

# Quantum Mechanics and Nilpotent Groups

## I. The Curved Magnetic Field

By

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### Abstract

The quantum mechanics of massive spinless particles in an external magnetic field polynomial in position variables is shown to be related to nilpotent Lie groups. By using the known representation structure of such groups, the Hilbert spaces of the quantum mechanical systems can be decomposed into irreducible representations of the nilpotent groups. Such a decomposition is given explicitly for constant and curved magnetic fields.

Since the Hamiltonian for polynomial magnetic fields is quadratic in the Lie algebra elements, its spectrum can be found using the representation structure of nilpotent groups. The explicit time dependence of the system can also be found by solving the heat equation on nilpotent groups. These ideas are worked out for the constant magnetic field, where the solution is well known, and the curved magnetic field, where it is not. Generalizations to other systems whose interaction terms are polynomial are also given.

### §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.

In this paper we will analyze quantum mechanical systems whose Hamiltonians are quadratic in generators of a Lie algebra. The class of such Hamiltonians is quite large; our concern will be with those Hamiltonians whose interaction terms are polynomial in the position variables. Such Hamiltonians are related to nilpotent Lie algebras. In this and succeeding papers, we will make

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use of the connection between polynomial Hamiltonians and Lie algebras to solve a variety of problems of physical interest. In all of these problems, we are interested in finding the spectrum of the Hamiltonian and the full Green's function which gives the time evolution of the system.

The spectrum is obtained by decomposing the physical space on which the Hamiltonian 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, also analyzed in this paper.

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.

The other sections of this paper are organized as follows: In Sect. 2 we convert the problem of a spinless particle in an external field polynomial in  $\hat{x}$  to a problem in the representation structure of nilpotent groups and algebras. Sections 3 and 4 deal with mathematical notation, and some general properties of operators, respectively, needed for this and other papers. Then in Sect. 5 we begin our analysis of nilpotent groups, while in Sect. 6 the decomposition of the constant and curved magnetic field examples are given. Section 7 provides a spectral analysis of the curved magnetic field example while in Sect. 8 the heat equation for the curved magnetic field is analyzed. We show that the curved field Hamiltonian decomposes as a direct integral over a single real parameter,  $-\infty < \alpha < \infty$ , such that each operator  $H_\alpha$  in the decomposition has a purely discrete spectrum, although each  $H_\alpha$  is obtained from a representation of a degenerate elliptic operator  $\tilde{A}$  on  $G$  with absolutely continuous spectrum.

An explicit trace formula is obtained for the operators  $e^{-tH_\alpha}$ ,  $t > 0$ ,  $\alpha \in \mathbf{R}$ .

There is a large amount of fairly recent work by B. Simon [Sim] and co-workers on the operator  $e^{-tH}$  for Schrödinger-Hamiltonians,  $H$ . Their work is quite different from ours: Firstly, their techniques are based on functional integration (the Feynman-Kac formula being central), and, secondly, the aim appears, for the most part, to be qualitative estimates. Their work includes a wider class of Schrödinger operators than does ours. Our work uses only integration on the line (or a finite number of copies of the line), and we get explicit formulas for a particular polynomial  $H$ .

§ 2. Physical Motivation

Consider a spinless particle of mass  $m$  in an external magnetic field  $\vec{B}(\vec{x})$ . The Hamiltonian for such a system is given by

$$H = \frac{1}{2m} \left( \vec{p} - \frac{e}{c} \vec{A} \right)^2, \tag{2.1}$$

where  $\vec{p} = \hbar/i \vec{\nabla}$  and  $\vec{A}$  is the vector potential satisfying  $\vec{B} = \vec{\nabla} \times \vec{A}$ . Consider the commutators

$$\begin{aligned} \left[ p_i - \frac{e}{c} A_i, p_j - \frac{e}{c} A_j \right] &= -\frac{\hbar}{i} \frac{e}{c} \epsilon_{ijk} B_k \\ \left[ p_i - \frac{e}{c} A_i, B_j \right] &= \frac{\hbar}{i} \frac{\partial B_j}{\partial x_i} \equiv \frac{\hbar}{i} B_{ij} \\ \left[ p_i - \frac{e}{c} A_i, B_{jk} \right] &= \frac{\hbar}{i} \frac{\partial B_{jk}}{\partial x_i} \equiv \frac{\hbar}{i} B_{ijk} \\ &\vdots \qquad \qquad \qquad \vdots \end{aligned} \tag{2.2}$$

If  $\vec{B}$  is a polynomial in  $\vec{x}$ , eventually the derivatives of  $\vec{B}$  will give zero, so that the set of commutators close. The resulting Lie algebra formed by  $p_i - e/c A_i, B_i, B_{ij}, \dots$  is a nilpotent Lie algebra, and the Hamiltonian (2.1) is quadratic in the Lie algebra elements  $(p_i - e/c A_i)$ .

To show how group theoretical methods can be used to analyze both the spectrum and the time evolution of systems with Hamiltonians that are quadratic sums of Lie algebra elements, we will, in this paper, analyze the simple cases of a constant magnetic field (whose spectrum and time evolution is known, see Ref. [L-L]) and the more complicated case of a magnetic field linear in  $\vec{x}$ , whose solution, both classically and quantum mechanically, is—to our knowledge—not known.

To connect the Hamiltonian (2.1) with specific groups and Lie algebras, it is best to make all quantities dimensionless. For the constant magnetic field, of magnitude  $b_0$ , the vector potential can be chosen to be  $A_y = b_0 x$ , with  $B_z = (\partial A_y / \partial x) = b_0$ . Then a natural unit of length is  $\sqrt{\hbar c / e b_0}$ , and a natural unit of energy,  $\hbar e b_0 / mc$ . So if  $b_0$  is chosen to be any convenient value, the magnitude of any constant magnetic field can be written as  $\gamma b_0$ , where  $\gamma$  is a real constant. Then a dimensionless Hamiltonian can be written as

$$H = \frac{1}{2} \left[ -\frac{\partial^2}{\partial x^2} - \left( \frac{\partial}{\partial y} - i\gamma x \right)^2 - \frac{\partial^2}{\partial z^2} \right],$$

or

$$-2H = \left[ \frac{\partial^2}{\partial x^2} + \left( \frac{\partial}{\partial y} - i\gamma x \right)^2 + \frac{\partial^2}{\partial z^2} \right]. \tag{2.3}$$

Consider the real nilpotent Lie group  $G = \{g(a, b, c, d)\}$ , where

$$g(a, b, c, d) = \begin{pmatrix} 1 & a & c & d \\ & 1 & b & 0 \\ & 0 & 1 & 0 \\ & & & 1 \end{pmatrix}. \quad (2.4)$$

As discussed in Sect. 3, Lie algebra elements are denoted by capital letters, so that  $[A, B] = C$  is the only nontrivial commutation relation in the Lie algebra of  $G$ . Further, as discussed in Sect. 6, a unitary representation for  $G$  can be given on  $\mathcal{L}^2(\mathbf{R}^3)$ , the quantum mechanical space for a spinless particle of mass  $m$ . This representation is induced from the subgroup of  $G$  given by  $\{g(0, 0, c, 0)\} \rightarrow e^{-i\gamma c}$ , where  $\gamma$  is an irreducible representation label. The representation is given by

$$(U_g f)(x, y, z) = e^{-i\gamma(c+xb)} f(x+a, y+b, z+d) \quad (2.5)$$

and has Lie algebra elements given by

$$\begin{aligned} dU(A) &= \frac{\partial}{\partial x} \\ dU(B) &= \frac{\partial}{\partial y} - i\gamma x \\ dU(C) &= -i\gamma \\ dU(D) &= \frac{\partial}{\partial z}, \\ [dU(A), dU(B)] &= dU(C) \end{aligned} \quad (2.6)$$

which give the Hamiltonian (2.3), i. e.,

$$-2H = (dU(A))^2 + (dU(B))^2 + (dU(D))^2, \quad (2.7)$$

a quadratic sum of Lie algebra elements. Note that  $\gamma$  is a representation label for  $G$ , which gives the strength of the magnetic field (relative to  $b_0$ ). Thus, dimensionless parameters in the Hamiltonian are related to representation labels. Note also that  $G$  is a direct product of the Heisenberg group and the translation group, reflecting the fact that the momentum in the direction of the magnetic field is conserved. In Sect. 6 it will be shown that the representation (2.5) is reducible; the reduction to irreducible representations will lead to a harmonic oscillator spectrum (see Ref. [L-L]).

The simplest nonconstant polynomial magnetic field is  $B_x = a_0 x$ ,  $B_y = -a_0 y$ ,  $B_z = 0$ , for which a suitable vector potential is  $A_z = a_0 x y$ . For this field a natural unit of length is  $(hc/ea_0)^{1/3}$ , and a natural unit of energy,  $1/m(ea_0 h^2/c)^{2/3}$ . Again, if  $a_0$  is chosen to be a convenient value, any other magnetic field of different

strength can be gotten from  $A_z = \gamma a_0 x y$ , where  $\gamma$  is again a real number. The dimensionless Hamiltonian is then

$$-2H = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \left( \frac{\partial}{\partial z} - i\gamma x y \right)^2. \tag{2.8}$$

Associated with this magnetic field is the nilpotent group  $G = \{g(a_1, a_2, a_3, b_1, b_2, c)\}$ , where

$$g(a_1, a_2, a_3, b_1, b_2, c) = \begin{pmatrix} 1 & a_1 & b_2 & c \\ & 1 & a_3 & b_1 \\ & 0 & 1 & a_2 \\ & & & 1 \end{pmatrix}; \tag{2.9}$$

the commutation relations for this nilpotent group are easily computed and are given in Sect. 5 (Ex. 5.3). A representation of  $G$  on  $\mathcal{L}^2(\mathbb{R}^3)$  (the ‘‘physical’’ space) can be obtained by inducing from the abelian subgroup  $\{g(0, 0, 0, b_1, b_2, c)\}$ , with one-dimensional representations  $e^{i(\beta_1 b_1 + \beta_2 b_2 - \gamma c)}$ :

$$\begin{aligned} (U_g f)(x, y, z) &= e^{i[\beta_1(b_1 + z a_2) + \beta_2(b_2 + x a_3)]} \\ &\times e^{-i\gamma(c + x b_1 - b_2 a_2 - b_2 y - x a_2 a_3 - x y a_3)} \\ &\times f(x + a_1, y + a_2, z + a_3), \\ &f \in \mathcal{L}^2(\mathbb{R}^3), g \in G. \end{aligned} \tag{2.10}$$

The infinitesimal generators are easily read off from (2.10):

$$\begin{aligned} dU(A_1) &= \frac{\partial}{\partial x} \\ dU(A_2) &= \frac{\partial}{\partial y} + i\beta_1 z \\ dU(A_3) &= \frac{\partial}{\partial z} - i\gamma x y + i\beta_2 x \\ dU(B_1) &= i\beta_1 + i\gamma x \\ dU(B_2) &= i\beta_2 - i\gamma y \\ dU(C) &= i\gamma; \end{aligned} \tag{2.11}$$

it is seen that this representation of the generators also satisfies the correct commutation relations.

However, most significant is the fact that if  $\beta_1 = \beta_2 = 0$ , then the Hamiltonian (2.8) can be written as

$$-2H = (dU(A_1))^2 + (dU(A_2))^2 + (dU(A_3))^2, \tag{2.12}$$

again a sum of squares of Lie algebra elements with the representation parameters specifying the (dimensionless) strength of the magnetic field. The proper representation labels have reproduced the correct vector potential for the curved magnetic field.

