^{1/2} .$$

Optimizing this last estimate over the possible paths α one deduces that

$$\|(I - U(g))\varphi\|_2 \leqq |g|' \left(\sum_{i=1}^{d'} \|B_i \varphi\|_2^2 \right)^{1/2} .$$

Therefore if $\psi \in L_1(G)$ is a positive function with $\|\psi\|_1 = 1$ one has

$$\|(I - U(\psi))\varphi\|_2 \leqq \int_G dg\, \psi(g)\, |g|' \left(\sum_{i=1}^{d'} \|B_i \varphi\|_2^2 \right)^{1/2} . \tag{12}$$

This bound together with Young's inequality now gives the Nash inequality.

Proposition 3.6. *Let $a_1, \ldots, a_{d_m}, \ldots, a_{d_m+k}$ be a weak Malcev basis passing through $\mathfrak{m}$ which has the ideal property* (3). *For each positive $\psi \in L_1(G)$ with $\|\psi\|_1 = 1$ and each algebraic basis $b_1, \ldots, b_{d'}$ of $\mathfrak{g}$,*

$$\|\varphi\|_2 \leqq \int_G dg\, \psi(g)\, |g|' \left(\sum_{i=1}^{d'} \|B_i \varphi\|_2^2 \right)^{1/2} + |||\psi|||_2 \|\varphi\|_1 \tag{13}$$

for all $\varphi \in L'_{2;1}(\mathbf{R}^k) \cap L_1(\mathbf{R}^k)$. In particular

$$\|\varphi\|_2 \leqq \varepsilon \left(\sum_{i=1}^{d'} \|B_i \varphi\|_2^2 \right)^{1/2} + (|||\psi_\varepsilon|||_2 / |||\psi_\varepsilon|||_1) \|\varphi\|_1 , \tag{14}$$

for each $\varepsilon > 0$ where ψ_ε denotes a non-zero, positive, integrable, function with support in the ball $B'_\varepsilon = \{g \in G : |g|' < \varepsilon\}$.

Proof. First, one has the obvious identity

$$\|\varphi\|_2 \leqq \|(I - U(\psi))\varphi\|_2 + \|U(\psi)\varphi\|_2 ,$$

and since $U(\psi)\varphi = \psi *_U \varphi$ the initial statement of the proposition follows from Proposition 3.1 and (12). The second statement is an immediate consequence of choosing $\psi = \psi_\varepsilon / |||\psi_\varepsilon|||_1$. □

The Nash inequalities (13) can in principle be optimized by minimizing the right-hand side with respect to the choice of ψ. The most practical way of tackling this problem appears to be through optimization of (14) with respect to ε and with ψ_ε a characteristic function. But this requires an efficient bound on $\varepsilon \mapsto |||\chi_\varepsilon|||_2 / |||\chi_\varepsilon|||_1$, where χ_ε is the characteristic function of the ball B'_ε. The L_1-norm $|||\chi_\varepsilon|||_1$ can be easily estimated because

$$|||\chi_\varepsilon|||_1 = \|\chi_\varepsilon\|_1 = |B'_\varepsilon| .$$

The main problem is to estimate $|||\chi_\varepsilon|||_2$. This is straightforward if $b_1, \ldots, b_{d'}$ is a vector space basis of $\mathfrak{g}$. Then the corresponding modulus $|g|'$ equals the full modulus $|g|$ and the image of $g \mapsto |g|$ under the exponential map is locally equivalent to the Euclidean norm on $\mathbf{R}^d$. Hence one has bounds

$$\alpha^{-1} \varepsilon^{d_m + k/2} \leqq |||\chi_\varepsilon|||_2 \leqq \alpha \varepsilon^{d_m + k/2}$$

for some $\alpha > 0$ and all $\varepsilon \in \langle 0, 1]$. Since one also has estimates $|||\chi_\varepsilon|||_1 \geqq \alpha' \varepsilon^d$ for small ε, with $d = d_{\mathfrak{m}} + k$ the dimension of the group, this gives bounds

$$|||\chi_\varepsilon|||_2 / |||\chi_\varepsilon|||_1 \leqq \alpha \varepsilon^{-k/2} \tag{15}$$

on the ratio which are valid for all $\varepsilon \in \langle 0, 1]$.

For an algebraic basis $b_1, \ldots, b_{d'}$ the $|||\chi_\varepsilon|||_1$ estimates are clear since one has estimates

$$\alpha^{-1}\varepsilon^{D'} \leqq |B'_\varepsilon| \leqq \alpha\varepsilon^{D'}$$

for $\varepsilon \in \langle 0, 1]$ and

$$\alpha_1^{-1}\varepsilon^{D} \leqq |B'_\varepsilon| \leqq \alpha_1\varepsilon^{D}$$

for $\varepsilon \geqq 1$, for appropriate $\alpha, \alpha_1 > 0$. The two dimensions D' and D are usually distinct and $D' = D$ if and only if G is stratified and $b_1, \ldots, b_{d'}$ spans the first subspace in its grading (see [VSC], Remark IV.5.9). The estimation of the L_2-norm is more difficult.

It is possible to make a crude estimate of $|||\chi_\varepsilon|||_2$ for small ε by remarking that there is a compact subset of $\mathbf{R}^d$ which contains the support of the images of $\chi_\varepsilon, \varepsilon \in \langle 0, 1]$ under the exponential map. Therefore

$$\alpha_2^{-1}\varepsilon^{D'} \leqq |||\chi_\varepsilon|||_2 \leqq \alpha_2\varepsilon^{D'/2}$$

for all $\varepsilon \in \langle 0, 1]$ and a suitable $\alpha_2 \geqq 0$. But a more precise estimate requires more detailed information on the relationship between the Malcev basis $a_1, \ldots, a_d$ and the algebraic basis $b_1, \ldots, b_{d'}$. For example, if G is stratified, $b_1, \ldots, b_{d'}$ is a basis for the first subspace of its grading and each a_i is a commutator in the b_j, then one can find good bounds on $|||\chi_\varepsilon|||_2$.

Our inability to establish good estimates on $|||\chi_\varepsilon|||_2$ limits the usefulness of the Nash inequalities for subelliptic operators. Nevertheless, the small ε estimates (15) yield inequalities which can be usefully applied to the analysis of strongly elliptic operators.

Let $b_1, \ldots, b_d$ be a vector space basis of $\mathfrak{g}$. Then combination of (14) and (15) gives bounds

$$\|\varphi\|_2 \leqq \varepsilon\left(\sum_{i=1}^{d}\|B_i\varphi\|_2^2\right)^{1/2} + \alpha\varepsilon^{-k/2}\|\varphi\|_1$$

for all $\varphi \in L_{2;1}(\mathbf{R}^k) \cap L_1(\mathbf{R}^k)$ and all $\varepsilon \in \langle 0, 1]$. But if one introduces the norms

$$\Gamma_{2,1}(\varphi) = \left(\sum_{i=1}^{d}\|B_i\varphi\|_2^2 + \gamma^2\|\varphi\|_2^2\right)^{1/2}$$

on $L_{2;1}(\mathbf{R}^k)$ with $\gamma \in \langle 0, 1]$ one then has bounds

$$\|\varphi\|_2 \leqq \varepsilon\Gamma_{2;1}(\varphi) + \alpha\varepsilon^{-k/2}\|\varphi\|_1$$

valid for all $\varepsilon \in \langle 0, 1]$ and for $\varepsilon \geqq 1/\gamma$. But these bounds can be simply modified to hold for all $\varepsilon > 0$ and then optimized over ε.

Corollary 3.7. *Let $a_1, \ldots, a_{d_m}, \ldots, a_{d_m+k}$ be a weak Malcev basis passing through $\mathfrak{m}$ with the ideal property* (3) *and let $b_1, \ldots, b_d$ a vector space basis for $\mathfrak{g}$. Then there is an $\alpha > 0$ such that*

$$\|\varphi\|_2 \leqq \varepsilon\Gamma_{2;1}(\varphi) + \alpha(\gamma\varepsilon)^{-k/2}\|\varphi\|_1$$

for all $\varphi \in L_{2;1} \cap L_1$, *all* $\varepsilon > 0$ *and all* $\gamma \in \langle 0, 1]$. *Consequently, there is an* $\alpha_1 > 0$ *such that*

$$\|\varphi\|_2 \leqq \alpha_1 (\Gamma_{2;1}(\varphi)/(\gamma\|\varphi\|_1))^{k/(k+2)} \|\varphi\|_1$$

for all $\varphi \in L_{2,1} \cap L_1$ *and all* $\gamma \in \langle 0, 1]$.

Remark 3.8. The above Nash inequalities are expressed, or are expressable, in terms of the C^1-seminorms $N_{2,1}$, or the C^1-norms $\| \cdot \|_{2,1}$ used in [Rob]. Similar results can, however, be formulated with the C^n-seminorms and C^n-norms by the use of embedding properties. In particular for each $n \in \{2, 3, \ldots\}$ there is an $\alpha_n > 0$ such that

$$N_{2;1}(\varphi) \leqq \varepsilon^{n-1} N_{2;n}(\varphi) + \alpha_n \varepsilon^{-1} \|\varphi\|_2$$

for all $\varphi \in L_{2;n}$ and all $\varepsilon \in \langle 0, 1]$ (see [Rob], Lemma III.3.3). Similarly,

$$\|\varphi\|_{2,1} \leqq \varepsilon^{n-1} \|\varphi\|_{2;n} + \alpha'_n \varepsilon^{-1} \|\varphi\|_2$$

for all $\varphi \in L_{2,n}$ and all $\varepsilon > 0$.

In the sequel we need a variation of the above results which is formulated in terms of a second representation U° of G associated with U. The action of U is given by (1) which can be reformulated with the notation of (2) as

$$(U(g)\varphi)(x) = e^{\imath\sigma_g(x)} \varphi(\theta_g(x)),$$

and then the action of U° is defined by

$$(U^\circ(g)\varphi)(x) = \varphi(\theta_g(x)).$$

It then follows as for U that U° is an isometric continuous representation on $L_p(\mathbf{R}^k)$ for $p \in [1, \infty]$. Note that if $b \in \mathfrak{g}$ and $B = dU(b)$ then

$$(B\varphi)(x) = \sum_{n=1}^{k} X_n(x) \frac{\partial \varphi}{\partial x_n}(x) + iY(x)\varphi(x)$$

with X_n and Y real polynomials. Hence if $B^\circ = dU^\circ(b)$ one has

$$(B^\circ \varphi)(x) = \sum_{n=1}^{k} X_n(x) \frac{\partial \varphi}{\partial x_n}(x),$$

i.e., B° is the principal part of the first-order partial differential operator B.

