HEAT KERNEL ASYMPTOTIC EXPANSIONS FOR THE HEISENBERG SUBLAPLACIAN AND THE GRUSHIN OPERATOR

DER-CHEN CHANG AND YUTIAN LI

Abstract. The subLaplacian on the Heisenberg group and the Grushin operator are typical examples of subelliptic operators. Their heat kernels are both given in the form of Laplace type integrals. By using Laplace's method, the method of stationary phase and the method of steepest descent, we derive the small-time asymptotic expansions for these heat kernels, which are related to the geodesic structure of the induced geometries.
Key words: heat kernel, Heisenberg group, Grushin operator, small-time asymptotics, saddle point method, geodesic, conjugate point
MS Classification (2010): Primary: 35K08; Secondary: 53B21

1. Introduction

1.1. **Heat kernel asymptotics for the Laplace-Beltrami operator.** It is well-known that much geometric information about a Riemannian manifold can be decoded from the small-time asymptotic expansions of the heat kernel (*i.e.*, fundamental solution of the heat operator) of the associated Laplace-Beltrami operator. Let (M, g) be a Riemannian manifold of n-dimension, $\rho(q_0, q)$ be the distance between two points $q_0, q \in M$, and Δ be the Laplace-Beltrami operator, and $p(t, x, y)$ be the heat kernel of Δ. The celebrated result of Varadhan [31, 32] reads

$$\lim_{t\to 0^+} t \log\big(p(t, q_0, q)\big) = -\frac{1}{2}\rho^2(q_0, q). \tag{1.1}$$

More precise small-time asymptotic approximations for $p(t, q_0, q)$ were investigated by many authors. As $t \to 0^+$, $p(t, q_0, q)$ has the following expansion

$$p(t, q_0, q) \sim \frac{1}{(2\pi t)^{n/2}} e^{-\frac{1}{2t}\rho^2(q_0,q)} \left\{a_0(q_0, q) + a_1(q_0, q)t^{1/2} + a_2(q_0, q)t + \cdots\right\}, \tag{1.2}$$

for q_0 and q are near points such that they are joined by a finite number of shortest geodesic along which they are not conjugate. The half-integer power terms vanish for manifold without boundary. If q_0 and q are conjugate to each other along the shortest geodesic, the asymptotic behavior of $p(t, q_0, q)$ will be different, namely, the leading power of t in the expansion changes from $t^{-n/2}$ to $t^{-(n+k)/2}$ for some positive number k. The number k appearing in the power is different for different situations. The details can be found in Molchanov's survey paper [26].

In the case when M is compact, consider the heat kernel trace,

$$\operatorname{trace}(p) = \int_M p(t, q, q)dV(q) = \sum_{j=1}^{\infty} e^{-t\lambda_j}, \tag{1.3}$$

where $0 < \lambda_1 \le \lambda_2 \le \cdots$ are the eigenvalues of the Laplace-Beltrami operator with vanishing Dirichlet condition if M has a nonempty boundary. M. Kac's famous question "can one hear the shape of a drum" [20] concerns the extraction of geometric information of M from the asymptotic expansion of the heat kernel trace. McKean-Singer [24] showed that

$$\sum_{j=1}^{\infty} e^{-t\lambda_j} \sim \frac{C_0}{t^{n/2}} + \frac{C_1}{t^{(n-1)/2}} + \frac{C_2}{t^{(n-2)/2}} + \cdots, \qquad t \to 0^+, \tag{1.4}$$

where C_0, C_1 and C_2 are all global geometric quantities given by

$$C_0 = \frac{\mathrm{vol}(M)}{(2\pi)^{n/2}}, \quad C_1 = \frac{A(\partial M)}{4(2\pi)^{(n-1)/2}}, \quad C_2 = \frac{\int_M R(x)dx}{6(2\pi)^{(n-2)/2}}, \tag{1.5}$$

with $\mathrm{vol}(M)$, $A(\partial M)$ and $R(x)$ being the volume of M, the volume of boundary of M, and the scalar curvature, respectively. By the Hardy-Littlewood tauberian theorem, the leading term in the expansion (1.4) yields the classical Weyl's asymptotic formula [35] for large eigenvalues

$$\lambda_n \sim \left(\frac{n}{\mathrm{vol}(M)}\right)^{2/n}, \qquad n \to \infty. \tag{1.6}$$

1.2. **Heat kernel asymptotics for subelliptic operators.** On an n-dimensional Riemannian manifold M, one needs n independent smooth vector fields $\{X_1, X_2, \cdots, X_n\}$ to introduce a metric g given by the $n \times n$ positive definite matrix $(g(X_i, X_j))_{n\times n} = (g_{ij})_{n\times n}$, and the Laplace-Beltrami operator is given by

$$\Delta = \frac{1}{2}(\det g)^{1/2} \sum_{i,j=1}^{n} \frac{\partial}{\partial x^i}\left(g^{ij} g^{-1/2} \frac{\partial}{\partial x^j}\right), \tag{1.7}$$

which is an elliptic operator. Here, (g^{ij}) is the inverse matrix of (g_{ij}). When one or several vector fields are missing, say, given $\{X_j\}_{j=1}^k$ with $k < n$, the possible generalizations of the elliptic operators, Riemannian geometries and their relations are of particular interest.

Hörmander [18] studied a class of operators called "sum of squares of vector fields" of the form

$$L = \frac{1}{2}\sum_{j=1}^{k} X_j^2, \qquad \text{with} \quad X_j = \sum_{i=1}^{n} a_{ij}(x)\frac{\partial}{\partial x^i}, \tag{1.8}$$

where $a_i(x)$'s are smooth functions on M. Hörmander showed that L is subelliptic (and hence hypoelliptic) if these vector fields satisfy the bracket-generating condition. The hypoellipticity means that $Lu = f$ has a smooth solution provided that f is smooth.

On the other hand, given a bracket generating vector fields $\{X_j\}_{j=1}^k$ with $k < n$, we can introduce a subRiemannian metric on M. The definition of the bracket generating condition and a brief description of the subRiemannian space $(M, \mathcal{D}, g)$ are provided in Appendix A.

It seems that subelliptic operators and subRiemannian geometries are natural generalizations of elliptic operators and Riemannian geometries. Now we return to our question, could one obtain geometric information of $(M, \mathcal{D}, g)$ from the small-time asymptotics of the heat kernel of L?

Leandre [21, 22] proved a result for the subelliptic heat kernels

$$\lim_{t\to 0^+} t \log\big(p(t, q_0, q)\big) = -\frac{1}{2}d^2(q_0, q). \tag{1.9}$$

Here, $d(q_0, q)$ denotes the subRiemannian distance between q_0 and q. This result could be regarded as a generalization of Varadhan's (1.1) to subelliptic operators. A refined asymptotic formula was then given by Ben Arous [4], who showed that

$$p(t, q_0, q) \sim \frac{1}{t^{n/2}} e^{-\frac{d^2(q_0,q)}{2t}} \left[a_0(q_0, q) + O(t^{1/2})\right], \qquad t \to 0^+. \tag{1.10}$$

for $q_0 \neq q$ and q is not on the cut-locus of q_0. This is an analogue to the elliptic case given in (1.2). The above results suggest that subelliptic heat kernels have the similar small-time behavior as elliptic ones. However, the subelliptic operators also show some new phenomena. On the diagonal, *i.e.* when $q_0 = q$, Ben Arous and Leandre [5, 6] proved

$$p(t, q, q) \sim \frac{C}{t^{Q/2}} + O(t^{(1-Q)/2}), \qquad t \to 0^+. \tag{1.11}$$

The asymptotic behavior of $p(t, q_0, q)$ is not known for $q \neq q_0$ and q is a cut point of q_0. The recent breakthrough is given by Barilari, Boscain and Neel [2], who showed that

$$p(t, q_0, q) \sim \frac{1}{(2\pi t)^{(n+k)/2}} e^{-\frac{1}{2t} d^2(q_0,q)} \left\{a_0(q_0, q) + o(1)\right\}, \qquad t \to 0^+, \tag{1.12}$$

if $q \neq q_0$ and q is a cut point as well as a conjugate point of q_0 along some shortest geodesic. Here, k is a positive number that reflects 'how conjugate' the two points are, in particular, when there is a k-parameter family of shortest geodesics. This result can be regarded as an extension of Molchanov's result [26] on elliptic operators to subelliptic operators. The investigations on the heat kernel asymptotics for some subelliptic heat kernels are also carried out in detail by Brockett and Mansouri [7] and Séguin and A. Mansouri [30].

Note that only the first term is derived in the above results on small-time asymptotic behavior of the subelliptic heat kernel. The results for the elliptic operator in (1.2) and (1.4)-(1.5) suggest the higher-order terms in the heat kernel asymptotic expansion will give interesting geometric quantities of the associated subRiemannian geometry. In the present paper, we shall use two examples as an illustration of how to derive the higher order terms in the heat kernel asymptotic expansions.

1.3. **Heat kernels for the Heisenberg subLaplacian and the Grushin operator.** Two typical and simple examples of subelliptic operators are the subLaplacian on Heisenberg group and the Grushin operator.

