5. The Heat Kernel

5.a. **The heat operator.**

5.1. The Dirichlet problem for the Laplace-Beltrami operator. We so far have worked with the Dirichlet Laplacian on a bounded domain in $\mathbb{R}^n$. We shall now also consider the case, where (Ω, g) is a smooth compact Riemannian manifold with boundary. In local coordinates we then define the Laplace-Beltrami operator, also denoted by Δ,

$$\Delta u(x) = \operatorname{div} \nabla u = \sqrt{\det g(x)}^{-1} \sum \partial_{x_j} (g^{jk}(x) \sqrt{\det g(x)} \partial_{x_k} u)(x).$$

Here one writes the metric locally as a matrix $g = g_{jk}$ and (g^{jk}) is the inverse matrix. This expression is in fact independent of the choice of coordinates. It defines a strongly elliptic second order differential operator in the interior of Ω. We additionally impose Dirichlet boundary conditions at the boundary. Then we have

$$\langle \Delta u, v \rangle_{L^2(\Omega)} = \langle \nabla u, \nabla v \rangle_{L^2(\Omega)}$$

for $u, v \in C^\infty(\Omega)$ with $u = 0$ on $\partial\Omega$. The right hand side extends to a closed semibounded form on $W_0^{1,2}(\Omega)$. We can therefore define $-\Delta_D$ as a selfadjoint operator on $L^2(\Omega)$ via Theorem 2.4. As before, the domain is $W^{2,2}(\Omega) \cap W_0^{1,2}(\Omega)$. It is not very difficult (the proof is basically as before) to see that $-\Delta_D$ is invertible and $(-\Delta_D)^{-1}$ is a compact operator on $L^2(\Omega)$. Therefore $-\Delta_D$ has a complete set of eigenfunctions $\{e_k : k \in \mathbb{N}\}$ for eigenvalues $0 < \lambda_1 \le \lambda_2 \le \ldots \to \infty$. It is also not hard to see that $\lambda_k \ge ck^{2/n}$ for a suitable constant c. In fact one can show that Weyl's formula also holds for this case - including the case when $\partial\Omega = \emptyset$.

5.2. The heat equation. The heat equation is the partial differential equation

$$\partial_t u - \Delta_D u = 0, \quad u(0) = u_0. \tag{1}$$

Here, u is considered a function of the variables $t \ge 0$ and $x \in \Omega$, where Ω is a bounded domain in $\mathbb{R}^n$ or a manifold with boundary, $-\Delta_D$ is the Dirichlet Laplacian, and u_0 is an initial value, say, $u_0 \in L^2(\Omega)$. Formally, the solution of the above equation is given by

$$u(t) = \exp(t\Delta_D)u_0,$$

and indeed this makes sense, as we shall see.

5.3. The heat kernel. Let Ω be a bounded domain in $\mathbb{R}^n$ or a compact manifold with boundary. Denote by $\{(e_k, \lambda_k) : k \in \mathbb{N}\}$ the set of eigenfunctions and eigenvalues, repeated according to multiplicity. We define the operator $\exp(t\Delta_D)$ by

$$\exp(t\Delta_D)u = \sum_{k=1}^{\infty} \exp(-t\lambda_k)\langle u, e_k \rangle e_k.$$

In view of the fact that $\lambda_k \ge ck^{2/n}$ the sum converges in $L^2(\Omega)$.
Moreover, $u(t,x) = \exp(t\Delta_D)u_0(x)$ solves the heat equation. In fact,

$$\partial_t u(t,x) = \sum_{k=1}^{\infty} \lambda_k \exp(-t\lambda_k)\langle u_0, e_k\rangle e_k = \Delta_D u(t,x), \quad u(0,x) = \sum_{k=1}^{\infty} \langle u_0, e_k\rangle e_k = u_0.$$

For $t > 0$ the operator $\exp(t\Delta_D)$ is an integral operator with the integral kernel

$$k_t = \sum_{k=1}^{\infty} \exp(-t\lambda_k) e_k \otimes \overline{e}_k.$$

Since $e_k \otimes \overline{e}_k$ has norm 1 in $L^2(\Omega \times \Omega)$, the sum converges in $L^2(\Omega \times \Omega)$.

5.4. Sobolev spaces on $\mathbb{R}^n$. For $s \in \mathbb{R}$, the space $H^s(\mathbb{R}^n)$ consists of all distributions u such that $\xi \mapsto (1+|\xi|^2)^{s/2}\hat{u}(\xi)$ is in L^2. Here $\hat{u}$ is the Fourier transform of u.
For $s \in \mathbb{N}_0$ this is equivalent to asking that u and its derivatives up to order s are in L^2. In particular for $s = 2$, we have

$$u \in H^2(\mathbb{R}^n) \Leftrightarrow (1+|\xi|^2)\hat{u}(\xi) \in L^2(\mathbb{R}^n) \Leftrightarrow (1-\Delta)u \in L^2(\mathbb{R}^n).$$

An important theorem is the Sobolev embedding theorem: $H^s(\mathbb{R}^n) \hookrightarrow C^k$ whenever $s > k + n/2$.