As with the constant magnetic field, the representation (2.10) is reducible and will be reduced to irreducibles in Sect. 6. But, the resulting Hamiltonian is not transparently solvable; it is, however, a Hamiltonian with a polynomial interaction, so that the group given in Eq. (2.9) can be used to solve the heat equation which in turn gives an expression for the Green's function of the curved magnetic field. This is done in Sect. 9. Before carrying out this analysis, we introduce notation (Sect. 3) and some further mathematical background (Sect. 4) which will be used in this series of papers.

### § 3. Notation

(i) Lower case Gothic letters,  $\mathfrak{g}$ ,  $\mathfrak{h}$ , etc. will denote finitedimensional Lie algebras over the reals  $\mathbf{R}$ . Elements in  $\mathfrak{g}$  will be denoted  $A, B$  etc. If  $B_1, \dots, B_d$  is a basis for  $\mathfrak{g}$ , then elements in  $\mathfrak{g}$  are expressed in the form  $\sum_i b_i B_i$ , where the  $b_i$ 's are *real* scalars. A subset of  $\mathfrak{g}$  consisting of elements,  $A_1, \dots, A_r$ , say, is said to generate  $\mathfrak{g}$  (as a Lie algebra) if the smallest Lie subalgebra  $\mathfrak{h}$  of  $\mathfrak{g}$  containing these elements equals  $\mathfrak{g}$ . If  $\mathfrak{h}$  is strictly contained in  $\mathfrak{g}$ , the set  $A_1, \dots, A_r$  may always be extended to a set of Lie generators. For many of our considerations it will suffice then to restrict attention to  $\mathfrak{g}$ .

(ii) The upper case Gothic  $\mathfrak{U}$  will be reserved for the universal enveloping algebra. If  $\mathfrak{g}$  is given as in (i), we shall denote  $\mathfrak{U}(\mathfrak{g})$  the complex (associative) enveloping algebra, with unit 1, over  $\mathfrak{g}$ . The Poincaré-Birkhoff-Witt theorem states that the monomials,  $B_1^{\alpha_1} B_2^{\alpha_2} \dots B_d^{\alpha_d}$ , where  $\alpha = (\alpha_1, \dots, \alpha_d)$ ,  $\alpha_i = 0, 1, \dots$ , is a multi-index, form a basis for  $\mathfrak{U}(\mathfrak{g})$ . (We have adopted the convention that the trivial multi-index,  $0 = (0, \dots, 0)$  corresponds to the identity 1 in  $\mathfrak{U}(\mathfrak{g})$ .) Each element in  $\mathfrak{U}(\mathfrak{g})$  may be expressed uniquely in the form  $\sum_{\alpha} c_{\alpha} B_1^{\alpha_1} \dots B_d^{\alpha_d}$ , where the coefficients  $c_{\alpha}$  are complex scalars, and the summation in  $\alpha$  is finite.

(iii) In the trivial case where we define the commutator Lie bracket  $[A, B] = 0$  for any pair of elements  $A, B$  in  $\mathfrak{g}$ , the corresponding universal algebra is called the symmetric (tensor) algebra, and it is denoted  $\mathfrak{S}(\mathfrak{g})$ . Choosing a basis,  $B_1, \dots, B_d$  for  $\mathfrak{g}$ , allows us to realize  $\mathfrak{S}(\mathfrak{g})$  as a polynomial algebra in  $d$  variables. Polynomials of degree  $\leq n$  give rise to a filtration  $\mathfrak{S}_n(\mathfrak{g})$  of  $\mathfrak{S}(\mathfrak{g})$ ; i.e., for elements  $a$  in  $\mathfrak{S}_n(\mathfrak{g})$  and  $b$  in  $\mathfrak{S}_m(\mathfrak{g})$ , the product,  $a \cdot b$  is in  $\mathfrak{S}_{n+m}(\mathfrak{g})$ .

According to the Poincaré-Birkhoff-Witt theorem,  $\mathfrak{U}(\mathfrak{g})$  and  $\mathfrak{S}(\mathfrak{g})$  are isomorphic as *linear* spaces. This isomorphism then gives rise to a filtration of elements in  $\mathfrak{U}(\mathfrak{g})$ . We have,  $\mathfrak{U}_n(\mathfrak{g}) \cdot \mathfrak{U}_m(\mathfrak{g}) \subset \mathfrak{U}_{n+m}(\mathfrak{g})$  since the corresponding inclusion holds for the  $\mathfrak{S}_n(\mathfrak{g})$ 's. We shall be particularly interested in second-order elements, i.e., the space,  $\mathfrak{U}_2(\mathfrak{g})$  because of its physical significance, cf. Sect. 2.

Dixmier [Dix 1] showed that the elements in the center of  $\mathfrak{U}(\mathfrak{g})$  serve as labels for the unitary irreducible representations of nilpotent, simply connected, Lie groups  $G$  with Lie algebra  $\mathfrak{g}$ . There is a canonical mapping from  $\mathfrak{U}(\mathfrak{g})$  into  $\mathfrak{S}(\mathfrak{g})$ . It transforms the center into a set of invariants contained in  $\mathfrak{S}(\mathfrak{g})$ , and Dixmier [Dix 1] showed, in the nilpotent case, that the restricted map is an isomorphism of algebras.

(iv) We shall need an additional structure for  $\mathfrak{U}(\mathfrak{g})$ : Using the universal property of  $\mathfrak{U}(\mathfrak{g})$ , it can easily be verified that there is a unique  $*$ -operation on  $\mathfrak{U}(\mathfrak{g})$  which satisfies,  $A^* = -A$  for  $A \in \mathfrak{g}$ . Recall that a  $*$ -operation is an involutive, complex-conjugate-linear, anti-automorphism.

(v) We shall consider representations  $\rho$  of  $\mathfrak{g}$ , and extensions,  $\tilde{\rho}$  say, to  $\mathfrak{U}(\mathfrak{g})$ : Let  $\mathcal{H}$  be a complex Hilbert space, and  $\mathcal{D} \subset \mathcal{H}$  a dense linear subspace. We shall consider the algebra  $\mathcal{A}$  of all linear operators  $T$  in  $\mathcal{H}$  with the following three properties:

- (a)  $T$  is defined on  $\mathcal{D}$ .
- (b)  $\mathcal{D}$  is invariant, i. e.,  $T\mathcal{D} \subset \mathcal{D}$ .
- (c) The adjoint operator,  $T^*$  is defined on  $\mathcal{D}$ .

The operator adjoint,  $*$  equips  $\mathcal{A}$  with the structure of a  $*$ -algebra.

A representation  $\rho$  of  $\mathfrak{g}$  is a linear map from  $\mathfrak{g}$  to  $\mathcal{A}$  satisfying,  $\rho([A, B]) = [\rho(A), \rho(B)]$  for  $A, B \in \mathfrak{g}$ , and, in addition, the identity,  $\rho(A) = -\rho(A)^*$  on  $\mathcal{D}$ ,  $A \in \mathfrak{g}$ . Using again the universal property of  $\mathfrak{U}(\mathfrak{g})$ , it can be checked that each representation  $\rho$  of  $\mathfrak{g}$  extends uniquely to a  $*$ -representation of  $\mathfrak{U}(\mathfrak{g})$ ,  $\tilde{\rho}$  say, i. e.,  $\tilde{\rho}$  satisfies the identity,  $\tilde{\rho}(a^*) = \tilde{\rho}(a)^*$  on  $\mathcal{D}$ , for  $a \in \mathfrak{U}(\mathfrak{g})$ .

(vi) Although the following lemma is well known ([Gär 1, Seg, Pou, J-M]), we make it explicit here for the benefit of the reader: Let  $G$  be a Lie group with Lie algebra  $\mathfrak{g}$ , and exponential map,  $\exp: \mathfrak{g} \rightarrow G$ . Let  $U$  be a strongly continuous unitary representation of  $G$  in a Hilbert space  $\mathcal{H}$ . Let  $dg$  be a fixed left-invariant Haar measure on  $G$ , and let  $C_c^\infty(G)$  be the algebra of all smooth compactly supported functions on  $G$ . Then the Gårding space  $\mathcal{D}$  is defined as the span of the vectors,

$$\psi_F = \int_G F(g)U(g)\psi dg, \tag{3.1}$$

where  $F \in C_c^\infty(G)$ , and  $\psi \in \mathcal{H}$ . Let  $\mathcal{A}$  be defined as in (v) above.

**Lemma 3.1.** *Let  $U$  be a unitary representation (strong continuity is always assumed) of  $G$ . Then there is a unique  $*$ -representation  $\rho$  of  $\mathfrak{U}(\mathfrak{g})$  which is specified by*

$$\rho(A)\psi_F = \frac{d}{dt}U(\exp(tA))\psi_F|_{t=0} \tag{3.2}$$

for  $A \in \mathfrak{g}$ ,  $\psi_F \in \mathcal{D}$ .

The representation  $\rho$  is called the infinitesimal representation, and is also

denoted  $dU$ . The special case where  $U$  is the left-regular representation  $L$ ,

$$(L(g)F)(g') = F(g^{-1}g'), \quad g, g' \in G, \tag{3.3}$$

is of particular interest. Let  $dL$  be the corresponding infinitesimal left-regular representation which is specified in Lemma 3.1, i. e.,

$$(dL(A)F)(g) = \frac{d}{dt} F(\exp(-tA) \cdot g) |_{t=0}. \tag{3.3'}$$

Then it can easily be checked that

$$U(g)(\phi_F) = \phi_{L(g)F}, \quad g \in G, \quad F \in C_c^\infty(G), \tag{3.4}$$

and

$$dU(A)(\phi_F) = \phi_{dL(A)F}, \quad A \in \mathfrak{g}. \tag{3.4'}$$

(The latter two formulas constitute the main steps in the proof of Lemma 3.1, see, for example, [Pou].)

#### § 4. Continuous Semigroups of Operators

In this paper, we shall study unitary one-parameter groups of operators in a fixed Hilbert space  $\mathcal{H}$ . If  $U(t)$  is such a group, then by Stone's theorem [D-S], it is of the form,  $U(t) = \exp(itH)$ ,  $H = H^*$ , and spectral resolutions,

$$U(t) = \int e^{it\lambda} dE(\lambda) \tag{4.1}$$

$$H = \int \lambda dE(\lambda) \tag{4.2}$$

exist. We shall focus attention on calculating explicitly the projection-valued measure  $E$  in the spectral resolution (4.2) for a class of semibounded Hamiltonians  $H$ , i. e.,  $H \geq 0$ . The semiboundedness allows us to restrict the integrals in (4.1)-(4.2) to the half-line  $[0, \infty)$ . Let  $A_0, A_1, \dots, A_r$  be a set of elements in  $\mathfrak{g}$ , and assume that  $A_0$  is in the real span of the  $A_k$ 's,  $k \geq 1$ . Let  $U$  be a unitary representation of  $G$ . We showed in [Jo] that the operator,  $H = -dU(iA_0 + \sum_{k=1}^r A_k^2)$ , is essentially self-adjoint on the Gårding space  $\mathcal{D}$ . In the special case when  $A_0 = 0$ , we have  $H \geq 0$ .