The m-th **Heisenberg group** is a nilpotent Lie group of step two on the manifold

$$\mathbb{H}^m \cong \mathbb{C}^m \times \mathbb{R} = \{(z, y) = (z_1, z_2, \cdots, z_m, y) : \; z \in \mathbb{C}^m, y \in \mathbb{R}\}, \tag{1.13}$$

with the group law

$$(z, y) \circ (w, s) = \Big(z + w, y + s + 2\,\mathrm{Im} \sum_{j=1}^{m} a_j z_j \overline{w_j}\Big), \tag{1.14}$$

where a_j's are positive parameters. For the sake of simplicity, we restrict ourselves on $\mathbb{H}^1 = \{(x_1 + ix_2, y)\}$, and assume $a_1 = 1/2$ without loss of generality. The vector fields

$$X_1 = \frac{\partial}{\partial x_1} + x_2 \frac{\partial}{\partial y}, \qquad X_2 = \frac{\partial}{\partial x_2} - x_1 \frac{\partial}{\partial y}, \tag{1.15}$$

are left-invariant under the group law and bracket-generating, that is $[X_1, X_2] = 2\frac{\partial}{\partial y}$ recovers the missing direction. Therefore, the subLaplacian

$$\Delta_H = \frac{1}{2}(X_1^2 + X_2^2), \tag{1.16}$$

is subelliptic by Hörmander's theorem. The heat kernel of Δ_H is well studied in literatures (see [15, 19, 3]). Thanks to the group structure, we can fix q_0 to be the origin and let the other point $q(x_1, x_2, y)$ vary, and the heat kernel $p_t(x_1, x_2, y)$ is given as a Laplace integral

$$p_t(x_1, x_2, y) = \frac{1}{(2\pi t)^2} \int_{-\infty}^{\infty} e^{-f(\tau)/t} V(\tau)\, d\tau, \tag{1.17}$$

where the phase function (also known as the modified complex action function) is

$$f(\tau) = -i\tau y + \frac{1}{2}\|x\|^2 \tau \coth \tau, \qquad \text{with} \quad \|x\|^2 = x_1^2 + x_2^2\,, \tag{1.18}$$

and the amplitude function (also known as the volume element) is

$$V(\tau) = \frac{\tau}{\sinh \tau}. \tag{1.19}$$

It is shown in [3] that the critical points of $f(\tau)$ and the geodesics joining $q(x_1, x_2, y)$ and the origin are one-one correspondence, and each of the critical value of $f(\tau)$ is equal to half of square of the length of corresponding geodesic.

The second example of subelliptic operators is introduced by Grushin [17]. Consider the following vector fields on $\mathbb{R}^{m+1} = \{(x_1, x_2, \cdots, x_m, y)\}$

$$X_j = \frac{\partial}{\partial x_j}, \qquad Y_j = x_j \frac{\partial}{\partial y}, \qquad 1 \le j \le m. \tag{1.20}$$

These vector fields give all $(m+1)$ directions on $\mathbb{R}^{m+1}$ except on y-axis, where their bracket $[X_j, Y_j] = \frac{\partial}{\partial y}$ gives the missing direction. The **Grushin operator**

$$\Delta_G = \frac{1}{2}\sum_{j=1}^{m}(X_j^2 + Y_j^2) = \frac{1}{2}\sum_{j=1}^{m}\frac{\partial^2}{\partial x_j^2} + \frac{1}{2}(x_1^2 + x_2^2 + \cdots + x_m^2)\frac{\partial^2}{\partial y^2} \tag{1.21}$$

is therefore subelliptic by Hörmander's theorem. When $m = 1$, Δ_G is the classical Grushin operator and its heat kernel is constructed in [11], the general case of $m \ge 1$ is studied in [10]. The heat kernel of Δ_G has the following form

$$p_t(q_0, q) = \frac{1}{(2\pi t)^{(m+2)/2}} \int_{-\infty}^{\infty} e^{-g(\tau)/t} W(\tau)\, d\tau, \tag{1.22}$$

where $q_0(x_0, y_0)$ and $q(x, y)$ are two points in $\mathbb{R}^{m+1}$, the phase function (the modified complex action function) is

$$g(\tau) = -i(y - y_0) + \frac{\tau}{2\sinh\tau}\left[(\|x\|^2 + \|x_0\|^2)\cosh\tau - 2\langle x, x_0\rangle\right] \tag{1.23}$$

and the amplitude function (the volume element) is

$$W(\tau) = \left(\frac{\tau}{\sinh\tau}\right)^{\frac{m}{2}}. \tag{1.24}$$

Note that the heat kernels (1.17) and (1.22) are both Laplace type integrals. To derive their small-time asymptotic expansions, we can use the techniques of integrals such as Laplace's method, the method of stationary phase and the method of steepest descent.

The aim of the present paper is to use these techniques to establish the asymptotic expansions for the heat kernels (1.17) and (1.22), and to compute the first few coefficients. This will shed some light on the connection between the heat kernel asymptotics of the subelliptic heat kernel and the subRiemannian geometry.

The remaining part of this paper is organized as follows.

2. Asymptotics for the heat kernel of the Heisenberg subLaplacian

For the heat kernel (1.17) of the Heisenberg group, we have the following result.

Theorem 1. *The heat kernel $p_t(x_1, x_2, y)$ of the Heisenberg group given in (1.17) has the following asymptotic expansions as $t \to 0^+$:*

(I) when $(x, y) = (\mathbf{0}, 0)$,

$$p_t(0,0,0) = \frac{1}{8t^2}; \tag{2.25}$$

(II) when $(x, y) = (\mathbf{0}, y)$ with $y \neq 0$,

$$p_t(0,0,y) \sim \frac{1}{2t^2} \sum_{k=1}^{\infty} e^{-\frac{k\pi y}{t}} (-1)^{k+1} k; \tag{2.26}$$

(III) when $x \neq \mathbf{0}$,

$$p_t(x_1,x_2,y) \sim \frac{1}{2\pi^2 t^{3/2}} e^{-\frac{d^2(x_1,x_2,y)}{2t}} \sum_{n=0}^{\infty} \Gamma\left(n + \frac{1}{2}\right) D_n t^n, \tag{2.27}$$

where $d(x_1, x_2, y)$ is the subRiemannian distance between the origin and the point (x_1, x_2, y), and the coefficients $D_n = \Gamma(n + \frac{1}{2}) C_{2n}$ with C_n given in (2.35) for $y = 0$ and in (2.51) – (2.52) for $y \neq 0$.

2.1. Case I: diagonal, i.e., $x_1 = x_2 = y = 0$.

In this case, $f(\tau) = 0$ and the integral in (1.17) reduces to

$$p_t(0,0,0) = \frac{1}{(2\pi t)^2} \int_{-\infty}^{\infty} \frac{\tau}{\sinh \tau} d\tau = \frac{1}{8t^2}. \tag{2.28}$$

2.2. Case II: $x = (x_1, x_2) = (0, 0)$ with $y \neq 0$.

Without loss of generality, we assume $y > 0$. Now the heat kernel is simply given as

$$p_t(0,0,y) = \frac{1}{(2\pi t)^2} \int_{-\infty}^{\infty} e^{i\tau y/t} \frac{\tau}{\sinh \tau} d\tau, \tag{2.29}$$

which can be evaluated via the residue calculation. Note that each $ik\pi$, $k = 1, 2, \ldots$, is a simple pole of $V(\tau)$ with the residue being $e^{-\frac{k\pi y}{t}} (-1)^k ik\pi$. Then, we have

$$p_t(0,0,y) = \frac{1}{(2\pi t)^2} \sum_{k=1}^{\infty} e^{-\frac{k\pi y}{t}} (-1)^{k+1} 2k\pi^2. \tag{2.30}$$

Note that $k\pi y = \ell_k^2/2$ with ℓ_k denoting the length of the k-th geodesic joining $(0, 0, y)$ and the origin so that ℓ_1 gives the subRiemannian distance between these two points. Therefore, the leading term asymptotic approximation reads

$$p_t(0,0,y) \sim \frac{1}{(2\pi t)^2} e^{-\frac{d^2(0,0,y)}{2t}} + \text{exponentially small terms}, \qquad t \to 0^+.$$

Here, $d(0, 0, y)$ stands for the subRiemannian distance between $(0, 0, y)$ and the origin.

2.3. **Case III-1:** $y = 0$**.** Now, the heat kernel (1.17) takes the form

$$p_t(x_1, x_2, y) = \frac{1}{(2\pi t)^2} \int_{-\infty}^{\infty} e^{-\frac{\tau \coth(\tau)\|x\|^2}{2t}} \frac{\tau}{\sinh \tau} d\tau. \tag{2.31}$$

Since the exponent $f(\tau)$ is real, the asymptotic expansion of the last integral as $t \to 0^+$ can be derived by Laplace's method. For a description of this method; see [34].

