Computation of heat asymptotics for nonminimal Laplace type operators: from theory to computer

(Work in progress with Bruno Iochum)

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Thierry Masson

Centre de Physique Théorique

The problem

- V a smooth hermitean vector bundle V (fiber $\mathbb{C}^N$) over a compact d-dimensional boundaryless Riemannian manifold (M, g).
- P a nonminimal Laplace type operator acting on smooth sections $\Gamma(V)$:

$$\begin{aligned} P &= -[g^{\mu\nu} u \partial_\mu \partial_\nu + v^\mu \partial_\nu + w] \\ &= -g^{\mu\nu} u \nabla_\mu \nabla_\nu - \big(p^\nu + g^{\mu\nu}(\nabla_\mu u) - \Gamma^\nu u\big)\nabla_\nu - q \end{aligned}$$

  - ∇_μ gauge (only) covariant derivative,
  - u, v^μ, w, p^μ, q are $M_N(\mathbb{C})$ matrix valued functions,
  - $u(x)$ positive and invertible (for any x),
  - u, p^μ, q have homogeneous gauge and diff. transformations (sections of $\mathrm{End}(V)$),
  - $\Gamma^\nu := g^{\mu\rho}\Gamma^\nu_{\mu\rho}$ where the $\Gamma^\nu_{\mu\rho}$ = Christoffel symbols of g.
- For any $a \in \Gamma(\mathrm{End}(V))$, consider the asymptotics of the heat-trace

$$\mathrm{Tr}[a e^{-tP}] \underset{t \downarrow 0^+}{\sim} \sum_{r=0}^{\infty} a_r(a, P)\, t^{(r-d)/2}$$

- **Compute $\mathcal{R}_r$ defined by**

$$a_r(a, P) = \int_M \mathrm{tr}[a(x)\mathcal{R}_r(x)]\, \mathrm{dvol}_g(x).$$

The key steps for the computation

Iochum, B. and Masson, T. (2017). Heat trace for Laplace type operators with non-scalar symbols. *Journal of Geometry and Physics* 116, pp. 90–118
Iochum, B. and Masson, T. (2018). Heat asymptotics for nonminimal Laplace type operators and application to noncommutative tori. *Journal of Geometry and Physics* 129, pp. 1–24

- $\mathrm{Tr}[ae^{-tP}] = \int \mathrm{d}x\ \mathrm{tr}[a(x)K(t,x,x)]$ with $K(t,x,x)$ diagonal of the kernel of e^{-tP}:
$$\int_M \mathrm{d}y\, K(t,x,y)s(y) = (e^{-tP}s)(x),\ \text{for any } s \in \Gamma(V)$$
- It is well known that
$$K(t,x,y) = (2\pi)^{-d} \int_{\mathbb{R}^d} \mathrm{d}\xi\, e^{-iy\cdot\xi}(e^{-tP}e^{ix\cdot\xi}) : \mathbb{C}^N \longrightarrow \mathbb{C}^N.$$
- One has (first trick):
$$-Pe^{ix\xi}s = -e^{ix\xi}[H+K+P]s,\ \text{with} \begin{cases} K := -i\xi_\mu\big(p^\mu + g^{\mu\nu}(\nabla_\nu u) - \Gamma^\mu u + 2g^{\mu\nu}u\nabla_\nu\big) \\ H := g^{\mu\nu}u\,\xi_\mu\xi_\nu \end{cases}$$
then, at fixed x, $K(t,x,x)$ is the linear operator (on $\mathbb{C}^N$):
$$\mathbb{C}^N \ni v \mapsto K(t,x,x)v = t^{-d/2}(2\pi)^{-d}\int_{\mathbb{R}^d} \mathrm{d}\xi\, e^{-H-\sqrt{t}K-tP}v.$$

The key steps (cont'd)

- One uses (second trick) the Volterra series

$$e^{A+B} = e^{A} + \sum_{k=1}^{\infty} \int_{\Delta_k} \mathrm{d}s\, e^{(1-s_1)A}\, B\, e^{(s_1-s_2)A} \dots e^{(s_{k-1}-s_k)A}\, B\, e^{s_k A},$$

where $\Delta_k := \{s = (s_1, \dots, s_k) \in \mathbb{R}_+^k \,|\, 0 \leq s_k \leq s_{k-1} \leq \cdots \leq s_2 \leq s_1 \leq 1\}$ ($\Delta_0 := \emptyset$)