The following more detailed information about  $H$  is available from [Jo]:

**Theorem 4.1** ([Jo]). *Let  $U$  be a unitary representation of  $G$ , and let  $A_0, A_1, \dots, A_r$  be elements in the Lie algebra  $\mathfrak{g}$  (no restriction on  $A_0$ ). Then  $dU(A_0 + \sum_{k=1}^r A_k^2)$  is the infinitesimal generator of a strongly continuous contraction  $^*semi$ -group  $\{V(t) : t \geq 0\}$  on  $\mathcal{H}$ .*

Applying this to the left-regular representation  $L$ , we get a semigroup  $\{V_L(t)\}$  of bounded operators on  $\mathcal{L}^2(G)$ =the space of all square integrable functions on  $G$ . It is proved in [Jo, Sect. 3] that  $V_L(t)$  is a convolution semigroup determined by a semigroup of probability measures  $\{p_t(g): t \geq 0\}$  on  $G$ , i. e.,

$$(V_L(t)f)(g') = \int_G p_t(g) f(g^{-1} \cdot g') dg,$$

or more briefly,

$$V_L(t)f = p_t * f \quad (\text{convolution}). \tag{4.3}$$

We recall that there is a heat kernel  $p_t(g)$ , corresponding to the Hamiltonian  $H$  of the curved magnetic field; we use this to give an explicit kernel for  $e^{-tH}$ . Spectral representations are also implied. We shall start from a physical representation  $U$ , decompose it into irreducibles, and then give a physical interpretation of the real parameter in the decomposition. When the semigroup,  $\exp(-tH)$  is obtained in the case when  $A_0=0$ , then the unitary group,  $e^{-itH}$ , may be obtained by analytic continuation in  $t$ .

The advantage of (4.3) is that the equation for  $p_t(g)$  is right invariant and "generalized" parabolic. Using right- $G$  invariance, we are able to solve the corresponding heat equation on  $G$ , although the operators in question are variable coefficients.

More specifically, set  $\tilde{A}_k = dL(A_k)$ , and  $\tilde{A} = \tilde{A}_0 + \sum_1^r \tilde{A}_k^2$ . Then  $p_t(g)$  is the solution to the Cauchy problem,

$$\frac{\partial F}{\partial t}(g, t) = \tilde{A}F(g, t) \tag{4.4a}$$

and

$$F(g, t)|_{t=0} = \delta(g), \tag{4.4b}$$

where  $\delta$  is the Dirac delta function on  $G$  corresponding to the unit mass at the neutral element  $e$  in  $G$ .

It is a consequence of [Jo, Thm. 3.1] that  $p_t(g)$  is supported on the closed subgroup of  $G$  which is generated by  $\{\exp(tA_k): t \in \mathbf{R}, 0 \leq k \leq r\}$ . Moreover,  $p_t(g)$  is of exponential decrease at infinity, and smooth in the  $g$ -variable. If  $A_0=0$ , it is smooth in both variables,  $\{(g, t): g \in G, t > 0\}$ ;  $p_t(g)$  is  $G$ -square integrable, and has analytic continuation to complex  $t$ ,  $\text{Re } t \geq 0$ . (Most of these properties are lost in the analytic continuation, although square integrability is known to hold for  $\text{Re } t > 0$ . Hence, we derive a considerable amount of information from the heat equation (4.4) on  $G$ . Before getting to this in Sect. 6, we describe the two nilpotent groups which are used in the analysis of the constant, respectively, curved, magnetic field.

§ 5. Nilpotent Lie Groups

Assume the Lie group  $G$  from Sect. 4 is simply connected and nilpotent. Let the elements  $A_1, \dots, A_r$  in  $\mathfrak{g}$  be fixed. We may assume without loss of generality (cf. Sect. 3) that these elements generate  $\mathfrak{g}$ . We shall assume that there is a one-parameter family of automorphisms  $\{\delta_s: s>0\}$  of  $G$  such that the infinitesimal Lie homomorphisms,  $d\delta_s: \mathfrak{g} \rightarrow \mathfrak{g}$ , satisfy  $d\delta_s(A_k) = s A_k, 1 \leq k \leq r$ . As discussed in [Goo, K-S, K-V], this is only a mild restriction.

**Lemma 5.1** ([Hul]). *Let the Lie groups  $G$  satisfy the assumptions above, and let  $\tilde{A} = \sum_1^r \tilde{A}_k^2$  be a sub-Laplacian constructed from elements  $A_k$  of  $\mathfrak{g}$  satisfying,  $(d\delta_s)(A_k) = s A_k$ . Then the heat kernel  $p_t(g)$ , solving the Cauchy problem (4.4a-b), scales as follows,*

$$p_t(g) = t^{-\nu/2} p_1(\delta_{t^{-1/2}}(g)), \quad t > 0, \quad g \in G \tag{5.1}$$

where  $\nu$  is the scaling constant of Haar measure, i.e.,  $d(\delta_s g) = s^\nu dg$ .

The following two examples will be used in our solution of the Schrödinger equation for the constant, respectively, the curved, magnetic field problem. The ingredients of Lemma 5.1 can all be calculated explicitly in the examples, and they enter into the integral kernel for the Schrödinger equation.

**Example 5.2**

The group  $G$  consists of upper triangular matrices  $g$  over the reals,

$$g = \begin{pmatrix} 1 & a & c & d \\ 0 & 1 & b & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Each of the four real parameters  $a, b, c,$  and  $d$  defines elements in the Lie algebra  $\mathfrak{g}$ . These elements will be denoted  $A, B, C,$  and  $D,$  respectively. They form a basis of  $\mathfrak{g}$ , and we have the simple nontrivial commutation relation,

$$[A, B] = C,$$

while all other commutators are zero. In particular, the center  $\mathfrak{z}$  of  $\mathfrak{g}$  is two dimensional and spanned by  $C$  and  $D$ .

We define the sub-Laplacian,  $\tilde{A}$  in the heat equation (4.4) to be,  $\tilde{A} = \tilde{A}^2 + \tilde{B}^2 + \tilde{D}^2$ , where

$$\tilde{A} = - \left( \frac{\partial}{\partial a} + b \frac{\partial}{\partial c} \right) \tag{5.2}$$

$$\tilde{B} = -\frac{\partial}{\partial b} \tag{5.3}$$

$$\tilde{D} = -\frac{\partial}{\partial d}. \tag{5.4}$$

(Note that formulas (5.2) through (5.4) are easy consequences of (3.2) and the particular matrix representation for  $G$ .)

There is a unitary representation  $U$  of  $G$  on  $\mathcal{H} = \mathcal{L}^2(\mathbb{R}^3)$  given in Eq. (2.5) such that [see, Eq. (2.6) with  $\gamma=1$ ]

$$dU(A) = \frac{\partial}{\partial x} \tag{5.5}$$

$$dU(B) = \frac{\partial}{\partial y} - iy \tag{5.6}$$

$$dU(D) = \frac{\partial}{\partial z}. \tag{5.7}$$

Hence, the constant field Hamiltonian  $H$  is,

$$2H = -dU(\mathcal{A}), \quad \mathcal{A} = A^2 + B^2 + D^2. \tag{5.8}$$

**Example 5.3**

The group  $G$  consists of upper triangular matrices  $g$  over  $\mathbb{R}$ .

$$g = \begin{pmatrix} 1 & a_1 & b_2 & c \\ 0 & 1 & a_3 & b_1 \\ 0 & 0 & 1 & a_2 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Each of the six real parameters  $a_1, a_2, a_3, b_1, b_2, c$  define elements,  $A_1, A_2, A_3, B_1, B_2, C$ , respectively, in the “infinitesimal” Lie algebra  $\mathfrak{g}$ . These six elements form a basis for  $\mathfrak{g}$ , and we have,

$$[A_3, A_2] = B_1$$

$$[A_1, A_3] = B_2$$

$$[A_1, B_1] = C$$

$$[A_2, B_2] = -C,$$

while all other commutators are zero. In particular, the center  $\mathfrak{z}$  of  $\mathfrak{g}$  is one dimensional, and spanned by the single element  $C$ .

The sub-Laplacian,  $\tilde{\Delta}$ , in the equation (4.4) is now,

$$\tilde{\Delta} = \sum_{k=1}^3 \tilde{A}_k^2,$$

where

$$\tilde{A}_1 = -\left(\frac{\partial}{\partial a_1} + a_3 \frac{\partial}{\partial b_2} + b_1 \frac{\partial}{\partial c}\right) \tag{5.9}$$

$$\tilde{A}_2 = -\frac{\partial}{\partial a_2} \tag{5.10}$$

$$\tilde{A}_3 = -\left(\frac{\partial}{\partial a_3} + a_2 \frac{\partial}{\partial b_1}\right) \tag{5.11}$$

There is a unitary representation  $U$  of  $G$  on  $\mathcal{L}^2(\mathbb{R}^3)$  given in Eq. (2.10) such that

$$dU(A_1) = \frac{\partial}{\partial x} \tag{5.12}$$

$$dU(A_2) = \frac{\partial}{\partial y} \tag{5.13}$$

$$dU(A_3) = \frac{\partial}{\partial z} - ixy. \tag{5.14}$$

Note that these formulas result as a special case from the system of equations (2.11), cf. Sect. 2, when the parameters  $(\beta_i, \gamma)$  in the latter formulas are specialized to:  $\beta_i=0$ , and  $\gamma=-1$ . The constant  $\gamma$  (field strength) is dimensionless, and we have set it equal to one below for simplicity. The explicit  $\gamma$ -dependence in the various formulas is worked out in Sect. 2, see, in particular, Eqs. (2.8) through (2.11).

Hence, the curved field Hamiltonian  $H$  is,

$$2H = -dU(\Delta), \quad \Delta = \sum_1^3 A_i^2. \tag{5.15}$$

It is easy to check that, in both examples, the Haar measure agrees with Lebesgue measure in four variables, respectively, six variables. In Example 5.2, the dilation  $\delta_s$  may be constructed subject to the following requirements on  $\sigma_s = d\delta_s$ :  $\sigma_s(X) = sX$ ,  $X = A, B, D$ , and  $\sigma_s(C) = s^2C$ . Hence, the scaling constant  $\nu$  for the Haar measure is  $\nu=5$ . In Example 5.3, the corresponding set of requirements on  $\sigma_s$  is,

$$\begin{aligned} \sigma_s(A_i) &= sA_i, \quad 1 \leq i \leq 3 \\ \sigma_s(B_j) &= s^2B_j, \quad 1 \leq j \leq 2 \\ \sigma_s(C) &= s^3C. \end{aligned}$$

Hence,  $\nu=10$  in this case.

### § 6. Decomposition of the Physical Representation

Recall [Ma 1, Puk, Kir] that a unitary representation  $U$  of a Lie group  $G$

is said to be *monomial* if it is induced from a one-dimensional representation of some subgroup of  $G$ . In this section we shall show that the physical representation  $U$ , from each of Examples 5.2 and 5.3, is monomial, and, moreover,  $U$  is a direct integral over a single real parameter of irreducibles where again each of the irreducible components in the direct integral is monomial. Moreover, we shall give explicit transforms, in each case, representing the integral decomposition.

In Example 5.2, we reduce  $H$  to an explicit integral of "copies" of the harmonic oscillator Hamiltonian in a single real variable, viz.,  $P^2+Q^2$  in  $\mathcal{L}^2(\mathbf{R})$  with  $P=-i d/dx$ ,  $Q=x$ (multiplication).

In Example 5.3, the components in the decomposition of  $H$  are given by

$$P_1^2+P_2^2+(\alpha+Q_1Q_2)^2, \tag{6.1}$$

where  $\alpha \in \mathbf{R}$  is the parameter in the decomposition. Recall, the latter Hamiltonian (6.1) acts in  $\mathcal{L}^2(\mathbf{R}^2)$ , where  $P_j=-i \partial/\partial x_j$ , and  $Q_j=x_j$  (multiplication),  $j=1, 2$ .

Since the Hermite-functions diagonalize  $P^2+Q^2$ , the constant field case is trivial.

*Proof. (The Constant Case).* The matrices  $g$  in Example 5.2 will be denoted,  $g=g(a, b, c, d)$  for typographical convenience, and we shall consider the following normal abelian subgroups,

$$N_1=\{g(a, b, c, d): a=b=d=0\}$$

and

$$N_3=\{g(a, b, c, d): a=0\}.$$

(The subscripts refer to the dimensions of the respective groups.)

