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Fundamental Solutions for a Family of Sub-elliptic PDEs

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Dedicated to Professor L. Simon on his sixtieth birthday

Abstract: In this article, we survey the behavior of the subRiemannian geodesics induced by a family of sub-elliptic partial differential equations, especially the sub-Laplacian on the Heisenberg group. In particular, we discuss the complex action function and volume element along the geodesics. Using this action function and the volume element, we obtain the fundamental solution and the heat kernel for the sub-Laplacian. We also give a brief discussion on applications on this theory to magnetic resonance imaging.
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1. Introduction

Function theory on the Heisenberg group was studied extensively by many mathematicians in the past 30 years. The Heisenberg group and its sub-Laplacian are at the cross-roads of many analysis and geometry domains. A few of these domains are nilpotent Lie groups theory, hypoelliptic second order partial differential equations, strongly pseudoconvex domains in complex analysis, probability theory of degenerate diffusion process, subRiemannian geometry, control theory

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and semiclassical analysis of quantum mechanics, see *e.g.,* [**4**], [**6**], [**12**], [**13**], [**14**], and [**19**]. Here we give a survey of the behavior of the subRiemannian geodesics induced by a family of sub-elliptic partial differential equations. We give special attention to the sub-Laplacian operating on the Heisenberg group and a step 4 subRiemannian manifold, which is the paradigm of the theory. This article is one of a series (see [**8**], [**9**], [**10**], [**11**], and [**12**]), whose aim is to study the subRiemannian geometry induced by the sub-Laplacian and its analytic consequences. We also give discuss the link between this theory and diffusion magnetic resonance imaging. In the last section, we give a detailed description of the quantization of energy.

2. Geometry induced by the sub-Laplacian

We start with m linearly independent vector fields $X_1, \dots, X_m$ on a n dimensional manifold $\mathcal{M}_n$ with $m \leq n$. In order to induce a geometry on $\mathcal{M}_n$, we consider an orthonormal set of "horizontal" vector fields $X = \{X_1, \dots, X_m\}$. If $m = n$, this yields a Riemannian geometry on $\mathcal{M}_n$. If $m < n$, we shall assume that a finite number of Lie brackets of $X_1, \dots, X_m$ generate the tangent bundle $T\mathcal{M}_n$; if one bracket suffices, we call X step 2, additional brackets indicate higher step. We invoke the Chow's bracket generating condition [**14**]. This implies that every 2 points of $\mathcal{M}_n$ may be connected by a horizontal curve, that is a curve, all of whose tangents can be represented as linear combinations of $X_1, \dots, X_m$. If γ is such a curve, and

$$\dot{\gamma} = \sum_{j=1}^{m} a_j X_j,$$

then

$$\ell(\gamma) = \int \sqrt{\sum_{j=1}^{m} a_j^2}$$

is the length of γ. By minimizing the lengths of horizontal curves between P, $Q \in \mathcal{M}_n$, we obtain the distance between P and Q. This is the Lagrangian formalism. Before we go further, let us point out that the Chow's condition is crucial to connect two points in $\mathcal{M}_n$ by a horizontal curve. For example, let us consider

$$X_1 = \frac{\partial}{\partial x_1}, \qquad X_2 = \frac{\partial}{\partial x_2} + x_1 x_3 \frac{\partial}{\partial x_3}$$

in $\mathbf{R}^3$. Then

$$[X_1, X_2] = x_3 \frac{\partial}{\partial x_3}, \qquad [X_2, [X_1, X_2]] = 0, \qquad [X_1, [X_1, X_2]] = 0.$$

This tells us that the tangent bundle cannot be generated by a finite number of Lie brackets on the plane $\{x_3 = 0\}$. Simple arguments show that a curve $\mathbf{c}(s) = (x_1(s), x_2(s), x_3(s))$ is horizontal if and only if $\dot{x}_3 = x_1 x_3 \dot{x}_2$. However, let P and Q be points in the half spaces $\{x_3 > 0\}$ and $\{x_3 < 0\}$ respectively. Assume that $\mathbf{c}$ is a horizontal curve connecting these two points with $\mathbf{c}(0) = P$ and $\mathbf{c}(1) = Q$. Then there is $\tau \in (0,1)$ such that $\mathbf{c}(\tau) = (x_1(\tau), x_2(\tau), 0)$, *i.e.,* $x_3(\tau) = 0$. Multiplying by the factor $e^{-\int x_1 \dot{x}_2 ds}$ in $\dot{x}_3 - x_1 x_3 \dot{x}_2 = 0$, we obtain

$$\left(x_3 e^{-\int x_1 \dot{x}_2 ds}\right)' = 0 \;\Leftrightarrow\; x_3 e^{-\int x_1 \dot{x}_2 ds} = C.$$

This implies that $x_3(s) = Ce^{\int x_1 \dot{x}_2 ds}$ and $x_3(0) = Ce^{\int_0^0 x_1 \dot{x}_2 ds} = C > 0$. Hence $x_3(\tau) > 0$ for all $\tau \in (0,1)$ which contradicts the assumption. But we also may conclude that any two points on the same half space $\{x_3 > 0\}$ or $\{x_3 < 0\}$ can be joined by a horizontal curve.

Now we shall work with the Hamiltonian formalism. Set

$$X_j = \sum_{k=1}^{n} a_{jk}(x) \frac{\partial}{\partial x_k}, \quad j = 1, \dots, m.$$

Then,

$$H = \frac{1}{2} \sum_{j=1}^{m} \Big(\sum_{k=1}^{n} a_{jk}(x) \xi_k \Big)^2$$

is the Hamiltonian function on the cotangent bundle $T^*\mathcal{M}_n$. A bicharacteristic curve $(\mathbf{x}(s), \xi(s)) \in T^*\mathcal{M}_n$ is a solution of the Hamiltonian system of differential equations:

$$\dot{x}_j(s) = H_{\xi_j}, \qquad \dot{\xi}_j(s) = -H_{x_j},$$

with boundary conditions

$$x_j(0) = x_j^{(0)}, \quad x_j(\tau) = x_j, \quad j = 1, \dots, n,$$

for given points $\mathbf{x}^{(0)}, \mathbf{x} \in \mathcal{M}_n$; one may think of τ as time. The projection $\mathbf{x}(s)$ of the bicharacteristic curve on $\mathcal{M}_n$ is a geodesic. When $m = n$ we have Riemannian geodesics and a Riemannian geometry, and when $m < n$ we talk about subRiemannian geodesics and subRiemannian geometry. SubRiemannian geometry is quite different from Riemannian geometry. In particular

(a) Every point P of a Riemannian manifold is connected to every other point in a sufficiently small neighborhood by a single, unique geodesic. On a subRiemannian manifold there will be points arbitrarily near P which are connected to P by an infinite number of geodesics (see *e.g.,* [**4**], [**9**], [**11**], and [**19**]). This strange phenomenon was first pointed out by Gaveau [**16**] and Strichartz [**25**], and it brings up the question of what "local" means in subRiemannian geometry. Control theorists (see *e.g.,* [**1**] and [**7**]) studying subRiemannian examples noticed that the Riemannian concepts of cut locus and conjugate locus behave badly in a subRiemannian context.