We recall some properties of the phase function (the modified complex function)

$$f(\tau) = \frac{1}{2}\|x\|^2 \tau \coth(\tau).$$

The function $f(\tau)$ is real positive and has only one minimum point at $\tau = 0$. That is $f'(\tau) = 0 \Leftrightarrow \tau = 0$. This critical point corresponds to the unique geodesic connecting the point $(x_1, x_2, 0)$ and the origin $(0, 0, 0)$, which is the line segment joining these two points. Moreover,

$$f(0) = \frac{1}{2}\|x\|^2 = \frac{1}{2} d^2(x_1, x_2, 0),$$

where $d(x_1, x_2, 0)$ denotes the subRiemannian distance between the point $(x_1, x_2, 0)$ and the origin. Now, f and V have the following Taylor's expansions at the point $\tau = 0$:

$$f(\tau) = \frac{1}{2}\|x\|^2 \tau \coth \tau = \sum_{k=0}^{\infty} \alpha_k \tau^k \tag{2.32}$$

$$V(\tau) = \frac{\tau}{\sinh \tau} = \sum_{k=0}^{\infty} \beta_k \tau^k, \tag{2.33}$$

where

$$\alpha_0 = \frac{\|x\|^2}{2}, \quad \alpha_2 = \frac{\|x\|^2}{6}, \quad \alpha_4 = -\frac{\|x\|^2}{90}, \quad \alpha_6 = \frac{\|x\|^2}{945}, \quad \cdots, \quad \alpha_{2j+1} = 0,$$

$$\beta_0 = 1, \quad \beta_2 = -\frac{1}{6}, \quad \beta_4 = \frac{7}{360}, \quad \beta_6 = -\frac{31}{15120}, \quad \cdots, \quad \beta_{2j+1} = 0.$$

By Laplace's method, we have the small t asymptotic expansion

$$\begin{aligned} p_t \sim & \frac{1}{(2\pi t)^2} e^{-\frac{f(0)}{t}} \sum_{n=0}^{\infty} 2\Gamma\left(\frac{n+1}{2}\right) C_n t^{\frac{n+1}{2}} \\ \sim & \frac{1}{2\pi^2 t^{3/2}} e^{-\frac{\|x\|^2}{2t}} \sum_{n=0}^{\infty} \Gamma\left(\frac{n+1}{2}\right) C_n t^{n/2} \end{aligned} \tag{2.34}$$

where the coefficients C_n can be expressed in terms of α_k and β_k with $0 \le k \le n$. The first few coefficients are given by

$$C_0 = \frac{\beta_0}{\alpha_0} = \frac{2}{\|x\|^2}, \quad C_1 = 0, \quad C_2 = \frac{1}{\alpha_0^3}\left(\beta_2 - \frac{3\alpha_2\beta_0}{\alpha_0}\right) = -\frac{28}{3\|x\|^6}, \quad C_3 = 0; \tag{2.35}$$

see [34]. Other coefficients can be obtained iteratively by the method in [33] or [23, eq. (28)].

2.4. **Case III-2:** $x \neq 0$ **and** $y \neq 0$**.** As $t \to 0^+$, the heat kernel in (1.17) is a Laplace type integral with $1/t$ playing the role of a large parameter. Note that the action function $f(\tau)$ is analytic in τ. Hence, we may apply Debye's method of steepest decent to derive the asymptotic expansion; see [34, Sec. II.4]. The basic idea is to deform the integration path to the steepest decent curve Γ, so that the following conditions hold:

(a) Γ passes the critical points of $f(z)$, *i.e.* points such that $f'(z) = 0$;

(b) the imaginary part of $f(\tau)$ is a constant along Γ, (here $\operatorname{Im} f(z) = 0$ on Γ).

The term *steepest descent* stems from condition (b) above, since $-\operatorname{Re} f(\tau)$ is steepest descent along the curve Γ.

We first recall the results on $f(\tau)$ in [3]. For $(x_1, x_2) \neq (0, 0)$, $f(\tau)$ has finitely many of critical points, all are purely imaginary. Denote these saddle points as $\tau_j = i\theta_j$, $j = 1, 2, \ldots, p$, with $0 < \theta_1 < \theta_2 < \cdots < \theta_p$, see Fig. 1 (b). It is known that

$$f(\tau_j) = \frac{1}{2}\ell_j^2, \qquad j = 0, 1, \ldots, p, \tag{2.36}$$

where ℓ_j is the length of the j-th geodesic joining (x_1, x_2, y) and the origin. In particular, the first critical point gives the smallest critical value,

$$f(\tau_1) = \frac{1}{2} d^2(x_1, x_2, y)$$

with $d(x_1, x_2, y) = \ell_1$ denoting the subRiemannian (Carnot-Carathéodory) distance between (x_1, x_2, y) and the origin. Since other critical values are larger than the first one, the contributions of these critical points are exponentially small compared with the first critical point. Write $\tau = a + ib$ with a, b both real. The imaginary part of $f(\tau)$ defined in (1.18) is

$$\operatorname{Im} f(\tau) = -ay + \frac{1}{2}\|x\|^2 \frac{-a \sin b \cos b + b \sinh a \cosh a}{\sinh^2 a + \sin^2 b}. \tag{2.37}$$

Note that $\operatorname{Im} f(\tau_1) = \operatorname{Im} f(i\theta_1) = 0$. The steepest descent path is plotted in Figure 1, where we choose $\|x\|^2 = 2$ and $y = 5$ for illustration: there are three critical points $\tau_j = i\theta_j$, $j = 1, 2, 3$ with $0 < \theta_1 < \pi < \theta_2 < \theta_3 < 2\pi$. They are the intersecting points of the steepest path with the imaginary axis.

The Taylor expansions of f and V and the first saddle point $\tau = \tau_1$ are

$$f(\tau) = \sum_{k=0}^{\infty} a_k (\tau - \tau_1)^k, \qquad V(\tau) = \sum_{k=0}^{\infty} b_k (\tau - \tau_1)^{k+\alpha-1}, \tag{2.38}$$

with $\alpha = 1$. By the method of steepest descent, we have

$$\begin{aligned} p_t(x_1, x_2, y) &\sim \frac{e^{-\frac{d^2}{2t}}}{(2\pi t)^2} \sum_{n=0}^{\infty} C_n \Gamma\Big(\frac{n+1}{2}\Big) t^{\frac{n+1}{2}} \\ &\sim \frac{e^{-\frac{d^2}{2t}}}{(2\pi)^2 t^{\frac{3}{2}}} \sum_{n=0}^{\infty} C_n \Gamma\Big(\frac{n+1}{2}\Big) t^{\frac{n}{2}}, \end{aligned} \tag{2.39}$$

where the coefficients C_n can be derived iteratively; see [34, §II.4]. We follow the method described in [23] to obtain these coefficients C_n. A simple calculation yields

$$f'(\tau) = -iy + i\frac{1}{2}\mu(-i\tau)\|x\|^2 \quad \text{and} \quad f''(\tau) = \frac{1}{2}\mu'(-i\tau)\|x\|^2, \tag{2.40}$$

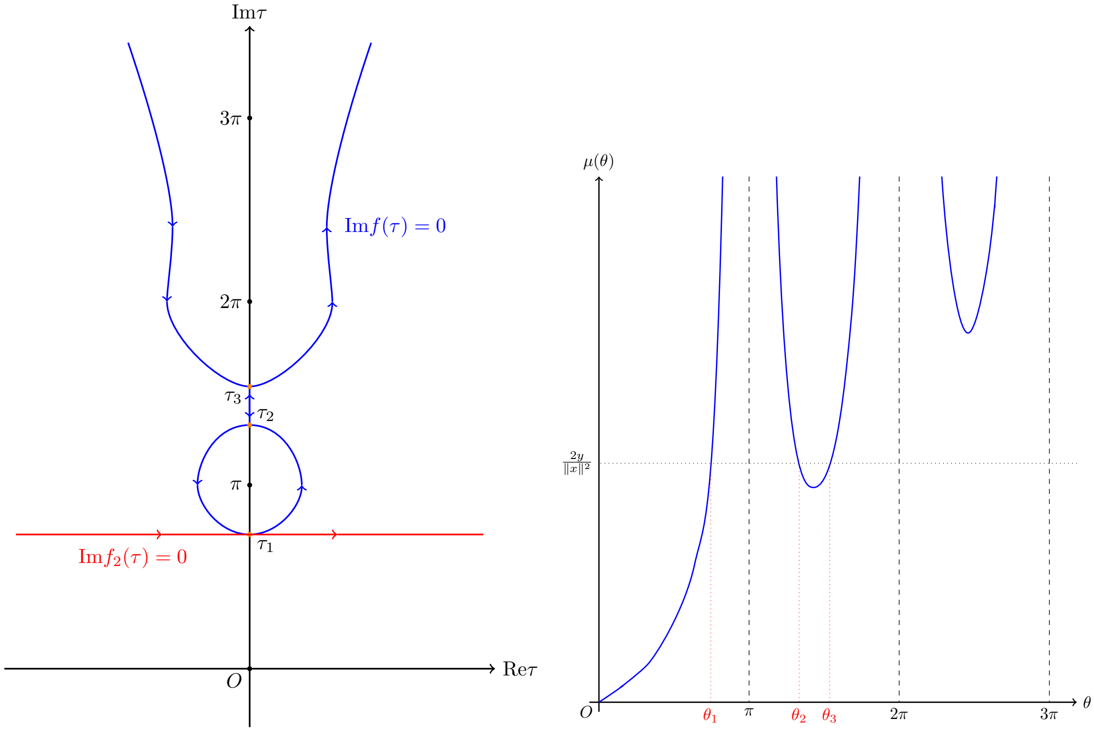

FIGURE 1. (a) Complex τ plane: the blue curve is the steepest descent path for $f(\tau)$; the red line is the steepest descent path for $f_2(\tau)$. (b) The function $\mu(\theta)$: the solutions of $\mu(\theta) = 2y/\|x\|^2$ give the saddle points $\tau_j = i\theta_j$. Parameters: $\|x\|^2 = 2$, $y = 5$.

where

$$\mu(\varphi) = \frac{\varphi}{\sin^2\varphi} - \cot\varphi; \tag{2.41}$$

see [3, eq. (1.26)]. By Lemma 1.33 of [3], we have $\mu'(\varphi) > 0$ for $0 < \varphi < \pi$, and hence $f^{(2)}(\tau_1) > 0$, which implies that $\tau = \tau_1$ is a saddle point of order one. Moreover, we also have $f^{(3)}(\tau_1) > 0$. Thus,

$$f(\tau) = f(\tau_1) + f^{(2)}(\tau_1)\frac{(\tau-\tau_1)^2}{2} + f^{(3)}(\tau_1)\frac{(\tau-\tau_1)^3}{6} + \cdots .$$