By Mackey's theorem [Ma 2-3, Oer, Kir], or alternatively, [Dix 1], the infinite-dimensional unitary irreducible representations of  $G$  are all monomial and induced from one-dimensional representations of  $N_3$ , hence, they are parametrized by the abelian dual group,  $\hat{N}_3 \cong \mathbf{R}^3$ . Elements in  $\hat{N}_3$  are denoted  $\chi=\chi(\beta, \gamma, \delta)$ , where  $(\beta, \gamma, \delta)$  are three real parameters:

$$\langle \chi, (b, c, d) \rangle = \exp i(\beta b + \gamma c + \delta d). \tag{6.2}$$

The physical representation  $U$ , in turn, is induced from  $N_1$  by the character,  $c \rightarrow e^{-1c}$ . This representation  $U$  is called "physical" because it transforms the three-vector fields, (5.9) through (5.11), into the corresponding operators, (5.12) through (5.14). The latter operators are expressed in the coordinates  $(x, y, z)$  with a direct physical meaning with reference to the field variables, and the constant  $\gamma$  referring to field strength. [Note that (5.14) changes into  $dU(A_3)=\partial/\partial z + \gamma xy$  for variable  $\gamma$ ]. An explicit calculation yields the formula,

$$(U(g)\phi)(x, y, z) = e^{-i(c+xb)}\phi(x+a, y+b, z+d) \tag{6.3}$$

$\phi \in \mathcal{L}^2(\mathbf{R}^3)$ ,  $g \in G$ . It is easy to check that the infinitesimal representation  $dU$

gives rise to the constant field, cf. formulas (5.5) through (5.7).

For each  $\chi \in \hat{N}_3$ , the induced representation  $U^\chi(g)$  acts on  $\mathcal{L}^2(\mathbf{R})$  since  $N_3 \backslash G \cong \mathbf{R}$ . It follows that each  $\phi(x, y, z) \in \mathcal{L}^2(\mathbf{R}^3)$  is a direct integral of functions in  $\mathcal{L}^2(\mathbf{R})$ . Let  $\phi \rightarrow f(s, \chi)$  be the corresponding integral transform.

Then we have,

$$\phi(x, y, z) = \iint e^{i(\beta y + \delta z)} f(x, \chi) d\beta d\delta, \tag{6.4}$$

where the integral is supported on the two real parameters  $\beta, \delta$ , and  $\chi = \chi(\beta, -1, \delta)$ , cf. formula (6.2).

Now, let  $\hat{\phi}$  denote the usual Euclidean Fourier transform in the last two variables  $y, z$ . Using Fourier inversion, it follows that,

$$f(s, \chi(\beta, -1, \delta)) = \hat{\phi}(s, \beta, \delta). \tag{6.5}$$

*Proof. (The Curved Case).* The matrices  $g$  in Example 5.3 will be denoted,  $g = g(a_1, a_2, a_3, b_1, b_2, c)$ , for typographical convenience. On occasion, we shall use the more compact terminology,  $g = g(a, b, c)$  where it is then understood that  $a$  and  $b$  are vector variables:

$$a = (a_1, a_2, a_3) \in \mathbf{R}^3, \quad b = (b_1, b_2) \in \mathbf{R}^2.$$

We shall consider the following two normal abelian subgroups,

$$N_3 = \{g(a, b, c) : a = 0\}$$

and

$$N_4 = \{g(a, b, c) : a_1 = a_2 = 0\}.$$

Note that  $N_3$  is parametrized by  $(b_1, b_2, c) \in \mathbf{R}^3$ , while  $N_4$  is coordinatized by  $(a_3, b_1, b_2, c) \in \mathbf{R}^4$ .

The characters on  $N_4$  again form a group  $\hat{N}_4$  which is naturally isomorphic to  $\mathbf{R}^4$ . We shall use the labels  $(\alpha_3, \beta_1, \beta_2, \gamma) \in \mathbf{R}^4$  for elements  $\chi \in \hat{N}_4$ , viz.,  $\chi = \chi(\alpha_3, \beta_1, \beta_2, \gamma)$ .

There is a well-known action of  $G$  on  $\hat{N}_4$  which we recall is defined by  $(\chi \cdot g) \in \hat{N}_4, g \in G$ , where

$$\begin{aligned} (\chi \cdot g)(n) &= \chi(g \cdot n \cdot g^{-1}) \\ \text{for } \chi &\in \hat{N}_4, \quad n \in \hat{N}_4, \quad g \in G. \end{aligned}$$

Introducing the parameters  $(\alpha_3, \beta_1, \beta_2, \gamma)$  on  $\hat{N}_4$ , this action takes the following form,

$$\begin{aligned} (\chi(\alpha_3, \beta_1, \beta_2, \gamma) \cdot g) &= \chi(\alpha_3 - \beta_1 \cdot a_2 + \beta_2 \cdot a_1 \\ &\quad - \gamma \cdot a_1 \cdot a_2, \beta_1 + \gamma \cdot a_1, \beta_2 - \gamma \cdot a_2, \gamma). \end{aligned}$$

The isotropy subgroup,  $G_\chi$  enters in Mackey's theory, where

$$G_\chi = \{g \in G : \chi \cdot g = \chi\}.$$

Let  $H$  be the subgroup of  $G$  which is given by  $H = \{g(a, b, c) : a_3 = b_1 = b_2 = c = 0\}$ . Then  $N_4 \cdot H = G$ ,  $N_4 \cap H = \{e\}$ , and,  $G_\chi \cap H = \{e\}$ , whenever  $\gamma \neq 0$  in  $\chi = \chi(\alpha_3, \beta_1, \beta_2, \gamma)$ . It follows [Ma 2] that the representations which are induced from  $\chi$  on  $N_4$  are irreducible when  $\gamma \neq 0$ .

In general, define  $H_\chi = H \cap G_\chi$ . Then  $G_\chi = N_4 \cdot H_\chi$ . It may happen that  $H_\chi \neq \{e\}$ . If so, let  $L \in \hat{H}_\chi$ , and consider the representation,  $(n, h) \rightarrow \chi(n)L(h)$ , of  $G_\chi$ . It is denoted  $\chi L$ , and it induces an irreducible representation  $U^{\chi L}$  of  $G$ ; and all the unitary irreducibles may be realized this way. (It is known, more generally, for simply connected nilpotent Lie groups, that all the irreducible representations are monomial induced from *some* subgroup; see, for example, [Puk] and [Kir].)

**Theorem 6.1.** *In the decomposition of the physical representation  $U$  of  $G$ , only irreducibles  $U^\chi$ ,  $\chi \in \hat{N}_4$ ,  $H_\chi = \{e\}$ , occur, and, moreover,  $U$  is a direct integral of the  $U^\chi$ 's, where  $\chi = \chi(\alpha_3, 0, 0, -1)$ ,  $\alpha_3 \in \mathbb{R}$ .*

Let  $\phi(x, y, z) \rightarrow f(x_1, x_2; \chi_{\alpha_3})$ , be the corresponding integral transform. Then we have,

$$\phi(x, y, z) = \int_{\mathbb{R}} e^{i\alpha_3 z} f(x, y; \chi_{\alpha_3}) d\alpha_3. \tag{6.6}$$

If  $\hat{\phi}(x_1, x_2, \alpha_3)$  denotes the Euclidean Fourier transform in the third variable, then

$$f(x_1, x_2; \chi_{\alpha_3}) = \hat{\phi}(x_1, x_2, \alpha_3). \tag{6.7}$$

*Proof.* We first note that the physical representation  $U$  in Example 5.3 is induced from  $N_3$  by the one-dimensional representation,  $(b_1, b_2, c) \rightarrow e^{-ic}$ . Hence, it is monomial, but certainly not irreducible. We shall denote by  $\chi$  this particular character of  $N_3$ . As an element in  $\hat{N}_3$ ,  $\chi_1$  has the label  $(0, 0, -1)$ . Using the isomorphism,  $N_3 \backslash G \cong \mathbb{R}^3$ , it follows that the induced representation,  $U = U^{\chi_1}$ , is realized on  $\mathcal{L}^2(\mathbb{R}^3)$  as,

$$(U(g)\phi)(x, y, z) = e^{-iEg} \phi(x + a_1, y + a_2, z + a_3)$$

for  $\phi \in \mathcal{L}^2(\mathbb{R}^3)$ , and  $g \in G$ , where

$$E = c - a_2 \cdot b_2 + (b_1 - a_2 \cdot a_3)x - b_2 \cdot y - a_3 \cdot xy.$$

(Compare formula (6.3) in the constant case.) It is also easy to check, by differentiation, that the infinitesimal representation  $dU$  gives rise to the curved field, cf. formulas (5.12) through (5.14) in Example 5.3.

Let  $A = \{\exp(\alpha A_3) : \alpha \in \mathbb{R}\}$ , and note that:  $N_4 = N_3 \cdot A$ , and  $N_3 \cap A = \{e\}$ , where each of the three groups,  $N_4$ ,  $N_3$ , and  $A$  is abelian. Recall that  $U$  acts on square-integrable functions  $F$  on  $G$  satisfying,

$$F(n \cdot g) = \chi_1(n)F(g), \quad n \in N_3, \quad g \in G. \tag{6.9}$$

If  $\chi = \chi(\alpha_3, \beta_1, \beta_2, \gamma) \in \hat{N}_4, \gamma \neq 0$ , the irreducible representation acts on the space of functions  $f(\cdot, \chi)$  on  $G$  satisfying

$$f(n \cdot g, \chi) = \chi(n)f(g, \chi), \quad n \in N_4, \quad g \in G. \tag{6.10}$$

Since,  $N_4 = N_3 \cdot A$ , the elements  $n$  in formula (6.10) factor as,  $n \cdot a$ , with  $n \in N_3, a \in A$ . Decomposition of  $F$  (satisfying (6.9), according to the Plancherel formula [Puk, Chapitre III]), leads to the result that the only components of  $F$  which contribute are of the form  $f(\cdot, \chi)$  where  $\chi \in \hat{N}_4$  satisfies,  $\chi_1(n)\chi(a) = \chi(na) = \chi(n)\chi(a)$  for all  $n \in N_3$ , and  $a \in A$ . If  $\chi = \chi(\alpha_3, \beta_1, \beta_2, \gamma)$ , it follows that,  $\chi_1(n) = \chi(n)$ , since  $\chi(a) \neq 0$ . Writing  $n = (b_1, b_2, c)$ , we conclude that  $\gamma = -1$ , and  $\beta_1 = \beta_2 = 0$ . Let  $\chi(\alpha_3, 0, 0, -1) \in \hat{N}_4$ . We have established the decomposition,

$$F(g) = \int_{\mathbf{R}} f(g, \chi_{\alpha_3}) d\alpha_3, \tag{6.11}$$

where  $F$ , respectively,  $f(\cdot, \chi)$ , satisfy (6.9), respectively, (6.10). Let  $\mathcal{A}(U^{\chi_1})$ , respectively,  $\mathcal{A}(U^{\chi_{\alpha_3}})$  denote the representation spaces specified by formula (6.9), respectively (6.10). It can easily be checked that the transformation,  $W: \phi(x, y, z) \rightarrow F(x, y, z, 0, 0, 0)$ , defines a unitary map of  $\mathcal{L}^2(\mathbf{R}^3)$  onto  $\mathcal{A}(U^{\chi_1})$ . Similarly,  $\phi(x_1, x_2) \rightarrow f(x_1, x_2, 0, 0, 0, 0, \chi_{\alpha_3})$ , realizes a unitary operator of  $\mathcal{L}^2(\mathbf{R}^2)$  onto  $\mathcal{A}(U^{\chi_{\alpha_3}})$  for all  $\alpha_3 \in \mathbf{R}$ .

