SOME SECOND-ORDER PARTIAL DIFFERENTIAL EQUATIONS ASSOCIATED WITH LIE GROUPS

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To Derek Robinson on the occasion of his 65th birthday

Abstract. In this note we survey results in recent research papers on the use of Lie groups in the study of partial differential equations. The focus will be on parabolic equations, and we will show how the problems at hand have solutions that seem natural in the context of Lie groups. The research is joint with D.W. Robinson, as well as other researchers who are listed in the references.

1. Introduction

When the Hamiltonian of a quantum-mechanical system is related to a Lie algebra, it is often possible to use the representation structure of the Lie algebra to decompose the Hilbert space of the quantum-mechanical system into simpler (irreducible) pieces. For example, if a Hamiltonian commutes with the generators of a Lie algebra, the Hilbert space of the system can be decomposed into irreducibles of the Lie algebra, and the Lie algebra elements themselves can be used as elements in a set of commuting observables.

We have aimed at making the present paper accessible to a wide audience of non-specialists, stressing the general ideas and motivating examples, as opposed to technical details.

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The class of such Hamiltonians is quite large: see [JoKl85] and [Jor88]. In this introduction we will review those Hamiltonians \( H \) whose interaction terms are polynomial in the position variables. Such Hamiltonians are directly and naturally related to nilpotent Lie algebras. The nilpotent case is studied in Section 2.

The spectrum of \( H \) is obtained by decomposing the physical space on which the Hamiltonian \( H \) acts into irreducible representations of the underlying nilpotent group. Sometimes this decomposition is decisive, as is the case with a particle in a constant magnetic field, where the decomposition leads to a harmonic-oscillator Hamiltonian. Sometimes the decomposition leads to a new Hamiltonian that requires further analysis, as is the case with a particle in a curved magnetic field.

The time evolution of the system is obtained by solving the heat equation of the underlying nilpotent Lie group. By writing the Hamiltonian as a quadratic sum of Lie-algebra elements and then using the representation of these Lie-algebra elements arising from the regular representation, it is possible to write \( e^{-tH} \) as the convolution of a kernel (which is a solution of the heat equation) with a representation acting on the physical Hilbert space; see [Jor88].

The simplest case of this spectral picture is as follows: Consider a nonrelativistic spinless particle of mass \( m \) in an external magnetic field \( \mathbf{B}(\mathbf{x}) \). The Hamiltonian for such a system is given by

\[
H = \frac{1}{2m} \left( \mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2,
\]

where \( \mathbf{p} = \frac{\hbar}{i} \nabla \) and \( \mathbf{A} \) is the vector potential satisfying \( \mathbf{B} = \nabla \times \mathbf{A} \). Consider the commutators

\[
\begin{align*}
[p_i - \frac{e}{c} a_i, p_j - \frac{e}{c} a_j] &= -\hbar \frac{e}{i c} \varepsilon_{ijk} b_k, \\
[p_i - \frac{e}{c} a_i, b_j] &= \frac{\hbar}{i} \frac{\partial b_j}{\partial x_i} \equiv \frac{\hbar}{i} b_{ij}, \\
[p_i - \frac{e}{c} a_i, b_{jk}] &= \frac{\hbar}{i} \frac{\partial b_{jk}}{\partial x_i} \equiv \frac{\hbar}{i} b_{ijk}, \\
&\vdots \quad \vdots \quad \vdots
\end{align*}
\]

where \( \mathbf{A} = (a_1, a_2, a_3) \), \( \mathbf{B} = (b_1, b_2, b_3) \), \( \mathbf{x} = (x_1, x_2, x_3) \). If \( \mathbf{B} \) is a polynomial in \( \mathbf{x} \), eventually the derivatives of \( \mathbf{B} \) will give zero, so that the set of commutators closes. The resulting Lie algebra formed by real linear combinations of the elements

\[
p_i - \frac{e}{c} a_i, b_i, b_{ij}, \ldots
\]
is therefore a nilpotent Lie algebra, and the Hamiltonian (1.1) is quadratic in the first three Lie algebra elements \( X_i := (p_i - \frac{e}{c}a_i), \ i = 1, 2, 3, \) from the list (1.3).