Follow the notations of [23],

$$m = \min\{k > 1\,;\, f^{(k)}(\tau_1) \neq 0\}, \qquad p = \min\{k > m\,;\, f^{(k)}(\tau_1) \neq 0\}. \tag{2.42}$$

In our case $m = 2$ and $p = 3$. Now, we split the phase function into two terms

$$f(\tau) = f_2(\tau) + \tau^3 f_3(\tau), \tag{2.43}$$

with

$$f_2(\tau) =: f(\tau_1) + \frac{f^{(2)}(\tau_1)}{2!}(\tau-\tau_1)^2, \tag{2.44}$$

$$f_3(\tau) := \frac{f(\tau) - f_2(\tau)}{\tau^3} = \frac{f^{(3)}(\tau_1)}{3!} + \frac{f^{(4)}(\tau_1)}{4!}(\tau-\tau_1) + \cdots . \tag{2.45}$$

The idea used in [23] is to deform the contour into a steepest descent path of $f_2(\tau)$ instead of that of $f(\tau)$, seeking for the simplicity. Notice that $f_2(\tau)$ is a polynomial of degree two, and Im $f_2(\tau_1) = \text{Im}\, f(\tau_1) = 0$, so the steepest descent path for $f_2(\tau)$ is the horizontal line, which is plotted in Figure 1 with a red line. This contour is divided into two semi-infinite lines

$$\Gamma_k = \left\{\tau \in \mathbb{C}; \quad \tau = \tau_1 + re^{ik\pi}, \quad r \geq 0\right\}, \qquad k = 0, 1. \tag{2.46}$$

Then the integral in (1.17) becomes an Laplace integral over r, and any method for computing the coefficients of Laplace's methods can be applied. Follow the approach in [23], the coefficients C_n in the expansion (2.39) are given by

$$C_n = c_n(0) + c_n(1), \tag{2.47}$$

with $c_n(1) = (-1)^n c_n(0)$ and the Laplace's coefficients $c_n(0)$ being calculated recursively by Wojdylo's method [33, p. 71]

$$c_n(0) = \frac{1}{m\Gamma(\frac{n+\alpha}{m})}\sum_{k=0}^{n} b_{n-k}\sum_{s=0}^{k}\frac{(-1)^s}{a_m^{(n+\alpha)/m+s}}\frac{B_{k,s}}{s!}\Gamma\left(\frac{n+\alpha}{m}+s\right). \tag{2.48}$$

Here, b_k is given in (2.38) and the partial ordinary Bell polynomials $B_{n,k}$ are defined by

$$B_{0,0} = 1, \quad B_{n,0} = 0, \qquad B_{n,k} = \sum_{j=k-1}^{n-p+m} a_{n+m-j}B_{j,k-1}, \qquad n \geq k \geq 1. \tag{2.49}$$

Recall that

$$a_n = \frac{1}{n!}f^{(n)}(\tau_1) = -\frac{(-i)^n}{2n!}\mu^{(n-1)}(-i\tau_1)\|x\|^2, \qquad n \geq 2. \tag{2.50}$$

The first few terms of $B_{n,k}$ are given by

$$B_{1,1} = \frac{1}{4}\|x\|^2\mu', \quad B_{2,1} = \frac{-i}{12}\|x\|^2\mu'', \quad B_{2,2} = \frac{1}{16}\|x\|^4(\mu')^2,$$

$$B_{3,1} = \frac{-1}{48}\|x\|^2\mu''', \quad B_{3,2} = \frac{-i}{24}\mu'\mu'', \quad B_{3,3} = \frac{1}{64}\|x\|^6(\mu')^3.$$

with $\mu' := \mu'(-i\tau_1)$, $\mu'' := \mu''(-i\tau_1)$ and $\mu''' := \mu'''(-i\tau_1)$. A slight calculation yields

$$C_0 = \frac{b_0}{a_2^{1/2}} = \frac{\tau_1}{\sinh\tau_1}\frac{2}{\|x\|}\sqrt{\frac{1}{\mu'(-i\tau_1)}} = \frac{\theta_1}{\|x\|}\sqrt{\frac{2\sin\theta_1}{\sin\theta_1 - \theta_1\cos\theta_1}}, \tag{2.51}$$

$$C_2 = \frac{b_2 - \frac{3}{2}b_1 - \frac{3}{2}\frac{a_3}{a_2}b_0 + \frac{15}{8}b_0}{a_2^{3/2}} \tag{2.52}$$

$$C_{2j+1} = 0, \qquad j = 0, 1, 2, 3, \cdots, \tag{2.53}$$

where

$$a_2 = \frac{\sin\theta_1 - \theta_1\cos\theta_1}{2\sin^3\theta_1}\|x\|^2, \quad a_3 = \frac{\theta_1 + 2\theta_1\cos^2\theta_1 + 3\sin\theta_1\cos\theta_1}{6\sin^4\theta_1}\|x\|^2,$$

$$b_0 = \frac{\theta_1}{\sin\theta_1}, \quad b_1 = \frac{\sin\theta_1 - \theta_1\cos\theta_1}{\sin^2\theta_1}, \quad b_2 = \frac{\theta_1(1+\cos^2\theta_1) - 2\sin\theta_1\cos\theta_1}{\sin^3\theta_1}.$$

2.5. **Some observations.** We have the following form of asymptotics for the heat kernel

$$p_t(x_1, x_2, y) \sim \frac{C}{t^{Q/2}} e^{-\frac{d^2}{2t}}, \tag{2.54}$$

where C and Q are constants and d is the Carnot-Carathéodory distance between (x_1, x_2, y) and the origin. We note that the power of t, α, varies. Namely,

$$2\alpha = \begin{cases} 4 = Q > n, & \text{when } x = 0, \quad y = 0, \quad \text{diagonal;} \\ 4 = n + 1, & \text{when } x = 0, \quad y \neq 0, \quad \text{off-diagonal and cut-conjugate;} \\ 3 = n, & \text{when } x \neq 0, \quad \text{off-diagonal and not cut-conjugate.} \end{cases} \tag{2.55}$$

Here, $n = 3$ is the topological dimension and Q is the Hausdorff dimension; cf. eq. (A.81). This agrees with the previous result on the asymptotics for the heat kernels on the diagonal, *i.e.* when the $(x_1, x_2, y) = (0, 0, 0)$; see [2, 4, 5, 6].

3. Asymptotics for the heat kernel of the Grushin operator

The geodesic structure of the Grushin plane is similar to the Heisenberg case. However, we do have exceptional geodesics in Grushin case, which do not correspond to the critical points of $g(\tau)$ but the singularities of $W(\tau)$, see [10, 11, 12]. All the geodesics correspond to $\tau_k = i\eta_k$ with $0 < \eta_1 \leq \eta_2 \leq \eta_3 \leq \cdots$ being a (finite or infinite) sequence of positive numbers. An exceptional geodesic corresponds to $\eta_k = j\pi$ for some positive integer j appears when (i) $x = x_0 \neq 0$ or (ii) $x = -x_0 \neq 0$. Moreover, the first geodesic is always generic in case (i), *i.e.* $0 < \eta_1 < \pi \leq \eta_2$. However, the first geodesic might be exceptional in case (ii), that is $\eta_1 = \pi = \eta_2$ or $\eta_1 = \pi < \eta_2$.

In this section, we shall derive the following result for the Grushin heat kernel with $m = 1$.

Theorem 2. *The heat kernel $p_t(x_0, y_0; x, y)$ of the Grushin operator given in (1.22) with $m = 1$ has the following asymptotic expansions as $t \to 0^+$:*

(I) when $x = x_0 = 0$ and $y = y_0$,

$$p_t(x, y; x, y) = \frac{1}{(2\pi t)^{3/2}} \int_{-\infty}^{\infty} \left(\frac{\tau}{\sinh \tau}\right)^{\frac{1}{2}} d\tau; \tag{3.56}$$

(II) when $x = x_0 \neq 0$ and $y = y_0$,

$$p_t(x, y; x, y) \sim \frac{2}{(2\pi)^{3/2} t} \sum_{s=0}^{\infty} \Gamma\Big(\frac{s+1}{2}\Big) c_{2s} t^s, \tag{3.57}$$

where c_s is given in (3.61);

(III) when $x = -x_0 \neq 0$ and $|y - y_0| = \frac{\pi}{2} x^2$,

$$p_t(x_0, y_0; x, y) \sim \frac{e^{-\frac{d^2(q_0, q)}{2t}}}{(2\pi)^{3/2} t^{5/4}} \sum_{s=0}^{\infty} \Gamma\Big(s + \frac{1}{4}\Big) D_s t^s; \tag{3.58}$$

(IV) other cases,

$$p_t(x_0, y_0; x, y) \sim \frac{e^{-\frac{d^2(q_0, q)}{2t}}}{(2\pi)^{3/2} t} \sum_{s=0}^{\infty} \Gamma\left(s + \frac{1}{2}\right) D_s t^s, \tag{3.59}$$

where $d(q_0, q)$ is the subRiemannian distance between the points $q_0(x_0, y_0)$ and $q(x, y)$, $D_s = C_{2s}$, and C_s can be computed by formulas in (2.47)-(2.49) with $m = 2$, $p = 3$, $\alpha = 1$ and a_s, b_s given in (3.73).

When $x = x_0 = 0$, $y = y_0$, the function $g(\tau)$ in (1.23) is identically equal to zero, the result in (3.56) follows immediately. In what follows, we shall derive the results in Cases (II)–(IV).