(b) In Riemannian geometry the unit ball is smooth. In subRiemannian geometry, among the many distances, there is a shortest one, often referred to as the Carnot-Carathéodory distance. In subRiemannian geometry the Carnot-Carathéodory unit ball is singular.

(c) The exponential map is smooth in Riemannian geometry, but often singular in subRiemannian geometry. The singularities occur at points connected to an "*origin*" by an infinite number of geodesics. These singular points constitute a submanifold whose tangents yields the "*missing directions*", that is the directions in $T\mathcal{M}_n$ not covered by the horizontal directions.

Our interest in subRiemannian geometry is a consequence of our wish to construct inverse kernels, *i.e.,* fundamental solutions, heat kernels, wave kernels, etc., for subelliptic partial differential operators of the form

$$\Delta_X = \frac{1}{2}\sum_{j=1}^{m} X_j^2.$$

The aim is to find explicit forms for these inverse kernels in terms of subRiemannian invariants which are induced by the horizontal vector fields $X_1, \dots, X_m$. If $m = n$, and X_j^* denote the L^2-dual of X_j in the induced Riemannian metric, then

$$\Delta_X = -\frac{1}{2}\sum_{j=1}^{n} X_j^* X_j$$

is elliptic. The operator Δ_X is the usual Laplace-Beltrami operator. When $m < n$ and the brackets of X_j yield all of $T\mathcal{M}_n$, according to a theorem of Hörmander [**20**], this implies that Δ_X is subelliptic. The number given by the minimum number of brackets necessary to generate $T\mathcal{M}_n$ plus 1 is referred to as the "step" of the operator Δ_X. In particular, an elliptic operator is step 1, one bracket generators are step 2, etc. To illustrate the proposed structure, we shall discuss a family of operators for which "explicit" fundamental solutions given in geometric terms are available. To simplify our notation, we will limit our discussion to 3 dimensional space, $\mathbf{x} = (t, x_1, x_2) = (t, x)$, with 2 vector fields

$$X_1 = \frac{\partial}{\partial x_1} + 2kx_2|x|^{2k-2}\frac{\partial}{\partial t}, \qquad X_2 = \frac{\partial}{\partial x_2} - 2kx_1|x|^{2k-2}\frac{\partial}{\partial t},$$

with $|x|^2 = x_1^2 + x_2^2$. The differential operator to invert is Δ_X which is step 2 at points $|x|^2 \neq 0$ and step $2k$ otherwise, see [**9**] and [**10**]. The fundamental solution $K(\mathbf{x}, \mathbf{x}^{(0)})$ of Δ_X is the distribution solution of

$$\Delta_{X,\mathbf{x}} K(\mathbf{x}, \mathbf{x}^{(0)}) = \delta(\mathbf{x} - \mathbf{x}^{(0)}).$$

We shall look for K in the form

$$K(\mathbf{x}, \mathbf{x}^{(0)}) = \int_{\mathbf{R}} \frac{E(\mathbf{x}, \mathbf{x}^{(0)}, \tau)v(\mathbf{x}, \mathbf{x}^{(0)}, \tau)}{g(\mathbf{x}, \mathbf{x}^{(0)}, \tau)} d\tau, \tag{2.1}$$

see [**3**] and [**5**], where the function g is a solution of the Hamilton-Jacobi equation

$$\frac{\partial g}{\partial \tau} + \frac{1}{2}\big(X_1 g\big)^2 + \frac{1}{2}\big(X_2 g\big)^2 = 0.$$

g is given by a modified action integral of a complex Hamiltonian problem. The associated energy

$$E = -\frac{\partial g}{\partial \tau}$$

is the first invariant of motion, and the volume element v is the solution of a transport equation, which is order 1 in the step 2 case, $k = 1$, and order 2 in the higher step case, $k \geq 2$. Let

$$H(\mathbf{x}, \xi) = \frac{1}{2}\big(\xi_1 + 2kx_2|x|^{2k-2}\theta\big)^2 + \frac{1}{2}\big(\xi_2 - 2kx_1|x|^{2k-2}\theta\big)^2$$

denote the Hamiltonian, where θ is the dual variable to t and ξ are the dual variables to $\mathbf{x}$. The complex bicharacteristics are solutions of the Hamiltonian system of differential equations

$$\dot{t} = H_\theta, \quad \dot{\theta} = -H_t, \quad \dot{x}_j = H_{\xi_j}, \quad \dot{\xi}_j = -H_{x_j}, \quad j = 1, 2,$$

with the nonstandard boundary conditions

$$x_1(0) = x_1^{(0)}, \quad x_2(0) = x_2^{(0)},$$
$$t(\tau) = t, \; x_1(\tau) = x_1, \quad x_2(\tau) = x_2, \quad \theta(0) = -i.$$

Then the energy E is

$$E = \frac{1}{2}\dot{x}_1^2 + \frac{1}{2}\dot{x}_2^2,$$

and the modified action g is given by

$$g = -it(0) + \int_0^\tau \Big[\xi_1(s)\dot{x}_1(s) + \xi_2(s)\dot{x}_2(s) - H(\mathbf{x}(s), \xi(s))\Big] ds.$$

We note that t, the “missing direction”, must be treated separately.

The volume element v is the solution of the following second order transport equation:

$$\Delta_X(Ev) + \frac{\partial}{\partial \tau}\Big[T(v) + (\Delta_X g)v\Big] = 0, \tag{2.2}$$

where

$$T = \frac{\partial}{\partial \tau} + \sum_{j=1}^{2} \big(X_j g\big) X_j$$

is differentiation along the bicharacteristic. Formula (2.1) has a simple geometric interpretation. The operator Δ_X has a characteristic variety in $T^*\mathcal{M}_n$ given by $H = 0$. Over every point $\mathbf{x} \in \mathcal{M}_n$, this is a line, parametrized by $\theta \in (-\infty, \infty)$,

$$\xi_1 = -2kx_2|x|^{2k-2}\theta, \qquad \xi_2 = 2kx_1|x|^{2k-2}\theta.$$

Consequently, K may be thought of as the $(\text{action})^{-1}$ summed over the characteristic variety with measure Ev. We note that, when Δ_X is elliptic, its characteristic variety is the zero section, so we do get simply $(\text{distance})^{-1}$, as expected. When Δ_X is sub-elliptic, τg behaves like the square of a distance function, even though it is complex. The following result can be found in [**12**].

Theorem 2.1. *The complex action is given by*

$$g(r, r_0, t, E, \tau) = -it + \frac{k-1}{k} E\tau + \frac{1}{k}\left(r\sqrt{\frac{E}{2} + k^2 r^{4k-2}} - r_0 \sqrt{\frac{E}{2} + k^2 r_0^{4k-2}} \right),$$

where $r = |x|$ and $r_0 = |x(0)|$.