Now if one defines a convolution product $\psi *_{U^\circ} \varphi$ by setting

$$\psi *_{U^\circ} \varphi = U^\circ(\psi)\varphi,$$

then the generalized Young inequality is again valid.

Proposition 3.9. *Let* $a_1, \ldots, a_{d_m}, \ldots, a_{d_m+k}$ *be a weak Malcev basis passing through* $\mathfrak{m}$ *which has the ideal property* (3). *If* $p, q, r \in [1, \infty]$ *and* $1 + 1/r = 1/p + 1/q$ *then* $(\psi, \varphi) \mapsto \psi *_{U^\circ} \varphi$ *from* $(\mathscr{L}_q \cap \mathscr{L}_1) \times (L_p(\mathbf{R}^k) \cap L_2(\mathbf{R}^k))$ *into* $L_r(\mathbf{R}^k)$ *extends to a map from* $\mathscr{L}_q \times L_p(\mathbf{R}^k)$ *into* $L_r(\mathbf{R}^k)$ *which satisfies*

$$\|\psi *_{U^\circ} \varphi\|_r \leqq \|\varphi\|_p \, |||\psi|||_q$$

for all $\varphi \in L_p(\mathbf{R}^k)$ *and* $\psi \in \mathscr{L}_q$.

Proof. The proof is very similar to that for the representation U but the starting point is now the identity

$$(U^\circ(\psi)\varphi)(x) = \int_{\mathbf{R}^{d_m}} dw \int_{\mathbf{R}^k} dy\, \psi(\beta(w)\gamma(y))\,\varphi(z_{w,x,y}),$$

which then gives

$$|(U^\circ(\psi)\varphi)(x)| \leqq \int_{\mathbf{R}^{d_m}} dw \int_{\mathbf{R}^k} dy |\psi(\beta(w)\gamma(y))| \cdot |\varphi(z_{w,x,y})|$$

in direct analogy with (8). The point is that the phase which distinguishes between the action of U and U° plays no role in this estimate or in the subsequent estimates that are essential in the proof. □

One can now derive a version of the Nash inequalities suited to the seminorms associated with the operators $B_i^\circ = dU^\circ(b_i)$. One has

$$\|(I - U^\circ(\psi))\varphi\|_2 \leqq \int_G dg\; \psi(g)|g| \left(\sum_{i=1}^{d} \|B_i^\circ \varphi\|_2^2\right)^{1/2}$$

in direct analogy with (12). Therefore if

$$\Gamma_{2;1}^\circ(\varphi) = \left(\sum_{i=1}^{d} \|B_i^\circ \varphi\|_2^2 + \gamma^2 \|\varphi\|_2^2\right)^{1/2}$$

with $\gamma \in \langle 0, 1]$ one obtains the following version of Corollary 3.7.

Corollary 3.10. *Let $a_1, \ldots, a_{d_m}, \ldots, a_{d_m+k}$ be a weak Malcev basis passing through $\mathfrak{m}$ with the ideal property* (3) *and let $b_1, \ldots, b_d$ a vector space basis for $\mathfrak{g}$. Then there is an $\alpha > 0$ such that*

$$\|\varphi\|_2 \leqq \varepsilon \Gamma_{2;1}^\circ(\varphi) + \alpha(\gamma\varepsilon)^{-k/2}\|\varphi\|_1$$

for all $\varphi \in L_{2;1} \cap L_1$, all $\varepsilon > 0$ and all $\gamma \in \langle 0, 1]$. Consequently, there is an $\alpha_1 > 0$ such that

$$\|\varphi\|_2 \leqq \alpha_1(\Gamma_{2;1}^\circ(\varphi)/(\gamma\|\varphi\|_1))^{k/(k+2)}\|\varphi\|_1$$

for all $\varphi \in L_{2;1} \cap L_1$ and all $\gamma \in \langle 0, 1]$.

The proof is a repetition of the previous arguments but with Proposition 3.1 replaced by Proposition 3.9.

4. Kernel Bounds: Small *t*

In this section we use the Nash inequalities to obtain bounds on the reduced kernel κ_t associated with the strongly elliptic semigroup S_t. Since the Nash inequalities are established for weak Malcev bases with the ideal property (3) we first derive kernel bounds in a representation realized with respect to such a basis. Subsequently we remove the ideal property by making a unitary transformation.

Our arguments are based on the Davies perturbation method as described in [Rob] Sect. IV.2. A complication occurs, however, since the present operators are in general not real. Therefore we have to work on the complex $L_p(\mathbf{R}^k)$ spaces. One cannot restrict attention to the subspaces spanned by the real-valued functions as in [Rob].

Let U be a basis realization on $L_2(\mathbf{R}^k)$ of the induced representation π and $b_1, \ldots, b_d$ a (vector space) basis of the Lie algebra $\mathfrak{g}$. If $B_j = dU(b_j)$ for $j \in \{1, \ldots, d\}$, then

$$(B_j\varphi)(x) = \sum_{n=1}^{k} X_{jn}(x)\frac{\partial\varphi}{\partial x_n}(x) + iY_j(x)\,\varphi(x)$$

with X_{jn} and Y_j real polynomials. Moreover, if U° is the representation of G defined at the end of Sect. 3, then $B_j^\circ = dU^\circ(b_j)$ is the principal part of B_j, i.e.,

$$(B_j^\circ\varphi)(x) = \sum_{n=1}^{k} X_{jn}(x)\frac{\partial\varphi}{\partial x_n}(x)\,.$$

Next, if $C = (c_{ij})$ is a real, symmetric, strictly positive-definite matrix we define

$$D_C = \{\psi \in C_c^\infty(\mathbf{R}^k) : \psi \text{ real valued and } \sum_{i,j=1}^{d} c_{ij}\,(B_i^\circ\psi)(x)\,(B_j^\circ\psi)(x) \leqq 1 \text{ for all } x \in \mathbf{R}^k\}\,,$$

and then the distance $d_{U,C} : \mathbf{R}^k \times \mathbf{R}^k \to [0,\infty\rangle$ is introduced by

$$d_{U,C}(x;y) = \sup_{\psi\in D_C} |\psi(x) - \psi(y)|\,.$$

The first theorem of this section gives kernel bounds for second-order operators

$$H = -\sum_{i,j=1}^{d} c_{ij}B_iB_j + \sum_{i=1}^{d} c_iB_i$$

with the matrix C as principal coefficients and with real first-order coefficients c_i. The large time behaviour of the bounds is governed by the smallest eigenvalue λ_1 of the self-adjoint principal part

$$H_0 = -\sum_{i,j=1}^{d} c_{ij}B_iB_j$$

of H acting on $L_2(\mathbf{R}^k)$, i.e.,

$$\begin{aligned}\lambda_1 &= \min\{(\varphi, H_0\varphi) : \varphi \in \mathcal{S}(\mathbf{R}^k) \text{ and } \|\varphi\|_2 = 1\}\\ &= \min\{(\varphi, H\varphi) : \varphi \in \mathcal{S}(\mathbf{R}^k) \text{ and } \|\varphi\|_2 = 1\}\,.\end{aligned}$$

Note that $\lambda_1 > 0$ since $k \geqq 1$. Indeed if $\lambda_1 = 0$ then the corresponding normalized eigenfunction φ_1 would satisfy

$$\sum_{i,j=1}^{d} c_{ij}(B_i\varphi_1, B_j\varphi_1) = 0$$

and, since C is strictly positive, $B_i\varphi_1 = 0$ for all $i \in \{1,\dots,d\}$. But this implies that $U(g)\varphi_1 = \varphi_1$ for all $g \in G$ which is impossible since U is irreducible and non-trivial. Further note that λ_1 is a unitary invariant, i.e., if U and $\widetilde{U}$ are unitarily equivalent representations, with $H, \widetilde{H}$ the corresponding strongly elliptic operators and $\lambda_1, \tilde{\lambda}_1$ the lowest eigenvalues then $\lambda_1 = \tilde{\lambda}_1$. This invariance will play a minor role in the following proof.

Theorem 4.1. *Let $l \in \mathfrak{g}^*$, $a_1,\dots,a_{d_{\mathfrak{m}}},\dots,a_{d_{\mathfrak{m}}+k}$ be a weak Malcev basis passing through a polarizing subalgebra $\mathfrak{m}$ of l and U the corresponding basis realization in $L_2(\mathbf{R}^k)$. Let H be a second-order operator associated with the real, symmetric, strictly positive-definite matrix $C = (c_{ij})$, the first-order coefficients $c_i \in \mathbf{R}$ and the basis $b_1,\dots,b_d$ of $\mathfrak{g}$. Further let κ_t denote the corresponding reduced kernel. Then there exists an $a > 0$, independent of the coefficients (C, c), such that*

$$|\kappa_t(x;y)| \leqq a(1 \wedge \varepsilon\mu t)^{-k/2} e^{-\lambda_1 t} \inf_{\rho \geqq 0} \exp\left(\rho^2(1+\varepsilon)t - \rho(d_{U,C}(x;y) - vt)\right)$$

uniformly for all $t > 0$, $x, y \in \mathbf{R}^k$ and $\varepsilon \in \langle 0, 1]$, where μ is the lowest eigenvalue of C,

$$\lambda_1 = \min\{(\varphi, H\varphi) : \varphi \in \mathscr{S}(\mathbf{R}^k) \text{ and } \|\varphi\|_2 = 1\}$$

and $v = |c|\mu^{-1/2}$ with $|c|$ the l_2-norm of the first-order coefficients.

Therefore if $d_{U,C}(x;y) \leqq vt$ then

$$|\kappa_t(x;y)| \leqq a(1 \wedge \varepsilon\mu t)^{-k/2} e^{-\lambda_1 t}$$

and if $d_{U,C}(x;y) \geqq vt$ then

$$|\kappa_t(x;y)| \leqq a(1 \wedge \varepsilon\mu t)^{-k/2} e^{-\lambda_1 t} \exp(-(d_{U,C}(x;y) - vt)^2(4(1+\varepsilon)t)^{-1})$$

for all $\varepsilon \in \langle 0, 1]$.

This result is the direct analogue of Theorem IV.2.2 for the universal kernel given in [Rob]. The proof is very similar although the complex structure introduces added complications.

These bounds on the reduced kernel give the optimal t-singularity for small t and the correct asymptotic behaviour for large t. In particular

$$\lim_{t\to\infty} -t^{-1}\log|\kappa_t(x;y)| \geqq \lambda_1 \,.$$

In addition the bounds give

$$\lim_{t\to 0} -t\log|\kappa_t(x;y)| \geqq d_{U,C}(x;y)^2/4 \,,$$

which is the optimal bound in the relative variable. (It is likely that both these bounds are identities.)

The principal weakness of the kernel bounds is that they fail to reflect the expected exponential decrease of the kernel on the diagonal. This will be established in the next section by an alternative set of bounds.