3.1. **Case II: $x = x_0 \neq 0$ and $y = y_0$.** Now, the phase function simplifies to

$$g(\tau) = x^2 \tau \tanh \frac{\tau}{2},$$

which is real positive-valued and has one minimum at $\tau = 0$. Therefore, we can use the Laplace's method to derive the asymptotic expansion for (1.22). Note that $g(\tau)$ and $W(\tau)$ are even functions, hence

$$p_t = \frac{2}{(2\pi t)^{3/2}} \int_0^\infty e^{-g(\tau)/t} W(\tau) d\tau.$$

The series expansion of g and W are

$$g(\tau) = \frac{x^2}{2}\tau^2 - \frac{x^2}{24}\tau^4 + \cdots = \sum_{k=0}^\infty a_k \tau^k, \quad W(\tau) = 1 - \frac{1}{12}\tau^2 + \cdots = \sum_{k=0}^\infty b_k \tau^k. \tag{3.60}$$

In the notations of (2.42), $m = 2$, $p = 4$. By Laplace's method

$$\begin{aligned} p_t \sim & \frac{2}{(2\pi t)^{3/2}} \sum_{s=0}^\infty \Gamma\Big(\frac{s+1}{2}\Big) c_s t^{\frac{s+1}{2}} \\ \sim & \frac{2}{(2\pi)^{3/2} t} \sum_{s=0}^\infty \Gamma\Big(\frac{s+1}{2}\Big) c_s t^{s/2}, \qquad t \to 0^+, \end{aligned}$$

where the coefficients c_s can be calculated by Wojdylo's formula in (2.48)-(2.49) with a_k and b_k given in (3.60). A slight calculation shows

$$c_0 = \frac{\sqrt{2}}{2|x|}, \quad c_1 = 0, \quad c_2 = \frac{\sqrt{2}}{24|x|^3}, \quad c_4 = \frac{-\sqrt{2}}{320|x|^5}, \quad c_5 = 0. \tag{3.61}$$

3.2. **Case III: $x = -x_0 \neq 0$ and $|y - y_0| = \frac{\pi}{2}x^2$.** Now,

$$g(\tau) = -i\tau(y - y_0) + x^2 \tau \coth \frac{\tau}{2} = \tau x^2 \left[\coth \frac{\tau}{2} - i\frac{\pi}{2}\right]. \tag{3.62}$$

It is readily seen that

$$g(\tau; x_0, y_0; x, y) = f(\tau/2; 2x, 0, y - y_0),$$

where f is the modified complex action function of the Heisenberg subLaplacian given in (1.18). Now $g(\tau)$ has only one saddle point $\tau_1 = i\pi$, which is also a branch point of $W(\tau)$. The saddle point corresponds to a generic geodesic, and the branch point corresponds to an exceptional geodesic, and these two geodesic coincide. The asymptoics of the heat kernel (1.22) can be derived in a similar method as that used in the Heisenberg case. The coalescing of a saddle point and a branch point is treated in [34, Ch. VII, §3]. The result in [23] also applies to this case. To this end, we first expand $g(\tau)$ and $W(\tau)$ at $\tau_1 = i\pi$,

$$g(\tau) - g(\tau_1) = \sum_{s=2}^\infty a_s (\tau - \tau_1)^s, \qquad W(\tau) = \sum_{s=0}^\infty b_s (\tau - i\pi)^{s-1/2}, \quad |\tau - i\pi| < \pi. \tag{3.63}$$

The first few coefficients are

$$a_0 = \frac{1}{2}\pi^2, \qquad a_1 = 0, \qquad a_2 = \frac{1}{2}, \qquad a_3 = -\frac{i\pi}{24},$$

$$b_0 = (-i\pi)^{1/2}, \qquad b_1 = \frac{1}{2\sqrt{\pi}}(-i)^{3/2}, \quad b_2 = \left(\frac{1}{8\pi^2} - \frac{1}{12}\right)(-i\pi)^{1/2}, \quad \cdots$$

In the notations of [23], $m = 2$, $p = 3$,p and $\alpha = \frac{1}{2}$. Then, the asymptotic expansion of the heat kernel is given by

$$\begin{aligned} p_t(x_0, y_0; x, y) &\sim \frac{e^{-g(\tau_1)/t}}{(2\pi t)^{3/2}} \sum_{s=0}^{\infty} \Gamma\Big(\frac{s}{2} + \frac{1}{4}\Big) C_s t^{\frac{s}{2}+\frac{1}{4}} \\ &\sim \frac{e^{-\frac{d^2(q_0,q)}{2t}}}{(2\pi)^{3/2} t^{5/4}} \sum_{s=0}^{\infty} \Gamma\Big(\frac{s}{2} + \frac{1}{4}\Big) C_s t^{\frac{s}{2}} \end{aligned} \tag{3.64}$$

as $t \to 0^+$. The coefficients C_s are calculated by the formulas in (2.47)-(2.49) with $m = 2$, $p = 3$ and $\alpha = 1/2$, and a_s, b_s given in (3.63).

3.3. **Case IV-1:** $x = x_0 = 0$ **and** $y \neq y_0$**.** We assume $y > y_0$ without loss of generality. Now, the heat kernel in (1.22) becomes

$$p_t(x_0, y_0; x, y) = \frac{1}{(2\pi t)^{\frac{3}{2}}} \int_{-\infty}^{\infty} e^{i\tau\frac{y-y_0}{t}} \left(\frac{\tau}{\sinh\tau}\right)^{\frac{1}{2}} d\tau. \tag{3.65}$$

Note that, $\tau_k = ik\pi$, $k = 1, 2, 3, \cdots$, are branch points of $W(\tau)$, and each of these singularities corresponds to a pair of geodesics joining $(0, y_0)$ and $(0, y)$. Since the contribution of all the other singularities is exponentially small compared with the first one, we just concentrate on the first one $\tau_1 = i\pi$. Recall the series expansion of $W(\tau)$ given in (3.63). By the change of variables

$$\tau \quad \mapsto \quad u: \qquad i(\tau - i\pi)\frac{y - y_0}{t} = u$$

and deforming the integral path to the Hankel loop reduce the integral in (3.65) to

$$p_t(x_0, y_0; x, y) = \frac{1}{(2\pi t)^{\frac{3}{2}}} e^{-\frac{\pi(y-y_0)}{t}} \int_{-\infty}^{(0+)} e^u \sum_{s=0}^{\infty} \left(\frac{-it}{y - y_0}\right)^{s+1/2} w_s u^{n-1/2} du \tag{3.66}$$

To derive the asymptotic expansion, we recall the Hankel's loop integral representation of the gamma function

$$\frac{1}{\Gamma(-\lambda)} = \frac{1}{2\pi i} \int_{-\infty}^{(0+)} u^{\lambda} e^u du; \tag{3.67}$$

see [28] or [29, eq. (5.9.2)]. Thus,

$$\begin{aligned} p_t(x_0, y_0; x, y) &\sim \frac{1}{(2\pi t)^{\frac{3}{2}}} e^{-\frac{\pi(y-y_0)}{t}} \sum_{s=0}^{\infty} \left(\frac{-it}{y - y_0}\right)^{s-1/2} w_s \frac{2\pi t}{y - y_0} \frac{1}{\Gamma(\frac{1}{2} - n)} \\ &\sim \frac{1}{2\pi t} e^{-\frac{\pi(y-y_0)}{t}} \sum_{s=0}^{\infty} \frac{\sqrt{2\pi}}{\Gamma(\frac{1}{2} - s)} \frac{(-i)^{s-1/2} w_s}{(y - y_0)^{s+1/2}} t^s \\ &\sim \frac{1}{2\pi t} e^{-\frac{d^2(q_0,q)}{2t}} \sum_{s=0}^{\infty} \frac{\sqrt{2\pi}}{\Gamma(\frac{1}{2} - s)} \frac{(-i)^{s-1/2} w_s}{(y - y_0)^{s+1/2}} t^s \end{aligned} \tag{3.68}$$

as $t \to 0^+$. Here, we have made use the fact that $\pi(y-y_0) = d^2(q_0;q)/2$ with $d(q_0;q)$ denoting the subRiemannian distance between the two points $q_0(0,y_0)$ and $q(0,y)$.

3.4. **Case IV-2:** $x = -x_0 \neq 0$ **and** $|y-y_0| > \frac{\pi}{2}x^2$**.** In this case, there are finitely many of geodesic connections, corresponding to $\tau_k = i\eta_k$ with $\eta_1 = \pi < \eta_2 \leq \cdots \leq \eta_p$. The shortest geodesic is the exceptional geodesic corresponding to $\tau_1 = i\pi$. From the integral point of view, the main contribution comes from the first singularity of $W(\tau)$, that is $\tau_1 = i\pi$.

The asymptotic expansion of (1.22) can be derived in a same manner as in Case (III-1). Make the change of variables

$$u = -\frac{g(\tau)-g(\tau_1)}{t} = \frac{1}{t}\sum_{s=1}^{\infty} g_s(\tau-\tau_1)^s, \qquad g_s = -\frac{g^{(s)}(\tau_1)}{s!}. \tag{3.69}$$

By the inverse function theorem,

$$\tau - \tau_1 = \sum_{s=1}^{\infty} \alpha_s t^s u^s.$$

Differentiating the last equation with respect to u and using (3.63), one has

$$W(\tau)\frac{d\tau}{du} = \sum_{s=0}^{\infty} c_s t^{\frac{s+1}{2}} u^{\frac{s-1}{2}}.$$

A slight calculation yields

$$c_0 = b_0\sqrt{\alpha_1} = \frac{b_0}{(-g_1)^{1/2}}, \qquad c_1 = \frac{3b_0\alpha_2 + 2b_1\alpha_1^2}{2\sqrt{\alpha_1}}. \tag{3.70}$$

Under the change of variables (3.69), the integral in (1.22) reduces to a Hankel's loop integral

$$p_t(x,y;x_0,y_0) = \frac{1}{(2\pi)^{3/2}t} e^{-\frac{d^2}{2t}} \int_{-\infty}^{(0+)} e^u \sum_{s=0}^{\infty} c_s t^{\frac{s}{2}} u^{\frac{s-1}{2}}\, du, \tag{3.71}$$

where $d^2/2 = g(\tau_1)$ and d is the subRiemannian distance between the two points (x_0,y_0) and (x,y). Using the integral representation in (3.67) and Watson's lemma, one has

$$p_t(x,y;x_0,y_0) \sim \frac{1}{2\pi t} e^{-\frac{d^2(q_0,q)}{2t}} \sum_{s=0}^{\infty} \frac{\sqrt{2\pi}}{\Gamma(\frac{1-s}{2})} c_s t^{s/2}, \tag{3.72}$$

as $t \to 0^+$. Indeed, all the terms with odd s vanish since $1/\Gamma(\frac{1-s}{2}) = 0$.