5.5. Theorem. *Let Ω be a bounded domain in $\mathbb{R}^n$ or a smooth compact Riemannian manifold with boundary.*

(a) *The eigenfunctions e_k of $-\Delta_D$ are smooth in the interior Ω° of Ω.*

(b) *For $t > 0$ the function $(t, x, y) \mapsto k_t(x, y)$ is smooth in $(0, 1) \times \Omega^\circ \times \Omega^\circ$.*

Proof. For simplicity assume $\Omega \subset \mathbb{R}^n$; the proof for manifolds works similarly.
(a) The fact that $e_k \in L^2(\Omega)$ and $-\Delta_D e_k = \lambda_k e_k \in L^2(\Omega)$ implies by iteration that, for every $\varphi \in C_c^\infty(\Omega)$ and every $m \in \mathbb{N}$, we have

$$(1-\Delta)^m(\varphi e_k) \in L^2(\mathbb{R}^n).$$

Taking the Fourier transform, $(1+|\xi|^2)^m(\varphi e_k)^\wedge \in L^2(\mathbb{R}^n)$, or, equivalently, $\varphi e_k \in H^{2m}(\mathbb{R}^n)$. By Sobolev's embedding theorem, $\varphi e_k \in C^\infty(\mathbb{R}^n)$. Hence e_k is smooth in Ω.
(b) We have

$$(1-i\partial_t)^l(1-\Delta_{D,x})^m(1-\Delta_{D,y})^{m'}k_t(x,y) = \sum_{k=1}^{\infty}(1+i\lambda_k)^l(1+\lambda_k)^m(1+\lambda_k)^{m'}e^{-t\lambda_k}e_k(x)\bar{e}_k(y).$$

We see that the sum of the L^2-norms of these derivatives converges, so that the above function is in L^2. Just as in the proof of (a) we obtain the smoothness. □

5.6. Remark. If the boundary is smooth, one can show the eigenfunctions are smooth up to the boundary (see Evans' book). It is hard to say what happens at the boundary, if that it not smooth.
In the sequel we will therefore work on a **smooth manifold with boundary, where the boundary might actually be empty.**

5.b. **The heat kernel on closed manifolds.** Let (Ω, g) be a closed[3] Riemannian manifold. Since $\partial\Omega = \emptyset$, we obtain from Theorem 5.6.

5.7. Corollary. *The heat kernel on a closed manifold Ω is a smooth function on $(0, 1) \times \Omega \times \Omega$.*

5.8. Lemma. *A function u on Ω belongs to $C^\infty(\Omega)$ if and only if its sequence of Fourier coefficients is rapidly decreasing.*

Proof. We have $u \in C^\infty(\Omega)$ if and only if $(1-\Delta)^m u \in L^2(\Omega)$ for every $k \in \mathbb{N}$. This in turn is equivalent to the fact that

$$(1+\lambda_k)^m\langle u, e_k\rangle \in \ell^2(\mathbb{N}) \text{ for all } m.$$

As $\lambda_k \sim k^{2/n}$, this shows the assertion. □

5.9. Proposition. *Let $u \in C^\infty(\Omega)$. Then $e^{t\Delta}u \to u$ in all (spacial) derivatives as $t \to 0^+$.*

[3]closed = compact and no boundary

Proof. We have

$$(1-\Delta)^m e^{t\Delta} u = \sum_{k=1}^{\infty} (1+\lambda_k)^m e^{-t\lambda_k} \langle u, e_k \rangle e_k.$$

As the Fourier coefficients of u are rapidly decreasing, we can take the limit $t \to 0^+$ under the summation and see that $(1-\Delta)^m e^{t\Delta} u \to (1-\Delta)^m u \in H^{2m}(\Omega)$ for all m. □

5.10. Lemma. *The heat kernel $k_t(x,y)$, considered as a smooth function on $(0,1)\times\Omega\times\Omega$ is uniquely determined by the facts that*

(i) $(1-\Delta)k_t(x,y) = 0$ *for all* $t>0, x, y \in \Omega$, *and*

(ii) *For* $f \in C^\infty(\Omega)$, $u(t,x) := \int k_t(\cdot,y) f(y)\, dS$ *converges to* f *in* $C(\Omega)$ *as* $t \to 0^+$.

Proof. We have seen that the heat kernel satisfies these properties.

Conversely, given $f \in C^\infty(\Omega)$, any function l_t with properties (i) and (ii) furnishes a function $u = u(t,x)$ which is smooth for $t>0$ with $\partial_t u = \Delta u$ and $\lim_{t\to 0} u(t,x) = f(x)$, i.e. a solution to the heat equation with initial value f. As the solution is unique (a fact we will not show here), $l_t = k_t$. □

5.11. The heat kernel on $\mathbb{R}^n$. We recall that on $\mathbb{R}^n$, the heat kernel is of the form

$$k_t(x,y) = (4\pi t)^{-n/2} \exp\Big(\frac{|x-y|^2}{4t}\Big).$$

Considering an initial heat distribution localized near a point, we may expect that, for small t, the heat kernel will approximately look this way. Following Grieser [3] we will show the theorem, below. It concerns the values of the heat kernel on the diagonal. It also holds in a neighborhood of it, but for later purposes, the diagonal values are the interesting ones:

5.12. Theorem. (*Minakshisumdaram and Pleijel, 1948*) *On a smooth Riemannian manifold the heat kernel, restricted to the diagonal in $\Omega\times\Omega$, has an asymptotic expansion*

$$k_t(x,x) \sim t^{-n/2}\big(a_0(x) + a_1(x)t + a_2(x)t^2 \ldots\big) \qquad \text{as } t \to 0^+.$$

The a_j are smooth functions on Ω and $a_j(x)$ is determined by the Riemannian metric and its derivatives in x.