Proof. We begin by assuming that the weak Malcev basis has the ideal property (3).

Let $\psi \in D_C$. For $\rho \in \mathbf{R}$ define the operator U_ρ on $L_2(\mathbf{R}^k)$ by $(U_\rho\varphi)(x) = e^{-\rho\psi(x)}\varphi(x)$ and the semigroup S^ρ by $S^\rho_t = U_\rho S_t U_\rho^{-1}$. Then the infinitesimal generator of S^ρ is the operator $H^\rho = U_\rho H U_\rho^{-1}$. Note that $U_\rho B_i U_\rho^{-1}\varphi = B_i\varphi + \psi_i\varphi$ for all $\varphi \in L_2(\mathbf{R}^k)$, where $\psi_i = B_i^\circ\psi$.

Let $\rho \in \mathbf{R}, \varphi \in L_2(\mathbf{R}^k)$ and set $\varphi_t = S^\rho_t\varphi$ for all $t > 0$. Then for all $t > 0$ one has

$$\begin{aligned}
\frac{d}{dt}\|\varphi_t\|_2^2 &= -2\,\mathrm{Re}(\varphi_t, H^\rho\varphi_t) \\
&= -2\,\mathrm{Re}\sum_{i,j=1}^d c_{ij}((B_i - \rho\psi_i)\varphi_t, (B_j + \rho\psi_j)\varphi_t) - 2\,\mathrm{Re}\sum_{i=1}^d c_i(\varphi_t, (B_i + \rho\psi_i)\varphi_t) \\
&= -2(\varphi_t, H_0\varphi_t) + 2\rho^2\sum_{i,j=1}^d c_{ij}(\psi_i\varphi_t, \psi_j\varphi_t) - 2\rho\sum_{i=1}^d c_i(\varphi_t, \psi_i\varphi_t) \\
&\leqq 2(\rho^2 - \lambda_1 + |\rho|v)\|\varphi_t\|_2^2\,.
\end{aligned}$$

(Here we have used the estimate

$$\sum_{i=1}^d\|\psi_i\varphi\|_2^2 \leqq \mu^{-1}\sum_{i,j=1}^d c_{ij}(\psi_i\varphi, \psi_j\varphi) \leqq \mu^{-1}\|\varphi\|_2^2$$

which is valid for all $\varphi \in L_2(\mathbf{R}^k)$.) Hence by integration one finds

$$\|S^\rho_t\|_{2\to 2} \leqq e^{(\rho^2 - \lambda_1 + |\rho|v)t} \tag{16}$$

for all $t > 0$.

Next we estimate $\|S^\rho_t\|_{2\to\infty}$. Let $\rho \in \mathbf{R}$ and $\varphi \in \bigcap_{p=1}^\infty L_p$. Then $\varphi_t = S^\rho_t\varphi \in \mathcal{S}(\mathbf{R}^k) \subset \bigcap_{p=1}^\infty L_p$. Thus if $p \geqq 2$ is an even integer,

$$\begin{aligned}
\frac{d}{dt}\|\varphi_t\|_{2p}^{2p} &= -2p\,\mathrm{Re}(\varphi_t^p, \varphi_t^{p-1}H^\rho\varphi_t) \\
&= -2p\,\mathrm{Re}\sum_{i,j=1}^d c_{ij}(B_i(\varphi_t^p\overline{\varphi_t}^{p-1}), B_j\varphi_t) + 2p\rho\,\mathrm{Re}\sum_{i,j=1}^d c_{ij}(\psi_i\varphi_t^p\overline{\varphi_t}^{p-1}, B_j\varphi_t) \\
&\quad - 2p\rho\,\mathrm{Re}\sum_{i,j=1}^d c_{ij}(B_i(\varphi_t^p\overline{\varphi_t}^{p-1}), \psi_j\varphi_t) + 2p\rho^2\,\mathrm{Re}\sum_{i,j=1}^d c_{ij}(\psi_i\varphi_t^p\overline{\varphi_t}^{p-1}, \psi_j\varphi_t) \\
&\quad - 2p\,\mathrm{Re}\sum_{i=1}^d c_i(\varphi_t^p\overline{\varphi_t}^{p-1}, B_i\varphi_t) - 2p\rho\,\mathrm{Re}\sum_{i=1}^d c_i(\varphi_t^p\overline{\varphi_t}^{p-1}, \psi_i\varphi_t)\,.
\end{aligned} \tag{17}$$

We estimate the six terms separately. Using the identity $B_i(\varphi\psi) = \psi B_i^\circ\varphi + \varphi B_i\psi$, together with the fact that B_i° is a derivation, one obtains for the first term

$$\begin{aligned}
(B_i(\varphi_t^p\overline{\varphi_t}^{p-1}), B_j\varphi_t) &= (B_i((|\varphi_t|^2)^{p-1}\varphi_t), B_j\varphi_t) \\
&= (p-1)(|\varphi_t|^{2p-4}\varphi_t\,B_i^\circ|\varphi_t|^2, B_j\varphi_t) + (|\varphi_t|^{2p-2}B_i\varphi_t, B_j\varphi_t) \\
&= (p-1)(|\varphi_t|^{2p-4}\,B_i^\circ|\varphi_t|^2, \chi_j) \\
&\quad + i(p-1)(|\varphi_t|^{2p-4}B_i^\circ|\varphi_t|^2, Y_j|\varphi_t|^2) + (|\varphi_t|^{p-1}B_i\varphi_t, |\varphi_t|^{p-1}B_j\varphi_t)\,,
\end{aligned}$$

where $\chi = (\overline{\varphi_t} B_1^\circ \varphi_t, \ldots, \overline{\varphi_t} B_d^\circ \varphi_t)$. The key point is that the second term is purely imaginary since B_i° is a real differential operator. Moreover, $|\varphi_t|^{2p-4} B_i^\circ |\varphi_t|^2$ is real. Hence using the identity $\chi_j + \overline{\chi_j} = B_j^\circ |\varphi_t|^2$ one deduces that

$$
\begin{aligned}
&-2p \operatorname{Re} \sum_{i,j=1}^{d} c_{ij}(B_i(\varphi_t^p \overline{\varphi_t}^{p-1}), B_j \varphi_t) \\
&\quad = -p(p-1) \sum_{i,j=1}^{d} c_{ij}(|\varphi_t|^{2p-4} B_i^\circ |\varphi_t|^2, \chi_j + \overline{\chi_j}) \\
&\qquad - 2p \sum_{i,j=1}^{d} c_{ij}(|\varphi_t|^{p-1} B_i \varphi_t, |\varphi_t|^{p-1} B_j \varphi_t) \\
&\quad = -p(p-1) \sum_{i,j=1}^{d} c_{ij}(|\varphi_t|^{2p-4} B_i^\circ |\varphi_t|^2, B_j^\circ |\varphi_t|^2) \\
&\qquad - 2p \sum_{i,j=1}^{d} c_{ij}(|\varphi_t|^{p-1} B_i \varphi_t, |\varphi_t|^{p-1} B_j \varphi_t) \\
&\quad = -4p^{-1}(p-1) \sum_{i,j=1}^{d} c_{ij}(B_i^\circ |\varphi_t|^p, B_j^\circ |\varphi_t|^p) - 2p \sum_{i,j=1}^{d} c_{ij}(|\varphi_t|^{p-1} B_i \varphi_t, |\varphi_t|^{p-1} B_j \varphi_t) \\
&\quad \leqq -2 \sum_{i,j=1}^{d} c_{ij}(B_i^\circ |\varphi_t|^p, B_j^\circ |\varphi_t|^p) - 2p \sum_{i,j=1}^{d} c_{ij}(|\varphi_t|^{p-1} B_i \varphi_t, |\varphi_t|^{p-1} B_j \varphi_t)
\end{aligned}
$$

because $p \geqq 2$.

Next we consider the second order terms on the right-hand side of (17) which are proportional to ρ. One has

$$
\begin{aligned}
2p \left| \rho \operatorname{Re} \sum_{i,j=1}^{d} c_{ij}(\psi_i \varphi_t^p \overline{\varphi_t}^{p-1}, B_j \varphi_t) \right| &= 2p|\rho| \left| \operatorname{Re} \sum_{i,j=1}^{d} c_{ij}(\psi_i |\varphi_t|^{p-1} \varphi_t, |\varphi_t|^{p-1} B_j \varphi_t) \right| \\
&\leqq \varepsilon p |\rho| \sum_{i,j=1}^{d} c_{ij}(|\varphi_t|^{p-1} B_i \varphi_t, |\varphi_t|^{p-1} B_j \varphi_t) \\
&\quad + \varepsilon^{-1} p |\rho| \sum_{i,j=1}^{d} c_{ij}(\psi_i |\varphi_t|^{p-1} \varphi_t, \psi_j |\varphi_t|^{p-1} \varphi_t) .
\end{aligned}
$$

Therefore choosing $\varepsilon = (2|\rho|)^{-1}$ one finds

$$
\begin{aligned}
2p \left| \rho \operatorname{Re} \sum_{i,j=1}^{d} c_{ij}(\psi_i \varphi_t^p \overline{\varphi_t}^{p-1}, B_j \varphi_t) \right| &\leqq 2^{-1} p \sum_{i,j=1}^{d} c_{ij}(|\varphi_t|^{p-1} B_i \varphi_t, |\varphi_t|^{p-1} B_j \varphi_t) \\
&\quad + 2p\rho^2 \|\varphi_t^p\|_2^2 .
\end{aligned}
$$

Alternatively,

$$
\begin{aligned}
(B_i(\varphi_t^p \overline{\varphi_t}^{p-1}), \psi_j \varphi_t) &= (p-1)(|\varphi_t|^{2p-4} \varphi_t B_i^\circ |\varphi_t|^2, \psi_j \varphi_t) + (|\varphi_t|^{2p-2} B_i \varphi_t, \psi_j \varphi_t) \\
&= 2p^{-1}(p-1)(B_i^\circ |\varphi_t|^p, \psi_j |\varphi_t|^p) + (|\varphi_t|^{p-1} B_i \varphi_t, |\varphi_t|^{p-1} \varphi_t \psi_j) .
\end{aligned}
$$

Hence estimating as before

$$2p\left|\rho\operatorname{Re}\sum_{i,j=1}^{d}c_{ij}(B_i(\varphi_t^p\overline{\varphi_t}^{p-1}),\psi_j\varphi_t)\right| \leqq 2\varepsilon(p-1)|\rho|\sum_{i,j=1}^{d}c_{ij}(B_i^\circ|\varphi_t|^p,B_j^\circ|\varphi_t|^p)$$

$$+2\varepsilon^{-1}(p-1)|\rho|\sum_{i,j=1}^{d}c_{ij}(\psi_i|\varphi_t|^p,\psi_j|\varphi_t|^p)$$

$$+\delta p|\rho|\sum_{i,j=1}^{d}c_{ij}(|\varphi_t|^{p-1}B_i\varphi_t,|\varphi_t|^{p-1}B_j\varphi_t)$$

$$+\delta^{-1}p|\rho|\sum_{i,j=1}^{d}c_{ij}(\psi_i|\varphi_t|^{p-1}\varphi_t,\psi_j|\varphi_t|^{p-1}\varphi_t)\,.$$

