On Carnot-Caratheodory Geometry, PDE-s and the Quartic Oscillator

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I shall start with the construction of geometrically invariant formulas for the fundamental solution and heat kernel of PDE's of the form

$$\Delta = \frac{1}{2}\sum_{j=1}^{m} X_j^2 + \cdots, \tag{1}$$

where $X_1, ..., X_m$ are vector fields on a manifold M_n of dimension n,

a) $m = n \Rightarrow \Delta$ is elliptic, assuming $X_1, \cdots, X_m$ are linearly independent,

b) $m < n$ and the brackets of the X_j's yield all of $TM_n \Rightarrow \Delta$ is subelliptic.

To illustrate the proposed structure, I shall discuss a family of operators for which "explicit" fundamental solutions given in geometric terms are available.

We are in 3 dimensions, $(x_1, x_2, y) = (x, y)$ with 2 vector fields,

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

and the differential operator one wants to invert is

$$\Delta = \frac{1}{2}(X_1^2 + X_2^2). \tag{2}$$

The fundamental solution $F(x, y; x^{(0)}, y^{(0)})$ is the distribution solution of

$$\Delta F = \delta(x - x^{(0)})\delta(y - y^{(0)}). \tag{3}$$

We note that

$$\Delta \int F(x, y; x^{(0)}, y^{(0)}) f(x, y) dx dy = f(x^{(0)}, y^{(0)}), \tag{4}$$

so the fundamental solution is the kernel of the integral operator which inverts, or solves Δ.

We shall look for F in the following form:

$$F = -\int_{\tau} \frac{v dg}{g}, \tag{5}$$

where the function g is a solution of the Hamilton-Jacobi equation

$$\frac{\partial g}{\partial \tau} + \frac{1}{2}(X_1 g)^2 + \frac{1}{2}(X_2 g)^2 = 0\,. \tag{6}$$

$g = g(x, y; x^{(0)}, y^{(0)}; \tau)$ is given by a modified action integral of a complex Hamiltonian problem and the volume element v is the solution of a transport equation. Let

$$H(x,\xi) = \frac{1}{2}(\xi_1 + 2kx_2|x|^{2k-2}\theta)^2 + \frac{1}{2}(\xi_2 - 2kx_1|x|^{2k-2}\theta)^2 \tag{7}$$

denote the Hamiltonian, where ξ and θ are the variables dual to x and y. The complex bicharacteristics are solutions of the Hamiltonian system of differential equations

$$\begin{aligned} &\dot{x}_j = H_{\xi_j}, \quad \dot{\xi}_j = -H_{x_j}, \quad j = 1,2, \\ &\dot{y} = H_\theta, \quad \dot{\theta} = -H_y \end{aligned} \tag{8}$$

with the unusual boundary conditions

$$\begin{aligned} \theta(0) &= -i, \\ x_1(0) &= x_1^{(0)}, x_2(0) = x_2^{(0)}, \\ y(\tau) = y, \quad x_1(\tau) &= x_1, \quad x_2(\tau) = x_2. \end{aligned}$$

Also

$$E = -\frac{\partial g}{\partial \tau} = \frac{1}{2}\dot{x}_1^2 + \frac{1}{2}\dot{x}_2^2, \tag{9}$$

is the energy where the modified action g is given by

$$g = -iy(0) + \int_0^\tau [\xi(s)\cdot\dot{x}(s) + \theta(s)\dot{y}(s) - H(x(s), y(s), \xi(s), \theta(s))]ds. \tag{10}$$

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

$$\Delta(Ev) + \frac{\partial}{\partial\tau}[Tv + (\Delta g)v] = 0, \tag{11}$$

where

$$T = \frac{\partial}{\partial\tau} + \sum_{j=1}^{2}(X_j g)X_j \tag{12}$$

is differentiation along the bicharacteristic. Now

$$F = \int_{\mathbb{R}} \frac{Ev\,d\tau}{g}$$

has a simple geometric interpretation. The operator Δ has a characteristic variety in T^*M_n given by $H = 0$. Over every point $x \in M_n$, this is a line, parametrized by $\theta \in (-\infty, \infty)$,

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

Consequently F may be thought of as the $(\text{action})^{-1}$ summed over the characteristic variety with measure Ev. I note that, when Δ is elliptic, its characteristic variety is the zero section, so we do get simply 1/distance, as expected; when

$$\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}$$

one has the Newton potential

$$F = (x, x^{(0)}) = \frac{-1/|S_2|}{|x - x^{(0)}|}.$$

$f = \tau g$ behaves like the square of a distance function even though it is complex; I recall that action $=(\text{distance})^2$.