When these unitary equivalences are introduced into (6.11), the desired integral formula (6.6) follows immediately, since

$$\begin{aligned} \phi(x, y, z) &= (W^*F)(x, y, z, 0, 0, 0) \\ &= \int_{\mathbf{R}} f(x, y, z, 0, 0, 0; \chi_{\alpha_3}) d\alpha_3 \\ &= \int_{\mathbf{R}} f((0, 0, z, -yz, 0, 0)(x, y, 0, 0, 0, 0); \chi_{\alpha_3}) d\alpha_3 \\ &= \int_{\mathbf{R}} e^{i\alpha_3 \cdot z} f(x, y, 0, 0, 0, 0; \chi_{\alpha_3}) d\alpha_3. \end{aligned}$$

Note that formula (6.7) follows directly from Fourier inversion in the  $z$ -variable. The net result is a reduction from the three physical  $(x, y, z)$  to the two variables  $(x_1, x_2)$ .

**Theorem 6.2.** *Under the decomposition in Theorem 6.1 above, the curved field Hamiltonian,*

$$H = P_x^2 + P_y^2 + (P_z - xy)^2$$

*decomposes according to the Fourier transform formula (6.6) as a direct integral over  $\alpha_3 \in \mathbf{R}$  of two-dimensional Hamiltonians,  $P_1^2 + P_2^2 + (\alpha_3 + Q_1 Q_2)^2$ , acting in  $\mathcal{L}^2(\mathbf{R}^2)$  relative to the variables  $x_1, x_2$ , where,  $P_j = -i\partial/\partial x_j$ , and  $Q_j = x_j, j=1, 2$ .*

*Proof.* If  $\chi \in \hat{N}_4$ ,  $\chi = \chi(\alpha_3, \beta_1, \beta_2, \gamma)$ , then the transformation,  $W : \phi(x_1, x_2) \rightarrow f(x_1, x_2, 0, 0, 0, 0, \chi)$ , defines a unitary of  $\mathcal{L}^2(\mathbf{R}^2)$  onto  $\mathcal{H}(U^\chi)$  as noted at the end of the proof of Theorem 6.1. The action of  $U^\chi$  on the space of functions,  $f(g) = f(g, \chi)$ , satisfying,

$$f(n \cdot g) = \chi(n)f(g), \quad n \in N_4, \quad g \in G,$$

is given by  $(U^\chi(g)f)(g') = f(g' \cdot g)$ . A direct calculation yields,

$$\begin{aligned} (U(g)\phi)(x_1, x_2) &= (W^*U^\chi(g)W)\phi(x_1, x_2) \\ &= e^{iE}\phi(x_1 + a_1, x_2 + a_2), \end{aligned} \tag{6.12}$$

where

$$\begin{aligned} E &= \alpha_3 a_3 + \beta_1 \{b_1 - a_3(x_2 + a_2)\} + \beta_2 \{b_2 + a_3 x_1\} \\ &\quad + \gamma \{c + b_1 x_1 - (b_2 + a_3 x_1)(x_2 + a_2)\}. \end{aligned} \tag{6.13}$$

For the corresponding infinitesimal representation,  $dU$ , we get by differentiating the above in the variables  $a_1, a_2, a_3$ :

$$dU(A_1) = iP_1 \tag{6.14.1}$$

$$dU(A_2) = iP_2 \tag{6.14.2}$$

and

$$dU(A_3) = i(\alpha_3 - \beta_1 Q_2 + \beta_2 Q_1 - \gamma Q_1 Q_2). \tag{6.14.3}$$

Specializing to  $(a_3, \beta_1, \beta_2, \gamma) = (\alpha_3, 0, 0, -1)$ , we finally get  $dU(A_3) = i(\alpha_3 + Q_1 Q_2)$ . The desired formula for the Hamiltonian now follows from (5.15) and Theorem 6.1.

In the next section we show that each  $H_\alpha$  has a purely discrete spectrum and give properties of the eigenfunctions.

### § 7. Spectral Theory of $P_1^2 + P_2^2 + (1 + Q_1 Q_2)^2$

**Theorem 7.1.** *The operator,  $H_\alpha = P_1^2 + P_2^2 + (\alpha + Q_1 Q_2)^2$ , has a purely discrete spectrum for all  $\alpha \in \mathbf{R}$ . Moreover, there are no bounded functions,  $\phi$  satisfying  $H_\alpha \phi = 0$ , other than the trivial zero-function.*

We shall give the proof only for  $\alpha = 1$ . Each step applies with only trivial modifications when  $\alpha \neq 1$ . The argument is based on [Sim 2].

Let  $U_1$  denote the representation which is induced from  $N_4$  by  $(1, 0, 0, -1) \in \hat{N}_4$ . It follows from [Jo, Corollary 2.1] that the space of  $C^\infty$ -vectors for  $U_1$  coincides with the Schwartz-space  $\mathcal{S}$  in the two variables  $x_1, x_2$ . Let  $H = P_1^2 + P_2^2 + (1 + Q_1 Q_2)^2$ , and  $\mathcal{D}(H)$  be the domain of  $H$ . Since  $H$  is self-adjoint, by [D-S; XII, 2.5, Thm. 6], we have,  $\mathcal{D}(H) = \{\phi \in \mathcal{L}^2(\mathbf{R}^2) : \int \lambda^2 \|dE(\lambda)\phi\|^2 < \infty\}$ . A similar fact holds for the domain of the  $n$ 'th power of  $H$ . We have ([Jo]),

$$C^\infty(U_1) = \mathcal{S} = \bigcap_{n=1}^\infty \mathcal{D}(H^n). \tag{7.1}$$

We first note that  $\lambda=0$  is not an eigenvalue. Assume that some  $\phi \in \mathcal{L}^2(\mathbf{R}^2)$  solves  $H\phi=0$ . It follows then that  $\phi$  belongs to each of the spaces in (7.1). In particular,  $\phi(x_1, x_2)$  is smooth and vanishes at  $\infty$  in  $\mathbf{R}^2$ . For  $j=1, 2, 3$ , we therefore have,

$$\begin{aligned} \|dU_1(A_j)\phi\|^2 &\leq \sum_j \|dU_1(A_j)\phi\|^2 \\ &= - \sum_j \langle dU_1(A_j)^2\phi, \phi \rangle \\ &= \langle H\phi, \phi \rangle \\ &= 0, \end{aligned}$$

where  $\langle \cdot, \cdot \rangle$  denotes the inner product in  $\mathcal{L}^2(\mathbf{R}^2)$ . Using the estimate above for  $j=1, 2$ , we get  $P_1\phi=P_2\phi=0$ . Since  $\phi$  is  $C^\infty$  by (7.1), it must be a constant. But this is a contradiction, unless the constant is zero.

We now show that there are also no nonzero-bounded solutions  $\phi$  to  $H\phi=0$ . Suppose  $\phi$  is such a function. The real part, and the imaginary part of  $\phi$ , will also be a solution, so we may assume  $\phi$  real. We shall show  $\phi \leq 0$ , using a simple maximum-principle. Since  $-\phi$  is also a solution, we are done. The proof is indirect: If  $\phi(x) > 0$ , for some  $x=(x_1, x_2) \in \mathbf{R}^2$ , then there is a local maximum,  $\phi(x^0) > 0$ , say. We have,  $H\phi = -\Delta\phi + V\phi = 0$ , where  $\Delta$  is the Laplace operator in  $\mathbf{R}^2$ , and  $V(x_1, x_2) = (1+x_1x_2)^2$ . Note that,  $(\Delta\phi)(x^0) \leq 0$ , since  $x^0$  is a maximum. We could not have,  $V(x^0) > 0$  at the point in question, since  $\Delta\phi = V\phi$  would then be positive at  $x^0$  which is a contradiction. Pick a neighborhood  $N$  of  $x^0$  such that  $\phi > 0$  in  $N$ . Since  $V \geq 0$ , we have  $\Delta\phi = V\phi \geq 0$  in  $N$ . Hence,  $\phi$  is subharmonic, and  $\phi(x^0) \leq \oint \phi$  for every contour in  $N$  which is centered at  $x^0$ . The curve integral  $\oint$  is here taken to be normalized, and we therefore also have  $\oint \phi \leq \phi(x^0)$ , recalling that  $\phi(x^0)$  is a maximum. Using  $\phi \leq \phi(x^0)$  in  $N$ , we conclude that  $\phi$  is constant in  $N$ . But then,  $\Delta\phi = 0 = V\phi$ . Since  $V$  is not identically zero in  $N$ , this contradicts the positivity of  $\phi$  in  $N$ .

We now show that  $H$  has discrete spectrum using a classical argument of H. Weyl. We shall show that the supremum of the real numbers  $\xi$  such that  $H$  has discrete spectrum under  $\xi$  is infinite. Let  $\xi \in \mathbf{R}$ , and assume that

$$(-\infty, \xi] \cap \sigma(H) = (-\infty, \xi] \cap \sigma_p(H), \tag{7.2}$$

where  $\sigma(H)$  denotes the spectrum of  $H$ , and  $\sigma_p(H)$  the set of eigenvalues. Since  $H \geq 0$ , the set  $D$  of all numbers  $\xi$ , satisfying (7.2), contains  $\mathbf{R}_-$ . For, if  $\xi < 0$ , then the intersection on both sides of (7.2) is the empty set. Let  $d$  be the supremum,  $d = \sup D$ . Clearly,  $0 \leq d$ . We claim that, in fact,  $d = \infty$ . This

follows from an application of Weyl's min-max theorem [Wey] and [Sim 2]. As proved in [Per, Thm. 2.1], the min-max theorem yields the following formula (7.3) below for  $d$ . For  $k > 0$ , let  $\mathcal{D}_k$  denote the compactly supported functions,  $\phi$  which vanish for  $x_1^2 + x_2^2 \leq k^2$ , i.e.,  $\phi$  is supported in the complement of a disk with radius  $k$  and center  $(0, 0)$ . Let  $d_k$  be the infimum of the expectation values,  $\langle H\phi, \phi \rangle = \iint (|\nabla\phi|^2 + V|\phi|^2) dx_1 dx_2$  when  $\phi \in \mathcal{D}_k$  has unit-norm, i.e.,  $\|\phi\| = \langle \phi, \phi \rangle^{1/2} = 1$ . Then, by [Per], we have,

$$d = \sup d_k, \quad k > 0. \tag{7.3}$$

*Proof of discreteness in Theorem 7.1.* The proof of discreteness of the spectrum in [Sim 2] ( $\alpha=0$ ) is based on earlier work of C. Fefferman and D. Phong [F-P]. The details for  $V = (1 + x_1 x_2)^2$  are as follows: Let  $C_j^\lambda$  ( $\lambda > 0$ ,  $j = (j_1, j_2) \in \mathbf{Z}^2$ ) be the square of side length  $\lambda^{-1/2}$ , centered at the point,  $j\lambda^{-1/2} = (j_1\lambda^{-1/2}, j_2\lambda^{-1/2})$ . Let  $\tilde{N}(\lambda)$  be the number of squares  $C_j^\lambda$  with  $\max_{x \in C_j^\lambda} V(x) \leq \lambda$ . The Fefferman-Phong-Simon theorem states that  $H = -\Delta_x + V$  has purely discrete spectrum if and only if  $\tilde{N}(\lambda) < \infty$  for all  $\lambda$ . For each  $C_j^\lambda$ , the maximum of  $V$  is attained at one of the corners. The orientation of the corner is independent of  $\lambda$ . Let  $p(j) = (j_1 \pm 1/2)(j_2 \pm 1/2)$ , where the signs  $\pm$  are determined by corner orientation. Then

$$\max_{C_k^\lambda} V = (1 + p(j)\lambda^{-1})^2$$

so we count the number of points  $j \in \mathbf{Z}^2$  such that  $(\lambda + p(j))^2 \leq \lambda^3$ . It follows that, for fixed  $\lambda > 0$ , the values for  $p(j)$  are restricted to the finite interval,

$$-\lambda - \lambda^{3/2} \leq p(j) \leq -\lambda + \lambda^{3/2}.$$

The set of values of  $p(j)$  in this interval is finite, and for each value,  $p$  say, the set of solutions of  $j \in \mathbf{Z}^2$ , to the equation,  $p(j) = p$  is again finite.