Therefore choosing $\delta=(2|\rho|)^{-1}$ and $\varepsilon=(2(p-1)|\rho|)^{-1}$ one concludes that

$$2p\left|\rho\operatorname{Re}\sum_{i,j=1}^{d}c_{ij}(B_i(\varphi_t^p\overline{\varphi_t}^{p-1}),\psi_j\varphi_t)\right|$$

$$\leqq\sum_{i,j=1}^{d}c_{ij}(B_i^\circ|\varphi_t|^p,B_j^\circ|\varphi_t|^p)+4(p-1)^2\rho^2\|\varphi_t^p\|_2^2$$

$$+2^{-1}p\sum_{i,j=1}^{d}c_{ij}(|\varphi_t|^{p-1}B_i\varphi_t,|\varphi_t|^{p-1}B_j\varphi_t)+2p\rho^2\|\varphi_t^p\|_2^2\,.$$

The fourth term on the right-hand side of (17) is straightforwardly estimated,

$$2p\,\rho^2\left|\operatorname{Re}\sum_{i,j=1}^{d}c_{ij}(\psi_i\varphi_t^p\overline{\varphi_t}^{p-1},\psi_j\varphi_t)\right|\leqq 2p\,\rho^2\|\varphi_t^p\|_2^2\,.$$

For the fifth term we use the skew-adjointness of B_i and B_i° to deduce that

$$-2p\operatorname{Re}\sum_{i=1}^{d}c_i(\varphi_t^p\overline{\varphi_t}^{p-1},B_i\varphi_t)=-2p\operatorname{Re}\sum_{i=1}^{d}c_i(|\varphi_t|^{2p-2}\varphi_t,B_i\varphi_t)$$

$$=2p\operatorname{Re}\sum_{i=1}^{d}c_i\,(B_i(|\varphi_t|^{2p-2}\varphi_t),\varphi_t)$$

$$=2p\operatorname{Re}\sum_{i=1}^{d}c_i(|\varphi_t|^{2p-2}B_i\varphi_t,\varphi_t)+2(2p-2)\operatorname{Re}\sum_{i=1}^{d}c_i(|\varphi_t|^{p-2}\varphi_tB_i^\circ|\varphi_t|^p,\varphi_t)$$

$$=2p\operatorname{Re}\sum_{i=1}^{d}c_i(|\varphi_t|^{2p-2}B_i\varphi_t,\varphi_t)+2(2p-2)\operatorname{Re}\sum_{i=1}^{d}c_i(B_i^\circ|\varphi_t|^p,|\varphi_t|^p)$$

$$=2p\operatorname{Re}\sum_{i=1}^{d}c_i(|\varphi_t|^{2p-2}B_i\varphi_t,\ \varphi_t)\,.$$

Therefore one concludes that

$$-2p\operatorname{Re}\sum_{i=1}^{d}c_i(\varphi_t^p\overline{\varphi_t}^{p-1},B_i\varphi_t)=0\,.$$

Finally,

$$2p \left| \rho \operatorname{Re} \sum_{i=1}^{d} c_i(\varphi_t^p \overline{\varphi_t}^{p-1}, \psi_i \varphi_t) \right| = 2p \left| \rho \sum_{i=1}^{d} c_i(|\varphi_t|^p, \psi_i |\varphi_t|^p) \right| \leqq 2p\, |\rho| v \|\varphi_t^p\|_2^2 .$$

Adding all these terms one derives the differential inequality

$$\begin{aligned} \frac{d}{dt}\|\varphi_t\|_{2p}^{2p} &\leqq - \sum_{i,j=1}^{d} c_{ij}(B_i^\circ |\varphi_t|^p, B_j^\circ |\varphi_t|^p) - p \sum_{i,j=1}^{d} c_{ij}(|\varphi_t|^{p-1} B_i \varphi_t, |\varphi_t|^{p-1} B_j \varphi_t) \\ &\quad + (4p^2 \rho^2 + 2p|\rho| v)\|\varphi_t^p\|_2^2 \\ &\leqq -\mu \sum_{i=1}^{d} \|B_i^\circ |\varphi_t|^p\|_2^2 + (4p^2 \rho^2 + 2p\, |\rho| v)\|\varphi_t^p\|_2^2 . \end{aligned} \tag{18}$$

Now using $\|\varphi_t^p\|_2^2 = \|\varphi_t\|_{2p}^{2p}$ one obtains

$$\frac{d}{dt}\|\varphi_t\|_{2p} \leqq -\mu(2p)^{-1}\|\varphi_t\|_{2p}^{1-2p} \sum_{i=1}^{d} \|B_i^\circ |\varphi_t|^p\|_2^2 + (2p\rho^2 + |\rho| v)\|\varphi_t\|_{2p} . \tag{19}$$

Finally, in terms of the norm $\Gamma_{2;1}^\circ$ introduced in Sect. 3,

$$\frac{d}{dt}\|\varphi_t\|_{2p} \leqq -\mu(2p)^{-1}\|\varphi_t\|_{2p}^{1-2p} \Gamma_{2,1}^\circ(|\varphi_t|^p)^2 + (2p\rho^2 + |\rho| v + \gamma^2 \mu (2p)^{-1})\|\varphi_t\|_{2p} .$$

This differential inequality is the same as inequality (IV.2.12) in [Rob], if one takes $\|C\| = 1$ in [Rob]. The important feature of the remaining part of the proof is the use of the Nash inequalities of Corollary 3.10 to estimate the terms in the sum. These estimates are in terms of L_1-, and L_2-, norms of $|\varphi_t|^p$. But $\||\varphi_t|^p\|_1 = \|\varphi_t\|_p^p$ and $\||\varphi_t|^p\|_2^2 = \|\varphi_t\|_{2p}^{2p}$. Therefore one can use the induction proof on pp. 262–264 in [Rob], starting from the L_2-estimate (16), to deduce bounds on $\|S_t^\rho\|_{2\to\infty}$. These bounds are the direct analogue of the bounds on p. 264 of [Rob],

$$\|S_t^\rho\|_{2\to\infty} \leqq ak(b\gamma^2 \varepsilon\mu t/k)^{-k/4} e^{-\lambda_1 t} e^{\rho^2(1+\varepsilon)t + |\rho| vt} e^{\gamma^2 \varepsilon \mu t} ,$$

and are valid for all $t > 0, \rho \in \mathbf{R}, \gamma \in \langle 0, 1]$ and $\varepsilon \in \langle 0, 1]$ with the values of a and b dependent only on the group, the basis $b_1, \ldots, b_d$ and the constant α in the Nash inequality Corollary 3.10. Now if $\varepsilon\mu t \leqq 1$ set $\gamma = 1$ and if $\varepsilon\mu t \geqq 1$ set $\gamma = (\varepsilon\mu t)^{-1/2}$. Then, with redefined values of a and ε, one obtains bounds

$$\|S_t^\rho\|_{2\to\infty} \leqq a(1 \wedge \varepsilon\mu t)^{-k/4} e^{-\lambda_1 t} e^{\rho^2(1+\varepsilon)t + |\rho| vt} \tag{20}$$

for all $t > 0, \rho \in \mathbf{R}$ and $\varepsilon \in \langle 0, 1]$. But by duality

$$\|S_t^\rho\|_{1\to\infty} \leqq \|S_{t/2}^\rho\|_{1\to 2} \|S_{t/2}^\rho\|_{2\to\infty} = \|S_{t/2}^{-\rho}\|_{2\to\infty} \|S_{t/2}^\rho\|_{2\to\infty} .$$

Hence one obtains bounds

$$\|S_t^\rho\|_{1\to\infty} \leqq a(1 \wedge \varepsilon\mu t)^{-k/2} e^{-\lambda_1 t} e^{\rho^2(1+\varepsilon)t + |\rho| vt}$$

for all $t > 0, \rho \in \mathbf{R}$ and $\varepsilon \in \langle 0, 1]$ and again a redefined value of a. Consequently

$$|\kappa_t(x; y)| \leqq a(1 \wedge \varepsilon\mu t)^{-k/2} e^{-\lambda_1 t} e^{\rho^2(1+\varepsilon)t + |\rho| vt + \rho(\psi(x) - \psi(y))}$$

for all $t > 0$ and $x, y \in \mathbf{R}^k$. The value of a now depends on the group, the dimension k, the basis $b_1, \ldots, b_d$ and the constant α in the Nash inequality Corollary 3.10, but is independent of the coefficients of H and of $\varepsilon \in \langle 0, 1]$. Minimizing over $\psi \in D_C$ one deduces that

$$|\kappa_t(x; y)| \leqq a(1 \wedge \varepsilon\mu t)^{-k/2} e^{-\lambda_1 t} e^{\rho^2(1+\varepsilon)t - |\rho| d_{U,C}(x;y) + |\rho| vt} .$$

This proves the first part of the theorem if the weak Malcev basis has the ideal property (3). We next remove this condition. By Lemma 2.2 there exists a weak Malcev basis $\tilde{a}_1, \ldots, \tilde{a}_{d_{\mathfrak{m}}+k}$ passing through $\mathfrak{m}$ which has the ideal property. Let c and σ be as in Lemma 2.3 and let κ_t and $\tilde{\kappa}_t$ be the two associated reduced kernels. Then it follows from the Gaussian bounds for $\tilde{\kappa}_t$ and Lemma 2.4 that

$$\begin{aligned} |\kappa_t(x; y)| &= |c^2 e^{i(\sigma(x) - \sigma(y))} \tilde{\kappa}_t(\theta(x); \theta(y))| \\ &\leqq c^2 a(1 \wedge \varepsilon\mu t)^{-k/2} e^{-\lambda_1 t} e^{\rho^2(1+\varepsilon)t - |\rho| d_{\tilde{U},C}(\theta(x),\theta(y)) + |\rho| vt} . \end{aligned}$$

Hence it remains to prove that $d_{\tilde{U},C}(\theta(x); \theta(y)) = d_{U,C}(x; y)$.