The asymptotic expansion holds uniformly in x and therefore can be integrated. In view of the fact that

$$\int_\Omega k_t(x,x)\, dS = \int_\Omega \sum e^{-t\lambda_k} |e_k(x)|^2\, dS = \sum e^{-t\lambda_k} \int_\Omega |e_k(x)|^2\, dS = \sum e^{-t\lambda_k}$$

we obtain

$$\sum_{k=1}^{\infty} e^{-t\lambda_k} \sim t^{-n/2} \sum_{j=0}^{\infty} \alpha_j t^j, \quad \textit{with } \alpha_j = \int_\Omega a_j(x)\, dS.$$

5.13. Outline. For the proof we follow Grieser [3], where also missing details can be found. We will construct a sequence of function $K_j = K_j(t,x,y)$ on $(0,\infty)\times\Omega\times\Omega$ that 'converges to the heat kernel in a certain sense which we will specify, below. We note two important features of the heat kernel on $\mathbb{R}^n$:

(i) it has the prefactor $(4\pi t)^{-n/2}$

(ii) It is a smooth function of the variable $X = |x-y|/\sqrt{t}$, $t>0$, exponentially decaying as $X \to \infty$.

We therefore introduce $C^\infty([0,\infty)_{1/2})$ as the space of all functions f on $[0,\infty)$ that are smooth as functions of $\sqrt{t}$, i.e. there exists a $g \in C^\infty([0,\infty))$ such that $f(s^2) = g(s)$. We will similarly write $C^\infty([0,\infty)_{1/2}\times\Omega\times\Omega)$, etc.

5.14. Definition. Let $\alpha \le 0$. By Ψ_H^α, we denote the space of all functions $A \in C^\infty((0,\infty)\times\Omega^2)$ such that

(i) If $x \neq y$, then $\partial_{t,x,y}^\gamma A(t,x,y) = O(t^\infty)$ for all γ as $t \to 0^+$ (off diagonal decay).

(ii) For every $x \in \Omega$, there exists a local coordinate system $U \subset \mathbb{R}^n$ for x and a function $\tilde{A} \in C^\infty([0,\infty)_{1/2} \times \mathbb{R}^n \times U)$ such that

(1) $$A(t,x,y) = t^{-\frac{n+2}{2}-\alpha}\tilde{A}\Big(t, \frac{x-y}{\sqrt{t}}, y\Big), \quad x,y \in U.$$

(we are using local coordinates on the right hand side.) In addition we require $\tilde{A}$ to be rapidly decreasing in the second variable, i.e.

(2) $$\partial_{t,X,y}^\gamma \tilde{A}(t,X,y) = O(|X|^{-\infty}) \text{ as } |X| \to \infty,$$

uniformly in t and y, t bounded.

5.15. Remark.

(a) In Definition 5.14, $\tilde{A}$ is not uniquely defined. In fact, for fixed $t > 0$, $X = (x-y)/\sqrt{t}$ takes values in a compact set. However, for $|x-y| = X\sqrt{t}$ small, condition (ii) lets us conclude that

(1) $$\tilde{A}(t,X,y) = t^{(n+2)/2+\alpha}A(t, X\sqrt{t}+y, y)$$

(b) (ii) implies (i) if both x and y belong to U.

(c) The choice of α is not well motivated at this point. It measures the flatness of A in t for $x = y$ as $t \to 0^+$; it will become clear later on.

(d) Since $\tilde{A}$ is required to be smooth as a function of $\sqrt{t}$ up to $t = 0$, we have $\Psi_H^{\alpha-1/2} \subset \Psi_H^\alpha$.

5.16. Definition. Given $A \in \Psi_H^\alpha$, we define the function $\Phi_\alpha(A)$ on $T\Omega$ as follows: Let $X \in T_y\Omega$ be a tangent vector and let $\gamma : (-\varepsilon,\varepsilon) \to \Omega$ be a curve with $\gamma(0) = y$ and $\gamma'(0) = X$. We then let

$$\Phi_\alpha(A)(X,y) = \lim_{t\to 0^+} t^{(n+2)/+\alpha}A(t,\gamma(\sqrt{t}),y).$$

In local coordinates, for $X\sqrt{t}$ small (here X is a tangent vector at y in $\mathbb{R}^n$), this is equivalent to setting

$$\Phi_\alpha(A)(X,y) = \tilde{A}(0,X,y)$$

with the function $\tilde{A}$ from 5.14(2).

The function $\Phi_\alpha(A)$ gives the leading term in the expansion of A.

This is a smooth function on TM; moreover, it decays rapidly in the fiber direction. We write $\Phi_\alpha(A) \in C_{\mathscr{S}}^\infty(T\Omega)$.

5.17. Lemma.

(a) *Let $A \in \Psi_H^\alpha$. Then $\Phi_\alpha(A) = 0$ if and only if $A \in \Psi_H^{\alpha-1/2}(A)$.*

(b) *For every function $F \in C_{\mathscr{S}}^\infty(T\Omega)$ there exists an $A \in \Psi_H^\alpha$ having F as its leading term.*

In other words we have a short exact sequence

$$0 \to \Psi_H^{\alpha-1/2}(\Omega) \to \Psi_H^\alpha(\Omega) \to C_{\mathscr{S}}^\infty(T\Omega) \to 0.$$

Proof. (a) Clearly, $\Phi_\alpha(A) = 0$ if $A \in \Psi_H^{\alpha-1/2}(A)$. Conversely, the fact that $\tilde{A}$ is smooth as a function of $\sqrt{t}$ implies that $\Psi_H^\beta \subset \Psi_H^\alpha$ only if $\beta = \alpha - k/2$ for some $k \in \mathbb{N}_0$. This shows (a).

(b) Define A by 5.15(1) for a function $\tilde{A}$ with $\tilde{A}(0,X,y) = \Phi_\alpha(A)$. $\square$

5.18. Definition. We define the $*$-product of two smooth functions A, B on $(0,\infty)\times\Omega^2$ by

$$(A*B)(t,x,y)=\int_0^t\int_\Omega A(t-s,x,z)B(s,z,y)\,dS(z)ds,$$

provided the integral makes sense.