We show further in [JoKl85] and [Jor88] that there is a unitary representation \( U \) of \( G \) on \( L^2(\mathbb{R}^3) \) such that

\[
2mH = dU \left( \sum_{i=1}^{3} \left( p_i - \frac{e}{c}a_i \right)^2 \right).
\]

If there is a constant of motion for the Lie-algebra elements \( p_i - \frac{e}{c}a_i \), then \( U \) is a direct integral over a corresponding spectral parameter \( \xi \). We then get \( H = \int d\xi H^{(\xi)} \) where \( H \) has absolutely continuous spectrum, while each \( H^{(\xi)} \) has purely discrete spectrum. If \( \lambda_0(\xi) \leq \lambda_1(\xi) \leq \cdots \) is the spectrum of \( H^{(\xi)} \), then each \( \xi \mapsto \lambda_i(\xi) \) is real analytic, and we get the following typical spectral picture.

In this paper we will focus attention on a more restricted case wherein the coefficients are periodic. As shown in Section 3, this case shares the spectral band structure with the polynomial-magnetic-field case. We show that in the periodic case the regularity of the coefficients may be relaxed, and in fact, our spectral-theoretic results will be valid when the operator has \( L^\infty \)-coefficients.

2. Periodic operators

We begin by recalling some elementary definitions and facts about stratified Lie groups from [FoSt82]. A real Lie algebra \( \mathfrak{g} \) is called
stratified if it has a vector-space decomposition

\begin{equation}
\mathfrak{g} = \bigoplus_{k=1}^{r} \mathfrak{g}^{(k)},
\end{equation}

for some \( r \), which we shall take finite here, i.e., all but a finite number of the subspaces \( \mathfrak{g}^{(k)} \) are nonzero,

\begin{equation}
[\mathfrak{g}^{(k)}, \mathfrak{g}^{(l)}] \subseteq \mathfrak{g}^{(k+l)}
\end{equation}

for all \( k, l \in \mathbb{N} \), and \( \mathfrak{g}^{(1)} \) generates \( \mathfrak{g} \) as a Lie algebra. Thus a stratified Lie algebra is automatically nilpotent, and if \( r \) is the largest integer such that \( \mathfrak{g}^{(r)} \neq 0 \), then \( \mathfrak{g} \) is said to be nilpotent of step \( r \). A Lie group is defined to be stratified if it is connected and simply connected and its Lie algebra \( \mathfrak{g} \) is stratified.

Let \( G \) be a stratified Lie group and \( \exp : \mathfrak{g} \to G \) the exponential map. The Campbell–Baker–Hausdorff formula establishes that

\[ \exp (X) \exp (Y) = \exp (H(X,Y)) \]

where \( H(X,Y) = X + Y + [X,Y]/2 + \) a finite linear combination of higher-order commutators in \( X \) and \( Y \). Thus \( X, Y \to H(X,Y) \) defines a group multiplication law on the underlying vector space \( V \) of \( g \) which makes \( V \) a Lie group whose Lie algebra is \( \mathfrak{g} \) and the exponential map \( \exp : \mathfrak{g} \to V \) is simply the identity. Then \( V \) with the group law is diffeomorphic to \( G \). Next let \( d_k \) denote the dimension of \( \mathfrak{g}^{(k)} \) and \( d \) the dimension of \( \mathfrak{g} \) and for each \( k \) choose a vector-space basis \( X^{(k)} = (X^{(k)}_1, \ldots, X^{(k)}_{d_k}) \) of \( \mathfrak{g}^{(k)} \) such that \( X_1, \ldots, X_d = X^{(1)}_1, \ldots, X^{(r)}_d \) is a basis of \( \mathfrak{g} \). If \( \xi_1, \ldots, \xi_d \) is the dual basis for \( \mathfrak{g}^* \), i.e., if \( \xi_k (X_l) = \delta_{k,l} \), define \( \eta_k = \xi_k \circ \exp^{-1} \). Then \( \eta_1, \ldots, \eta_d \) are a system of global coordinates for \( G \), and the product rule on \( G \) becomes

\[ \eta_k(xy) = \eta_k(x) + \eta_k(y) + P_k(x,y), \quad x, y \in G, \]

where \( P_k(x,y) \) is a finite sum of monomials in \( \eta_i(x), \eta_i(y) \) for \( i < k \) with degree between 2 and \( m \). It follows that both left and right Haar measure on \( G \) can be identified with Lebesgue measure \( d\eta_1 \cdots d\eta_d \).