Now let V be the unitary map as in Lemma 2.3. Further let $\psi \in C_c^\infty(\mathbf{R}^k)$ and set $\Psi = \psi \circ \theta$. Then $(V^* \Psi)(x) = c^{-1} e^{-i\sigma(x)} \psi(x)$. So

$$\begin{aligned} (\tilde{B}_i \Psi)(\theta^{-1}(x)) &= (V B_i V^* \Psi)(\theta^{-1}(x)) = c e^{i\sigma(x)} (B_i V^* \Psi)(x) \\ &= (B_i \psi)(x) - i(B_i^\circ \sigma)(x) \psi(x) \end{aligned}$$

for all $x \in \mathbf{R}^k$. Hence $(\tilde{B}_i^\circ \Psi)(\theta^{-1}(x)) = (B_i^\circ \psi)(x)$ and $\tilde{B}_i^\circ \Psi = (B_i^\circ \psi) \circ \theta$. From this identity one easily derives the transformation formula for the distances and the proof of the first part of the theorem is complete. The second part follows by minimizing over ρ. □

There is another description of the distance $d_{U,C}$ which allows one to reformulate the statement of the theorem in a more geometric manner.

Each B_i° is a vector field on $\mathbf{R}^k$. But the algebra generated by the B_i consists of all differential operators with polynomial coefficients, ([CoG] Theorem 4.1.1(i)), and the differential operator $\partial/\partial x_j$ has no constant term. It follows that the vector fields $B_1^\circ, \ldots, B_d^\circ$ generate the tangent space at any point of $\mathbf{R}^k$. We now define a geometric distance on $\mathbf{R}^k$ as in [NSW]. For $\delta > 0$ let $C(\delta)$ be the set of all absolutely continuous functions $\gamma : [0, 1] \to G$ which satisfy the differential equation

$$\dot{\gamma}(t) = \sum_{i=1}^{d} \gamma_i(t) B_i^\circ \Big|_{\gamma(t)} ,$$

almost everywhere, with

$$\sum_{i,j=1}^{d} (C^{-1})_{ij} \gamma_i(t) \gamma_j(t) < \delta^2$$

for all $t \in [0, 1]$, where C denotes the matrix of coefficients. Then define the distance $d^{\mathrm{g}}_{U,C}(x; y)$ between two elements $x, y \in \mathbf{R}^k$ by

$$d^{\mathrm{g}}_{U,C}(x\,; y) = \inf\{\delta > 0 : \exists_{\gamma \in C(\delta)} [\gamma(0) = x \text{ and } \gamma(1) = y]\} .$$

The distance $d^{\mathrm{g}}_{U,C}$ induces the Euclidean topology on $\mathbf{R}^k$.

Lemma 4.2. *The distances $d_{U,C}$ and $d^{\mathrm{g}}_{U,C}$ are equal.*

Proof. Let $x, y \in \mathbf{R}^k, \psi \in D_C, \delta > 0$ and $\gamma \in C(\delta)$ with $\gamma(0) = x$ and $\gamma(1) = y$. Write

$$\dot\gamma(t) = \sum_{i=1}^{d} \gamma_i(t)\, B_i^\circ\,|_{\gamma(t)} \;,$$

with

$$\sum_{i,j=1}^{d} (C^{-1})_{ij}\, \gamma_i(t)\, \gamma_j(t) < \delta^2$$

for almost every $t \in [0,1]$.

Now denote the inner product on $\mathbf{R}^d$ by $\langle \,\cdot\, , \,\cdot\, \rangle$, the norm by $|\cdot|$, set $[(B^\circ\psi)(z)] = ((B_1^\circ\psi)(z), \ldots, (B_d^\circ\psi)(z)) \in \mathbf{R}^d$ for all $z \in \mathbf{R}^k$ and $[\dot\gamma(t)] = (\gamma_1(t), \ldots, \gamma_d(t))$. Then

$$\begin{aligned} |\psi(y) - \psi(x)| &= \left| \int_0^1 dt \frac{d}{dt}\psi(\gamma(t)) \right| = \left| \int_0^1 dt \sum_{i=1}^{d} \gamma_i(t)(B_i^\circ\psi)(\gamma(t)) \right| \\ &\leqq \int_0^1 dt |\langle C^{-1/2}[\dot\gamma(t)], C^{1/2}[(B^\circ\psi)(\gamma(t))]\rangle| \\ &\leqq \int_0^1 dt |C^{-1/2}[\dot\gamma(t)]|\, |C^{1/2}[(B^\circ\psi)(\gamma(t))]| \leqq \int_0^1 dt\, \delta \cdot 1 = \delta \,. \end{aligned}$$

Therefore $d_{U,C}(x;y) \leqq d^{\mathrm{g}}_{U,C}(x;y)$.

Alternatively, fix $x_0, y_0 \in \mathbf{R}^k$ and let $n = d^{\mathrm{g}}_{U,C}(x_0;y_0) + 1$. Define $\varphi_n : \mathbf{R} \to \mathbf{R}$ by

$$\varphi_n(x) = \begin{cases} |x| & \text{if } |x| \leqq n \,, \\ 2n - |x| & \text{if } n < |x| \leqq 2n \,, \\ 0 & \text{if } |x| > 2n \,. \end{cases}$$

Then $\varphi_n \in C_c(\mathbf{R})$ and $|\varphi_n(x) - \varphi_n(y)| \leqq |x - y|$ for all $x, y \in \mathbf{R}$. Define $\chi_n : \mathbf{R}^k \to \mathbf{R}$ by $\chi_n(x) = \varphi_n(d^{\mathrm{g}}_{U,C}(x;y_0))$. Then $\chi_n \in C_c(\mathbf{R}^k)$ and $|\chi_n(x_1) - \chi_n(x_2)| \leqq d^{\mathrm{g}}_{U,C}(x_1;x_2)$ for all $x_1, x_2 \in \mathbf{R}^k$.

Next we regularize χ_n. Fix a positive $\tau \in C_c^\infty(\mathbf{R}^k)$ with integral equal to one. For $m \in \mathbf{N}$ define $\tau_m \in C_c^\infty(\mathbf{R}^k)$ by $\tau_m(x) = m^k \tau(m^{-1}x)$ and $\psi_{nm} : \mathbf{R}^k \to \mathbf{R}$ by

$$\psi_{nm} = \tau_m * \chi_n \,.$$

Here $*$ is the convolution on the commutative group $\mathbf{R}^k$. Then $\psi_{nm} \in C_c^\infty(\mathbf{R}^k)$. Moreover one has

$$\lim_{m\to\infty} \psi_{nm}(x_0) = \varphi_n(d^{\mathrm{g}}_{U,C}(x_0;y_0)) = d^{\mathrm{g}}_{U,C}(x_0;y_0) \,.$$

For all $i \in \{1, \ldots, d\}$, $x \in \mathbf{R}^k$ and $t > 0$ one has

$$|\chi_n(\exp(-tB_i^\circ)(x)) - \chi_n(x)| \leqq d^{\mathrm{g}}_{U,C}(\exp(-tB_i^\circ)(x);x) \leqq ((C^{-1})_{ii})^{1/2} t \,.$$

Since the representation V on $L_\infty(\mathbf{R}^k)$ defined by $(V_t\omega)(x) = \omega(\exp(-tB_i^\circ)(x))$ is weakly* continuous it follows that χ_n is in the domain of the operator B_i°, viewed as an operator on $L_\infty(\mathbf{R}^k)$. Next we argue that $\sum_{i,j=1}^d c_{ij}(B_i^\circ\chi_n)(x)(B_j^\circ\chi_n)(x) \leqq 1$ for all $x \in \mathbf{R}^k$. One has for all $x \in \mathbf{R}^k$:

$$\left(\sum_{i,j=1}^d c_{ij}(B_i^\circ\chi_n)(x)(B_j^\circ\chi_n)(x)\right)^{1/2} = |C^{1/2}[(B^\circ\chi_n)(x)]|$$

$$= \sup_{\substack{\xi\in\mathbf{R}^d \\ |\xi|=1}} \langle \xi, C^{1/2}[(B^\circ\chi_n)(x)]\rangle = \sup_{|\xi|=1} C^{1/2}\xi \cdot [(B^\circ\chi_n)(x)] \, .$$

Now for all $t > 0$ the path $\gamma(s) = \exp(stC^{1/2}\xi \cdot B^\circ)(x)$ is a C^∞-path from x to $\exp(tC^{1/2}\xi \cdot B^\circ)(x)$ and $[\dot\gamma(s)] = tC^{1/2}\xi$ for all s. So

$$\langle[\dot\gamma(s)], C^{-1}[\dot\gamma(s)]\rangle = \langle tC^{1/2}\xi, C^{-1}tC^{1/2}\xi\rangle = t^2 \, ,$$

and hence $\gamma \in C(t)$. Therefore $d^{g}_{U,C}(\exp(tC^{1/2}\xi \cdot B^\circ)(x); x) \leqq t$ and $C^{1/2}\xi \cdot [(B^\circ\chi_n)\,(x)] \leqq 1$ by an estimate as we used above for the proof that χ_n is differentiable.

Next, note that the representation V leaves $C_c^\infty(\mathbf{R}^k)$ invariant. For all $f \in L_1(\mathbf{R}^k)$ and $\omega \in C_c^\infty(\mathbf{R}^k)$ define

$$F = \{\psi \in D(B_i^\circ) : (f, (B_i^\circ\omega) * \psi) = (\tilde\omega * f, B_i^\circ\psi)\} \, ,$$

where $\tilde\omega(x) = \omega(-x)$. Then $C_c^\infty(\mathbf{R}^k) \subset F$ and F is weakly* closed in $D(B_i^\circ)$, so $F = D(B_i^\circ)$. Therefore

$$B_i^\circ(\omega * \psi) = (B_i^\circ\omega) * \psi = \omega * B_i^\circ\psi$$

for all $\psi \in D(B_i^\circ)$. In particular:

$$B_i^\circ\psi_{nm} = \tau_m * B_i^\circ\chi_n \, ,$$

and for all $x \in \mathbf{R}^k$ one obtains

$$\left(\sum_{i,j=1}^d c_{ij}(B_i^\circ\psi_{nm})(x)(B_j^\circ\psi_{nm})(x)\right)^{1/2} = |C^{1/2}[(B^\circ\psi_{nm})(x)]|$$

$$= \sup_{|\xi|=1}\langle\xi, C^{1/2}[(B^\circ\psi_{nm})(x)]\rangle = \sup_{|\xi|=1}(\tau_m * \langle\xi, C^{1/2}[B^\circ\chi_m]\rangle)(x)$$

$$\leqq \sup_{|\xi|=1}\|\tau_m\|_1|\xi|\||C^{1/2}[B_i^\circ\chi_m]|\|_\infty \leqq 1 \, .$$

Hence $\psi_{nm} \in D_C$ and $d^{g}_{U,C}(x_0; y_0) \leqq d_{U,C}(x_0; y_0)$. □

It follows from the general theory of strongly elliptic operators that the semigroup generated by a closed strongly elliptic operator with real principal coefficients is holomorphic in the open right half-plane. Then, by the discussion in Sect. 3, the corresponding reduced kernel extends to a function which is analytic in the half-plane. Therefore it is of interest to examine bounds on the kernel for complex t. This is particularly simple if there are no first-order terms, i.e., if $c_i = 0$. In this case the bounds of Theorem 4.1 give

$$|\kappa_t(x; y)| \leqq a(1 \wedge \varepsilon\mu t)^{-k/2}e^{-\lambda_1 t}\exp(-d_{U,C}(x; y)^2(4(1+\varepsilon)t)^{-1})$$

for all $t > 0$ and $\varepsilon \in \langle 0, 1]$. These bounds have the following analogue.