3.5. **Case IV-3: other cases.** What left are the following cases:
(a) $x \neq \pm x_0$. Here, x_0 or x can be zero;
(b) $x = -x_0 \neq 0$ and $|y-y_0| < \frac{\pi}{2}x^2$;
(c) $x = x_0 \neq 0$.

The geodesics in Cases (a) and (b) are all generic geodesics. There might be exceptional geodesic(s) in case (c), but the shortest geodesic is generic. In all these three cases, the action function $g(\tau)$ has finite number of critical points (saddle points) $\tau_k = i\eta_k$, $k = 1,2,\cdots,p$, with $0 < \eta_1 < \pi \leq \eta_2 < \cdots \leq \eta_p$. Here, p is a positive integer. The first saddle point τ_1 will give the main contribution in the asymptotic approximation of (1.22), and all the other saddle points contribute exponentially small and hence negligible. At the first saddle point τ_1, g and W have the following Taylor expansions,

$$g(\tau) - g(\tau_1) = \sum_{s=2}^{\infty} a_s (\tau - \tau_1)^s, \qquad W(\tau) = \sum_{s=0}^{\infty} b_s (\tau - \tau_1)^s. \tag{3.73}$$

Then, the method of saddle point yields

$$\begin{aligned} p_t(x, y; x_0, y_0) &\sim \frac{e^{-\frac{d^2}{2t}}}{(2\pi t)^{3/2}} \sum_{n=0}^{\infty} C_n \Gamma\Big(\frac{n+1}{2}\Big) t^{\frac{n+1}{2}} \\ &\sim \frac{e^{-\frac{d^2}{2t}}}{(2\pi)^{3/2} t} \sum_{n=0}^{\infty} C_n \Gamma\Big(\frac{n+1}{2}\Big) t^{\frac{n}{2}}, \end{aligned} \tag{3.74}$$

as $t \to 0^+$. Here, $d^2/2 = g(\tau_1)$ and d is the subRiemannian distance between the two points (x_0, y_0) and (x, y). The coefficients of C_n can be obtained by the same manner as in Section 2. The C_n's can be computed by formulas in (2.47)-(2.49) with $m = 2$, $p = 3$, $\alpha = 1$ and a_s, b_s given in (3.73).

3.6. **Some observations.** The heat kernel of the Grushin operator has the small-time asymtotics in the following form

$$p_t(x_0, y_0; x, y) \sim \frac{C}{t^\alpha} e^{-\frac{d^2}{2t}},$$

where C is a constant, d is the subRiemannian distance between the points $q_0(x_0, y_0)$ and $q(x, y)$, and

$$2\alpha = \begin{cases} 3 = Q > n, & x = x_0 = 0, \quad y = y_0, \quad \text{diagonal;} \\ 2 = Q = n, & x = x_0 \neq 0, \quad y = y_0, \quad \text{diagonal;} \\ 5/2 = n + 1/2, & x = -x_0 \neq 0, \quad |y - y_0| = \pi x^2/2, \\ & \text{off-diagonal and cut-conjugate;} \\ 2 = n, & \text{off-diagonal and not cut-conjugate points.} \end{cases}$$

Here, $n = 2$ is the topological dimension and Q is the Hausdorff dimension. We see that in most of the cases $\alpha = Q/2$. The case of $2\alpha = 5/2$ corresponds to the situation when (x_0, y_0) and (x, y) are cut-conjugate points; see [2].

Case II two is the diagonal case, for which we have

$$p_t(x, y; x, y) \sim \frac{1}{2\pi t |x|} \left(1 + \frac{1}{24|x|^2} t + \cdots \right), \qquad \text{as} \quad t \to 0^+.$$

The second term here is related to the scalar curvature in the sense that $\frac{1}{24|x|^2} = -\frac{R(x,y)}{96}$. The scalar curvature $R(x, y)$ is calculated in Appendix C.

4. Uniform asymptotic expansions, the discontinuity of α

4.1. **Heisenberg subLaplacian.** Let us consider the Heisenberg case first. We have shown that the leading power of t in the small-time asymptotic expansion for the heat kernel (1.17) varies as the point (x_1, x_2, y) varies. To be precise, as (x_1, x_2) approaches $(0, 0)$, the power α of t changes from $3/2$ to 2; see eqs. (2.54)-(2.55). From the integral point of view, the discontinuity of α is due to the coalescing of the two saddle points τ_1 and τ_2 to the same value $i\pi$ as $\|x\| \to 0$. Note that $\theta_1 < \pi < \theta_2$ for $\|x\| \neq 0$, and that θ_1 and

θ_2 both tend to π as $\|x\| \to 0$, and $\tau = i\pi$ is also a simple pole of the phase function $f(\tau)$. For such a case, Frenzen and Wong [14] derived a uniform asymptotic approximation in terms of Bessel function; see also [34, Ch. VII]. Their idea is to introduce a rational mapping $\tau \mapsto u$ by

$$-2f(i\eta) = u - \frac{A^2(\sigma)}{u}, \tag{4.75}$$

where $\sigma = \frac{2y}{\|x\|^2}$ and the function $A(\sigma)$ is determined as follows. Note that

$$-2if_\eta(i\eta)\frac{d\tau}{du} = 1 + \frac{A(\sigma)^2}{u^2}.$$

In order to have a one-to-one mapping in the region of interest, one requires $\frac{d\eta}{du} \neq 0$ or ∞. Note that $f_\eta(i\eta_1) = 0$ and $f_\eta(i\eta_2) = 0$, thus we let τ_1 and τ_2 correspond to $u = iA(\sigma)$ and $u = -iA(\sigma)$, respectively. Therefore,

$$A(\sigma) = if(i\eta_1) = i\frac{d^2}{2}, \tag{4.76}$$

where d is the subRiemannian distance between (x, y) and the origin. Here, we have made use of the fact that $f(i\eta_1) = d^2/2$. By the transformation $\tau \mapsto u$, the heat kernel (1.17) reduces to

$$p_t(x, y) = \frac{1}{(2\pi t)^3}\int u^{-1}h(u)\exp\left\{\frac{1}{t}\left(u - \frac{A(\sigma)^2}{u}\right)\right\}du, \tag{4.77}$$

where

$$h(u) = uV\big(\tau(u)\big)\frac{d\tau}{du} \tag{4.78}$$

is analytic near $u = 0$. Recall Schläfli's integral representation of the Bessel function $J_\nu(z)$ (see [29, eq. (10.9.19)])

$$J_\nu(z) = \frac{1}{2\pi i}\left(\frac{z}{2}\right)^\nu \int_{-\infty}^{(0+)} t^{-(\nu+1)}\exp\left\{t - \frac{z^2}{4t}\right\}dt.$$

The change of variables $t = \lambda u/2$ leads to

$$J_\nu(\lambda z) = \frac{z^\nu}{2\pi i}\int_{-\infty}^{(0+)} u^{-(\nu+1)}\exp\left\{\frac{\lambda}{2}\left(u - \frac{z^2}{u}\right)\right\}du. \tag{4.79}$$

Comparing the last equation with (4.77) yields

$$p_t(x, y) \sim \frac{1}{t^2}J_0\left(\frac{A(\sigma)}{t}\right)a_0(x, y) + O(t^{-1}), \qquad \text{as} \quad t \to 0^+,$$

where $a_0(x, y)$ is a function of x, y. Follow the approach of Fenzen and Wong [14], we can derive an asympttoic expansion of the form

$$p_t(x_1, x_2, y) \sim \frac{1}{t^2}\left\{J_0\left(A(\sigma)/t\right)\sum_{s=0}^{\infty}a_s t^s + \frac{J_1\left(A(\sigma)/t\right)}{A(\sigma)}\sum_{s=0}^{\infty}b_s t^{s+1},\right\} \tag{4.80}$$

as $t \to 0^+$.

4.2. **Grushin operator.** In the small-time asymptotics of the heat kernel of the Grushin operator, we see that the leading power of t, α, changes from 1 to $5/4$ as q approaches the cut-conjugate point of q_0. From the integral point of view, this discontinuity of α is due to the coalescing of the saddle point τ_1 and the singularity of $W(\tau)$ at $\tau = i\pi$. The treatment of such coalesce of critical points can be found in Wong [34, Ch. VII, §3], and the uniform asymptotic expansion involves parabolic cylinder functions. The discontinuous change of α from $3/2$ to 1 can be smoothed out in a same manner as in the Heisenberg case. Since there is no alternation in the methods, we omit the details here.