- Then

$$e^{-H-\sqrt{t}K-tP} v = e^{-H} v + \sum_{k=1}^{\infty} (-1)^k f_k(\xi)[(\sqrt{t}K + tP) \otimes \cdots \otimes (\sqrt{t}K + tP)] v$$

where, for any $k \in \mathbb{N}$, the map $f_k(\xi) : M_N[\xi, \nabla]^{\otimes^k} \longrightarrow M_N[\xi]$ is defined by

$$f_k(\xi)[B_1 \otimes \cdots \otimes B_k] := \int_{\Delta_k} \mathrm{d}s\, e^{(s_1-1)H}\, B_1\, e^{(s_2-s_1)H}\, B_2\, e^{(s_3-s_2)H} \dots B_k\, e^{-s_k H},$$

$$f_0(\xi)[z] := z\, e^{-H}, \quad \text{for } z \in \mathbb{C} =: M_N^{\otimes^0}.$$

- The B_i are matrix-valued diff. op. in ∇_μ depending on x and (polynomials in) ξ.

The key steps (cont'd)

- Then one has to compute:

$$a_0(a,P)(x) = \operatorname{tr} \frac{|g|^{-1/2}}{(2\pi)^d} a(x) \int_{\mathbb{R}^d} d\xi\, f_0[1],$$

$$a_2(a,P)(x) = \operatorname{tr} \frac{|g|^{-1/2}}{(2\pi)^d} a(x) \int_{\mathbb{R}^d} d\xi\, (f_2[K \otimes K] - f_1[P]),$$

$$a_4(a,P)(x) = \operatorname{tr} \frac{|g|^{-1/2}}{(2\pi)^d} a(x) \int_{\mathbb{R}^d} d\xi\, (f_2[P \otimes P] - f_3[K \otimes K \otimes P] - f_3[K \otimes P \otimes K] - f_3[P \otimes K \otimes K] + f_4[K \otimes K \otimes K \otimes K]),$$

etc.

- Strategy for the computation:
  1. Compute and characterize the operators $f_k : M_N[\xi, \nabla]^{\otimes^k} \longrightarrow M_N[\xi]$;
  2. Take care of the operators ∇_μ in the arguments…

Let us use the notations:

$$H^{\mu\nu} := g^{\mu\nu} u, \qquad L^\mu := p^\mu + g^{\mu\nu}(\nabla_\nu u) - \Gamma^\mu u, \qquad K^\mu := -i\big(L^\mu + 2H^{\mu\nu}\nabla_\nu\big),$$

$$H = H^{\mu\nu}\xi_\mu\xi_\nu, \qquad K = K^\mu \xi_\mu, \qquad P = -H^{\mu\nu}\nabla_\mu\nabla_\nu - L^\mu\nabla_\mu - q.$$

The universal operators

- Define the functions of $r_i \in$ spectrum of $u(x)$ (x is fixed):
$$I_{\alpha,k}(r_0, r_1, \dots, r_k) := \int_{\Delta_k} \mathrm{d}s\, [(1 - s_1) r_0 + (s_1 - s_2) r_1 + \cdots + s_k r_k]^{-\alpha}$$
- Define the associated (x-dependent) operators $X_{\alpha,k} \in \mathcal{B}(M_N^{\otimes^k}, M_N)$ by
$$X_{\alpha,k}[B_1 \otimes \cdots \otimes B_k] := I_{\alpha,k}(r_0, \dots, r_k)\, E_0 B_1 E_1 \cdots B_k E_k$$
with summation over $k+1$-uplets $(r_0, \dots, r_k)$ of spectral values of $u(x)$, E_i the spectral projection of $u(x)$ associated to r_i.
- One has
$$X_{d/2+p,k,\mu_1\dots\mu_{2p}} := G_{\mu_1\dots\mu_{2p}} X_{d/2+p,k} = \frac{1}{g_d} \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \mathrm{d}\xi\, \xi_{\mu_1} \cdots \xi_{\mu_{2p}}\, f_k(\xi)$$
with
$$G_{\mu_1\dots\mu_{2p}} := \frac{1}{2^{2p}\, p!} \sum_{\rho \in S_{2p}} g_{\mu_{\rho(1)}\mu_{\rho(2)}} \cdots g_{\mu_{\rho(2p-1)}\mu_{\rho(2p)}}$$
(S_{2p} = symm. group of perm. on $2p$ elements) and $g_d = \dfrac{|g|^{1/2}}{2^d\, \pi^{d/2}}$.
- **Everything here depend only on u and $g^{\mu\nu}$, not on P.**