Corollary 4.3. *Let $l \in \mathfrak{g}^*$, $a_1, \ldots, a_{d_{\mathfrak{m}}}, \ldots, a_{d_{\mathfrak{m}}+k}$ be a weak Malcev basis passing through a polarizing subalgebra $\mathfrak{m}$ of l and U the corresponding basis realization in $L_2(\mathbf{R}^k)$. Let H be a pure second-order operator associated with the real, symmetric, strictly positive-definite matrix $C = (c_{ij})$, and the basis $b_1, \ldots, b_d$ of $\mathfrak{g}$. Further let κ denote the corresponding reduced kernel. Then there exists an $a > 0$, independent of the coefficients C, such that*

$$|\kappa_z(x;y)| \leqq a(\varepsilon \cos\theta)^{-k/2}(1 \wedge \varepsilon\mu \operatorname{Re} z)^{-k/2} e^{-\lambda_1 \operatorname{Re} z}$$
$$\times \exp\left(-d_{U,C}(x;y)^2 \operatorname{Re}(4(1+\varepsilon)z)^{-1}\right)$$

for all $z \in \mathbf{C}$ with $\operatorname{Re} z > 0$ and all $\varepsilon \in \langle 0, 1]$, where $\theta = \arg z$.

Proof. We adapt the general reasoning of Davies [Dav2], Lemma 3.4.6 and Theorem 3.4.8.

First remark that if $z = t + is$ then

$$\|S_z\|_{1\to 2} = \|S_t\|_{1\to 2} = \|S_t\|_{2\to\infty} = \|S_{\bar{z}}\|_{2\to\infty}$$

because H is self-adjoint on $L_2(\mathbf{R}^k)$. Therefore

$$\|S_z\|_{1\to\infty} \leqq \|S_{z/2}\|_{1\to 2}\|S_{z/2}\|_{2\to\infty} = (\|S_{t/2}\|_{2\to\infty})^2 .$$

Hence, by (20) with $\rho = 0$ and $\varepsilon = 1$, one has bounds

$$|\kappa_z(x;y)| \leqq \|S_z\|_{1\to\infty} \leqq a(1 \wedge \mu t)^{-k/2} e^{-\lambda_1 t} ,$$

with a redefined value of a, for all $z \in \mathbf{C}$ with $t = \operatorname{Re} z > 0$. Then since $(1 \wedge t) \geqq (1 - e^{-t})$ this gives

$$|\kappa_z(x;y)| \leqq a(1 - e^{-\mu t})^{-k/2} e^{-\lambda_1 t} .$$

Alternatively, one can rephrase the bounds of Theorem 4.1 as

$$|\kappa_t(x;y)| \leqq a(1 - e^{-\varepsilon\mu t})^{-k/2} e^{-\lambda_1 t} e^{-d_{U,C}(x;y)^2(4(1+\varepsilon)t)^{-1}} ,$$

uniformly for all $t > 0$ and $\varepsilon \in \langle 0, 1]$.

Next for fixed $x, y \in \mathbf{R}^k, \varepsilon \in \langle 0, 1]$ and $\varphi \in \langle 0, \pi/2\rangle$ define the analytic function F in the open right half-plane by

$$F(z) = \kappa_{z^{-1}}(x;y) e^{\lambda_1 z^{-1}} (1 - e^{-\varepsilon\mu z^{-1}})^{k/2} e^{b_\varphi e^{\iota(\pi/2-\varphi)} d_{U,C}(x;y)^2 z} ,$$

where $b_\varphi = (4(1+\varepsilon)\sin\varphi)^{-1}$. Then

$$|F(t)| \leqq a$$

for all $t > 0$. Now it follows from a Duhamel estimate that

$$|1 - e^{-se^{-\iota\varphi}}| \leqq |se^{-\iota\varphi}| \left|\int_0^1 d\lambda\, |e^{-\lambda s e^{-\iota\varphi}}|\right| = s\int_0^1 d\lambda\, e^{-\lambda s\cos\varphi}$$

$$= (\cos\varphi)^{-1}(1 - e^{-s\cos\varphi}) = (\cos\varphi)^{-1}(1 - e^{-\operatorname{Re} se^{-\iota\varphi}})$$

for all $s > 0$. Hence

$$|F(te^{\iota\varphi})| \leqq a(1 - e^{-\mu \operatorname{Re} t^{-1} e^{-\iota\varphi}})^{-k/2} |1 - e^{-\varepsilon\mu t^{-1} e^{-\iota\varphi}}|^{k/2}$$

$$\leqq a(1 - e^{-\varepsilon\mu \operatorname{Re} t^{-1} e^{-\iota\varphi}})^{-k/2} |1 - e^{-\varepsilon\mu t^{-1} e^{-\iota\varphi}}|^{k/2}$$

$$\leqq a(\cos\varphi)^{-k/2} .$$

Moreover, if $\theta \in [0, \varphi]$ then

$$|F(te^{i\theta})| \leqq a(\cos\theta)^{-k/2} e^{b_\varphi d_{U,C}(x;y)^2 t \sin(\varphi-\theta)} \leqq a(\cos\varphi)^{-k/2} e^{b_\varphi d_{U,C}(x;y)^2 t \sin\varphi} .$$

Therefore the Phragmén–Lindelöf theorem implies that

$$|F(z)| \leqq c(\cos\varphi)^{-k/2}$$

for all z with $\arg z \in [0, \varphi]$, for a suitable $c > 0$, depending only on a. Similar reasoning leads to an identical bound for z with $\arg z \in [-\varphi, 0]$. But since

$$\kappa_z(x;y) = F(z^{-1})(1 - e^{-\varepsilon\mu z})^{-k/2} e^{-\lambda_1 z} e^{-b_\varphi z^{-1} e^{i(\pi/2-\varphi)} d_{U,C}(x;y)^2} ,$$

one concludes that

$$|\kappa_z(x;y)| \leqq c(\cos\varphi)^{-k/2} |1 - e^{-\varepsilon\mu z}|^{-k/2} e^{-\lambda_1 \operatorname{Re} z} e^{-b_\varphi d_{U,C}(x,y)^2 t^{-1} \sin(\varphi - |\theta|)}$$

for all $z = te^{i\theta} \in \mathbf{C}$ with $|\arg z| \leqq \varphi$. Now, however, $1 - e^{-\operatorname{Re} z} \leqq |1 - e^{-z}|$ for all $z \in \mathbf{C}$ with $\operatorname{Re} z > 0$, by the triangle inequality. In addition $1 \wedge t \leqq (1 - e^{-1})^{-1}(1 - e^{-t})$ for all $t > 0$. Therefore

$$|\kappa_z(x;y)| \leqq c(\cos\varphi)^{-k/2} (1 \wedge \varepsilon\mu \operatorname{Re} z)^{-k/2} e^{-\lambda_1 \operatorname{Re} z} e^{-b_\varphi d_{U,C}(x,y)^2 t^{-1} \sin(\varphi - |\theta|)}$$

for all $z = te^{i\theta} \in \mathbf{C}$ with $|\arg z| \leqq \varphi$.

Next for $z \in \mathbf{C}$ with $\operatorname{Re} z > 0$ and $\operatorname{Im} z \neq 0$ choose $\varphi \in \langle 0, \pi/2 \rangle$ such that $\varepsilon \tan\varphi = \tan|\theta|$. Then $\sin(\varphi - |\theta|)(\sin\varphi)^{-1} = (1 - \varepsilon)\cos\theta$ and $\cos\varphi = \varepsilon(\varepsilon^2 + \tan^2\theta)^{-1/2} \geqq \varepsilon\cos\theta$, so

$$|\kappa_z(x;y)| \leqq c(\varepsilon\cos\theta)^{-k/2} (1 \wedge \varepsilon\mu \operatorname{Re} z)^{-k/2} e^{-\lambda_1 \operatorname{Re} z} e^{-(1-\varepsilon) d_{U,C}(x;y)^2 \operatorname{Re}(4(1+\varepsilon)z)^{-1}} .$$

Finally, set $\delta = 2\varepsilon(1 - \varepsilon)^{-1}$ so that $(1 + \varepsilon)(1 - \varepsilon)^{-1} = (1 + \delta)$. Then $\varepsilon = \delta(2 + \delta)^{-1} \geqq \delta/3$ for $\delta \in \langle 0, 1]$ and

$$|\kappa_z(x;y)| \leqq c3^k (\delta\cos\theta)^{-k/2} (1 \wedge \delta\mu \operatorname{Re} z)^{-k/2} e^{-\lambda_1 \operatorname{Re} z} e^{-d_{U,C}(x;y)^2 \operatorname{Re}(4(1+\delta)z)^{-1}}$$

for all $z \in \mathbf{C}$ with $\operatorname{Re} z > 0$ and $\theta = \arg z$ and for all $\delta \in \langle 0, 1]$. Thus the statement of the corollary is established by a change of notation. □

The estimates of Theorem 4.1 depend critically on the reality of the principal coefficients (c_{ij}) but less critically on the reality of the first-order coefficients c_i. One can adapt the foregoing arguments to bound the reduced kernels associated with second-order operators with complex-valued c_i at the cost of forfeiting control over the large t behaviour.

Corollary 4.4. *Let $l \in \mathfrak{g}^*, a_1, \ldots, a_{d_\mathfrak{m}}, \ldots, a_{d_\mathfrak{m}+k}$ be a weak Malcev basis passing through a polarizing subalgebra $\mathfrak{m}$ of l and U the corresponding basis realization in $L_2(\mathbf{R}^k)$. Let H be a second-order operator associated with the real symmetric matrix of principal coefficients $C = (c_{ij})$, the first-order coefficients $c_i \in \mathbf{C}$ and the basis $b_1, \ldots, b_d$ of $\mathfrak{g}$. Further let κ_t denote the corresponding reduced kernel. Then for all $\varepsilon \in \langle 0, 1]$ there exists an $a_\varepsilon > 0$ and $\omega_\varepsilon \geqq 0$ such that*

$$|\kappa_t(x;y)| \leqq a_\varepsilon t^{-k/2} e^{\omega_\varepsilon t} e^{-d_{U,C}(x;y)^2 (4(1+\varepsilon)t)^{-1}}$$

uniformly for all $t > 0$ and $x, y \in \mathbf{R}^k$.