5.19. Proposition. *Let $A\in\Psi_H^\alpha$, $B\in\Psi_H^\beta$, $\alpha,\beta<0$. Then $A*B$ is defined and furnishes an element in $\Psi_H^{\alpha+\beta}$.*
In addition, we have he formula

$$\Phi_{\alpha+\beta}(A*B)(X,y)=\int_0^1\int_{\mathbb{R}^n}(1-\sigma)^{(n+2)/2-\alpha}\sigma^{(n+2)/2-\beta}\Phi_\alpha\Big(\frac{X-Z}{\sqrt{1-\sigma}}\Big)\Phi_\beta\Big(\frac{Z}{\sqrt{\sigma}}\Big)\,dZd\sigma.$$

Proof. Computation. □

5.20. Proposition. *Let $A\in\Psi_H^\alpha$ for $\alpha\le -1$. Then $(\partial_t-\Delta)A\in\Psi_H^{\alpha+1}$ and*

$$\Phi_{\alpha+1}(\partial_t-\Delta)A)(X,y)=\left[-\frac{n+2}{2}-\alpha-\frac{1}{2}X\partial_X-\Delta_X^{0,y}\right]\Phi_\alpha(A)(X,y).$$

Here $X\partial_X=\sum_{j=1}^n X_j\partial_{X_j}$ and $\Delta_X^{0,y}=\sum_{jk}g^{jk}\partial_{X_j}\partial_{X_k}$.

Proof. Write $A(t,x,y)=t^{-l}\tilde A(t,(x-y)/\sqrt{t},y)$ with $l=(n+2)/2+\alpha$. Then

$$\begin{aligned}\partial_tA(t,x,y) &= -lt^{-l-1}\tilde A(t,(x-y)/\sqrt{t},y)\\ &\quad -t^{-1}\partial_X\tilde A(t,(x-y)/\sqrt{t})\frac{1}{2}\frac{x-y}{t^{3/2}}+t^{-l}\partial_t\tilde A(t,(x-y)/\sqrt{t},y)\\ &= t^{-l-1}\left(-l-\frac{1}{2}X\partial_X\right)\tilde A(t,(x-y)/\sqrt{t},y)+R(t,x,y),\end{aligned}$$

where $R\in\Psi_H^{\alpha+1/2}$. In view of the fact that $\partial_{x_j}(t^{-l}A)=t^{-l-1/2}\partial_{X_j}\tilde A$ we find

$$\begin{aligned}\Delta_xA(t,x,y) &= t^{-l-1}\sum_{jk}g^{jk}(x)\partial_{X_j}\partial_{X_k}\tilde A+t^{-l-1/2}\sum_{j=1}^n b_j(x)\partial_{X_j}\tilde A\\ &= t^{-l-1}\sum_{jk}g^{jk}(y)\partial_{X_j}\tilde A+R_2\end{aligned}$$

with $R_2\in\Psi_H^{\alpha+1/2}$. Note that we have changed the argument of g^{jk}. In fact, a Taylor expansion shows that $g^{jk}(x)=g^{jk}(y)+h^{jk}(x,y)(x-y)$ with $(n\times n)$-matrix valued functions h^{jk}, so that we may write

$$g^{jk}(x)-g^{jk}(y)=\sqrt{t}h^{jk}(y+X\sqrt{t},y)X$$

The term R_2 consists of the term on the right hand side plus the sum of the terms $b_j(x)\partial_{X_j}\tilde A=b_j(y+X\sqrt{t})\partial_{X_j}\tilde A$ and therefore is an element of $\Psi_H^{\alpha+1/2}$. In particular, R_1 and R_2 do not contribute to $\Phi_\alpha(A)$. □

We will next see what happens at $t=0$. The first result:

5.21. Lemma. (a) *Let $A\in\Psi_H^{-1}$ and $f\in C^\infty(\Omega)$, Then*

$$Af(t,x)=\int_\Omega A(t,x,y)f(y)\,dS(y)$$

defines an element of $C^\infty([0,\infty)_{1/2}\times\Omega)$ and

$$Af(0,x)=f(x)\int_{T_x\Omega}\Phi_{-1}(A)(X,x)\,dX.$$

(b) *If* $A \in \Psi_H^\alpha(\Omega)$ *for some* $\alpha < -1$, *then* $Af(0,x) = 0$.

Proof. In local coordinates in $\mathbb{R}^n$ we compute

$$\int A(t,x,y)f(y)\,dy = t^{-(n+2)/2-\alpha}\tilde{A}(t,(x-y)/\sqrt{t},y)\,dy \overset{X=(x-y)/\sqrt{t}}{=} t^{-1-\alpha}\int \tilde{A}(t,X,x-X\sqrt{t})f(x-X\sqrt{t})\,dX.$$

It is clear that this defines a smooth function of $\sqrt{t}$ and x for $\alpha \le -1$ and that Af vanishes for $t = 0$ whenever $\alpha < -1$. For $\alpha = -1$, we have

$$Af(0,x) = \int \tilde{A}(0,X,x)f(x)\,dz = f(x)\int \Phi_{-1}(A)(X,x)\,dX.$$

□

Now we will see how to construct an exact solution.