Propagation of the ∇_μ

- To compute $\mathcal{R}_r$, we start with terms of the form

$$\frac{1}{(2\pi)^d} \int \mathrm{d}\xi\, \xi_{\mu_1} \cdots \xi_{\mu_{2p}}\, f_k(\xi) [(B_1 \otimes \cdots \otimes B_k)^{\mu_1 \cdots \mu_{2p}}] = g_d X_{d/2+p,k,\mu_1\dots\mu_{2p}} [(B_1 \otimes \cdots \otimes B_k)^{\mu_1 \cdots \mu_{2p}}]$$

- Let $Q[A]$ be a matrix-valued function written as a polynomial in the A_μ and their derivatives (∇_μ repeatedly acting on $v \in \mathbb{C}^N$). One main result is

$$\begin{aligned} &X_{d/2+p,k,\mu_1\dots\mu_{2p}} [(B_1 \otimes \cdots \otimes B_i \nabla_\nu \otimes \cdots \otimes B_k)^{\mu_1 \cdots \mu_{2p}}] Q[A] \\ &= \sum_{j=i+1}^{k} X_{d/2+p,k,\mu_1\dots\mu_{2p}} [(B_1 \otimes \cdots \otimes (\nabla_\nu B_j) \otimes \cdots \otimes B_k)^{\mu_1 \cdots \mu_{2p}}] Q[A] \\ &\quad - \sum_{j=i}^{k} X_{d/2+p+1,k+1,\mu_1\dots\mu_{2(p+1)}} [(B_1 \otimes \cdots \otimes B_j \otimes (\nabla_\nu H^{\mu_{2p+1}\mu_{2p+2}}) \otimes \cdots \otimes B_k)^{\mu_1 \cdots \mu_{2p}}] Q[A] \\ &\quad + X_{d/2+p,k,\mu_1\dots\mu_{2p}} [(B_1 \otimes \cdots \otimes B_i \otimes \cdots \otimes B_k)^{\mu_1 \cdots \mu_{2p}}] (\nabla_\nu Q[A]). \end{aligned}$$

Use repeatedly ➞ all the ∇_ν are applied...

Computation of $\mathcal{R}_2$

$$H^{\mu\nu} := g^{\mu\nu} u, \qquad L^\mu := p^\mu + g^{\mu\nu}(\nabla_\nu u) - \Gamma^\mu u, \qquad K^\mu := -i\big(L^\mu + 2H^{\mu\nu}\nabla_\nu\big),$$
$$H = H^{\mu\nu}\xi_\mu\xi_\nu, \qquad K = K^\mu \xi_\mu, \qquad P = -H^{\mu\nu}\nabla_\mu\nabla_\nu - L^\mu\nabla_\mu - q.$$

- Start with
$$\mathcal{R}_2 = \frac{1}{2^d\, \pi^{d/2}} \left(X_{d/2+1,2,\mu_1\mu_2}[K^{\mu_1} \otimes K^{\mu_2}] - X_{d/2,1}[P] \right).$$
- Propagate the ∇_μ ➡ **24 terms** (after simplifications).
- Replace $H^{\mu\nu}$, L^μ and their derivatives (use normal coordinates)…

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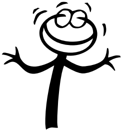
$$\mathcal{R}_2 = \frac{1}{2^d\,\pi^{d/2}}\Big(X_{d/2+1,2,\mu_1\mu_2}[K^{\mu_1}\otimes K^{\mu_2}] - X_{d/2,1}[P]\Big).$$