This leads to the estimate  $\tilde{N}(\lambda) \leq c \cdot \lambda^{3/2} \cdot \ln \lambda$  which coincides with an estimate which is known [Sim 2] for the special case  $\alpha = 0$ .

**Corollary 7.2.** *For the operator  $H_\alpha = -\Delta_x + (\alpha + x_1 x_2)^2$ , the number  $d$  in (7.3) is infinite.*

**Conjecture 7.3.** *Let  $\{\lambda_n(\alpha) : n = 0, 1, \dots\}$  be the spectrum of  $H_\alpha$  for each  $\alpha \in \mathbf{R}$ . We conjecture that each  $\lambda_n(\cdot)$  is continuous in  $\alpha$ .*

An answer would be interesting since,  $H_\alpha = -1/2 dU^\alpha(\Delta)$ , where the unitary representations  $U^\alpha$  of  $G$  are mutually inequivalent. We show in Corollary 8.2 that trace  $(e^{-tH_\alpha})$  is a continuous function of  $\alpha \in \mathbf{R}$  for  $t > 0$ .

§ 8. Irreducible Representations

We continue our study of the Hamiltonian,  $H=P_1^2+P_2^2+(1+Q_1Q_2)^2$ . Recall that  $H=-\Delta+V$ , where  $\Delta=(\partial/\partial x_1)^2+(\partial/\partial x_2)^2$  is the Laplace operator, and,  $V(x_1, x_2)=(1+x_1x_2)^2$ , is the potential studied in the previous section. We shall really need a one-parameter family,  $V_\alpha=(\alpha+x_1x_2)^2$ , indexed by  $\alpha \in \mathbf{R}$ . But we set  $\alpha=1$  for notational convenience. The modifications for  $\alpha \neq 1$  are easy and will be postponed.

Recall from Sect. 5, formula (5.15), that we defined  $H$  as

$$-2H=dU(\Delta),$$

where  $\Delta=\sum_{k=1}^3 A_k^2 \in \mathfrak{U}_2(\mathfrak{g})$ . In Sect. 3, formulas (3.3), we introduced the left-regular representation  $L$ . For each  $X \in \mathfrak{g}$ , we have the right-invariant vector field  $\tilde{X}=dL(X)$ . Similarly, the operator

$$\tilde{\Delta}=dL(\Delta)=\sum_{k=1}^3 dL(A_k)^2=\sum_{k=1}^3 \tilde{A}_k^2 \tag{8.1}$$

is right invariant. It is the so-called sub-Laplacian [Jo, J-M, Hul, Goo, K-S, K-V]. While it is not elliptic (the metric is degenerate semidefinite [O-R]), it is known to be hypoelliptic, i. e., the equation,  $\tilde{\Delta}u=f$  has only smooth solutions  $u$  in open sets where the right hand side  $f$  is smooth. Recall from formulas (5.9) through (5.11) that  $\tilde{\Delta}$  has the following representation in local coordinates:

$$\begin{aligned} \tilde{\Delta} &= (\partial/\partial a_1 + a_3 \partial/\partial b_2 + b_1 \partial/\partial c)^2 \\ &+ (\partial/\partial a_2)^2 + (\partial/\partial a_3 + a_2 \partial/\partial b_1)^2. \end{aligned} \tag{8.2}$$

Since,

$$dU_1(A_j)=iP_j, \quad j=1, 2, \tag{8.3}$$

the two variables  $a_1, a_2$  correspond in the representation  $dU_1$  to  $x_1, x_2$ , and hence they play a special role. The following labels for  $g=g(a_1, a_2, a_3, b_1, b_2, c)$ , cf. (2.9) and Example 5.3, will simplify the formulas and calculations to follow. Write  $A$  for  $(a_1, a_2)$ , and  $B$  for the remaining four coordinates,  $(a_3, b_1, b_2, c)$ . For the Haar measure on  $G$ , we then get  $dg=dAdB$ , where  $da=da_1da_2$ , and  $dB=da_3db_1db_2dc$ .

Functions  $\phi(x_1, x_2)$  of vector variables  $x=(x_1, x_2)$  will be written  $\phi(X)$ , and the translated function,  $\phi(X+A)$ , where the addition  $X+A$  agrees with the usual one in  $\mathbf{R}^2$ , i. e.,  $(x_1+a_1, x_2+a_2)$ . Note that the use of upper case letters,  $A, B \dots$  is consistent with Sect. 3 since the corresponding coordinate expressions may also be regarded as representing elements in the Lie algebra  $\mathfrak{g}$  of  $G$ .

The fundamental solution  $p_t(g)$  to the heat equation (4.4) on  $G$  may then be regarded as a function of  $A, B$  via  $g=g(A, B)$ . We have

$$\begin{cases} \partial \tilde{F}(g, t) / \partial t = \tilde{J} \tilde{F}(g, t) \\ \tilde{F}(\cdot, 0) = \delta(\cdot) \text{ (Dirac function at } e), \end{cases} \tag{8.4}$$

where  $p_t(g) = p_t(A, B)$ ,  $g \in G$ ,  $t > 0$ .

**Theorem 8.1.** *Let  $H = P_1^2 + P_2^2 + (1 + Q_1 Q_2)^2$ , and let the function  $K_t(X, A)$  be defined on  $\mathbf{R}_+ \times \mathbf{R}^2 \times \mathbf{R}^2$  by,*

$$K_t(X, A) = \int_{\mathbf{R}^4} p_t(A - X, B) e^{i\Omega(A, B, X)} dB, \tag{8.5}$$

where

$$\Omega(A, B, X) = a_3 - c - b_1 x_1 + a_2 \cdot (b_2 + a_3 x_1).$$

Then  $K$  is an integral kernel for the operator  $e^{-tH}$  on  $\mathcal{L}^2(\mathbf{R}^2)$  in the usual sense,

$$(e^{-tH} \phi)(X) = \int_{\mathbf{R}^2} K_t(X, A) \phi(A) dA.$$

and

$$K_t(X, A) = \mathcal{O}(t^{-1}), \tag{8.6}$$

at  $t \rightarrow +\infty$ ; and  $e^{-tH}$  is a positivity preserving semigroup.

*Proof.* The infinitesimal representation,  $dU_1$  is determined by formulas (8.3), and it follows from Sect. 6 that  $dU_1$  exponentiates to a representation of  $G$  on  $\mathcal{L}^2(\mathbf{R}^2)$ . We saw in formulas (6.12) and (6.13) that

$$(U_1(g)\phi)(X) = \phi(X + A) e^{iE}, \tag{8.7}$$

with  $E = a_3 - \{c + b_1 x_1 - (b_2 + a_3 x_1)(x_2 + a_2)\}$ , for  $\phi \in \mathcal{L}^2(\mathbf{R}^2)$ ,  $g = (A, B) \in G$ .

By [Jo, Proposition 3.2], we also have

$$\begin{aligned} (e^{-tH} \phi) &= \int_G p_t(g) (U_1(g)\phi)(X) dg \\ &= \iint p_t(A, B) \phi(X + A) e^{iE} dA dB \\ &= \iint p_t(A - X, B) \phi(A) e^{i\Omega(A, B, X)} dA dB \\ &= \iint \{ p_t(A - X, B) e^{i\Omega(A, B, X)} dB \} \phi(A) dA, \end{aligned}$$

where Fubini's theorem was used in the last step. Formula (8.5) follows from this.

We now use Lemma 5.1 in the proof of the asymptotic property (8.6).

Starting with (8.5), we have

$$\begin{aligned}
 K_t(X, A) &= \int p_t(A-X, B) e^{i\Omega(A, B, X)} dB \\
 &= \int t^{-5} p_1(t^{-1/2}(A-X), \delta_{t^{-1/2}}(B)) e^{i\Omega(A, B, X)} dB \\
 &= \int t^{-1} p_1(t^{-1/2}(A-X), B) e^{i\Omega(A, \delta_{t^{1/2}}(B), X)} dB,
 \end{aligned}$$

where we have used the scaling factor  $\nu$  in formula (5.1); from Lemma 5.1,  $\nu=10$  for this group, and  $dB=d(\delta_{t^{-1/2}}(B))t^4$ . We have then transformed the integral in the variables collected in  $B$ . An estimate of the resulting integral yields,

$$|K_t(X, A)| \leq t^{-1} \int p_1(t^{-1/2}(A-X), B) dB,$$

where we have used positivity of the heat kernel on  $G$ . Since,  $p_1(\cdot) \in \mathcal{L}^1(G) \cap C^\infty(G)$ , and of exponential decay at  $\infty$ , we conclude, for  $t \rightarrow \infty$ , that,

$$p_1(t^{-1/2}(A-X), B) \longrightarrow p_1(0, B),$$

and

$$\iint p_1(t^{-1/2}(A-X), B) dB \longrightarrow \iint p_1(0, B) dB,$$

where the last integral is finite.

The conclusion (8.6) follows. To see that  $e^{-tH}$  is positivity preserving (a known fact), recall that  $H = -\Delta + V$ , where  $V \geq 0$ . If  $E_X$  denotes the expectation value relative to the Wiener measure for paths  $\omega(t)$  in  $\mathbf{R}^2$  starting at  $X$ , then we have, by the Feynman-Kac formula [B-R],

$$e^{-tH} \phi(X) = E_X \{ \phi(\omega(t)) e^{-\int_0^t V(\omega(s)) ds} \}, \tag{8.8}$$

and positivity is immediate. Comparison of Theorem 8.1 with (8.8) yields direct information about the kernel in the Feynman-Kac formula.

**Corollary 8.2.** *The operator  $e^{-tH_\alpha}$ , for  $t > 0$ , and  $H_\alpha = P_1^2 + P_2^2 + (\alpha + Q_1 Q_2)^2$ , is trace class. If  $\hat{p}_t$  denotes the Fourier transform of  $p_t(a_1, a_2, a_3, b_1, b_2, c)$  in the last four variables, then*

$$\text{trace}(e^{-tH_\alpha}) = \int_{\mathbf{R}^2} \hat{p}_t(0, 0, \alpha + a_1 a_2, -a_1, a_2, -1) da_1 da_2. \tag{8.9}$$

and it follows that  $\text{trace}(e^{-tH_\alpha})$  is continuous in the  $\alpha$ -variable.

*Proof.* Substitution into (8.5) yields

$$K_t(A, A) = \int_{\mathbf{R}^4} p_t(0, B) e^{i\Omega(A, B, A)} dB,$$

where  $dB = da_3 db_1 db_2 dc$ , and  $A = (a_1, a_2)$ . (The fact that  $K_t$  is a trace class

operator follows from [Jo, Theorem 2.1] and standard regularity results of Rellich type. For a discussion of this, see, for example, [Sim 1].) By Mercer's theorem, and Theorem 8.1, we therefore have

$$\begin{aligned} \text{trace}(e^{-tH_\alpha}) &= \int_{\mathbb{R}^6} p_t(0, 0, a_3, b_1, b_2, c) \\ &\times e^{i(\alpha a_3 - c - b_1 a_1 + a_2(b_2 + a_1 a_3))} da_1 da_2 da_3 db_1 db_2 dc. \end{aligned}$$

When Fubini is used, and the integrations are carried out in the order  $c, b_2, b_1, a_3$ , the desired formula follows.