5.22. Lemma. *Suppose that* $K_1 \in \Psi_H^{-1}$ *satisfies*

(1) $$(\partial_t - \Delta_x)K_1(t,x,y) = R(t,x,y) \in \Psi_H^{-1+1/2}(\Omega) \text{ and } \lim_{t\to 0^+} K_1(t,x,y) = \delta_x(y)$$

and that $S \in \Psi_H^\beta$ *for* $\beta < 0$. *Then*

$$(\partial_t - \Delta_x)(K_1 * S) = S + R * S \text{ and } \lim_{t\to 0^+} K_1 * S = 0.$$

Proof. By definition

$$(K_1 * S)(t,x,y) = \int_0^t \int_\Omega K_1(t-s,x,z)S(s,z,y)dzdy.$$

Since $\partial_t \int_0^t h(t,s)ds = h(t,t) + \int_0^t \partial_t h(t,s)\,ds$ for continuous h, the first assertion is immediate (the convergence of the integral is seen as in the proof of Lemma 5.21). The second assertion follows from Lemma 5.21(b) together with the fact that $K_1 * S \in \Psi_H^{-1+\beta}$. □

5.23. Lemma. *Assume that* 5.22(1) *holds with* $R \in \Psi_H^{-1/2}$. *Define*

$$K = \sum_{j=0}^\infty (-1)^j K_1 * R^{*j} = K_1 + K_1 * R + K_1 * R * R + \dots.$$

Then (a) *The series converges*[4] *in* $C^\infty([0,\infty)\times\Omega\times\Omega)$.
(b) K *satisfies* 5.22(1) *with* $R = 0$, *i.e.* K *solves the heat equation in the distributional sense.*
(c) *The series gives an asymptotic expansion in that* $K_1 * R^{j*} \in \Psi_H^{-1-j/2}$.

Proof. (a) Let $j \ge n/2+1$ and $S = R^{j*} \in \Psi_H^{-j/2}$. In particular, S is continuous in t up to $t = 0$. Then

$$S^{m*}(t,x,y) = \int_{0\le t_1\le\ldots\le t_{m-1}\le t}\int_{\Omega^{m-1}} S(t-t_1,x,z_1)S(t_1-t_2,z_1,z_2)\dots \times S(t_{m-1},z_{m-1},y)dz_1\dots dz_{m-1}dt_1\dots dt_{m-1}$$

Let us show that this integral converges for $(t,x,y) \in M = [0,T]\times\Omega^2$ as $m\to\infty$ together with all derivatives for all $T > 0$. Suppose first we have no derivatives. Let $C = \max_M |S(t,x,y)|$.

[4]It is not a function in $C^\infty([0,\infty)\times\Omega\times\Omega)$, however, since the first terms are not in this space

The integral with respect to t is over an $m-1$-simplex of size T. Its volume is $T^{m-1}/(m-1)!$. We therefore estimate

$$\max_M |S^{m*}(t,x,y)| \le \frac{T^{m-1}(\operatorname{vol}\Omega)^{m-1}C^m}{(m-1)!}.$$

Since $|R^{(j+k)*}|$ is bounded on M for $k=0,1,\ldots,j$, say by C', we obtain a corresponding bound also for $\max_M |R^{(jm+k)*}|$. Hence the series converges uniformly.

Using the fact that functions in $A\in\Psi_H^\alpha$ are of the form $A(t,x,y)=t^{-(n+2)/2-\alpha}\tilde A(t,(x-y)/\sqrt t,y)$ for $\tilde A$ smooth in $\sqrt t$, we find a corresponding estimate also for the derivatives in t,x and y (we have to take j larger as the number of derivatives increases). Hence the series converges in C^∞ (note, however, that the full series is not in C^∞ since the first terms are not due to the factor $t^{-n/2}$ in K_1).

(b) The fact that K_1 satisfies 5.22(1) together with Lemma 5.22 implies by iteration that $(\partial_t-\Delta_x)K_1=R$ and $(\partial_t-\Delta_x)(K_1*R^{j*})=R^{j*}+R^{(j+1)*}$ for $j\ge1$. We therefore have

$$(\partial_t-\Delta_x)\Big(\sum_{j=0}^k(-1)^jK_1*R^{*j}\Big)=R^{(k+1)*}.$$

According to (a) the series converges to zero.

(c) follows from the fact that $\Psi_H^\alpha*\Psi_H^\beta\subseteq\Psi_H^{\alpha+\beta}$, see Proposition 5.19. □

5.24. Lemma. *In local coordinates on Ω define*

$$K_1(t,x,y)=(4\pi t)^{-n/2}\exp\Big(\frac{|x-y|^2_{g(y)}}{4t}\Big),$$

where $|x|^2_{g(y)}=\sum_{j,k=1}^n g_{jk}(y)x_jx_k$. Then K_1 satisfies the assumptions of Lemma 5.22 and therefore furnishes the heat kernel via the above process.

Proof. Write $K(t,x,y)=t^{-n/2}(4\pi)^{-n/2}\exp\Big(\sum g_{jk}(y)X_jX_k/4\Big)$. Hence $K_1\in\Psi_H^{-1}(\Omega)$. A computation analogous to that in 5.20 shows that $\Phi_0((\partial_t-\Delta)K_1)=0$ and therefore $(\partial_t-\Delta_x)K_1\in\Psi_H^{-1/2}$. Moreover, for $f\in C^\infty(\Omega)$,

$$\begin{aligned}\lim_{t\to0^+}\int_\Omega K_1(t,x,y)f(y)dS(y)&=f(x)\int_{T_x\Omega}\Phi_{-1}K_1(X,x)\,dX\\&=(4\pi)^{-n/2}\int_{T_x\Omega}\exp\Big(|X|^2_{g(x)}/4\Big)\,dX\,f(x)=f(x),\end{aligned}$$

since $\int_{\mathbb R}\exp(-t^2)\,dt=\sqrt\pi$. Hence $\lim K_1(t,x,y)=\delta_x(y)$. □