k = 1: The Heisenberg group

Here

$$X_1 = \frac{\partial}{\partial x_1} + 2x_2\frac{\partial}{\partial y}, \quad X_2 = \frac{\partial}{\partial x_2} - 2x_1\frac{\partial}{\partial y},$$

referred to as the "horizontal vector fields", are left-invariant with respect to the Heisenberg translation

(13) $$(x, y) \circ (x', y') = (x + x', y + y' + 2[x_2x_1' - x_1x_2']).$$

Therefore

(14) $$F(x, y; x^{(0)}, y^{(0)}) = F((-x^{(0)}, -y^{(0)}) \circ (x, y); 0, 0).$$

and

$$F(x, y; 0, 0) = \int_{\mathbb{R}} \frac{Evd\tau}{g},$$

where

$$g = |x|^2 \coth(2\tau) - iy,$$
$$E = -\frac{\partial g}{\partial \tau} = \frac{2|x|^2}{\sinh^2(2\tau)},$$
$$v = -\frac{1}{4\pi^2}\frac{\sinh(2\tau)}{|x|^2}.$$

We also have the heat kernel:

(15) $$P = ker(e^{t\Delta}) = \frac{1}{(2\pi t)^2}\int_{\mathbb{R}} e^{-\frac{f}{t}} V d\tau,$$
$$V = Ev, \quad f = \tau g.$$

In particular, one has

(16) $$\frac{\partial P}{\partial t} - \Delta P = \delta(t)\delta(x).$$

$f = \tau g$ has geometric significance.

Heisenberg Geometry

On the Heisenberg group, every neighbourhood of the origin contains points which are connected to the origin by a finite number of geodesics, more than one, and also points which are connected to the origin by an infinite number of geodesics. This is true for all Carnot-Caratheodory geometries.

1 Theorem. *On H_1, there are a finite number of geodesics connecting (x, y) to $(0,0)$ if and only if $x \neq 0$. Among their lengths, $d_j(x,y), j = 1, 2, \cdots$ the shortest is the so-called "classical action" and we shall denote it by $d_c(x,y)$. Every point of the line $(0,y)$ is connected to the origin by an infinite number of geodesics.*

A geodesic is the projection of a bicharacteristic, i.e. solution of the Hamiltonian system of differential equations (8) with end conditions

$$x(0) = 0, \quad y(0) = 0, \quad x(\tau) = x, \quad y(\tau) = y, \tag{17}$$

onto the base manifold. We set

$$f = \tau g. \tag{18}$$

f is a "complex distance".

2 Theorem. *Let $\tau_j(x,y), j=1,2,\cdots$ denote the critical points of $f(x,y,\tau)$ with respect to τ, i.e.*

$$f_\tau(x,y,\tau_j(x,y)) = 0. \tag{19}$$

Then

$$f(x,y,\tau_j(x,y)) = \frac{1}{2}d_j(x,y)^2, \quad j=1,2,\cdots \tag{20}$$

This remarkable result has important consequences. Recall the heat kernel

$$P = \frac{1}{(2\pi t)^2}\int_{\mathbb{R}} e^{-f/t} V d\tau.$$

One may obtain the small time asymptotic of P by the stationary phase method which picks out the first critical point $\tau_1(x,y)$ of f. Then (20) yields $f_\tau(x,y,\tau_1(x,y)) = \frac{1}{2}d_c(x,y)^2$.

3 Theorem. *(i) Given a fixed point (x,y) with $x \neq 0$, one has*

$$P(x,y;t) = \frac{1}{(2\pi t)^2} e^{-\frac{d_c(x,y)^2}{2t}}[\Theta(x,y)\sqrt{2\pi t} + O(t)], \tag{21}$$

as $t \to 0^+$, where

$$\Theta(x,y) = \left(\frac{1}{f''(\tau_1)}\right)^{1/2} V(\tau_1),$$

$f''(\tau) = \partial^2 f/\partial\tau^2$.

(ii) At points $(0,y), y \neq 0$, one has

$$P(0,y;t) = \frac{1}{4\pi t^2} e^{-\frac{d_c(0,y)^2}{2t}}\left[1 + O\left(e^{-\frac{d_c(0,y)^2}{2t}}\right)\right], \tag{22}$$

as $t \to 0^+$.