5. Discussions

We have derived small-time asymptotic expansions for the heat kernels of the Heisenberg subLaplacian and the Grushin operator. Our derivation is based on the integral representations, and $1/t$ serves as a large parameter as $t \to 0^+$. The techniques in deriving asymptotics of integrals, such as the methods of stationary phase and steepest descent, are the main tools here. The leading power of t in the expansions of $p_t(q_0; q)$ is different for different situations of q_0 and q. This discontinuity of the power α can be smoothed out by the uniform expansion techniques. As all the known subelliptic heat kernels have Laplace-type integral representations, the techniques described here can also be applied to such cases. The two examples we take here are both subelliptic operators on non-compact manifold. On the other hand, elliptic heat kernel asymptotics show that the compact cases pose more interesting properties, since their eigenvalues are discrete and one can investigate the trace asymptotic expansions. In the future work, we shall consider subelliptic heat kernel asymptotics on compact manifolds, such as the subLaplacians on the odd-dimension spheres S^{2n+1} considered in [16].

Appendix A. SubRiemannian geometry

The term **bracket-generating condition** is the following condition on the vector fields $\{X_j\}_{j=1}^k$, or equivalently, on the distribution $\mathcal{D} := \text{span}\,\{X_j\}_{j=1}^k$. Recall that the Lie bracket of two vector fields X_i and X_j is $[X_i, X_j] = X_iX_j - X_jX_i$. One can define a sequence of distributions $\{\mathcal{D}^s\}_{s=1}^\infty$ recursively by $\mathcal{D}^1 = \mathcal{D}$ and $\mathcal{D}^{s+1} = \mathcal{D} \cup [\mathcal{D}, \mathcal{D}^s]$ for $s = 1, 2, \cdots$. Note that $\mathcal{D}^s \subset TM$ for each $s \geq 1$, here TM denotes the tangent bundle of M. If there exists a positive integer S, such that $\mathcal{D}^S = TM$, then we say the vector fields $\{X_j\}_{j=1}^k$ are **bracket-generating**. The smallest integer S such that $\mathcal{D}^S = TM$ is called the **step** of these vector fields.

Assume $\{X_j\}_{j=1}^k$ are bracket-generating vector fields on the n-dimensional manifold M. Since $k < n$, we have several directions missing. However, Chow's theorem [13] showed that one can define a nature metric on M. To start, consider a curve $\gamma(s) : [0, 1] \to M$ whose tangent is in $\mathcal{D} = \text{span}\,\{X_1, \cdots, X_k\}$ and given by

$$\gamma'(s) = \sum_{j=1}^k a_j(s)X_j.$$

By assuming $\{X_j\}_{j=1}^k$ are orthonormal, one can define the length

$$\ell(\gamma) = \int_0^1 \sqrt{a_1(s)^2 + a_2(s)^2 + \cdots + a_k(s)^2}\, ds.$$

Such curves with tangents being in $\mathcal{D}$ are called **horizontal curves** or **admissible curves**. Chow's theorem says the following: if the vector fields $\{X_j\}_{j=1}^k$ are bracket-generating, then any two points $q_0, q \in M$ can be joined by at least one horizontal curve. By minimizing all the lengths of the horizontal curves joining these two points, one can define the distance between q_0 and q. This distance $d(q_0, q)$ is known as the Carnot-Carathéodory distance (or subRiemannian distance). Therefore, Chow's theorem shows that one can define a metric structure g on M, but this is not a Riemannian metric. The metric space $(M, \mathcal{D}, g)$ is called **subRiemannian geometry** or **Carnot-Carathéodory space**.

Despite of the similarity in the names, subRiemannian geometries are very different from Riemannian ones. For instance, the geodesic structures are different, the local uniqueness of the shortest geodesics for the Riemannian geometries is no longer valid in subRiemannian geometries. Another difference is the Hausdorff dimension. The Hausdorff dimension of the Riemannian geometry equals to n, however the Haussdorff dimension of subRiemannian geometry is larger than n. Mitchell [25] showed that the Hausdorff dimension of $(M, \mathcal{D}, g)$ can be calculated as

$$Q = \sum_{s=1}^{S} (\dim \mathcal{D}^s - \dim \mathcal{D}^{s-1}) s, \qquad \text{with} \quad \dim \mathcal{D}^0 = 0. \tag{A.81}$$

Appendix B. Cut points and conjugate points

Fix a point $q_0 \in M$, a point q is a **conjugate point** of q_0 if there exists a nonzero Jacobi fields $\mathcal{J}$ along one geodesic joining q_0 and q such that $\mathcal{J}(q_0) = \mathcal{J}(q) = 0$. An equivalent definition of the conjugate point is by the exponential map, see for example, [1]. If q is a conjugate point of q_0 along a shortest geodesic γ, this geodesic will not be shortest any more after this point q. This indicates that the distance $d(q_0, q)$ as a function of q is not smooth at a conjugate point, and the loss of smoothness of $d(q_0, q)$ explains why the heat kernel asymptotic behavior changes at a conjugate point.

Take the Grushin plane as an example. Given a fixed point $q_0(x_0, y_0)$ with $x_0 \neq 0$, a point $q(x, y)$ is a conjugate point of q_0 if and only if $|y - y_0| = \frac{k\pi}{2} x^2$ and $x = (-1)^k x_0$ for some positive integer k. However, the small-time asymptotic expansion for the heat kernel changes only at the first two conjugate points corresponding to $k = 1$. The explanation is as follows. The first two conjugate points here are also cut points, that is $q \in \mathrm{Cut}(q_0) \cup \mathrm{Conj}(q_0)$. Here, $\mathrm{Cut}(q_0)$ and $\mathrm{Conj}(q_0)$ denote the cut locus (the set of all cut points) and the conjugate locus (the set of all conjugate points) of q_0, respectively. To be clear, we recall that q is a **cut point** of q_0 if: (i) there are more than one shortest geodesic joining q and q_0; or (ii) q is a conjugate point of q_0 along one shortest geodesic. Therefore, for a given point q_0, there might be points are cut points but not conjugate points, and vice versa. Take the Grushin plane as an example for illustration. The cut locus of $q_0(0, y_0)$ is $\{(0, y);\ y \neq y_0\}$, but these points are not conjugate points. For the point $q_0(x_0, y_0)$ with $x_0 \neq 0$, the conjugate points are given above as $\{(x, y);\ |y - y_0| = \frac{k\pi}{2} x^2,\ x = (-1)^k x_0,\ k = 1, 2, 3, \cdots\}$, but only the first two conjugate points associated with $k = 1$ are cut points, all the others are not in the cut locus of q_0. Our result here confirms the observation of Barilari, Boscain and Neel [2], that the leading power of t in the subelliptic heat kernel asymptotics changes at the point $q \in \mathrm{Conj}(q_0) \cup \mathrm{Cut}(q_0)$. This fact is also noticed by Molchanov [26] for Riemannian case. How about the other conjugate points $q \in \mathrm{Conj}(q_0) \setminus \mathrm{Cut}(q_0)$? This happens when q is conjugate along a non-shortest geodesic. If we consider all the contributions from each geodesic, these conjugate points will change the behavior of exponentially small terms, which can not be seen from the asymptotic expansion we consider here.

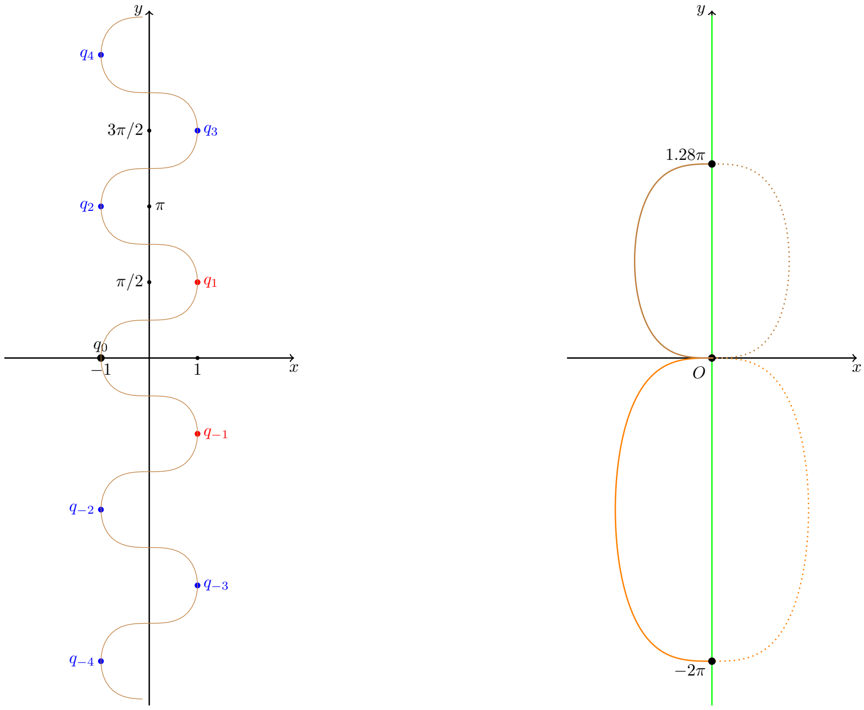

FIGURE 2. Cut points and conjugate points of q_0 in the Grushin plane. (a) $q_0 = (-1, 0)$: $\mathrm{Conj}(q_0) = \{q_{\pm 1}, \ldots q_{\pm k}, \ldots\}$, these points are conjugate with q_0 along the geodesic plotted in the brown curve; $\mathrm{Cut}(q_0) = \{q_1, q_{-1}\}$, so q_1 and q_{-1} are the only cut-conjugate points of q_0.
(b) $q_0 = (0, 0)$: $\mathrm{Cut}(q_0) = \{(0, y); y \neq 0\}$ and $\mathrm{Conj}(q_0) = \emptyset$, any point $q(0, y)$ is joined with q_0 by two shortest geodesics plotted in a solid and a dotted curves, illustration is done for $q = (0, -2\pi)$ and $q = (0, 1.28\pi)$.