5.25. Proposition. *On closed manifolds, only integer powers appear in the heat kernel expansion at the diagonal $x=y$.*

Proof. Let $L\in\Psi_H^\alpha(\Omega)$, for some $\alpha\in-\mathbb N_0/2$. Write $L(t,x,y)=t^{-(n+2)/2-\alpha}\tilde L(t,X,y)$, where $X=\frac{x-y}{\sqrt t}$ and $\tilde L$ is assumed to be a smooth function of $\sqrt t$, so that it has a Taylor expansion

$$\tilde L(t,X,y)\sim\sum_{j=0}^\infty k_j(X,y)t^{j/2}.$$

Call L even, if k_j is even in X for $j/2+\alpha$ integer and odd in X if $j/2+\alpha$ is non-integer. One notices

- ∂_t and ∂_{x_j} and multiplication by smooth functions of x map even functions to even functions
- The convolution of even functions is even.

Next we observe that the function $K_1 \in \Psi_H^{-1}$ in Lemma 5.24 is even and thus the construction shows that the heat kernel is even. Since odd functions vanish at the origin, evaluation at $t = 0$ shows that $k_j(0, y) = 0$ for j odd. □

5.26. Theorem. *The leading coefficient $a_0(x)$ of the heat trace expansion in Theorem 5.12 is constant $(4\pi)^{-n/2}$. Hence $\alpha_0 = \int_\Omega a_0(x)\, dS = (4\pi)^{-n/2}\mathrm{vol}\,\Omega$.*

Proof. According to Lemma 5.23 and Lemma 5.21 only the term K_1 contributes to the zero order coefficient. It is $(4\pi)^{-n/2}\exp(0) = (4\pi)^{-n/2}$. □

5.c. **The heat kernel on manifolds with boundary.** In the case of manifolds with boundary we have the following analog of Theorem 5.12:

5.27. Theorem. *(Minakshisundaram and Pleijel) Let (Ω, g) be a smooth compact manifold with boundary. Then there exists a unique Dirichlet heat kernel, i.e. a function $K \in C^\infty((0,\infty)\times \Omega \times \Omega)$ with the following properties:*

(i) $(\partial_t - \Delta)K(t, x, y) = 0$, $t > 0$, $x, y \in \Omega$,

(ii) $K(t, x, y) = 0$ *whenever* $x \in \partial\Omega$,

(iii) $\lim_{t\to 0^+} K(t, x, y) = \delta_x(y)$.

Moreover,

$$K(t, x, x) = t^{-n/2}(A(t, x) + B(t, x)) \tag{1}$$

with $A \in C^\infty([0,\infty) \times \Omega)$ and a function B supported in a small neighborhood of the boundary, which, in local coordinates $(x', x_n) \in U' \times [0, \varepsilon)$, $U' \subseteq \mathbb{R}^{n-1}$ is of the form

$$B(t, x) = b(t, x', x_n/\sqrt{t}), \qquad b \in C^\infty([0,\infty)_{1/2} \times U' \times \overline{\mathbb{R}}_+)$$

with $b(t, x', \xi_n)$ rapidly decreasing as $\xi_n \to \infty$, uniformly in $t \in [0, 1]$, $x' \in U'$.

5.28. Remark.

(a) As $t \to 0^+$ we therefore obtain an expansion in half-integer powers of t by using the Taylor expansion of A and B as $t \to 0+$.

(b) In view of the fact that b vanishes rapidly away from the boundary, we see that the expansion at a point x in the interior of Ω is given by the expansion of A, which is the same as in the case without boundary.

(c) While the expansion of A only furnishes integer powers of t, B now contributes terms in $\sqrt{t}$.

5.29. Corollary. *As $t \to 0^+$ we have an asymptotic expansion*

$$\int_\Omega K(t, x, x)\, dS = t^{-n/2}(\alpha_0 + \beta_0 + \beta_{1/2}t^{1/2} + (\alpha_1 + \beta_1)t + \ldots),$$

where $\beta_0 = 0$ and α_j is as before for $j \in \mathbb{N}_0$. In particular, the leading term is $(4\pi t)^{-n/2}\mathrm{vol}\Omega$.

Why do these additional terms arise? We recall that on $\mathbb{R}^n$ the heat kernel is

$$K(t, x, y) = (4\pi t)^{-n/2}\exp\Big(-\frac{\|x - y\|^2}{4t}\Big).$$

On the halfspace $\overline{\mathbb{R}}^n_+$ with coordinates $x = (x', x_n)$, $x' \in \mathbb{R}^{n-1}$, $x_n \geq 0$, it has the form

$$E_1(t, x, y) = (4\pi t)^{-n/2}\Big(\exp\Big(-\frac{\|x - y\|^2}{4t}\Big) - \exp\Big(-\frac{\|x^* - y\|^2}{4t}\Big)\Big),$$

where $x^* = (x', -x_n)$. One finds this solution by the standard trick of the mirror image across the interface $x_n = 0$.

In the new variables

$$X' = \frac{x' - y'}{\sqrt{t}},\ \xi_n = \frac{x_n}{\sqrt{t}},\ \eta_n = \frac{x_n}{\sqrt{t}}.$$

E_1 has the form

$$E_1(t,x,y) = (4\pi t)^{-n/2} \exp\Big(\frac{-|X'|^2}{4}\Big)\Big(\exp(-(\xi_n - \eta_n)^2/4) - \exp(\xi_n + \eta_n)^2/4\Big).$$

5.30. Definition. The boundary heat calculus, denoted $\Psi^{\alpha}_{H,\partial}(\Omega)$, $\alpha \le 0$, consists of all smooth functions A on $(0,\infty) \times \Omega \times \Omega$ such that

(a) If $x \ne y$, then $\partial^{\gamma}_{t,x,y} A(t,x,y) = O(t^{\infty})$ for all γ as $t \to 0^+$ (off diagonal decay).