The convergence of the two-dimensional integral on the right-hand side of formula (8.9) may be established by a direct argument, or by an indirect one. The direct argument is an easy consequence of [Jo, Prop. 3.1], whereas the indirect argument may be based on Mercer's theorem, and the known multiplicity estimate,  $\dim E_\alpha(0, \lambda) \leq c_\alpha \lambda^{3/2} \ln \lambda$ ,  $H_\alpha = \int \lambda dE_\alpha(\lambda)$ , cf., the proof of Theorem 7.1, and [Sim 2, F-P]. Since  $\text{trace}(e^{-tH_\alpha}) = \sum_\lambda e^{-t\lambda}$ , where the summation is over the spectrum of  $H_\alpha$ , the multiplicity estimate yields,

$$\text{trace}(e^{-tH_\alpha}) \leq c_\alpha e^{2t}(e^t - 1)^{-3}.$$

The latter estimate follows from the above and

$$\begin{aligned} &\sum_\lambda e^{-\lambda t} \dim E_\alpha(\{\lambda\}) \\ &= \sum_n \sum_{n < \lambda \leq n+1} e^{-\lambda t} \dim E_\alpha(\{\lambda\}) \\ &\leq \sum_n e^{-nt} \sum_{n < \lambda \leq n+1} \dim E_\alpha(\{\lambda\}) \\ &\leq \sum_n e^{-nt} \dim E_\alpha(0, n+1] \\ &\leq c_\alpha \sum_n (e^{-t})^n (n+1)^{3/2} \ln(n+1). \end{aligned}$$

But, for high-energy behavior ( $t \rightarrow 0_+$ ), a better estimate

$$\text{trace}(e^{-tH_\alpha}) \leq \text{const } t^{-5/2} |\ln t|$$

may be available.

### § 9. The Heat Equation

It is immediate from (8.2) that the sub-Laplacian  $\tilde{\Delta}$  has a semidefinite degenerate metric  $(g_{ij})$  relative to the six real variables  $(a_1, a_2, a_3, b_1, b_2, c)$  which label the points  $g$  in the six-dimensional group  $G$  from Example 5.3. If we regard  $(g_{ij})$  as a  $6 \times 6$  matrix, and write  $\tilde{\Delta} = \nabla^T (g_{ij}) \nabla$ , then it can easily be checked that the eigenvalues of  $(g_{ij})$  are  $\{0, 1 + a_3^2 + b_1^2, 1, 1 + a_2^2\}$ , where  $\lambda = 0$  has multiplicity 3. The gradient  $\nabla$  is defined relative to the group coordinates,  $\nabla = (\partial/\partial a_1, \partial/\partial a_2, \partial/\partial a_3, \partial/\partial b_1, \partial/\partial b_2, \partial/\partial c)$ , and  $\nabla^T$  denotes the transposed vector.

In a sequel paper, we will carry out the harmonic analysis of  $\tilde{A}$  and use this to solve explicitly the equation

$$\tilde{A}p_t(a_1, a_2, a_3, b_1, b_2, c, t) = \frac{\partial}{\partial t} p_t$$

with  $p_t(\cdot) = \delta(\cdot)$  on  $G$ . The solution is the kernel which was denoted,

$$p_t(g) = p_t(a, b, c) = p_t(A, B)$$

in Theorem 8.1. Recall that  $A = (a_1, a_2)$  and  $B = (a_3, b_1, b_2, c)$  in the expression for  $p_t$  in Sect. 8.

The following is immediate from this and [Jo, Prop. 3.1]:

**Corollary 9.1.** *The heat equation kernel  $p_t(a, b, c)$  is of exponential decay at  $\infty$  in each of the variables  $a, b,$  and  $c$ . Moreover,*

$$(e^{-tH}\phi)(X) = \int K_t(X, A)\phi(A)dA = \mathcal{O}(t^{-1/2})$$

uniformly in  $X$ ; and the kernel  $K_t(X, A)$  is of Carleman type.

*Proof.* We are using the terminology of Theorem 8.1. In particular,  $H = P_1^2 + P_2^2 + (1 + Q_1Q_2)^2$ ,  $\phi \in \mathcal{L}^2(\mathbf{R}^2)$ , with  $X$  denoting vectors in  $\mathbf{R}^2$ .

We saw that for  $\phi \in \mathcal{L}^2(\mathbf{R}^2)$ , the solution  $u(X, t)$  to the analytically continued Schrödinger equation,

$$-H_x u(X, t) = \frac{\partial u}{\partial t}(X, t)$$

is given by

$$u(X, t) = (e^{-tH}\phi)(X) = \int K_t(X, A)\phi(A)dA,$$

where the integral in the  $A$ -variable runs over  $\mathbf{R}^2$ , and  $dA = da_1 da_2$ . Using formula (8.5) for  $K_t(X, A)$ , we get the following estimates,

$$|(e^{-tH}\phi)(X)| \leq \left\{ \int |K_t(X, A)|^2 dA \int |\phi(A)|^2 dA \right\}^{1/2}$$

and

$$\begin{aligned} \int |K_t(X, A)|^2 dA &\leq \int \left\{ \int p_t((A-X), B) dB \right\}^2 dA \\ &= \int \left\{ \int p_t(A, B) dB \right\}^2 dA \\ &= t^{-10} \int \left\{ \int p_1(\delta_{t^{-1/2}}(A, B)) dB \right\}^2 dA \\ &= t^{-1} \int \left\{ \int p_1(A, B) dB \right\}^2 dA. \end{aligned}$$

The last integral is finite in view of the first part of the corollary.

It follows that the  $\mathcal{L}^2$ -norm  $\|K_t(X, \cdot)\|_2$  is finite for all  $X \in \mathbf{R}^2$ , and  $t > 0$ . Moreover,

$$\|K_t(X, \cdot)\|_2 = \mathcal{O}(t^{-1/2}) \tag{9.4}$$

at  $t \rightarrow +\infty$ , uniformly in  $X$ , as claimed.

In the next corollary, we use (9.4) to give an asymptotic estimate on the eigenfunctions for  $H = P_1^2 + P_2^2 + (1 + Q_1 Q_2)^2$ . We saw in Sect. 7 that  $H$  is self-adjoint,  $H \geq 0$ , with purely discrete spectrum.

Using the theory of generalized eigenfunctions, we shall now go into more detailed properties of the spectrum of the different operators. We refer to [B-J-S, Suppl. I], [G-S, vol. 3, Chap. IV], [Mau], and [B-S] for background material on generalized eigenfunctions. It follows from Theorem 7.1 that  $H$  has a complete set of eigenfunctions  $\{\phi_n(\lambda, x)\}$ , indexed by  $n = 1, 2, \dots$  (finite),  $\lambda > 0$ ,  $\lambda \in \mathbf{R}$ . By elliptic regularity, it follows that each  $\phi_n(\lambda, \cdot)$  is  $C^\infty$  on  $\mathbf{R}^2$ , and is a solution of the partial differential equation,

$$(-\Delta_x + (1 + x_1 x_2)^2)\phi_n(\lambda, x) = \lambda \phi_n(\lambda, x) \tag{9.5}$$

in the strong sense. The functions  $\phi_n(\lambda, x)$  are specified by the choice of a canonical diagonalization for  $H$ . If  $H = \int_0^\infty \lambda dE(\lambda)$ , then  $E$  is discrete, and  $\dim E(0, \lambda] = 0(\lambda^{3/2} \ln \lambda)$ . Let  $\mathcal{H}$  be the Hilbert space of functions  $F(\lambda) = (F_1(\lambda), F_2(\lambda), \dots)$  with  $d(\lambda)$  denoting the multiplicities and with inner product,

$$\langle F, F \rangle = \sum_\lambda \sum_{n=1}^{d(\lambda)} |F_n(\lambda)|^2,$$

where the summation  $\sum_\lambda$  is over the discrete point spectrum. Then, by [Gå 2], there is a unitary spectral representation,  $U : \mathcal{L}^2(\mathbf{R}^2) \rightarrow \mathcal{H}$ , satisfying  $(U\phi)(\lambda) \in \mathcal{H}$  for all  $\phi \in \mathcal{L}^2(\mathbf{R}^2)$ , and,

$$\|\phi\|^2 = \sum_\lambda |\langle U\phi \rangle(\lambda)|^2, \tag{9.6}$$

$$(U\phi)_n(\lambda) = \int_{\mathbf{R}^2} \phi(x) \overline{\phi_n(\lambda, x)} dx, \tag{9.7}$$

$$|\langle U\phi \rangle(\lambda)|^2 = \sum_{n=1}^{d(\lambda)} |(U\phi)_n(\lambda)|^2, \tag{9.8}$$

$$U[e^{-tH}\phi](\lambda) = e^{-t\lambda} \langle U\phi \rangle(\lambda). \tag{9.9}$$

Note that formula (9.7) makes sense as it stands for  $\phi \in \mathcal{S}(\mathbf{R}^2)$  (the Schwartz space), and it extends to a unitary map by virtue of (9.6). We also note that, because of (7.1),  $e^{-tH}\phi \in \mathcal{S}$ , for  $t > 0$ , and  $\phi \in \mathcal{L}^2(\mathbf{R}^2)$ , so that

$$U[e^{-tH}\phi]_n(\lambda) = \int_{\mathbf{R}^2} (e^{-tH}\phi)(x) \overline{\phi_n(\lambda, x)} dx = e^{-t\lambda} (U\phi)_n(\lambda).$$

Since the potential,  $V=(1+x_1x_2)^2$ , in (9.5) is real valued, we may assume without loss of generality that the functions  $\phi_n(\lambda, \cdot)$  are real valued as well.

**Corollary 9.2.** *For the eigenfunctions,  $\phi_n(\lambda, \cdot)$ ,  $n=1, 2, \dots, \lambda>0$ , we have the estimate,*

$$\sum_{\lambda} \sum_{n=1}^{d(\lambda)} e^{-2\lambda t} |\phi_n(\lambda, x)|^2 \leq \text{const} \times t^{-1}, \tag{9.10}$$

where the constant is independent of the variables  $t(>0)$ ,  $n$ , and  $x$ .

**Remark 9.3.** We saw in Theorem 7.1 that the generalized eigenfunctions are not always bounded in the  $x$ -variable. The estimate (9.10) shows that the functions nonetheless satisfy a property which is ‘‘similar’’ to boundedness.

*Proof.* We showed, in (9.4), that  $\|K_t(x, \cdot)\|^2 = \mathcal{O}(t^{-1})$  at  $t \rightarrow +\infty$ , and that this estimate is uniform in  $x(\in \mathbf{R}^2)$ . It follows that

$$\begin{aligned} \|K_t(x, \cdot)\|^2 &= \sum_{\lambda} \sum_{n=1}^{d(\lambda)} |U[K_t(x, \cdot)]_n(\lambda)|^2 \\ &= \sum_{\lambda} \sum_n |\langle K_t(x, \cdot), \phi_n(\lambda, \cdot) \rangle|^2 \\ &= \sum_{\lambda} \sum_n |(e^{-tH} \phi_n(\lambda, \cdot))(x)|^2 \\ &= \sum_{\lambda} e^{-2t\lambda} \sum_{n=1}^{d(\lambda)} |\phi_n(\lambda, x)|^2 \leq C t^{-1}, \end{aligned}$$

where the constant  $C$  is independent of  $t, n$ , and  $x$ . In particular,

$$\sum_{\lambda} e^{-2t\lambda} |\phi_n(\lambda, x)|^2 \leq C \cdot t^{-1},$$

as claimed. In the calculation of  $\|K_t(x, \cdot)\|^2$  above, we used (9.6), (9.7), (9.8), (9.9), and (9.4), in this order.