Length and distance

Given a curve

(23) $$x(s) = (x_1(s), \cdots, x_n(s)), \qquad 0 \leqq s \leqq t$$

in $\mathbb{R}^n$, its length is

$$l = \int_0^t \sqrt{\dot{x}_1(s)^2 + \cdots + \dot{x}_n(s)^2} ds.$$

Here

$$\dot{x}(s) = \sum_{j=1}^{n} \dot{x}_j(s) \frac{\partial}{\partial x_j}$$

is the tangent vector to the curve $x(s)$. More generally, given horizontal vectorfields $X = (X_1, \cdots, X_m)$ on M_n, $m \leqq n$, we introduce a metric by calling X an orthonormal set. Given a curve $x(s)$, $0 \leqq s \leqq t$, we write

(24) $$\dot{x}(s) = \sum_{j=1}^{m} \gamma_j(s) X_j(s),$$

and then

(25) $$l = \int_0^t \sqrt{\gamma_1(s)^2 + \cdots + \gamma_m(s)^2} ds$$

is its length. The distance of 2 points A and B is the minimum of the lengths of all connecting curves. Here a problem arises. Consider the horizontal vectorfields $\partial/\partial x$ and $\partial/\partial y$ in $\mathbb{R}^3 = \{(x, y, z)\}$. Then 2 points with different z-components do not have a horizontal connection, that is a curve all of whose tangents are linear combination of $\partial/\partial x$ and $\partial/\partial y$; in particular, we cannot assign a distance to two such points.

4 Theorem. *(W. L. Chow, 1939) Given vectorfields $X_1, \cdots, X_m$, let*

(26) $$X_1, \cdots, X_m, \ [X_i, X_j], \ [[X_i, X_j], X_k], \cdots$$

generate the tangent space after a finite number of steps. Then 2 points always have a horizontal connection.

In particular we can assign a distance to 2 arbitrary points and this yields a Carnot-Caratheodory geometry. (26) is often referred to as Hörmander's bracket generating condition (1967).

Missing directions

What is the analogue of the Heisenberg y-axis, the center of the group, or the missing direction, for general Carnot geometries ? We start with an example.

Let

$$X = \frac{\partial}{\partial x} + y^2 \frac{\partial}{\partial t}, \qquad Y = \frac{\partial}{\partial y} \tag{27}$$

denote two vector fields in $\mathbb{R}^3$.

" How many geodesics induced by X *and* Y *join two given points* (x_0, y_0, t_0) *and* (x, y, t) *?"*

5 Theorem. $y_0 > 0$. *Every point* $P(x, y, t)$, $y > 0$, *can be joined to* $P(0, y_0, 0)$ *by at least one local geodesic. The number of these local geodesics is finite if and only if*

(*i*) $y \neq y_0$, or

(*ii*) $y = y_0$ and $t + y_0^2 x \neq 0$.

6 Theorem. $y_0 > 0$. *When* $y = y_0$ *and* $t + y_0^2 x = 0$, *then* $P(x, y_0, t)$ *is joined to* $P(0, y_0, 0)$ *by a discrete infinity of local geodesics.*

7 Theorem. $y_0 = 0$. *Every point* $P(x, y, t)$ *is connected to the origin by at least one geodesic. The number of geodesics joining* $P(x, y, t)$ *to the origin is finite if and only if* $y \neq 0$. *When* $y = 0$, *every point of the "canonical submanfold"* $\{(x, 0, 0), x \neq 0\}$ *is joined to the origin by a continuous infinity of geodesics, while every point of the complement* $\{(x, 0, t), t \neq 0\}$ *is joined to the origin by a discrete infinity of geodesics.*

When $y \neq 0$, $[Y, X] = YX - XY = 2y\partial/\partial t$ yields $T\mathbb{R}^3$. When $y = 0$ we also need $[Y, [Y, X]] = 2\partial/\partial t$ for $T\mathbb{R}^3$. So $\mathbb{R}^3$ breaks up naturally into the domains $y > 0$, $y < 0$ and their boundary $y = 0$. A geodesic connecting 2 points in $y > 0$ is local if it stays in $y > 0$, otherwise it is nonlocal. The line $y = y_0$, $t + y_0^2 x = 0$ is called the canonical curve and its tangent space may replace the missing direction not covered by the horizontal vectorfields X and Y. Note that the canonical curve goes into the x-axis as $y_0 \to 0$.