(b) For every $x \in \operatorname{int}\Omega$, there exists a local coordinate system $U \subset \mathbb{R}^n$ for x and a function $\tilde{A} \in C^{\infty}([0,\infty)_{1/2} \times \mathbb{R}^n \times U)$ such that

$$A(t,x,y) = t^{-\frac{n+2}{2}-\alpha} \tilde{A}\Big(t, \frac{x-y}{\sqrt{t}}, y\Big), \quad x, y \in U \tag{1}$$

(we are using local coordinates on the right hand side.) In addition we require $\tilde{A}$ to be rapidly decreasing in the second variable, i.e.

$$\partial^{\gamma}_{t,X,y} \tilde{A}(t,X,y) = O(|X|^{-\infty}) \text{ as } |X| \to \infty \tag{2}$$

uniformly in t and y. (i.e. at interior points we have the same properties as before). Moreover

(c) For each boundary point there exists a local coordinate neighborhood $U = U' \times [0,\varepsilon)$ and functions

$$\tilde{A}^{\rm dir} \in C^{\infty}([0,\infty)_{1/2} \times \mathbb{R}^n \times U)$$
$$\tilde{A}^{\rm refl}, \tilde{A}^{bd} \in C^{\infty}([0,\infty)_{1/2} \times \mathbb{R}^{n-1} \times \overline{\mathbb{R}}_+ \times U')$$

such that, for $t > 0$ and $x = (x', x_n), y = (y', y_n) \in U$

$$\begin{aligned} A(t,x,y) &= t^{-\frac{n+2}{2}-\alpha}\Big(\tilde{A}^{\rm dir}\Big(t, \frac{x-y}{\sqrt{t}}, y\Big) - \tilde{A}^{\rm refl}\Big(t, \frac{x'-y'}{\sqrt{t}}, \frac{x_n}{\sqrt{t}}, \frac{y_n}{\sqrt{t}}, y'\Big)\Big) \\ &= t^{-\frac{n+2}{2}-\alpha}\Big(\tilde{A}^{\rm bd}\Big(t, \frac{x'-y'}{\sqrt{t}}, \frac{x_n}{\sqrt{t}}, \frac{y_n}{\sqrt{t}}, y'\Big) \end{aligned} \tag{3}$$

with rapid decay for $\tilde{A}^{\rm dir}$ as in (2) and

$$\tilde{A}^{\rm refl}(t, X', \xi_n, \eta_n, y') = O((|X'| + \xi_n + \eta_n)^{-\infty})$$

together with all derivative, uniformly for bounded t.

5.31. Remark.

(a) Using the coordinates X', ξ_n, η_n we can write

$$\tilde{A}^{\rm bd}(t, X', \xi_n, \eta_n, y') = \tilde{A}^{\rm dir}(t, X', \xi_n - \eta_n, y', \eta_n\sqrt{t}) - \tilde{A}^{\rm refl}(t, X', \xi_n, \eta_n, y')$$

(b) Note that (c) implies (b) for y near an interior point (i.e. $y_n \ge c > 0$). Namely, let

$$\tilde{A}(t,X,y) = \tilde{A}^{\rm dir}(t,X,y) - \tilde{A}^{\rm refl}(t, X', X_n + y_n/\sqrt{t}, y_n/\sqrt{t}, y').$$

Then $A(t,x,y) = t^{-(n+2)/2-\alpha}\tilde{A}(t,X,y)$ and $\tilde{A}$ is smooth in $\sqrt{t}$. Since $y_n \ge c > 0$, $\tilde{A}^{\rm refl}$ decays to zero rapidly as $t \to 0^+$. Hence, for the smoothness in t near $t = 0$ we may ignore $A^{\rm refl}$, and $\tilde{A} = \tilde{A}^{\rm dir}$ is smooth in $\sqrt{t}$.

Leading terms.

5.32. Definition. To $A \in \Psi^{\alpha}_{H,\partial}(\Omega)$ we associate two leading terms, $\Phi^{\mathrm{int}}_{\alpha}(A)$ and $\Phi^{\mathrm{bd}}_{\alpha}(A)$: The interior leading term $\Phi^{\mathrm{int}}_{\alpha}(A)$ is as in the case without boundary, while the boundary leading term $\Phi^{\mathrm{bd}}_{\alpha}(A)$ is defined by

$$\Phi^{\mathrm{bd}}_{\alpha}(X', \xi_n, \eta_n, y') = \tilde{A}^{\mathrm{bd}}(0, X', \xi_n, \eta_n, y).$$

5.33. Coordianate invariance. Similarly as before, $\tilde{A}^{\mathrm{dir}}$ and $\tilde{A}^{\mathrm{refl}}$ are not uniquely defined. We know, however, that this is the case for $\Phi^{\mathrm{int}}_{\alpha}(A)$ which is an element of $C^{\infty}_{\mathscr{S}}(T\Omega)$, the smooth functions on $T\Omega$ which are rapidly decreasing in the fibers.

In order to obtain an invariant definition of $\Phi^{\mathrm{bd}}_{\alpha}(A)$ we introduce the bundle E over $\partial\Omega$ by letting, for $p \in \partial\Omega$,

$$E_p = (T_p\Omega \times T_p\Omega)/T_p\partial\Omega$$

where we identify (u, v) and (u', v') in $T_p\Omega \times T_p\Omega$ whenever $u - u' = v - v' \in T_p\partial\Omega$. We denote the equivalence class of (u, v) by $[u, v]$. We also introduce the map $\beta : E_p \to T_pM$, given by

$$\beta([u, v]) = u - v.$$

Each E_p is a $(2n - (n - 1)) = (n + 1)$-dimensional vector space. The E_p then define a vector bundle of rank $n + 1$. It has as a subset the $E^+_p = (T^+_p\Omega \times T^+_p\Omega)/T_p\partial\Omega$ of all $[u, v]$, where u and v are inward-pointing.