Proof. The proof is an elaboration of the proof of Theorem 4.1. We briefly comment on the extra features.

First, in the calculation of $d\|\varphi_t\|_2^2/dt$ one has additional terms

$$X_1 = 2\,\mathrm{Re}\sum_{i=1}^{d} c_i(\varphi_t, (B_i + \rho\psi_i)\varphi_t)\,.$$

But these can be handled by $(\varepsilon, \varepsilon^{-1})$-estimates. For example, one readily finds that

$$\begin{aligned}|X_1| &\leqq \varepsilon\mu\sum_{i=1}^{d} \|B_i\varphi_t\|_2^2 + \varepsilon^{-1}v^2\|\varphi_t\|_2^2 + 2|\rho|v\|\varphi_t\|_2^2\\ &\leqq \varepsilon(\varphi_t, H_0\varphi_t) + (\varepsilon^{-1}v^2 + 2|\rho|v)\|\varphi_t\|_2^2\,.\end{aligned}$$

Therefore choosing $\varepsilon = 2$ and using the previous estimates one finds that

$$\frac{d}{dt}\|\varphi_t\|_2^2 \leqq 2(|\rho| + v/2)^2\|\varphi_t\|_2^2\,,$$

and then, by integration,

$$\|S_t^\rho\|_{2\to 2} \leqq e^{(|\rho|+v/2)^2 t}$$

for all $t > 0$ and $\rho \in \mathbf{R}$.

Similar modifications are necessary for the estimation of $d\|\varphi_t\|_{2p}^{2p}/dt$. Now one has additional terms

$$\begin{aligned}W_1 &= -2p\,\mathrm{Re}\sum_{i=1}^{d} c_i(\varphi_t^p\overline{\varphi_t}^{p-1}, (B_i + \rho\psi_i)\varphi_t)\\ &= -2p\,\mathrm{Re}\sum_{i=1}^{d} c_i(|\varphi_t|^{p-1}\varphi_t, |\varphi_t|^{p-1}B_i\varphi_t) - 2p\rho\,\mathrm{Re}\sum_{i=1}^{d} c_i(|\varphi_t|^p, \psi_i|\varphi_t|^p)\,.\end{aligned}$$

Hence

$$\begin{aligned}|W_1| &\leqq \varepsilon p v\sum_{i,j=1}^{d} c_{ij}(|\varphi_t|^{p-1}B_i\varphi_t, |\varphi_t|^{p-1}B_j\varphi_t) + \varepsilon^{-1}pv\|\varphi_t^p\|_2^2 + 2p|\rho|v\|\varphi_t^p\|_2^2\\ &= p\sum_{i,j=1}^{d} c_{ij}(|\varphi_t|^{p-1}B_i\varphi_t, |\varphi_t|^{p-1}B_j\varphi_t) + (pv^2 + 2p|\rho|v)\|\varphi_t^p\|_2^2\end{aligned}$$

if one chooses $\varepsilon = v^{-1}$. Finally, one obtains a differential inequality which differs from the earlier one for pure second-order operators only in the terms proportional to $\|\varphi_t\|_{2p}$. Now one deduces that

$$\frac{d}{dt}\|\varphi_t\|_{2p}^{2p} \leqq -\mu\sum_{i=1}^{d} \|B_i^\circ|\varphi_t|^p\|_2^2 + (4p^2\rho^2 + 2p|\rho|v + pv^2)\|\varphi_t\|_2^2\,,$$

instead of the inequality (18) and

$$\frac{d}{dt}\|\varphi_t\|_{2p} \leqq -\mu(2p)^{-1}\|\varphi_t\|_{2p}^{1-2p}\sum_{i=1}^{d} \|B_i^\circ|\varphi_t|^p\|_2^2 + (2p\rho^2 + |\rho|v + v^2/2)\|\varphi_t\|_{2p}\,,$$

which is the direct analogue of (19). The coefficient $2p\rho^2$ is replaced by $2p\rho^2 + |\rho|v + v^2/2$. Hence the bounds on the reduced kernel become

$$|\kappa_t(x;y)| \leqq a_\varepsilon t^{-k/2} e^{(\rho^2+\rho v)(1+\varepsilon)t-\rho d_{U,C}(x;y)} e^{4^{-1}v^2(1+\varepsilon)t}$$

$$\leqq a_\varepsilon t^{-k/2} e^{\rho^2(1+2\varepsilon)t-\rho d_{U,C}(x;y)} e^{w^2(1+\varepsilon^{-1}(1+\varepsilon)^2)t},$$

uniformly for all $\rho, t, \varepsilon > 0$ where $w = v/2$. Hence minimizing over ρ, replacing 2ε by ε and redefining a_ε gives the desired bounds. □

There is also an analogue of Corollary 4.5 for operators with real principal coefficients and purely imaginary first-order coefficients. The resulting H is still self-adjoint on $L_2(\mathbf{R}^k)$ and hence one has bounds

$$\|S_z\|_{1\to\infty} \leqq \|S_{z/2}\|_{1\to 2}\|S_{z/2}\|_{2\to\infty} = (\|S_{t/2}\|_{2\to\infty})^2$$

for all $z \in \mathbf{C}$ with $t = \operatorname{Re} z > 0$. Thus it follows from Corollary 4.4 that one has bounds

$$|\kappa_z(x;y)| \leqq a t^{-k/2} e^{\omega t}$$

for all $z \in \mathbf{C}$ with $t = \operatorname{Re} z > 0$ uniformly for $x, y \in \mathbf{R}^k$. Now the arguments of Davies [Dav2], Sect. 3.4, apply directly to give the analogue of Corollary 4.3.

Corollary 4.5. *Let $l \in \mathfrak{g}^*$, $a_1, \ldots, a_{d_{\mathfrak{m}}}, \ldots, a_{d_{\mathfrak{m}}+k}$ be a weak Malcev basis passing through a polarizing subalgebra $\mathfrak{m}$ of l and U the corresponding basis realization in $L_2(\mathbf{R}^k)$. Let H be a second-order operator associated with the real, symmetric, strictly positive-definite matrix $C = (c_{ij})$, the imaginary first-order coefficients c_i and the basis $b_1, \ldots, b_d$ of $\mathfrak{g}$. Further let κ_t denote the corresponding reduced kernel. Then for all $\varepsilon \in \langle 0, 1]$, there exists an $a_\varepsilon > 0$, independent of the coefficients C, and an $\omega_\varepsilon \geqq 0$ such that*

$$|\kappa_z(x;y)| \leqq a_\varepsilon (\cos\theta)^{-k/2} (\operatorname{Re} z)^{-k/2} e^{\omega_\varepsilon \operatorname{Re} z} e^{-d_{U,C}(x;y)^2 \operatorname{Re}(4(1+\varepsilon)z)^{-1}}$$

for all $z \in \mathbf{C}$ with $\operatorname{Re} z > 0$, where $\theta = \arg z$.

Finally we note that for strongly elliptic operators of order $m > 2$ the method of this section does not work. The first problem is that there is no description of higher order strongly elliptic operators in terms of positivity of a matrix of principal coefficients. This can be bypassed by using the method of Sect. III.4 in [Rob]. But then one encounters m^{th} order derivatives on the functions ψ used in the perturbation argument. One could define inductively $D_1 = D_{U,C}$ and

$$D_n = \{\psi \in D_{n-1} : B_i^\circ \psi \in D_{n-1} \quad \text{for all} \quad i \in \{1, \ldots, d\}\}$$

for all $n \geqq 2$ and

$$d_n(x;y) = \sup_{\psi \in D_n} |\psi(x) - \psi(y)|.$$

Then it is readily verified that d_n is non-degenerate and is a distance on $\mathbf{R}^k$. One can then obtain Gaussian type bounds for the reduced kernel of the semigroup generated by an m^{th} order operator with the distance on $\mathbf{R}^k$ equal to d_m. In the situation of Sect. III.4 of [Rob] the corresponding distances $d_1, d_2, \ldots$ are all equivalent (see pp. 200–203), but in the present setting with the irreducible unitary representations the distance d_m is not equivalent to $d_1 = d_{U,C} = d_{U,C}^{\mathfrak{g}}$ if m is large, in general.

One can prove bounds on the reduced kernels corresponding to m^{th} order operators by exploiting the Nash inequalities Corollary 3.7 as in [Rob] Chapter III and one obtains that

$$\|\kappa_t\|_\infty = \|S_t\|_{1\to\infty} \leqq a t^{-k/m} e^{\omega t}$$

for some $a > 0$ and $\omega \in \mathbf{R}$, valid for all $t > 0$. If the strongly elliptic operator is self-adjoint, with smallest eigenvalue λ_1 then $\|S_t\|_{2\to 2} \leqq e^{-\lambda_1 t}$ by spectral theory. So using the decomposition $S_t = S_1 \circ S_{t-2} \circ S_1 : L_1 \to L_2 \to L_2 \to L_\infty$ one deduces that

$$\|\kappa_t\|_\infty = \|S_t\|_{1\to\infty} \leqq a(1\wedge t)^{-k/m} e^{-\lambda_1 t}$$

for some $a > 0$, valid for all $t > 0$.

The same situation occurs if one attempts to derive Gaussian bounds for the higher order derivatives of the reduced kernel, even for second order operators. We are only able to derive Gaussian bounds in terms of the distance $d_{U,C}$ for the first-order derivatives of the reduced kernels of semigroups generated by second-order operators:

$$|(B_i\kappa_t)(x;y)| \leqq a t^{-(k+1)/2} e^{-b d_{U,C}(x;y)^2 t^{-1}}$$

uniformly for all $i \in \{1,\ldots,k\}, t \in \langle 0,1]$ and $x,y \in \mathbf{R}^k$. Since we are not able to prove higher order kernel bounds with the distance $d_{U,C}$ we omit the proof.

5. Kernel Bounds: Large *t*

In this section we use spectral theory in combination with embedding arguments to establish bounds on the reduced kernel κ_t associated with the semigroup S generated by an m^{th} order, formally self-adjoint operator. The arguments apply equally well to strongly elliptic operators or subelliptic operators. Self-adjointness is the important characteristic. There are two main features of these bounds. First, they still give the optimal decrease, $\exp(-\lambda_1 t)$, as a function of t. Secondly, they establish that the kernel is "exponentially" decreasing on the diagonal. The earlier bounds did not give any estimate on the decrease of the kernel along the diagonal.