The following statement may be correct under rather general circumstances.

"Given m *vectorfields on* M_n *whose brackets generate* TM_n, *for every point* $P_0 \in M_n$ *there is an* $n - m$ *dimensional submanifold* $S_0, P_0 \in S_0$, *characterized by having all its points connected to* P_0 *by an infinite number of geodesics".*

The quartic oscillator

The name "quartic oscillator" refers to the following differential operator:

$$-\frac{d^2}{dx^2} + x^4; \tag{28}$$

recall that the harmonic oscillator is

$$-\frac{d^2}{dx^2} + x^2. \tag{29}$$

They are special instances of a class of operators of the form

$$-\frac{d^2}{dx^2} + a_1 x^2 + a_2 x^4 + \cdots + a_k x^{2k}. \tag{30}$$

A great deal is known about the harmonic oscillator, almost nothing about operators of the form (30), in particular about the quartic oscillator; one has asymptotic information about (28) but until lately no inverse formulas of any kind. (30) is not a hypergeometric equation, it is called Heun's equation.

In 1983 Voros wrote a famous 300 page paper with the title: "The quartic oscillator". He claimed some very interesting results but the arguments were unconvincing. Pham and his coworkers in Nice tried to elucidate Voros' results but did not get beyond the harmonic oscillator. Voros based his work on articles written by the physicists Balian and Bloch in the 1960-s, who extended heat kernels to complex phase functions. Also in 1972-73 Colin de Verdiere used ideas from these physics papers to obtain results on closed geodesics for elliptic operators. I should also mention that Kawai and coworkers at RIMS in Kyoto have been working on Voros' ideas on the quartic oscillator; mainly trying to understand the asymptotics via Borel summation, Ecalle's resurgence, WKB method (Wentzel-Kramers-Brillouin), Airy functions, Kelvin lines, etc.

The mathematical description of the quantum mechanical problem of the double well potential leads to the differential operator

$$-\frac{d^2}{dx^2} + (x^2 - a^2)^2. \tag{31}$$

Inverting (28) and (31) are equivalent problems. Recall the sub-elliptic Laplacian for the vectorfields (27):

$$\Delta = \frac{1}{2}\left(\frac{\partial}{\partial x} - y^2\frac{\partial}{\partial t}\right)^2 + \frac{1}{2}\left(\frac{\partial}{\partial y}\right)^2; \tag{32}$$

the change of sign in the first vectorfield is irrelevant. Taking the Fourier transform of (32) in the x and t variables we obtain

$$-\frac{d^2}{dy^2}+(\xi^2-y^2\tau^2)^2 \tag{33}$$

which agrees with (31). To use these ideas on the quartic oscillator we regularize (28):

$$-\frac{d^2}{\partial x^2}+x^4\eta^2, \tag{34}$$

and this is the Fourier transform in y of the subelliptic operator

$$\Delta=\left(\frac{\partial}{\partial x}\right)^2+\left(x^2\frac{\partial}{\partial y}\right)^2; \tag{35}$$

subelliptic because at $x=0$ we only have 1 vectorfield $\partial/\partial x$ in $\mathbb{R}^2$. To invert (35) we introduce

$$R=\frac{1}{2}(x^6+(x')^6+9|y-y'|^2),$$
$$\rho=\frac{|xx'|^3}{R},$$
$$v=\operatorname{sgn}(xx')=\frac{xx'}{|xx'|}.$$

8 Theorem. *(35) has the fundamental solution $F(x,y-y';x')$, where*

$$F=-\frac{1}{8\sqrt{\pi}}\frac{G}{R^{1/3}} \tag{36}$$

with

$$G=\frac{1}{\Gamma(1/4)}\int_0^1\int_0^1\frac{K(v,\sqrt{u_1u_2}\rho)du_1du_2}{u_1^{5/6}u_2^{1/3}(1-u_1)^{3/4}(1-u_2)^{3/4}},$$
$$K(v,z)=\frac{\varphi_-(z^2)}{\sqrt{\varphi_+(z^2)-2z^{1/3}v}},$$
$$\varphi_+(z^2)=(1+\sqrt{1-z^2})^{1/3}+(1-\sqrt{1-z^2})^{1/3}$$
$$\varphi_-(z^2)=\frac{(1+\sqrt{1-z^2})^{1/3}-(1-\sqrt{1-z^2})^{1/3}}{\sqrt{1-z^2}}.$$

9 Corollary. *The inverse kernel of the quartic oscillator (28) is*

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-iy} F(x, y; x')\,dy, \tag{37}$$

where F is given by (36).