- Propagate the ∇_μ ➞ **24 terms** (after simplifications).
- Replace $H^{\mu\nu}$, L^μ and their derivatives (use normal coordinates)...
- Final result, with $\widehat{\nabla}_\mu$ the "full covariant derivative" (gauge + Riemannian):

$$\begin{aligned}\mathcal{R}_2 = \frac{1}{2^d\,\pi^{d/2}}\Big(&\tfrac{1}{6}\mathfrak{R}\, X_{d/2,1}[u] + X_{d/2,1}[q] - X_{d/2+1,2}[u\otimes \widehat{\nabla}_\mu p^\mu] \\ &+ \frac{1}{2}\, g^{\mu\nu}\, X_{d/2+1,2}[(\widehat{\nabla}_\mu u + p_\mu)\otimes(\widehat{\nabla}_\nu u - p_\nu)] \\ &- \frac{d+2}{2}\, g^{\mu\nu}\, X_{d/2+2,3}[u\otimes \widehat{\nabla}^2_{\mu\nu} u \otimes u] \\ &- \frac{d+2}{2} g^{\mu\nu}\, X_{d/2+2,3}[u\otimes \widehat{\nabla}_\mu u\otimes(\widehat{\nabla}_\nu u - p_\nu)] \\ &- \frac{d+2}{2} g^{\mu\nu}\, X_{d/2+2,3}[(\widehat{\nabla}_\mu u + p_\mu)\otimes \widehat{\nabla}_\nu u \otimes u] \\ &+ \frac{(d+2)(d+4)}{2}\, g^{\mu\nu}\, X_{d/2+3,4}[u\otimes \widehat{\nabla}_\mu u \otimes \widehat{\nabla}_\nu u\otimes u]\Big).\end{aligned}$$



Computation of $\mathcal{R}_4$

- Start with

$$\mathcal{R}_4 = \frac{1}{2^d\,\pi^{d/2}}\Big(X_{d/2,2}[P \otimes P] - X_{d/2+1,3,\mu_1\mu_2}[K^{\mu_1} \otimes K^{\mu_2} \otimes P] - X_{d/2+1,3,\mu_1\mu_2}[K^{\mu_1} \otimes P \otimes K^{\mu_2}] - X_{d/2+1,3,\mu_1\mu_2}[P \otimes K^{\mu_1} \otimes K^{\mu_2}] + X_{d/2+2,4,\mu_1\mu_2\mu_3\mu_4}[K^{\mu_1} \otimes K^{\mu_2} \otimes K^{\mu_3} \otimes K^{\mu_4}]\Big).$$

- Propagate the ∇_μ ➞ **3771 terms** (after simplifications!).

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$\mathcal{R}_4$: computer enters the game...

- All the manipulations in the method are "symbolic" and "combinatorial".
- A computer algebra system should do the work for us!
- Requirements:
  - Derivations (∇_μ);
  - Noncommutative products (matrix algebra)...
  - mixed with commutative products (metric...);
  - Tensor products;
  - Riemannian tensor manipulations (in normal coordinates);
  - Gauge field strength and its derivatives;
  - Contractions of indices;
  - Simplification of expressions combining all these structures...

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- First tentative: Mathematica...

  ➞ Not easy to make it understand all these requirements!
- Present tentative: **home made object oriented software**.
  - We manipulate (programmed) "objects" that reproduce our (math.) "objects"...
  - Can be written in lot of languages: we (I) chose Javascript with Node.
    (I am used to Javascript, favorable benchmarks compared to Python...)

Problems and benefits...

- We (Bruno and me) are not specialist in “formal mathematical manipulations” on computers...
  - How to simplify?
  - How to tell the software that we want a expression instead of another?
- How to be sure that the software computes what we want?

- The software is designed for the method and we can add filters, post operations (simplifications), etc...
- LaTeX exportation...

Some preliminary results...

- The 3771 terms can be sorted according to the only 5 values of $Q[A]$: $\mathbb{1}$ (2026 terms), $\nabla_{\nu_1}\mathbb{1}$ (1296 terms), $\nabla^2_{\nu_1\nu_2}\mathbb{1}$ (382 terms), $\nabla^3_{\nu_1\nu_2\nu_3}\mathbb{1}$ (62 terms), and $\nabla^4_{\nu_1\nu_2\nu_3\nu_4}\mathbb{1}$ (5 terms).