If \( X_i \) denotes one of the (abstract) Lie generators, we denote by \( A_i \) the corresponding right-invariant vector field on \( G \), i.e., \( A_i \) on a test function \( \psi \) on \( G \) is given by \( A_i^{(l)} = dL (X_i) \), or more precisely,

\begin{equation}
\left( A_i^{(l)} \psi \right) (g) = \frac{d}{dt} \psi (\exp (-tX_i) g) \big|_{t=0}, \quad g \in G,
\end{equation}

and similarly \( A_i^{(r)} = dR (X_i) \) given by

\begin{equation}
\left( A_i^{(r)} \psi \right) (g) = \frac{d}{dt} \psi (g \exp (tX_i)) \big|_{t=0}.
\end{equation}
Since we can pass from left to right with the adjoint representation,
the formulas may be written in one alone, and we will work with \( A_i^{(l)} \),
and denote it simply \( A_i \).

If \( 1 \leq j \leq d_1 \) we will need the functions \( y_j \) on \( G \) defined by
\[
y_j \left( \exp \left( \sum_{k=1}^{d} \eta_k X_k \right) \right) = \eta_j.
\]
These functions satisfy the following system of differential equations:
\[
-A_i^{(l)} y_j = A_i^{(r)} y_j = \delta_{i,j}.
\]
It follows by the standard ODE existence theorem that the functions \( y_i \) on \( G \) are determined uniquely by (2.6) and the “initial” conditions
\( y_i(e) = 0 \). Also note that (2.6) is consistent only for the differential
equations defined from a sub-basis \( A_1, \ldots, A_{d_1} \), and that they would
be overdetermined had we instead used a basis: hence the distinction
between subelliptic and elliptic.

In addition, we have given a discrete subgroup \( \Gamma \) in \( G \) such that
\( M = G/\Gamma \) is compact. It is well-known that it then has a unique (up
to normalization) invariant measure \( \mu \). The corresponding Hilbert space is \( L^2(M, \mu) \), and the invariant operators on \( G \) pass naturally to invariant operators on \( M \); see \[BBJR95\]. Let \( X_1, \ldots, X_{d_1} \)
be the generating Lie-algebra elements. Then the corresponding invariant vector fields on \( G \) will be denoted \( A_1, \ldots, A_{d_1} \), and those on \( M \)
will be denoted \( B_1, \ldots, B_{d_1} \). Functions \( c_{i,j} \in L^\infty(G) \) are given, and we
form the quadratic form
\[
h(f) = \sum_{i,j=1}^{d_1} \langle A_i f \mid c_{i,j} A_j f \rangle.
\]
If further
\[
c_{i,j}(g\gamma) = c_{i,j}(g) \quad \text{for } g \in G, \ \gamma \in \Gamma;
\]
then we have a corresponding form \( h_M \) on \( M = G/\Gamma \).

Introducing
\[
c_{i,j}^\varepsilon(x) = c_{i,j}(\varepsilon^{-1}x), \quad \varepsilon > 0,
\]
we get for each \( \varepsilon \) a periodic problem corresponding to the period lattice
\( \varepsilon \Gamma \). To speak about \( \varepsilon \Gamma \) for \( \varepsilon \in \mathbb{R}_+ \), we must have an action of \( \mathbb{R}_+ \) on
\( G \) which generalizes the familiar one
\[
\varepsilon: (x_1, \ldots, x_d) \mapsto (\varepsilon x_1, \ldots, \varepsilon x_d)
\]
of \( \mathbb{R}^d \). It turns out that this can only be done if \( G \) is stratified, and so in
particular nilpotent; see \[FoSt82, Jor88\]. In that case it is possible to
construct a group of automorphisms \( \{\delta_\varepsilon\}_{\varepsilon \in \mathbb{R}_+} \) of \( G \) which is determined by the differentiated action \( d\delta_\varepsilon \) on the Lie algebra \( \mathfrak{g} \). If \( \mathfrak{g} \) is specified as in (2.1)–(2.2), then
\[
d\delta_\varepsilon \left( X^{(1)} \right) = \varepsilon X^{(1)}, \quad X^{(1)} \in \mathfrak{g}^{(1)}, \quad \varepsilon \in \mathbb{R}_+.
\]