Corollary 2.2. *The complex action starting at the origin is given by*

$$g = -it + \frac{1}{k}\left((k-1)E\tau + |x|\sqrt{\frac{E}{2} + k^2 (x_1^2 + x_2^2)^{2k-1}} \right).$$

In the step 2 case the energy E depends on $|x|$ and is given by

$$E = \frac{2|x|^2}{\sinh^2(2\tau)} = -\frac{\partial g}{\partial \tau}.$$

Corollary 2.3. *When $k = 1$, the complex action starting from the origin is given by*

$$g = -it + (x_1^2 + x_2^2)\coth(2\tau).$$

In this case, the volume element v is the solution of the following transport equation

$$\frac{\partial v}{\partial \tau} + \sum_{j=1}^{2} (X_j g)(X_j v) + (\Delta_X g) v = 0,$$

which can be calculated explicitly:

$$v(\mathbf{x}, \tau) = -\frac{1}{4\pi^2} \frac{\sinh(2\tau)}{|x|^2}.$$

Therefore,

$$K(x, t) = \frac{1}{8\pi^2} \int_{-\infty}^{\infty} \frac{1}{|x|^2 \cosh(s) - it\sinh(s)} ds.$$

Denote

$$R = (|x|^4 + t^2)^{\frac{1}{4}} \quad \text{and} \quad e^{-i\phi} = R^{-2}(|x|^2 - it)$$

where $\phi \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$. Using the identity

$$\cosh(s + i\phi) = \cosh(s)\cos\phi + i\sinh(s)\sin\phi,$$

one has

$$K(x,t) = \frac{1}{8\pi^2}\int_{-\infty}^{\infty} \frac{1}{R^2\cosh(s+i\phi)}ds. \tag{2.3}$$

Changing the contour, the formula (2.3) becomes

$$K(x,t) = \frac{1}{8\pi^2}\frac{1}{R^2}\int_{-\infty}^{\infty} \frac{1}{\cosh(s)}ds.$$

The above integral can be evaluated as follows:

$$K(\mathbf{x},t) = C(|x|^2+it)^{-\frac{1}{2}}(|x|^2-it)^{-\frac{1}{2}} = C(|x|^4+t^2)^{-\frac{1}{2}}.$$

This coincides with the result obtained by Folland and Stein [**15**] on the Heisenberg group. On general non-isotropic Heisenberg groups, we may obtain the fundamental solutions by using Laguerre calculus which are given in the form (2.1). See *e.g.,* [**6**] and [**18**]. The reason is that the fundamental solution must include all the distances, which necessitates the use of g and the summation over all the distances means integration on τ.

3. Heisenberg group

An n-dimensional non-isotropic Heisenberg group is a nilpotent Lie group with the group law

$$\mathbf{x}\circ\mathbf{y} = [x_1+y_1,\dots,x_{2n}+y_{2n}, t+s-2\sum_{j=1}^{n} a_j(x_jy_{j+n}-y_jx_{j+n})],$$

with $a_j < 0$ for $j = 1,\dots,n$, numbered so that

$$0 < a_1 \le a_2 \le \cdots \le a_\ell < a_{\ell+1} = \cdots = a_n.$$

Here $\mathbf{x} = (\mathbf{x}', t) = (x_1,\dots,x_{2n}, t)$ and $\mathbf{y} = (\mathbf{y}', s) = (y_1,\dots,y_{2n}, s)$. This structure is the Heisenberg group $\mathbf{H}_n$. The vector fields $X = \{X_1, X_2,\dots,X_{2n}\}$ with

$$X_j = \frac{\partial}{\partial x_j} - 2a_jx_{n+j}\frac{\partial}{\partial t}, \qquad X_{n+j} = \frac{\partial}{\partial x_{n+j}} + 2a_jx_j\frac{\partial}{\partial t}$$

form a basis of the Heisenberg Lie algebra. Note that

$$\left[X_{2j-1}, X_{2j}\right] = -4a_j\frac{\partial}{\partial t},$$

and $\mathbf{H}_n$ is step 2. The group $\mathbf{H}_n$ implements the Heisenberg canonical commutation relations of quantum physics in terms of the Lie bracket $[\cdot,\cdot]$ of the Heisenberg Lie algebra $\mathcal{H}_n$ consisting of the infinitesimal generators of $\mathbf{H}_n$. Transition to the vector fields of directional derivatives presents the canonical commutation relations in terms the Poisson bracket $\{\cdot,\cdot\}$ on the space of all real-valued smooth functions.

Evidence that the t-axis is the "*canonical submanifold*" through the origin follows from calculating the number of geodesics connecting 2 points. In this case (see [**2**], [**4**] and [**12**]):

$$K(\mathbf{x}', t; \mathbf{0}) = \frac{2(n-1)!}{(2\pi)^{n+1}} \int_{-\infty}^{+\infty} \frac{v(\tau)d\tau}{g^n(\mathbf{x}', t; \tau)}$$

where

$$g(\mathbf{x}', t; \tau) = \sum_{j=1}^{n} a_j(x_j^2 + x_{n+j}^2) \coth(a_j\tau) - it$$

and

$$v(\tau) = \prod_{j=1}^{n} \frac{2a_j}{\sinh(2a_j\tau)}.$$

Theorem 3.1. *Let*

$$f(\mathbf{x}', t; \tau) = \tau g(\mathbf{x}', t; \tau) = \tau \sum_{j=1}^{n} a_j\big(x_j^2 + x_{n+j}^2\big) \coth(a_j\tau) - i\tau t$$

denote a complex distance on $\mathbf{H}_n$*. Assuming that* $\mathbf{x}' \neq 0$*, the number of critical points of* f *with respect to* τ*, i.e.,*

$$\frac{\partial f}{\partial \tau}(\mathbf{x}', t; \tau) = 0,$$

given by $\tau_1, \dots, \tau_N$*, agrees with the number of geodesics connecting* $(\mathbf{x}', t)$ *to* $(\mathbf{0}, 0)$*. Moreover, the numbers*

$$\zeta_k = 2i \int_0^{\tau_k} \sum_{j=1}^{n} \big(x_j^2(s) + x_{n+j}^2(s)\big)\, ds, \quad k = 1, \dots, N,$$

satisfy the equation

$$\frac{t}{|\mathbf{x}'|^2} = \mu(-\zeta_k),$$

where

$$\mu(z) = \frac{z}{\sin^2 z} - \cot z. \tag{3.4}$$

Furthermore,

$$f\big(\mathbf{x}', t; \tau_k(\mathbf{x}', t)\big) = \frac{1}{2}\ell_k^2 = \frac{1}{2}\nu(\zeta_k)\Big(|t| + |\mathbf{x}'|^2\Big), \quad k = 1, \dots, N,$$

where ℓ_k *is the length of that geodesic and*

$$\nu(z) = \frac{z^2}{z + \sin^2 z - \sin z \cos z}.$$

Such invariant formulas also yield full Hadamard-Kodaira expansions for the parametrix of step 2 subelliptic operators on Heisenberg manifolds. A Heisenberg manifold is an odd dimensional manifold together with a subbundle of the tangent bundle of one lower dimension, and with the first bracket generating property. The behavior of the function μ given by (3.4) is very important in understanding the subRiemannian geometry of the Heisenberg group. The function μ is a monotone increasing diffeomorphism of the interval $(-\pi, \pi)$ onto $\mathbf{R}$. On each interval $(m\pi, (m+1)\pi)$, $m = 1, 2, \ldots$, μ has a unique critical point x_m. On this interval μ decreases strictly from $+\infty$ to $\mu(x_m)$ and then increases strictly from $\mu(x_m)$ to $+\infty$. Moreover

$$\mu(x_m) + \pi < \mu(x_{m+1}), \quad m = 1, 2, \ldots$$

Hence, we know that the number of geodesics connecting the point $(\mathbf{x}', t)$ and the origin is increasing without bound. In fact, given any point $(0, t)$ on the t-axis with $t \neq 0$, there are infinitely many geodesics connected this point and the origin. In general, we have the following result.