The higher step case, k > 1

No group structure, and the complex bicharacteristics run between 2 arbitrary points $(x^{(0)}, y^{(0)})$ and (x, y). We obtain 2 invariants of the motion, the energy E and the angular momentum Ω, and g and v may be found in terms of E and Ω. In particular

$$g = -i(y - y^{(0)}) + \left(1 - \frac{1}{k}\right)E\tau + \frac{1}{2k}\operatorname{sgn}\tau\left[(2E|x|^2 + W(|x|^2)^2)^{1/2} - (2E|x^{(0)}|^2 + W(|x^{(0)}|^2)^2)^{1/2}\right],$$

where one uses the principal branch of the square roots, and

(38) $$W(u) = 2ku^k - \Omega, \qquad \Omega = \Omega(x, y; x^{(0)}, y^{(0)}; \tau).$$

10 Theorem. $k > 1$. *The fundamental solution* $F(x, y; x^{(0)}, y^{(0)})$ *of* Δ *has the following invariant representation:*

(39) $$F = \int_{\mathbb{R}} \frac{Ev\,d\tau}{g},$$

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

(40) $$v = \frac{-i}{4k\pi^3}(A_+ - g)^{-\frac{1}{2}}(A_+ + g)^{-\frac{1}{2}}L(q_+, q_-),$$

(41) $$A_\pm = \frac{1}{k}\Omega_\pm + g_\pm, \qquad \Omega_\pm = \lim_{\tau\to\pm\infty}\Omega, \qquad g_\pm = \lim_{\tau\to\pm\infty} g,$$

(42) $$q_\pm = \frac{2^{1/k}(x_1 \pm ix_2)(x_1^{(0)} \mp ix_2^{(0)})}{(A_\pm \mp g)^{1/k}},$$

and $L(q_+, q_-)$ *is a hypergeometric function of 2 variables,*

(43) $$L(q_+, q_-) = \frac{1}{\pi}\int_0^1\int_0^1 \frac{ds_+ ds_-}{s_+ s_-}\left(\frac{s_+}{1 - s_+}\right)^{\frac{1}{2}}\left(\frac{s_-}{1 - s_-}\right)^{\frac{1}{2}} \frac{1 - q_+q_-(s_+s_-)^{1/k}}{(1 - q_+s_+^{1/k})(1 - q_-s_-^{1/k})(1 - (q_+q_-)^k s_+s_-)}$$

Heat kernels

There exist no explicit heat kernel for a higher step operator as yet. For the examples of this lecture we are looking for a heat kernel in the form

$$P = \frac{1}{t^2}\int_{\mathbb{R}} e^{-\frac{f}{t}} W(-f_\tau d\tau) = -\frac{1}{t^2}\int_{f_-}^{f_+} e^{-\frac{f}{t}} W(f)\,df, \qquad f_\pm = \lim_{\tau\to\pm\infty} f, \tag{44}$$

where $f = \tau g$. f_τ turns out to be a constant of motion, just like $g_\tau = -E$ is; i.e. a constant along the bicharacteristics. Then W is a solution of

$$\tau(T + \Delta g)\frac{\partial W}{\partial \tau} - f_\tau \Delta W = 0, \tag{45}$$

where

$$T = \frac{\partial}{\partial \tau} + Xg\cdot X \tag{46}$$

is derivation along the bicharacteristic curve. (45) may be put in the following form:

$$\tau\left[(T + \Delta g)\frac{\partial W}{\partial \tau} - g_\tau \Delta W\right] = g\Delta W, \qquad f = \tau g. \tag{47}$$

This should be compared to the equation for the volume element v of (40) given by

$$(T + \Delta g)\frac{\partial v}{\partial \tau} - g_\tau \Delta v = 0. \tag{48}$$

We note that (48) may be reduced to an Euler-Poisson-Darboux equation by a clever choice of coordinates. Thus to find a higher step heat kernel we need a solution to (47). (48) suggests that one may try to find such a solution as a perturbation of the volume element of the fundamental solution.

Remark. Although I worked with examples only, all our formulas and differential equations are invariant and apply to general sub-elliptic operators.

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