Let \( H \), respectively \( H_\varepsilon \), be the selfadjoint operators associated to the period lattices \( \Gamma \) and \( \varepsilon \Gamma \) (see [BBJR95] or [Rob91]), and let \( S_t = e^{-tH} \), \( S^\varepsilon_t = e^{-tH_\varepsilon} \).

We now turn to the homogenization analysis of the limit \( \varepsilon \to 0 \) which leads to our comparison of the variable-coefficient case to the constant-coefficient one. It should be stressed that in the Lie case, even the “constant-coefficient” operator \( \sum_{i,j} A_i \hat{c}_{i,j} A_j \) is not really constant-coefficient, as the vector fields \( A_i \) are variable-coefficient.

Take even the simplest example where \( G \) is the three-dimensional Heisenberg group of upper triangular matrices of the form
\[
g = \begin{pmatrix} 1 & x & z \\ 0 & 1 & y \\ 0 & 0 & 1 \end{pmatrix}, \quad x, y, z \in \mathbb{R}.
\]

In this case, \( \dim \mathfrak{g}^{(1)} = 2 \), and \( \dim \mathfrak{g}^{(2)} = 1 \), with \( \mathfrak{g}^{(2)} \) spanned by the central element in the Lie algebra. Differentiating matrix multiplication (2.10) on the left as in (2.3), we get the following three identities:
\[
A_1 = \frac{\partial}{\partial x} + y \frac{\partial}{\partial z} = -dL \left( X_1 \right),
\]
\[
A_2 = \frac{\partial}{\partial y} = -dL \left( X_2 \right),
\]
\[
A_3 = \frac{\partial}{\partial z} = -dL \left( X_3 \right),
\]
where the first vector field is of course variable coefficients.

We will use standard tools [ZKO94] (see also [Dau92], [Tho73], [Wil78]) on homogenization.

**Theorem 2.1.** [BBJR95] Suppose the system \( c_{i,j} \in L^\infty \) is given and assumed strongly elliptic. Then there is a \( C_0 \)-semigroup \( \hat{S}_t \) on \( L^2 \left( G, dx \right) \) with constant coefficients, where \( dx \) is left Haar measure, such that
\[
\lim_{\varepsilon \to 0} \left\| \left( S^\varepsilon_t - \hat{S}_t \right) f \right\|_2 = 0
\]
for all \( f \in L^2 \left( G, dx \right) \) and \( t > 0 \).

The constant coefficients of the limit operator \( \hat{c}_{i,j} \) may be determined as follows: We show in [BBJR95] that if
\[
c_{i,j} \left( g \right) := h \left( g_i - y_i, g_j - y_j \right)
\]
and if \( C(g) \) is the corresponding quadratic form, then the problem

\[
\inf_g C(g) =: \hat{C}
\]

(2.13)

has a unique solution, i.e., the infimum is attained at \( f_1, \ldots, f_{d_1} \) such that

\[
C(f) = \hat{C}.
\]

(2.14)

The order relation which is used in the infimum consideration (2.13) is the usual order on hermitian matrices: For every \( g \), the matrix \( C(g) := (c_{i,j}(g))_{i,j=1}^{d_1} \) is hermitian, and the matrix inequality \( C(g) \geq \hat{C} \) may thus be spelled out as follows:

\[
\sum_{i,j} \bar{z}_i c_{i,j}(g) z_j \geq \sum_{i,j} \bar{z}_i \hat{c}_{i,j} z_j \quad \text{for all } z_1, \ldots, z_{d_1} \in \mathbb{C}.
\]

Solvability of this variational problem is part of the conclusion of our analysis in [BBJR95], i.e., the existence of the minimizing functions \( f_1, \ldots, f_{d_1} \).