Theorem 3.2. *On a general non-isotropic Heisenberg group* $\mathbf{H}$, *i.e.,* $\ell > 0$, *every point* $(\mathbf{0}, t)$ *is connected to the origin by an infinite number of geodesics. Every point* $(\mathbf{x}', t)$ *with*

$$\tilde{\mathbf{x}} = (x_{2\ell+1}, x_{2\ell+2}, \ldots, x_{2n}) \neq 0$$

is connected to the origin by a finite number of geodesics.

On the other hand, there are points $(\mathbf{x}', t)$, *with* $\mathbf{x}' \neq \mathbf{0}$, *but* $\tilde{\mathbf{x}} = 0$, *which are connected to the origin an infinite number of geodesics.*

If $(\mathbf{x}', t)$, $\mathbf{x}' \neq \mathbf{0}$, *is connected to the origin by an infinite number of geodesics, then the infinity of the number of geodesics connecting* $(\mathbf{x}', t)$ *to* $(\mathbf{0}, 0)$ *is "smaller" than the infinity of the number of geodesics connecting* $(\mathbf{0}, t)$ *to* $(\mathbf{0}, 0)$*; this can be made precise (see [**4**] and [**12**]).*

From the Heisenberg group law, we know that $\mathbf{H}_1$ admits a realization by a faithful matrix representation $\mathbf{H}_1 \to \mathbf{SL}(3, \mathbf{R})$:

$$\mathbf{H} = \left\{ \begin{bmatrix} 1 & x_1 & t \\ 0 & 1 & x_2 \\ 0 & 0 & 1 \end{bmatrix} \right\}$$

with the group law

$$\begin{bmatrix} 1 & x_1 & t \\ 0 & 1 & x_2 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & y_1 & s \\ 0 & 1 & y_2 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & x_1 + y_1 & t + s + x_1 y_2 \\ 0 & 1 & x_2 + y_2 \\ 0 & 0 & 1 \end{bmatrix}.$$

It is easy to see that $\mathbf{H}_1$ is a closed subgroup of the symplectic group $\mathbf{Sp}(4, \mathbf{R})$. The embedding of $\mathbf{H}_1$ under its basic representation $\mathbf{H}_1 \hookrightarrow \mathbf{Sp}(4, \mathbf{R})$ displays the symplectic structure associated to $\mathbf{H}_1$. The symplectic structure of $\mathbf{H}_1$ inherited from $\mathbf{Sp}(4, \mathbf{R})$ is of main issue for the application to quantum holography and

Fourier magnetic resonance imaging (MRI). For more detailed discussion, see *e.g.,* [**23**], [**24**] and references therein. Directional derivatives, or linear magnetic field gradients operating on the L^2-sections of a homogeneous hologram line bundle are the source of the spatial encoding in diffusion MRI.

The action of the symplectic gradients forms that the bracket transition $\Psi : [\cdot,\cdot] \rightsquigarrow \{\cdot,\cdot\}$ from Poisson manifolds to symplectic manifolds. This is very important to the structure-function problem of diffusion MRI because it provides the Hamiltonian action of $\mathbf{H}_1$ which provides the trace filter encoding of quantum holography. It is known that a diffeomorphism of the sympletic affine cross section $\mathbf{H}_1/\mathcal{C}$, the center of the group, preserves the Poisson bracket $\{\cdot,\cdot\}$ if and only if it preserves the system of Hamilton-Jacobi equations. Here the Poisson bracket is defined as follows:

$$\{f,g\} = \frac{\partial f}{\partial x_2}\frac{\partial g}{\partial x_1} - \frac{\partial f}{\partial x_1}\frac{\partial g}{\partial x_2}$$

for $f,g \in C^\infty(\mathbf{R} \bigoplus \mathbf{R})$.

The operator Δ_X plays the central role in the mathematical model of diffusion MRI. Indeed, the natural symplectic affine structure of the flat radial cross section $\mathbf{H}_1/\mathcal{C}$ derives via the natural planar connection from the group of isometries of the subRiemannian geometry of $\mathbf{H}_1$. It allows to translate the Larmor frequency equation for the precession dispersion of spin isochromats into the language of subelliptic geometrical analysis. The Hamiltonian on the cotangent bundle $T^*(\mathbf{H}_1)$ of the operator Δ_X provides the Heisenberg helices which are the projections onto the (x,y,z)-space of solutions of the Hamilton-Jacobi equation. These helices are the subRiemannian geodesics of $\mathbf{H}$ under the natural left-invariant subRiemannian metric of the group. This metric which is left-invariant under the transitive Hamiltonian action of $\mathbf{H}_1$, is obtained as a subelliptic bundle form on the tangent bundle $T(\mathbf{H}_1)$ from the Hamiltonian of the left-invariant sub-Laplacian Δ_X by the Legendre transform

$$T(\mathbf{H}_1) \to T^*(\mathbf{H}_1).$$

The isometries of the subRiemannian manifold $\mathbf{H}_1$ allow to tune the grating arrays of the traces of Heisenberg helices in order to perform the tracial encoding of image contrast within the quantum hologram inside the transverse plane $\mathbf{H}_1/\mathcal{C}$.

4. Higher step cases

When $k > 1$, there is no group structure and the complex bicharacteristics run between two arbitrary points $\mathbf{y}$ and $\mathbf{x}$. We obtain 2 invariants of the motion, the energy E and the angular momentum Ω. One cannot calculate them explicitly, but we know their analytic properties, and g and v may be found in terms of E and Ω. We state the result as follows (see [**2**] and [**3**]).