Let U be the basis realization of the nilpotent Lie group G corresponding to a weak Malcev basis $a_1,\ldots,a_{d_{\mathfrak{m}}},\ldots,a_{d_{\mathfrak{m}}+k}$ passing through a polarizing subalgebra $\mathfrak{m}$ for an $l \in \mathfrak{g}^*$ and let C be a strongly elliptic, formally self-adjoint, m^{th} order form. Set $H = dU(C)$ and let κ be the corresponding reduced kernel. It follows from the general theory of elliptic operators that H is self-adjoint on $L_2(\mathbf{R}^k)$. Moreover, it follows from Kirillov theory that the kernel κ_t belongs to the Schwartz space $\mathcal{S}(\mathbf{R}^k \times \mathbf{R}^k)$. Therefore the self-adjoint semigroup S generated by H is trace class and H has compact resolvent (see Theorem 2.5). Now we exploit these spectral properties to derive bounds on κ_t.

Since κ_t belongs to the Schwartz space $\mathcal{S}(\mathbf{R}^k \times \mathbf{R}^k)$ it is polynomial decreasing, together with all its derivatives. But more is true, the kernel is "exponentially" decreasing.

Theorem 5.1. *Let U be the basis realization in $L_2(\mathbf{R}^k)$ of the nilpotent Lie group corresponding to $l \in \mathfrak{g}^*$ and a weak Malcev basis passing through a polarizing subalgebra $\mathfrak{m}$ of l. Further, let κ be the reduced semigroup kernel corresponding to a self-adjoint, m^{th} order, strongly elliptic operator H. Then there exist $\alpha \in [2,\infty\rangle$*

and $b > 0$ such that for all $z \in \mathbf{C}$ with $t = \operatorname{Re} z > 0$ and all multi-indices β and γ there exists $c_{\beta,\gamma,t} > 0$ such that

$$|(D_x^\beta D_y^\gamma \kappa_z)(x; y)| \leqq c_{\beta,\gamma,t}\, e^{-\lambda_1 t} e^{-b|x|^{1/\alpha} - b|y|^{1/\alpha}}$$

uniformly for all $x, y \in \mathbf{R}^k$, where λ_1 denotes the smallest eigenvalue of the operator H. Moreover, the constants $c_{\beta,\gamma,t}$ can be chosen such that

$$\sup_{t \geqq 1} c_{\beta,\gamma,t} < \infty$$

for all β and γ.

Proof. Let $\lambda_1 \leqq \lambda_2 \leqq \ldots$ denote the eigenvalues of the operator H, repeated according to multiplicity and let $\varphi_1, \varphi_2, \ldots$ be a corresponding orthonormal basis of eigenfunctions. Then $\varphi_j \in D^\infty(H) = \mathscr{S}(\mathbf{R}^k)$ for all j. We obtain bounds on κ_t by examining the spectral decomposition

$$\kappa_z(x; y) = \sum_{j=1}^{\infty} e^{-\lambda_j z} \varphi_j(x) \overline{\varphi_j(y)} \tag{21}$$

of the semigroup S_z generated by H. This series converges in the L_2-sense, by general theory, but we will establish that the convergence is uniform. The estimates we obtain will even demonstrate that it converges in the L_p-sense for all $p \in [1, \infty]$.

Let P_j and Q_j, $j \in \{1, \ldots, k\}$, be the self-adjoint operators on $L_2(\mathbf{R}^k)$ such that $(P_j f)(x) = i\partial_j f(x)$ and $(Q_j f)(x) = x_j f(x)$ for all $f \in \mathscr{S}(\mathbf{R}^k)$ and $x \in \mathbf{R}^k$. There exists, by [CoG] Theorem 4.1.1, an $n \in \mathbf{N}$ such that each P_j and Q_j is a linear combination of monomials of order at most n in the B_i on the Schwartz space. Hence, by [Rob] Corollary I.6.7, there exists $c \geqq 1$ such that $D(H^n) \subseteq D(H_0)$ and

$$\|H_0 \varphi\|_2^2 \leqq c(\|H^n \varphi\|_2^2 + \|\varphi\|_2^2)$$

for all $\varphi \in D(H^n)$, where

$$H_0 = \sum_{j=1}^{k} P_j^2 + Q_j^2 \,.$$

So $H_0^2 \leqq c(H^{2n} + I)$. Let $N(\lambda)$ and $N_0(\lambda)$ denote the number of eigenvalues of H and H_0 which are less than or equal to λ, counted according to their multiplicity. Then it follows from the minimax theorem that

$$N(\lambda) \leqq N_0((c(\lambda^{2n} + 1))^{1/2}) \leqq N_0(2c\lambda^n)$$

for all $\lambda \geqq \max(|\lambda_1|, 1)$. One can easily estimate N_0 and one has $N_0(\lambda) \leqq ((\lambda - 1)/2)^k$ for all $\lambda \geqq 1$. So $N(\lambda) \leqq c^k \lambda^{kn}$ if $\lambda \geqq \max(|\lambda_1|, 1)$. Then $j \leqq N(\lambda_j) \leqq c^k \lambda_j^{kn}$ and hence

$$\lambda_j \geqq (c^{-k} j)^{1/(kn)} \tag{22}$$

for all $j \in \mathbf{N}$ with $\lambda_j \geqq \max(|\lambda_1|, 1)$.

Alternatively, there exists $c > 0$ such that $c\|H\varphi\| \leqq \|H_0^{mr}\varphi\|$ for all $\varphi \in D(H_0^{mr})$, where r is the rank of the Lie algebra $\mathfrak{g}$. Then

$$N(\lambda) \geqq N_0(c^{1/(mr)} \lambda^{1/(mr)}) \geqq 2^{-1}(c^{1/(mr)} \lambda^{1/(mr)} - k) \geqq c' \lambda^{1/(mr)}$$

for all λ sufficiently large. Hence

$$|\lambda_j| \leqq b j^{mr}$$

for some $b > 0$, first for all sufficiently large j, but then by increasing b, if necessary, for all $j \in \mathbf{N}$.

Next we consider bounds on the eigenfunctions φ_j. If $T_1, \ldots, T_q$ are operators in $L_2(\mathbf{R}^k)$ and $\lambda > 0$ then we define the Gevrey space $G_\lambda(T_1, \ldots, T_q)$ by

$$G_\lambda(T_1, \ldots, T_q) = \bigcup_{s>0} G_{\lambda;s}(T_1, \ldots, T_q) ,$$

where $G_{\lambda;s}(T_1, \ldots, T_q)$ is the normed space of all $\varphi \in \bigcap_{p=0}^{\infty} \bigcap_{i_1,\ldots,i_p \in \{1,\ldots,q\}} D(T_{i_1} \cdots T_{i_p})$ such that

$$\sup_{p \in \mathbf{N}_0} \sup_{i_1,\ldots,i_p \in \{1,\ldots,q\}} (s^p p!^\lambda)^{-1} \|T_{i_1} \cdots T_{i_p} \varphi\| < \infty .$$

Using the eigenvalue estimates one deduces

$$\begin{aligned}\|H^p \varphi_j\|_2 = |\lambda_j|^p &\leqq (b j^{mr})^p = b^p ((j^{1/(2kn)})^p)^{2kmnr} \\ &\leqq b^p (e^{j^{1/(2kn)}} p!)^{2kmnr} = e^{2kmnr\, j^{1/(2kn)}} b^p p!^{2kmnr}\end{aligned}$$

uniformly for all $p \in \mathbf{N}_0$ and $j \in \mathbf{N}$, so $\varphi_j \in G_{2kmnr,b}(H)$, with norm bounded by $e^{2kmnr\, j^{1/(2kn)}}$. It then follows from [E1R], Theorem 6.1, that

$$G_{2kmnr}(H) = G_{2knr}(B_1, \ldots, B_d) \subseteq G_{2kn^2r}(P_1, \ldots, P_k, Q_1, \ldots, Q_k) = S^{\alpha,\ldots,\alpha}_{\alpha,\ldots,\alpha} ,$$

where $\alpha = 2kn^2 r$ and $S^{\alpha,\ldots,\alpha}_{\alpha,\ldots,\alpha}$ denotes the Gel'fand–Shilov space on $\mathbf{R}^k$ (see [GeS] Chapter IV). Now each function $\varphi \in S^{\alpha,\ldots,\alpha}_{\alpha,\ldots,\alpha}$ is infinitely differentiable and there exists $b' > 0$ (depending on φ) such that for every multi-index β there exists $c' > 0$ such that

$$|(D^\beta \varphi)(x)| \leqq c' e^{-b'|x|^{1/\alpha}}$$

uniformly for all $x \in \mathbf{R}^k$. So

$$|(D^\beta \varphi_j)(x)| \leqq c_{\beta,j} e^{-b_j |x|^{1/\alpha}}$$

for some constants $b_j, c_{\beta,j} > 0$. But if one traces the various constants then it follows that b_j depends only on b since each $\varphi_j \in G_{r;b}(H)$ and $c_{\beta,j}$ can be estimated by a function which depends linearly on the norm of φ_j in the space $G_{r;b}(H)$. So $c_{\beta,j} \leqq c_\beta e^{2kmnr\, j^{1/(2kn)}}$ for some c_β, independent of j. Thus

$$|(D^\beta \varphi_j)(x)| \leqq c_\beta e^{2kmnr\, j^{1/(2kn)}} e^{-b_0 |x|^{1/\alpha}}$$

for some constant $b_0 > 0$, uniformly for all multi-indices β, all $j \in \mathbf{N}$ and $x \in \mathbf{R}^k$.

It now easily follows that for all multi-indices β, γ the series

$$(D_x^\beta D_y^\gamma \kappa_z)(x; y) = \sum_{j=1}^{\infty} e^{-\lambda_j z} (D^\beta \varphi_j)(x) \overline{(D^\gamma \varphi_j)(y)}$$

converges by the estimates (22) and that

$$|(D_x^\beta D_y^\gamma \kappa_z)(x; y)| \leqq c_{\beta,\gamma,t} e^{-\lambda_1 t} e^{-b_0 |x|^{1/\alpha} - b_0 |y|^{1/\alpha}}$$

with $t = \mathrm{Re}\, z$ and

$$c_{\beta,\gamma,t} = c_\beta\, c_\gamma \sum_{j=1}^{\infty} e^{-(\lambda_j - \lambda_1)t} e^{2kmnrj^{1/(2kn)}} < \infty .$$

Note that $\sup_{t \geqq 1} c_{\beta,\gamma,t} < \infty$. □

The foregoing estimates establish that the spectral decomposition (21) of the semigroup generated by H is uniformly convergent. But as the estimates also give an exponentially decreasing bound it follows that the series is L_p-convergent for all p. This is a direct consequence of the Lebesgue dominated convergence theorem. Note that uniform convergence can also be deduced from cross-norm estimates on the semigroup by arguments similar to those on p. 247 of [Rob].

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