Then the coefficients of the homogenized operator can also be computed with the aid of the coordinates \( y_i, i = 1, \ldots, d_1 \), introduced in (2.5) and (2.6). One has the representation

\[
\hat{c}_{i,j} = \int_Y dy \sum_{k,l=1}^{d_1} (A_k(f_i(y) - y_i)) c_{k,l}(y) (A_l(f_j(y) - y_j))
\]

(2.15) \[= h_Y(f_i - y_i, f_j - y_j),\]

where \( h \) denotes the sesquilinear form associated with \( H \), and the subscript \( Y \) refers to the region of integration. Specifically, \( Y \) is a fundamental domain for the given lattice \( \Gamma \) in \( G \). For example, we may take \( Y \) to be defined by

\[
Y = \bigcap_{\gamma \in \Gamma} \{ x \in G : |x| \leq |x\gamma^{-1}| \},
\]

(2.16) and \( |\cdot| \) defined relative to a geodesic distance \( d \), \( |x| := d(x,e), x \in G \). Then

(i) \( \bigcup_{\gamma \in \Gamma} Y\gamma = G \), and
(ii) \( \text{meas}(Y\gamma_1 \cap Y\gamma_2) = 0 \) whenever \( \gamma_1 \neq \gamma_2 \) in \( \Gamma \).

(These are the axioms for fundamental domains of given lattices, but we stress that (2.16) is just one choice in a vast variety of possible choices.)

The simplest case of the construction is \( G = \mathbb{R} \), and it was first considered in [Dav97] by Brian Davis. This is the simplest possible
heat equation, and we then have the conductivity represented by a periodic function \( c \), say

\[
c(x + p_0) = c(x), \quad x \in \mathbb{R},
\]

where \( p_0 \) is the period. Then \( H = -\frac{d}{dx}c(x) \frac{dx}{c(x)} \), and it can be checked that

\[
\hat{c} = \left( \frac{1}{p_0} \int_0^{p_0} \frac{dx}{c(x)} \right)^{-1}.
\]

**Theorem 2.2.** [BBJR95] Adopt the assumptions of Theorem 2.1. Then

\[
\lim_{t \to \infty} t^{D/2} \text{ess sup}_{|x|^2 + |y|^2 \leq a t} |K_t(x ; y) - \hat{K}_t(x ; y)| = 0
\]

for each \( a > 0 \) where \( |x| = d_c(x ; e) \), and where

\[
d_c(x ; y) = \sup \left\{ \psi(x) - \psi(y) ; \psi \in C^\infty_c(G) ,
\sum_{i,j=1}^{d_1} c_{i,j} (A_i \psi) (A_j \psi) \leq 1 \text{ pointwise} \right\}
\]

and \( A_i \psi \) refers to the Lie action of the vector field \( A_i \) on \( \psi \) from (2.3).

The number \( D \) is the homogeneous degree defined from the given filtration \( \mathfrak{g}^{(i)} \) of the nilpotent Lie algebra \( \mathfrak{g} \). As spelled out in [Jor88] and [FoSt82], there are numbers \( \nu_i \) depending on the Lie-structure coefficients such that

\[
D = \sum_i \nu_i \dim \mathfrak{g}^{(i)}.
\]

To be specific, the numbers \( \nu_i \) are determined in such a way that we get a group of scaling automorphisms \( \{ \delta_\varepsilon \}_{\varepsilon \in \mathbb{R}_+} \) of \( \mathfrak{g} \), and therefore on \( G \), and it is this group which is fundamental in the homogenization analysis. Specifically, \( \delta_\varepsilon : \mathfrak{g} \to \mathfrak{g} \) is defined by

\[
(2.17) \quad \delta_\varepsilon (X^{(i)}) = \nu_i X^{(i)}, \quad X^{(i)} \in \mathfrak{g}^{(i)},
\]

and then extended to \( \mathfrak{g} \) by linearity via (2.1), in such a way that

\[
(2.18) \quad \delta_\varepsilon ([X,Y]) = [\delta_\varepsilon (X), \delta_\varepsilon (Y)], \quad X,Y \in \mathfrak{g}, \quad \varepsilon \in \mathbb{R}_+.
\]