Theorem 4.1. *For $k > 1$, the fundamental solution $K(\mathbf{x}', \mathbf{y}', t-s)$ of Δ_X has the following invariant representation*

$$K(\mathbf{x}', \mathbf{y}', t-s) = \int_{\mathbf{R}} \frac{E(\mathbf{x}', \mathbf{y}', t-s; \tau) v(\mathbf{x}', \mathbf{y}', t-s; \tau)}{g(\mathbf{x}', \mathbf{y}', t-s; \tau)} d\tau,$$

where the second order transport equation (2.2) may be reduced to an Euler-Poisson-Darboux equation and solved explicitly as a function of E and Ω. Namely,

$$v = -\frac{e^{i\pi/2}}{2\pi^3 k} \frac{F(\mathcal{P}_+, \mathcal{P}_-)}{\sqrt{(\mathcal{A}_+ - g)(\mathcal{A}_- - g)}},$$

where

$$\mathcal{A}_+ = \overline{\mathcal{A}}_- = |\mathbf{x}'|^{2k} + |\mathbf{y}'|^{2k} - i(t-s) = \frac{\Omega_+}{k} + g_+,$$

and

$$\mathcal{P}_+ = \overline{\mathcal{P}}_- = \frac{2^{1/k}(x_1 + ix_2)(y_1 - iy_2)}{\mathcal{A}_+^{1/k}} = \left(1 + \frac{g_+}{\Omega_+/k}\right)^{-1/k},$$

with

$$\Omega_\pm = \lim_{\tau \to \pm\infty} \Omega.$$

Here F is a hypergeometric function of 2 variables,

$$\begin{aligned} F(\mathcal{P}_+, \mathcal{P}_-) =& \frac{2}{\pi} \int_0^1 \int_0^1 \frac{1 - |\mathcal{P}_+|^2 (\zeta\eta)^{1/k}}{(1 - \mathcal{P}_+ \zeta^{1/k})(1 - \mathcal{P}_- \eta^{1/k})(1 - |\mathcal{P}_+|^{2k} \zeta\eta)} \\ & \times \frac{d\zeta d\eta}{\sqrt{\zeta\eta(1-\zeta)(1-\eta)}}. \end{aligned}$$

In particular, when $k = 2$, the fundamental solution $K(\mathbf{x}', \mathbf{y}', t-s)$ has the following simple form (see [**6**] and [**13**]):

$$K(\mathbf{x}', \mathbf{y}', t-s) = \frac{i}{2\pi^2 d} \log \Big[\frac{|1 - \mathcal{P}^2| - i(\mathcal{P} + \overline{\mathcal{P}})}{1 + |\mathcal{P}|^2} \Big],$$

where

$$d = 2|\mathcal{A}| \sqrt{(1 - \mathcal{P}^2)(1 - \bar{\mathcal{P}}^2)},$$

and

$$\mathcal{P} = \frac{(x_1 y_1 + x_2 y_2) + i(x_1 y_2 - x_2 y_1)}{\mathcal{A}^{1/2}},$$

and

$$\mathcal{A} = \frac{1}{2} \left(|\mathbf{x}'|^4 + |\mathbf{y}'|^4 + i(t-s) \right).$$

In this case, we have (see [**10**])

Proposition 4.2. *Let τ_j denote the critical points of the modified complex action $f(\tau) = \tau g(\tau)$. Setting $\zeta_j = \mathcal{F}(i\tau_j)$, the lengths of the geodesics between the origin and the point (x,t), $|\mathbf{x}'| \neq 0$ are given by*

$$\ell_j^4 = \nu(\zeta_j)\big(|t| + |\mathbf{x}'|^4\big).$$

Here the function $\mathcal{F}$ has the following expression:

$$\mathcal{F}(z) = \frac{1+\sqrt{3}}{4^{1/3}}z - 3^{1/2}\,2^{-2/3}z - \frac{1}{2}\tan^{-1}\left(\frac{sd(2^{4/3}\,3^{1/4}z)}{2\cdot 3^{1/4}}\right)$$
$$+\frac{1}{2}\left[u\left\{\mathcal{E}(am^{-1}\omega, k') + \left[\left(\frac{2\pi}{\Gamma(\frac{1}{6})\Gamma(\frac{1}{3})}\right)^2 - \frac{3-\sqrt{3}}{6}\right]am^{-1}\omega\right\} + \frac{i}{2}\log\frac{\theta_4(x-iy)}{\theta_4(x+iy)}\right],$$

with $u = 2^{4/3}\,3^{1/4}\,z$ and $am^{-1}\omega = sn^{-1}(\sqrt{3}-1, k')$.

Here $amv = \int_0^v \mathrm{dn}\gamma\, d\gamma$ and θ_4 stands for Jacobi's zeta function. For definitions, see [**21**]. We omit the detail here.

5. The diffusion equation

Next we write the heat kernel associated to the sub-Laplacian Δ_X on the Heisenberg group in terms of the distance function $f = \tau g$ as follows (see [**2**], [**3**], [**4**], and [**14**]):

$$e^{-\Delta_X u}\psi(\mathbf{x}', t, u) = \int_{\mathbf{H}_1} P_u((\mathbf{y}', s)^{-1} \circ (\mathbf{x}', t))\psi(\mathbf{y}', s)dyds,$$

where

$$P_u(x,t) = \frac{1}{(2\pi u)^2}\int_{\mathbb{R}} e^{-\frac{f(x,t,\tau)}{u}}V(\tau)d\tau.$$

Here

$$f(x,t,\tau) = \tau g(x,t,\tau) = \tau\coth(2\tau)|x|^2 - i\tau t$$

is the complex action and

$$V(\tau) = \frac{2\tau}{\sinh(2\tau)}$$

is the Van Vleck determinant. Using the modified complex action function $f(x,t,\tau)$, one may discuss the small time behavior of the heat kernel. Then we have the following theorems.

Theorem 5.1. *Given a fixed point (x,t), $x \neq 0$, let θ_c denote the solution of equation (3.4) in the interval $[0, \pi/2)$. Then the heat kernel on $\mathbf{H}_1$ has the following small time behavior:*

$$P_u(x,t) = \frac{1}{(2\pi u)^2}e^{-\frac{d_c^2(x,t)}{2u}}\left\{\Theta(x,t)\sqrt{2\pi u} + \mathcal{O}(u)\right\}, \qquad u \to 0^+,$$

where

$$\Theta(x,t) = \frac{\theta_c}{|x|\sqrt{[1 - 2\theta_c \coth(2\theta_c)]}},$$

and d_c denotes the Carnot-Carathéodory distance.

Theorem 5.2. *At points $(0,t)$ with $t > 0$, we have the following expansion*

$$P(0,t;u) = \frac{1}{4u^2}\sum_{k=1}^{\infty}(-1)^{k+1} k e^{-\ell_k^2(0,t)/2u}$$

as $u \to 0^+$.