- $Q[A] = \nabla_{\nu_1}\mathbb{1}$: no gauge homogeneous expression ➙ should be 0. This is what the computer returns!

- $Q[A] = \nabla^4_{\nu_1\nu_2\nu_3\nu_4}\mathbb{1}$: the only gauge homogeneous expression is $F_{\mu\nu}F^{\mu\nu}$. The computer produces (directly) only one term:
$$\frac{1}{12}\,X_1[u]\,F^{\nu_1\nu_2}F_{\nu_1\nu_2}.$$
Special case $u = \mathbb{1}$: this reduces to $\frac{1}{12}\,F^{\nu_1\nu_2}F_{\nu_1\nu_2}$ and agrees with results in Gilkey, P. B. (2003). *Asymptotic formulae in spectral geometry.* CRC press.

Some preliminary results (cont'd)...

- $Q[A] = \nabla^3_{\nu_1 \nu_2 \nu_3} \mathbb{1}$: let $\mathcal{X}_{(3)}[a] := \frac{1}{6} X_1[a] - X_3[u \otimes a \otimes u]$, then

$$
\begin{aligned}
&- 4\, g^{\nu_1 \nu_2} g^{\nu_3 \nu_4}\, X_5[(\widehat{\nabla}_{\nu_4} u) \otimes u \otimes u \otimes u \otimes u]\, (\widehat{\nabla}_{\nu_1} F_{\nu_2 \nu_3}) \\
&+ d\, g^{\nu_1 \nu_2} g^{\nu_3 \nu_4}\, X_5[u \otimes (\widehat{\nabla}_{\nu_4} u) \otimes u \otimes u \otimes u]\, (\widehat{\nabla}_{\nu_1} F_{\nu_2 \nu_3}) \\
&- d\, g^{\nu_1 \nu_2} g^{\nu_3 \nu_4}\, X_5[u \otimes u \otimes u \otimes (\widehat{\nabla}_{\nu_4} u) \otimes u]\, (\widehat{\nabla}_{\nu_1} F_{\nu_2 \nu_3}) \\
&+ 4\, g^{\nu_1 \nu_2} g^{\nu_3 \nu_4}\, X_5[u \otimes u \otimes u \otimes u \otimes (\widehat{\nabla}_{\nu_4} u)]\, (\widehat{\nabla}_{\nu_1} F_{\nu_2 \nu_3}) \\
&- g^{\nu_1 \nu_2}\, \mathcal{X}_{(3)}[p^{\nu_3}]\, (\widehat{\nabla}_{\nu_1} F_{\nu_2 \nu_3}).
\end{aligned}
$$

  ➞ more simplifications to expect?

- $Q[A] = \nabla^2_{\nu_1 \nu_2} \mathbb{1}$: work in progress, we analyze what the software has returned. "Post-production" on 31 terms...

- $Q[A] = \mathbb{1}$: that's the big piece of the cake!
  - Use normal coordinates up to 4-th derivatives of $H^{\mu\nu}$...
  - Replace gauge covariant derivatives with full covariant derivatives...
  - Introduce derivations of Riemann and Ricci tensors...
  - Self (full) contractions of Riemann tensor and Ricci tensor...
  - Lot of work to be done "in post production" to get (human) readable expression...

Conclusions

- The method gives "universal" formulas in terms of universal operators.
- These formulas can be instantiated to specific situations:
  - "diagonal" case $u = \mathbb{1}$ ➞ know results...
  - Noncommutative Torus ➞ we confirm results by Connes, Tretkoff, Moscovici, Fathizadeh, Khalkhali... (avoid NC pseudodifferential calculus).

- Search for "hidden" structures (patterns) in the result.
  Wait and see what $\mathcal{R}_4$ will tell us...

- The software could help compute $\mathcal{R}_r$ for large r...
  with the help of a powerful computer?

- The method could (should!) work in NCG:
  spectral decompositions, algebraic constructions, traces...

- Only work with leading term $-g^{\mu\nu} u \nabla_\mu \nabla_\nu$ in P...