We conclude this section by showing that the spectrum of the sub-Laplacian  $\tilde{\mathcal{A}}$  is absolutely continuous with uniform multiplicity.

**Theorem 9.4.** *The spectrum of  $\tilde{\mathcal{A}} = \sum_1^3 \tilde{\mathcal{A}}_j^2$  is absolutely continuous with uniform multiplicity.*

*Proof.* On  $\mathcal{L}^2(G)$ , we define a family of unitary operators  $\{V_s : s>0\}$  as follows

$$(V_s f)(g) = f(\partial_s(g)) s^5, \quad g \in G, \quad s > 0.$$

A direct calculation shows that  $V_s$  is indeed unitary relative to the norm on  $\mathcal{L}^2(G)$  coming from Haar measure on  $G$ .

We have,

$$V_s \tilde{\mathcal{A}} V_s^* = s^{-2} \tilde{\mathcal{A}}$$

by virtue of Lemma 5.1. Writing the spectral representation for  $-\tilde{D}$  in the form,

$$-\tilde{D} = \int_0^\infty \lambda \, de(\lambda),$$

we get

$$V_s de(\lambda) V_s^* = de(s^2\lambda). \tag{9.11}$$

Working with the multiplicative group  $\mathbf{R}_+$ , this may, in turn, be expressed as saying that the transform,  $de(s^2\lambda)$  of  $de(\lambda)$ , is quasi-equivalent to  $de(\lambda)$ . By Mackey's theorem on quasi-equivalent measures, [Ma 1], this means that  $de(\lambda)$  is absolutely continuous relative to the Haar measure on  $\mathbf{R}_+$ . Since the latter Haar measure is just  $d\lambda/\lambda, \lambda > 0$ , the desired conclusion follows, taking into account the  $s^2$ -factor in (9.11).

There is, therefore, a spectral representation  $R$  say, as in (9.6)-(9.9), a separable Hilbert space  $\mathfrak{U}$  such that  $R: \mathcal{L}^2(G) \rightarrow \mathcal{L}^2(\mathbf{R}_+, \mathfrak{U}, d\lambda/\lambda)$  is unitary onto, and

$$(Rf)_n(\lambda) = (f, e_n(\lambda, \cdot)), \quad n=1, 2, \dots, \lambda \geq 0.$$

In particular,

$$\int_G |f(g)|^2 dg = \int_0^\infty |(Rf)(\lambda)|^2 \frac{d\lambda}{\lambda}.$$

(Details of this construction are contained in a sequel paper by the first-named author.)

### § 10. Conclusion

Whenever the Hamiltonian of a quantum mechanical system is a polynomial in elements of a Lie algebra, it is possible to analyze the system by using the representation structure of the Lie algebra. Such an analysis can generally be broken into two parts. First, since the Hilbert space of the system is a representation space of the Lie algebra (or Lie group), if the Hilbert space is reducible, it can be decomposed into irreducible representation spaces; the Hamiltonian on these irreducible spaces will generally differ from the original Hamiltonian. Such was the case for both the constant and curved magnetic fields discussed in this paper. The Hamiltonian for the constant magnetic field [Eq. (2.3)] acting on a reducible representation space of the group given by Eq. (2.4) became, as shown in Sects. 5 and 6, the harmonic oscillator Hamiltonian, while for the curved magnetic field, the Hamiltonian, Eq. (2.8), associated with the group given in Eq. (2.9), became the Hamiltonian given in Eq. (6.11). In both of these cases a decomposition occurred because some (generalized) momenta were conserved quantities.

Second, if the Hamiltonian is a quadratic sum of Lie algebra elements, it is possible to use the solution of the heat equation of the underlying Lie group to compute the time dependent Green's function for the time evolution of the

quantum mechanical system. This computation proceeds in the following way. Let  $\phi_0$  be the wave function for the system at  $t=0$ ; we wish to find the wave function of the system  $\phi_t$ , at  $t>0$ , by writing  $\phi_t=e^{-iHt}\phi_0$ . To explicitly compute  $e^{-iHt}$ , we look instead at  $e^{-2Ht}$ . Then [Jo] shows that if  $H$  is a quadratic sum of Lie algebra elements, it follows that

$$e^{-2Ht}\phi_0=\int_G dg p_t(g)U_g \phi_0,$$

where  $U_g$  is the representation of  $G$  acting on the physical Hilbert space  $\mathcal{H}$ , and  $p_t(g)$  is the ‘‘heat kernel’’ satisfying

$$\frac{\partial p_t}{\partial t}=\tilde{\mathcal{L}}p_t, \quad p_0(g)=\delta(g),$$

and  $\tilde{\mathcal{L}}$  is the sub-Laplacian defined in Eq. (4.4a). Finally, using analytic continuation, the time evolution is given by

$$e^{-iHt}\phi_0=\int_G dg p_{it/2}(g)U_g\phi_0.$$

For the case of the curved magnetic field, the representation  $U_g$  on the physical Hilbert space is given by Eq. (2.10). Combining these results gives

$$\begin{aligned} (e^{-2Ht}\phi_0)(x, y, z) &= \int_G dg p_t(g)(U_g\phi_0)(x, y, z) \\ &= \int_{\mathbb{R}^6} db_1 db_2 dc da_1 da_2 da_3 \\ &\quad \times e^{-i\gamma(a_2 b_2 + a_2 a_3 x + a_3 x y)} e^{i\gamma(c + b_1 x - b_2 y)} \\ &\quad \times p_t(a_1, a_2, a_3, b_1, b_2, c)\phi_0(x + a_1, y + a_2, z + a_3) \\ &= \int_{\mathbb{R}^6} db_1 db_2 dc da_1 da_2 da_3 \\ &\quad \times e^{-i\gamma((a_2 - y)b_2 + (a_2 - y)(a_3 - z)x + (a_3 - z)xy)} e^{i\gamma(c + b_1 x - b_2 y)} \\ &\quad \times p_t(a_1 - x, a_2 - y, a_3 - z, b_1, b_2, c)\phi_0(a_1, a_2, a_3). \end{aligned}$$

It follows that  $e^{-2tH}$  is an integral operator with kernel,

$$\begin{aligned} K_t(x, y, z; a_1, a_2, a_3) &= \hat{p}_t(a_1 - x, a_2 - y, a_3 - z, \gamma x, -\gamma a_2, \gamma) \\ &\quad \times e^{-i\gamma(a_3 - z)a_2 x}, \end{aligned}$$

where  $\hat{p}_t$  refers to the Euclidean Fourier transform in the last three variables  $b_1, b_2, c$ .

Letting  $2t$  go to  $i$ , we then get the kernel for the Schrödinger operator  $e^{-itH}$ , given by,

$$\begin{aligned} K_t^s(x, y, z; a_1, a_2, a_3) &= \hat{p}_{it/2}(a_1 - x, a_2 - y, a_3 - z, \gamma x, -\gamma a_2, \gamma) \\ &\quad \times e^{-i\gamma(a_3 - z)a_2 x}, \end{aligned}$$

reflecting the explicit time-dependence of the system. (The problem of evaluating the heat kernel  $p_t$  at purely imaginary time is discussed in [Jo, Prop. 3.3], and [J-M, Chap. 3].) Also note that the conserved quantity  $p_z$  plays a special role in the kernel. This result, along with the spectral analysis of the reduced Hamiltonian given in Sects. 7, 8, and 9 are the major results of our paper.

To conclude, we wish to point out that the analysis carried out in this paper can be generalized to many systems with polynomial interactions. Consider, for example, the Hamiltonian

$$H = \frac{1}{2} \sum_{i=1}^n p_i^2 + V(x_1, \dots, x_n),$$

where  $V$  is a polynomial in  $x_1, \dots, x_n$ . Then the commutators

$$\begin{aligned} \left[ \frac{\partial}{\partial x_i}, V \right] &= \frac{\partial V}{\partial x_i} \equiv V_i \\ \left[ \frac{\partial}{\partial x_i}, V_j \right] &= \frac{\partial V_j}{\partial x_i} \equiv V_{ij} \\ &\vdots \qquad \qquad \qquad \vdots \qquad \qquad \qquad \vdots \end{aligned}$$

generate Lie algebra elements  $\partial/\partial x_i, V_i, V_{ij}, \dots$  that finally close to give a nilpotent Lie algebra, because of the polynomial nature of  $V$ .

For example, the Hamiltonian

$$H = \frac{p^2}{2} + \frac{x^2}{2} + \alpha x^4$$

generates a nilpotent Lie algebra consisting of elements  $p, x^2, x$ , and 1; the underlying nilpotent group is given by the matrices

$$\begin{pmatrix} 1 & a & a^2/2 & b_0 \\ & 1 & a & b_1 \\ & \mathbf{0} & 1 & b_2 \\ & & & 1 \end{pmatrix}$$

and the Hamiltonian is a quadratic sum of Lie algebra elements. Further, the Hilbert space  $\mathcal{L}^2(\mathbf{R})$  for this Hamiltonian is an irreducible representation space for the underlying nilpotent group.

Similarly, the Henon-Hailes potential

$$V = \frac{1}{2} x_1^2 + \frac{1}{2} x_2^2 + x_1 x_2^2 - \frac{1}{3} x_2^3$$

generates a nilpotent Lie algebra. If the Lie algebra includes the elements  $p_1, p_2, x_1, x_2$ , and  $x_0 = x_1 x_2^2 - (1/3)x_2^3$ , then the Hamiltonian can be written as  $2H = p_1^2 + p_2^2 + x_1^2 + x_2^2 + x_0$ , so that it is again possible to use the structure of the heat equation (Thm. 4.1) of the underlying nilpotent Lie group to find the time evolu-

tion of the system. Both the quartic, and Henon-Hailes, potentials will be investigated in forthcoming papers.

Another class of systems with polynomial interactions is given by a quantum mechanical particle in an external electromagnetic field. In this case the Hamiltonian is of the form

$$H = \frac{1}{2}(\vec{p} - \vec{A})^2 + \phi,$$

where  $\phi$  is the electrostatic potential. Consider as Lie algebra elements

$$\frac{1}{i} \frac{\partial}{\partial x_j} - A_j, \quad j=1, 2, 3$$

and  $\phi$ ; then  $[p_j - A_j, p_k - A_k]$  generates, as shown in Eq. (2.2), the magnetic field and its derivatives. If the magnetic field is a polynomial in the coordinates, then these commutators will close. Also, if  $\phi$  is a polynomial in the coordinates, the commutators generating  $[p_i - A_i, \phi]$  will eventually close, and again a nilpotent Lie algebra is generated. In this paper we have analyzed the simplest systems of this form, where  $\phi=0$  and the magnetic field is either a constant or varies linearly with the coordinates. In a forthcoming paper, we will analyze a more realistic example which includes a constant electric field.

In all of these cases, the nilpotent group structure plays a crucial role in analyzing the quantum mechanical system. Since our unitary representations are induced representations [Dix 1, Puk], it is generally straightforward to find the inducing subgroup of the given nilpotent group that yields the physical Hilbert space. Such was the case for the constant and curved magnetic fields, where the inducing structure is given in Eqs. (2.5) and (2.10).

Finally, we point out that several of the problems we are considering—such as the curved magnetic field analyzed in this paper—have classical solutions that are of interest. Thus, another problem to be investigated is the relationship between the heat kernel generated by nilpotent groups and appropriate classical limits.

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