One also has

Theorem 5.3. *The heat kernel $P_u(x,t)$ on $\mathbf{H}_1$ has the following sharp upper bound:*

$$|P_u(x,t)| \le \frac{C}{u^2} e^{-\frac{d_c^2(x,t)}{2u}} \cdot \min\left\{1, \sqrt{\frac{u}{|x| d_c(x,t)}}\right\}.$$

For the proofs of Theorems 5.1, 5.2 and 5.3, see [**4**] and [**12**]. There exists no explicit heat kernel for a higher step heat operator as yet. For the examples of this paper we are looking for a heat kernel of the form;

$$P(\mathbf{x};u) = \frac{1}{u^2}\int_{\mathbb{R}} e^{-\frac{f}{u}} V\left(-\frac{\partial f}{\partial \tau} d\tau\right) = -\frac{1}{u^2}\int_{f_-}^{f_+} e^{-\frac{f}{u}} V(f) df,$$

where $f = \tau g$ and $f_\pm = \lim_{\tau \to \pm\infty} f$. $\frac{\partial f}{\partial \tau}$ turns out to be a constant of motion, just like $\frac{\partial g}{\partial \tau} = -E$ is; *i.e.,* a constant on the bicharacteristics. Then V is a solution of

$$\tau(T + \Delta_X g)\frac{\partial V}{\partial \tau} - \frac{\partial f}{\partial \tau}\Delta_H V = 0, \tag{5.5}$$

where

$$T = \frac{\partial}{\partial \tau} + (X_1 g)X_1 + (X_2 g)X_2$$

is derivation along the bicharacteristic curve. The equation (5.5) may be put in the following form:

$$\tau\left[(T + \Delta_X g)\frac{\partial V}{\partial \tau} - \frac{\partial g}{\partial \tau}\Delta_X V\right] = g\Delta_X V. \tag{5.6}$$

This should be compared to the equation for the volume element v of (2.2) which is a solution of

$$(T + \Delta_X g)\frac{\partial v}{\partial \tau} - \frac{\partial g}{\partial \tau}\Delta_X v = 0. \tag{5.7}$$

As we mentioned earlier, the above equation may be reduced to an Euler-Poisson-Darboux equation by a clever choice of coordinates. To find a higher step heat kernel we need a solution of equation (5.6). Equation (5.7) suggests that one may try to find such a solution as a perturbation of the volume element of the fundamental solution.

6. Quantification of energy

• **The harmonic oscillator.** Let us start with an simple example. Consider a unit mass particle under the influence of force $F(x) = x$. The Newton's equation is $\ddot{x} = x$. This is the equation which describes the dynamics of an inverse pendulum in an unstable equilibrium, for a small angle x, see Figure 1.

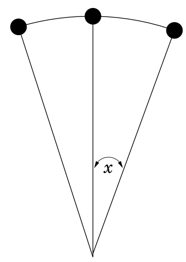

Figure 1: The inverse pendulum problem.

The potential energy is

$$U(x) = -\int_0^x F(u)\, du = -\frac{x^2}{2}.$$

The Lagrangian $L : T\mathbf{R} \to \mathbf{R}$ is the difference between the kinetic and the potential energy

$$L(x, \dot{x}) = K - U = \frac{1}{2}\dot{x}^2 + \frac{1}{2}x^2.$$

The momentum is $p = \frac{\partial L}{\partial \dot{x}} = \dot{x}$ and the Hamiltonian associated with the above Lagrangian is obtained using the Legendre transform: $H : T^*\mathbf{R} \to \mathbf{R}$

$$H(x, p) = p\dot{x} - L(x, \dot{x}) = p^2 - \frac{1}{2}p^2 - \frac{1}{2}x^2 = \frac{1}{2}p^2 - \frac{1}{2}x^2.$$

Adapting some of Xavier and de Aguiar [**27**] ideas, we consider the following complexification

$$x = x_1 + ip_2, \quad p = p_1 + ix_2.$$

Hence $H : T^*\mathbb{C} \to \mathbb{C}$ and

$$\begin{aligned} H(x, p) =& \frac{1}{2}p^2 - \frac{1}{2}x^2 = \frac{1}{2}(p_1 + ix_2)^2 - \frac{1}{2}(x_1 + ip_2)^2 \\ =& \frac{1}{2}(p_1 + ix_2)^2 + \frac{1}{2}(ix_1 - p_2)^2 = \frac{1}{2}(p_1 + ix_2)^2 + \frac{1}{2}(p_2 - ix_1)^2. \end{aligned}$$

Replacing $\theta = -i$, we get

$$H(x, p; \theta) = \frac{1}{2}(p_1 - \theta x_2)^2 + \frac{1}{2}(p_2 + \theta x_1)^2.$$

Quantizing, $p_1 \to \partial_{x_1}$, $p_2 \to \partial_{x_2}$, $\theta \to 2\partial_t$ and hence $H \to \Delta_X$, where

$$\Delta_X = \frac{1}{2}\big(\partial_{x_1} - 2x_2\partial_t\big)^2 + \frac{1}{2}\big(\partial_{x_2} + 2x_1\partial_t\big)^2$$

is the sub-Laplacian on the Heisenberg operator.

In general, the Hamiltonian for a spinless nonrelativistic planar particle in a magnetic field perpendicular to the plane with signed magnitude B is:

$$H = -\frac{\hbar^2}{2m}\Big\{\big(\frac{\partial}{\partial x} - i\frac{e}{\hbar}A_x(x,y)\big)^2 + \big(\frac{\partial}{\partial y} - i\frac{e}{\hbar}A_y(x,y)\big)^2\Big\}. \tag{6.8}$$

Here e is the charge, m is the mass of the particle and $\hbar$ is the Planck's constant (see [**26**]). The vector potential for B is $A = A_x dx + A_y dy$ so that $B = \frac{\partial A_x}{\partial y} - \frac{\partial A_y}{\partial x}$. In other words, $B\, dx \wedge dy = dA$. If the magnetic field is a constant $B = B_0$, then the ground state energy is

$$E_1 = \frac{\hbar^2}{2m}\frac{|e|\|B_0\|}{\hbar}.$$

If B is not a constant, we assume that the magnetic field is bounded away from zero by some constant B_0 then it is known that the particle's ground state energy $E_1(e/\hbar)$ satisfies

$$E_1(e/\hbar) \geq \frac{|e|\|B_0\|}{\hbar}.$$

This tells us that when the magnetic field B is not constant but instead satisfies an estimate $B < B_0$ (or less than $-B_0$ when B is negative) then this energy is a lower bound for the true energy. Montgomery showed [**22**] that the energy satisfies the following estimates

$$E_j(e) \sim \frac{\hbar^2}{m}\Big\{\big(\frac{|e|\|b_0\|}{\hbar}\big)^{2/3}E_* + o(1)\Big\},$$

when the field B vanishes along a curve $\mathcal{C}$ with nonzero constant gradient $\|b_0\| = \|\nabla B\|$. Here E_* is the infimum of the ground state energies $E(a)$ of the anharmonic oscillator family $-\frac{d^2}{dx^2} + (\frac{x^2}{2} - a)^2$. Replacing $\frac{\hbar^2}{m}$ by 1 and setting $-i\frac{e}{\hbar} = \theta$, the Hamiltonian function

$$H(\mathbf{x},\xi) = \frac{1}{2}\Big\{(\xi_1 + 2kx_2|x|^{2k-2}\theta)^2 + (\xi_1 - 2kx_1|x|^{2k-2}\theta)^2\Big\}$$

becomes a special case of the equation (6.8). In this section, we are going to discuss the energy associated to our model by studying subRiemannian geometry.