Hence if (2.2) holds, then it follows from (2.17) and (2.18) that \( \nu_i = i \) for \( i = 1, 2, \ldots \). In the case of the Heisenberg Lie algebra \( \mathfrak{g} \), we have \( [X,Y] = Z \) as the relation on the basis elements; \( Z \) is central. Then \( \mathfrak{g}^{(1)} = \text{span} (X,Y) \), \( \mathfrak{g}^{(2)} = \mathbb{R}Z \), \( \nu_1 = 1 \), \( \nu_2 = 2 \), so \( D = 4 \).
Let $K_t$ and $\hat{K}_t$ be the respective integral kernels for the semigroups $S_t$ and $\hat{S}_t$, and set
\[
\|K\|_p = \text{ess sup}_{x \in G} \left( \int_G dy \left| K(x, t) \right|^p \right)^{1/p}
\]
and
\[
\|K\|_\infty = \text{ess sup}_{x, y \in G} \left| K(x, y) \right|.
\]

Then
\[
\text{Theorem 2.3. \cite{BBJR95}} \quad \text{Adopt the assumptions of Theorem 2.1. Then}
\]
\[
\lim_{t \to \infty} t^{D/2} \left\| K_t - \hat{K}_t \right\|_\infty = 0, \quad \lim_{t \to \infty} \left\| K_t - \hat{K}_t \right\|_1 = 0.
\]

3. $G = \mathbb{R}^d$

The case $G = \mathbb{R}^d$ was considered in \cite{BJR99}, where we further showed that the limit $S_t^\varepsilon \to \hat{S}_t$ then holds also in the spectral sense. In that case, we scale by $\varepsilon = 1/n, n \to \infty$, and then identify the limit operator as having absolutely continuous spectral type, and we prove spectral asymptotics. (A general and classical reference for periodic operators is \cite{Eas73}.)

Starting with an equation which is invariant under the $\mathbb{Z}^d$-translations, we then use the Zak transform \cite{Dau92} to write $S_t = e^{-tH}$ as a direct integral over $\mathbb{T}^d (= \mathbb{R}^d/\mathbb{Z}^d)$, viz.,
\[
S_t = \int_{\mathbb{T}^d} S_t^{(z)} d^z
\]
and we establish continuity of $z \mapsto S_t^{(z)}$ in the strong topology \cite[Lemma 2.2]{BJR99}. Pick a positive $C^\infty$-function $\tau$ on $\mathbb{R}^d$ of integral one, and set
\[
c_{i,j}^{(n)}(x) = n^d \int_{\mathbb{R}^d} dy \tau(ny) c_{i,j}(x - y),
\]
and form the corresponding $C_0$-semigroup
\[
S_t^{(n)} = e^{-tH^{(n)}},
\]
where $H^{(n)}$ is defined from $c_{i,j}^{(n)}$. We then show in \cite{BJR99} that $S_t^{(n)}$ approximates $S_t$, not only in the strong topology, but also in a spectral-theoretic sense. Using this, we establish the following connection between $S_t = e^{-tH}$ and $S_t^{(z)} = e^{-tH^{(z)}}$ in (3.1). Setting $z = (e^{i\theta_1}, \ldots, e^{i\theta_d})$, we get
Theorem 3.1. If \( \lambda_n(z) \) denotes the eigenvalues of \( H_z \) then

\[
\lim_{N \to \infty} \left\{ N^2 \lambda_n(w) ; w^N = z, \ n = 0, 1, \ldots \right\} = \left\{ \langle (n - \theta) \ | \ \hat{C} (n - \theta) \rangle ; n \in \mathbb{Z}^d \right\},
\]

where the limit is in the sense of pointwise convergence of the ordered sets, and where \( \hat{C} = (\hat{c}_{i,j}) \) is the constant-coefficient homogenized case.

The rate of convergence of the eigenvalues in (3.2) can be estimated further by a trace norm estimate.

We refer the reader to [BJR99] for details of proof, but the arguments in [BJR99] are based in part on the references [Aus96], [DaTr82], [Eas73], and [ZKON79]. In addition, we mention the papers [Aus96], [AMT98], and [TERo99], which contain results which are related, but with a different focus.

Finally, we mention that our result from [BJR99], Theorem 3.1, has since been extended in several other directions: see, e.g., [Sob99] and [She00].

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