APPENDIX C. SCALAR CURVATURE

Recall that the scalar curvature is the trace of the Ricci curvature tensor

$$R = \sum_{i,j} g^{ij} R_{ij}, \tag{C.82}$$

where the Ricci tensor can be calculated via the Christoffel symbols

$$R_{ij} = \sum_{\ell} \left[\frac{\partial \Gamma^{\ell}_{ij}}{\partial x^{\ell}} - \frac{\partial \Gamma^{\ell}_{i\ell}}{\partial x^{j}} + \sum_{m} \left(\Gamma^{m}_{ij} \Gamma^{\ell}_{\ell m} - \Gamma^{m}_{i\ell} \Gamma^{\ell}_{jm} \right) \right] \tag{C.83}$$

and

$$\Gamma^{m}_{ij} = \frac{1}{2} \sum_{k} g^{mk} \left(\frac{\partial g_{ki}}{\partial x^{j}} + \frac{\partial g_{kj}}{\partial x^{i}} - \frac{\partial g_{ij}}{\partial x^{k}} \right). \tag{C.84}$$

Consider the Grushin vector fields in (1.20) for $m = 1$, and the coordinates (x, y) are understood as (x^1, x^2) in the above formulas. The metric is given by

$$(g_{ij}) = \begin{pmatrix} 1 & 0 \\ 0 & x^{-2} \end{pmatrix}, \qquad (g^{ij}) = (g_{ij})^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & x^2 \end{pmatrix}. \tag{C.85}$$

A slight calculation shows

$$R(x, y) = -\frac{4}{x^2}, \qquad x \neq 0. \tag{C.86}$$

Acknowledgement

This research project was initiated when the authors visited the National Center for Theoretical Sciences (NCTS), Hsinchu, Taiwan during January 2013, and the final version of the paper was completed while the authors visited NCTS during July 2014. They would like to express their profound gratitude to the Director of NCTS, Professor Winnie Li, for her invitation and for the warm hospitality extended to them during their stay in Taiwan. The work of D.-C. Chang is partially supported by Hong Kong RGC competitive earmarked research grants #600607, #601410 and a competitive research grant at Georgetown University. The work of Y. Li is partially supported by a General Research Fund from Hong Kong Research Grant Committee (Grant no. 201513).

References

[1] A. A. Agrachev, Exponential mappings for contact sub-Riemannian structures, *J. Dynam. Control Systems* **2** (1996), 321-358. doi: 10.1007/BF02269423

[2] D. Barilari, U. Boscain, and R.W. Neel, Small-time heat kernel asymptotics at the sub-Riemannian cut locus, *J. Differential Geom.* **92** (2012), 373-416. Article

[3] R. Beals, B. Gaveau and P. C. Greiner, Hamilton-Jacobi theory and the heat kernel on Heisenberg groups, *J. Math. Pures Appl.* **79** (2000), 633-689. doi: 10.1016/S0021-7824(00)00169-0

[4] G. Ben Arous: Développement asymptotique du noyau de la chaleur hypoelliptique sur la diagonale, *Ann. Inst. Fourier* **39** (1989), 73-99. Article

[5] G. Ben Arous and R. Léandre, Décroissance exponentielle du noyau de la chaleur sur la diagonale I, *Probab. Th. Rel. Fields* **90** (1991), 175-202. doi: 10.1007/BF01192161

[6] G. Ben Arous and R. Léandre, Décroissance exponentielle du noyau de la chaleur sur la diagonale II, *Probab. Th. Rel. Fields* **90** (1991), 377-402. doi: 10.1007/BF01193751

[7] R.W. Brockett and A. Mansouri, Short-time asymptotics of heat kernels for a class of hypoelliptic operators, *Amer. J. Math.* (2009), 1795-1814. doi: 10.1353/ajm.0.0081

[8] O. Calin and D.-C. Chang, SubRiemannian geometry, a variational approach, *J. Differential Geom.* **80** (2008), 23-43. Article

[9] O. Calin, D.-C. Chang, and P. Greiner, *Geometric Analysis on the Heisenberg Group and Its Generalizations*, American Mathematical Society, Providence, RI; International Press, Somerville, MA, 2007.

[10] O. Calin, D.C. Chang, J. Hu, and Y. Li, On heat kernels of a class of degenerate elliptic operators, *J. Nonlinear Convex Anal.*, **12** (2011), 309-340. Article

[11] C.-H. Chang, D.-C. Chang, B. Gaveau, P. Greiner, and H.-P. Lee, Geometric analysis on a step 2 Grusin operator, *Bull. Inst. Math. Acad. Sin. (N.S.)* **4** (2009), 119-188. Article

[12] D.-C. Chang and Y. Li, SubRiemannian geodesics in the Grushin plane, *J. Geom. Anal.* **22** (2012), 800-826. doi: 10.1007/s12220-011-9215-y

[13] W. L. Chow, Über Systeme von Linearen partiellen Differentialgleichungen erster Ordnung, *Math. Ann.* **117** (1939), 98-105. Article

[14] C. L. Frenzen and R. Wong, Uniform asymptotic expansions of Laguerre polynomials. *SIAM J. Math. Anal.* **19** (1988), 1232-1248. doi: 10.1137/0519087

[15] B. Gaveau, Principe de moindre action, propagation de la chaleur et estimées sous-elliptiques sur certains groupes nilpotents, *Acta Math.* **139** (1977), 95-153. doi: 10.1007/BF02392235

[16] P. Greiner, A Hamiltonian approcah to the heat kernel of a subLaplacian on S^{2n+1}, *Anal. Appl.*, **11** (2013), aricle no.: 1350035, 62pp. doi: 10.1142/S0219530513500358
[17] V.V. Grushin, On a class of hypoelliptic operators, *Math. USSR Sb.* **12** (1970), 456-473. doi: 10.1070/SM1970v012n03ABEH000931
[18] L. Hörmander, Hypoelliptic second order differential equations, *Acta Math.*, **119** (1967), 147-171. doi: 10.1007/BF02392081
[19] A. Hulanicki, The distribution of energy in the Brownian motion in the Gausssian field and analytic hypoellipticity of certain subelliptic operators on the Heisenberg group, *Studia Math.* **56** (1976), 165-173. Article
[20] M. Kac, Can one hear the shape of a drum? *Amer. Math. Monthly* **73** (1966), 1-23. doi: 10.2307/2313748
[21] R. Léandre, Majoration en temps petit de la densité dune diffusion dégénérée, *Probab. Theory Related Fields* **74** (1987), 289-294. doi: 10.1007/BF00569994
[22] R. Léandre, Minoration en temps petit de la densité dune diffusion dégénérée, *J. Funct. Anal.* **74** (1987), 399-414. doi: 10.1016/0022-1236(87)90031-0
[23] J. L. López and P. J. Pagola, An explicit formula for the coefficients of the saddle point method, *Constr. Approx.*, **33** (2011), 145-162. doi: 10.1007/s00365-010-9089-4
[24] H. P. McKean, Jr. and I. M. Singer, Curvature and the eigenvalues of the Laplacian, *J. Differential Geom.* **1** (1967), 43-69. Article
[25] J. Mitchell, On Carnot-Carathéodory metrics, *J. Differential Geom.*, **21** (1985), 35-45. Article
[26] S. A. Molchanov, Diffusion processes and Riemannian geometry, *Russian Math. Surveys* **30** (1975), 1-63. doi: 10.1070/RM1975v030n01ABEH001400
[27] G. Nemes, An explicit formula for the coefficients in Laplace's method, *Constr. Approx.*, **38** (2013), 471-487. doi: 10.1007/s00365-013-9202-6
[28] F. W. J. Olver, *Asymptotics and Special Functions*, A. K. Peters, Wellesley, MA, 1997.
[29] F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark, *NIST Handbook of Mathematical Functions*, Cambridge University Press, New York, 2010. `http://dlmf.nist.gov`
[30] C. Séguin and A. Mansouri, Short-time asymptotics of heat kernels of hypoelliptic Laplacians on unimodular Lie groups, *J. Funct. Anal.* **262** (2012), 3891-3928. doi: 10.1016/j.jfa.2012.02.004
[31] S. R. S. Varadhan, On the behaviour of the fundamental solution of the heat equation with variable coefficients, *Comm. Pure Appl. Math.* **20** (1967), 431-455. doi: 10.1002/cpa.3160200210
[32] S. R. S. Varadhan, Diffusion processes in a small time interval, *Comm. Pure Appl. Math.* **20** (1967), 659-685. doi: 10.1002/cpa.3160200404
[33] J. Wojdylo, Computing the coefficients in Laplace's method, *SIAM Rev.*, **48** (2006), 76-96. doi: 10.1137/S0036144504446175
[34] R. Wong, *Asymptotic Approximation of Integrals*, Academic Press, Boston, 1989; Reprinted by SIAM, Philadelpha, 2001.
[35] H. Weyl, Über die asymptotische Verteilung der Eigenwerte, *Nachrichten der Königlichen Gesellschaft der Wissenschaften zu Göttingen*, (1911), 110-117. Article

Department of Mathematics and Department of Computer Sciences, Georgetown University, Washington D.C. 20057, USA, and Department of Mathematics, Fu Jen Catholic University, Taipei 242, Taiwan, ROC
E-mail address: `chang@georgetown.edu`

Department of Mathematics, Hong Kong Baptist University, Kowloon, Hong Kong
E-mail address: `yutianli@hkbu.edu.hk`