We shall do this in two parts. First, we consider the geodesic in unit speed parametrization and find the length of geodesics. As the lengths do not depend on the parametrization, we shall consider in the second part a parametrization by interval $[0,1]$. We use the fact that the square of the length is twice the energy. As the lengths are quantized, so the energy will be.

• **The lengths of geodesics.** In this section we shall make use of the arc length parametrization, in which $\dot{x}_1^2 + \dot{x}_2^2 = 1$. The Hamiltonian becomes

$$H = \frac{1}{2}(\dot{x}_1^2 + \dot{x}_2^2) = \frac{1}{2}.$$

Set $x_1 = r\cos\phi$, $x_2 = r\sin\phi$. Then the conservation of energy law becomes

$$\dot{r}^2 + 4k^2\theta^2 r^{2(2k-1)} = 1,$$

which can be written as

$$\frac{dr}{\sqrt{1 - 4k^2\theta^2 r^{2(2k-1)}}} = \pm ds.$$

As the geodesic starts at the origin, $r(0) = 0$. Then we shall consider the positive sign in the right side. Integrating

$$\int_0^{r(s)} \frac{dx}{\sqrt{1 - 4k^2\theta^2 x^{2(2k-1)}}} = s.$$

The substitution $u = x^2$ yields

$$\int_0^{r^2(s)} \frac{du}{\sqrt{u(1 - 4k^2\theta^2 u^{2k-1})}} = 2s.$$

Let $v = u(4k^2\theta^2)^{\frac{1}{2k-1}}$. Then $du = (4k^2\theta^2)^{-\frac{1}{2k-1}}\, dv$ and the above integral equation becomes

$$\int_0^{\sigma(s)} \frac{dv}{\sqrt{v(1 - v^{2k-1})}} = 2(2k\theta)^{\frac{1}{2k-1}} s, \tag{6.9}$$

where $\sigma(s) = (4k^2\theta^2)^{\frac{1}{2k-1}}$ and we considered $\theta > 0$. The above integral can be written in terms of Barnes's extended hypergeometric function

$$\int_0^{\sigma(s)} \frac{dv}{\sqrt{v(1 - v^{2k-1})}} = 2\sqrt{\sigma(s)}\, F\Big(\Big[\frac{1}{2}, \frac{1}{2(2k-1)}\Big], \Big[1 + \frac{1}{2(2k-1)}\Big], \sigma(s)^{2k-1}\Big).$$

Using $2\sqrt{\sigma(s)} = 2\,(2k\theta)^{\frac{1}{2k-1}}\, r(s)$, the equation (6.9) becomes

$$r(s)\, F\Big(\Big[\frac{1}{2}, \frac{1}{2(2k-1)}\Big], \Big[1 + \frac{1}{2(2k-1)}\Big], \sigma(s)^{2k-1}\Big) = s. \tag{6.10}$$

The function

$$z \to F\Big(\Big[\frac{1}{2}, \frac{1}{2(2k-1)}\Big], \Big[1 + \frac{1}{2(2k-1)}\Big], z\Big)$$

is increasing on the interval $[0,1]$, see Figure 2. The minimum and maximum values are

$$F\Big(\Big[\frac{1}{2}, \frac{1}{2(2k-1)}\Big], \Big[1 + \frac{1}{2(2k-1)}\Big], 0\Big) = 1,$$

$$F\Big(\Big[\frac{1}{2}, \frac{1}{2(2k-1)}\Big], \Big[1 + \frac{1}{2(2k-1)}\Big], 1\Big) = \frac{1}{2}\int_0^1 \frac{dv}{\sqrt{v(1-v^{2k-1})}} = M.$$

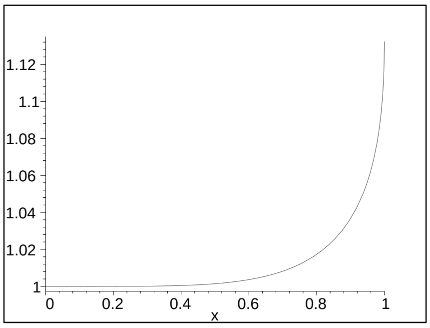

Figure 2. The graph of $z \to F\Big(\Big[\frac{1}{2}, \frac{1}{2(2k-1)}\Big], \Big[1 + \frac{1}{2(2k-1)}\Big], z\Big)$.

Choose $r(s)$ such that the hypergeometric function (6.10) reaches the maximum

$$r(s) = \Big(\frac{1}{2k\theta}\Big)^{\frac{1}{2k-1}}.$$

This has to be the same as r_{max}. Indeed, taking $E = \frac{1}{2}$

$$r_{max} = \Big(\frac{E}{2k^2\theta^2}\Big)^{\frac{1}{2(2k-1)}} = \Big(\frac{1}{2k\theta}\Big)^{\frac{1}{2k-1}}.$$

Denote by s_1 the arc length parameter for which $r_{max} = r(s_1)$. Then (6.10) yields

$$r_{max}\, M = s_1. \tag{6.11}$$

At $r(s_1)$ the trajectory starts to bounce back and at $s = 2s_1$ reaches the t-axis again, *i.e.,* $r(2s_1) = 0$. Hence, the shortest geodesic will have the length

$$\ell_1 = 2s_1 = 2r_{max}\, M. \tag{6.12}$$

If the geodesic winds m times around the t-axis, joining $(0,0,0)$ and $(0,0,t)$, the length is

$$\ell_m = 2ms_1 = 2m\, r_{max}\, M. \tag{6.13}$$

The momentum θ depends on the boundary condition t. This relationship will be found below.

From Hamilton's equation

$$\dot{t} = H_\theta = -2r^{2k}\dot{\phi}.$$

Consider boundary conditions for the argument angle

$$\phi_0 = \phi(0), \qquad \phi_1 = \phi(2ms_1).$$

As we considered $\theta > 0$, the angle ϕ moves clockwise, *i.e.,* decreasing. After one complete loop

$$\phi(2s_1) = -\frac{\pi}{2k-1},$$

and hence after m loops

$$\phi_1 = m\phi(2s_1) = -\frac{m\pi}{2k-1}.$$

Integrating between ϕ_0 and ϕ_1, yields

$$t(\phi_1) - t(\phi_0) = -2\int_{\phi_0}^{\phi_1} r^{2k}(\phi)\,d\phi.$$

Using the boundary conditions for $t(s)$

$$t(\phi_0) = 0, \quad t(\phi_1) = t,$$

and the formula in polar coordinates for the solution, we have

$$t = -2r_{max}^{2k}\int_{\phi_0}^{\phi_1} \sin((2k-1)(\phi-\phi_0))^{\frac{2k}{2k-1}}\,d\phi.$$

Substituting $v = (2k-1)(\phi - \phi_0)$, yields

$$t = \frac{2r_{max}^{2k}}{2k-1}\int_0^{m\pi} \sin(v)^{\frac{2k}{2k-1}}\,dv = \frac{2mr_{max}^{2k}}{2k-1}\int_0^{\pi} \sin(v)^{\frac{2k}{2k-1}}\,dv,$$

and hence

$$r_{max}^{2k} = \frac{(2k-1)t}{mQ}, \tag{6.14}$$

where

$$Q = 2\int_0^{\pi} \sin(v)^{\frac{2k}{2k-1}}\,dv.$$

Substituting (6.14) in (6.13) leads to the following result.

Theorem 6.1. *The lengths ℓ_m of the geodesics joining the origin and the point $(0,0,t)$ on the t-axis satisfy*

$$\ell_m^{2k} = \frac{(2k-1)m^{2k-1}(2M)^{2k}|t|}{Q}, \; m = 1, 2, \ldots \tag{6.15}$$

The Carnot-Carathéodory distance between $(0,0,0)$ and $(0,0,t)$ is ℓ_1, with

$$\ell_1^{2k} = \frac{(2k-1)(2M)^{2k}|t|}{Q}. \tag{6.16}$$

• **Particular cases:** (1) *The step* 2 *case.*

If $k = 1$,

$$\ell_m^2 = \frac{m(2M)^2|t|}{Q},$$

with

$$2M = \int_0^1 \frac{dv}{\sqrt{v(1-v)}} = \arcsin(2v-1)\Big|_0^1 = \pi,$$

then,

$$Q = 2\int_0^\pi \sin^2 v\, dv = \pi.$$

Hence, the lengths in the Heisenberg case are

$$\ell_m^2 = m\pi|t|, \quad m = 1, 2, 3, \dots$$

(2) *The step* 4 *case.*

If $k = 2$, the lengths satisfy

$$\ell_m^4 = \frac{3m^3(2M)^4}{Q}|t|.$$

We shall compute the constants $2M$ and Q.

$$2M = \int_0^1 \frac{dv}{\sqrt{v(1-v^3)}} = \frac{1}{2\sqrt{3}}\mathcal{B}\Big(\frac{1}{6}, \frac{1}{3}\Big) = \frac{1}{2\sqrt{3}} \frac{\Gamma\Big(\frac{1}{6}\Big)\Gamma\Big(\frac{1}{3}\Big)}{\sqrt{\pi}} = \frac{\sqrt{\pi}}{3}\frac{\Gamma\Big(\frac{1}{6}\Big)}{\Gamma\Big(\frac{2}{3}\Big)},$$

where $\mathcal{B}(\alpha, \beta)$ is a Bessel function. Here we used

$$\Gamma\Big(\frac{1}{3}\Big) = \frac{2\pi\sqrt{3}}{3\Gamma\Big(\frac{2}{3}\Big)}.$$

$$Q = 2\int_0^\pi \sin^{4/3} u\, du = 2\int_0^1 \frac{x^{1/6}\, dx}{\sqrt{1-x}} = 2\mathcal{B}\Big(\frac{7}{6}, \frac{1}{2}\Big) = \frac{1}{2}\frac{\Gamma\Big(\frac{1}{6}\Big)}{\Gamma\Big(\frac{2}{3}\Big)}\sqrt{\pi}.$$

Hence

$$\ell_m^4 = 2|t|\left(\frac{m\sqrt{\pi}\,\Gamma\Big(\frac{1}{6}\Big)}{3\Gamma\Big(\frac{2}{3}\Big)}\right)^3, \quad m = 1, 2, 3, \dots$$

• **The energies.** The lengths are the same for all parametrizations. In this section we shall consider geodesics $\gamma : [0,1] \to \mathbf{R}^3$ joining the origin and the point $(0,0,t)$. As the Hamiltonian is preserved along the solutions, the velocity has constant length in the subRiemannian metric (in which X_1 and X_2 are orthonormal), and hence we have identity in Cauchy's inequality

$$\ell(\gamma) = \int_0^1 |\dot\gamma(s)|\,ds = \Big(\int_0^1 ds\Big)^{1/2}\Big(\int_0^1 |\dot\gamma(s)|^2\,ds\Big)^{1/2} = \sqrt{2E}.$$

Hence the energies of a unit mass particle moving along the geodesic are given by

$$E_m = \frac{1}{2}\ell_m^2, \quad m = 1,2,3,\dots$$

Theorem 6.2. *The particle has discrete energies* $0 < E_1 < E_2 < \dots$, *given by*

$$(E_m)^k = \frac{(2k-1)m^{2k-1}(2\,M^2)^k|t|}{Q}, \quad m = 1,2,3\dots$$

For $k = 1$,

$$E_m = \frac{m\pi}{2}|t|,$$

and for $k = 2$,

$$E_m^2 = \frac{|t|}{2}\left(\frac{m\sqrt{\pi}\,\Gamma\Big(\frac{1}{6}\Big)}{3\Gamma\Big(\frac{2}{3}\Big)}\right)^3, \quad m = 1,2,3,\dots$$

E_1 is the ground-state energy, *i.e.,* the lowest energy of the particle. All the other energy levels correspond to excited states. If the electron is in ground-state, then it can be excited up to the level of energy E_m if it receives energy from a photon with energy $\hbar\nu_m = E_m - E_1$, where $\hbar$ is Planck's constant and ν_m is the frequency of the photon.

The difference $E_{m+1} - E_m$ gives the distance between the energy levels. In the step 2 case, the energy levels are equidistant

$$E_2 - E_1 = E_3 - E_2 = \dots = E_{m+1} - E_m = \frac{\pi}{2}|t|.$$

For step $k > 2$, the energy levels become more and more distant as m increases

$$0 < E_2 - E_1 < E_3 - E_2 < \dots < E_{m+1} - E_m < \dots$$

Let $f_k(x) = C_k x^{2-\frac{1}{k}}$, where the constant

$$C_k = 2M\left(\frac{(2k-1)|t|}{Q}\right)^{1/k}.$$

Then

$$E_{m+1} - E_m = f_k(m+1) - f_k(m) = f_k'(\xi_m),$$

with $m < \xi_m < m+1$. Hence, the difference between two consecutive energy levels is estimated as

$$\Big(2 - \frac{1}{k}\Big) C_k m^{1-\frac{1}{k}} < E_{m+1} - E_m < \Big(2 - \frac{1}{k}\Big) C_k (m+1)^{1-\frac{1}{k}}.$$

In particular, when $k = 2$, we have,

$$\frac{3}{2} C_2 \sqrt{m} < E_{m+1} - E_m < \frac{3}{2} C_2 \sqrt{m+1},$$

with

$$C_2 = \sqrt{\frac{|t|}{2}} \left(\frac{\sqrt{\pi}\, \Gamma\Big(\frac{1}{6}\Big)}{3\Gamma\Big(\frac{2}{3}\Big)} \right)^{3/2} \approx 2.676\sqrt{|t|}.$$

Using $3C_2/2 \approx 4.014\sqrt{|t|}$, yields

$$4\sqrt{m|t|} < E_{m+1} - E_m, \quad m = 1, 2, 3, \ldots$$

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