One can then show that $\Phi^{\mathrm{bd}}_{\alpha}(A)$ is an element of

$$\begin{aligned} C^{\infty}_{\mathrm{bd}}(E^+) \;=\; & \{\phi^{\mathrm{bd}} \in C^{\infty}(E^+) : \phi^{\mathrm{bd}} = \beta^*\phi^{\mathrm{dir}} - \phi^{\mathrm{refl}} \text{ for suitable} \\ & \phi^{\mathrm{dir}} \in C^{\infty}_{\mathscr{S}}(T_{\partial\Omega}\Omega), \phi^{\mathrm{refl}} \in C^{\infty}_{\mathscr{S}}(E)\}. \end{aligned}$$

Then $\Phi^{\mathrm{bd}}_{\alpha}(A)$ is invariantly defined as an element of $C^{\infty}_{\mathrm{bd}}(E^+)$.

In the definition of $C^{\infty}_{\mathrm{bd}}(E^+)$, ϕ^{dir} is determined by ϕ^{bd} through

$$\phi^{\mathrm{dir}}(X, p) = \lim_{w} \phi^{\mathrm{bd}}([X + w, w], p),$$

where the limit is over all $w \in T^+_p gO$ whose class in $T^+_p\Omega$ tends to ∞ (informally for $p = (y', 0)$: $\tilde{A}^{\mathrm{dir}}(0, X', X_n, y', 0) = \lim_{r\to\infty} \tilde{A}^{\mathrm{bd}}(0, X', X_n + r, r, y')$).

One therefore introduces the space $C^{\infty}_{\Phi,\partial}(\Omega)$ as the space of all pairs $(\Phi^{\mathrm{int}}_{\alpha}(A), \Phi^{\mathrm{bd}}_{\alpha}(A))$ such that $\Phi^{\mathrm{int}}_{\alpha}(A)_{|T_{\partial\Omega}\Omega} = \phi^{\mathrm{dir}}$, where ϕ^{dir} is determined by $\Phi^{\mathrm{bd}}_{\alpha}(A)$ as noted above.

With these definitions one obtains the short exact sequence

$$0 \to \Psi^{\alpha-1/2}_{H,\partial}(\Omega) \to \Psi^{\alpha}_{H,\partial}(\Omega) \to C^{\infty}_{\Phi,\partial}(\Omega) \to 0. \tag{1}$$

From this point on, the argument proceeds very much like in the case without boundary.

5.34. Proposition.

(a) *For $A \in \Psi^{\alpha}_{H,\partial}(\Omega)$ and $B \in \Psi^{\beta}_{H,\partial}(\Omega)$ with $\alpha, \beta < 0$ the convolution $A * B$ is defined and an element of $\Psi^{\alpha+\beta}_{H,\partial}$.*

(b) *Let $A \in \Psi^{\alpha}_{H,\partial}(\Omega)$, $\alpha \le -1$. Then $(\partial_t - \Delta)A \in \Psi^{\alpha+1}_{H,\partial}(\Omega)$ with $\Phi_{\alpha+1}(\partial_t - \Delta)A)(X, y)$ as in Proposition 5.20 and*

$$\begin{aligned} &\Phi^{bd}_{\alpha+1}(\partial_t - \Delta)A)(X', \xi_n, \eta_n, y') \\ &\quad = \Big(-\frac{n+2}{2} - \alpha - \frac{1}{2}X'\partial_{X'} - \frac{1}{2}\xi_n\partial_{\xi_n} - \frac{1}{2}\eta_n\partial_{\eta_n} - \Delta^{0,y}_{X',\xi_n}\Big)\Phi^{bd}_{\alpha}(A)(X', \xi_n, \eta_n, y'). \end{aligned}$$

Proof. See Grieser. □

We are almost there. However, we still need to take care of the boundary condition. We therefore introduce the subclass

$$\Psi^\alpha_{H,\mathrm{Dir}} = \{A \in \Psi^\alpha_{H,\partial}(\Omega) : A(t,x,y) = 0 \text{ if } x \in \partial\Omega\}.$$

5.35. Lemma.

(a) *For $A \in \Psi^\alpha_{H,Dir}(\Omega)$ and $B \in \Psi^\beta_{Dir}H,\partial(\Omega)$ with $\alpha, \beta < 0$ the convolution $A * B$ is an element of $\Psi^{\alpha+\beta}_{H,Dir}$.*

(b) *There is a short exact sequence for $\Psi^\alpha_{\mathrm{Dir}}(\Omega)$ with boundary leading parts vanishing at $\xi_n = 0$.*

(c) *The value of Af at $t = 0$ can be determined as in Lemma 5.21 from the interior leading part alone.*

Proof. (a) is obvious. (b) follows from the fact that $\xi_n = x_n/\sqrt{t}$. (c) is as before. □

5.36. Proposition. *Assume $K_1 \in \Psi^{-1}_{H,\partial}$ satisfies*

(i) $(\partial_t - \Delta)K_1 = R \in \Psi^{-1/2}_{H,\partial}(\Omega)$

(ii) *$K_1(t,x,y) = 0$ for $x \in \partial\Omega$.*

(iii) $\lim_{t\to 0^+} K_1(tax, y) = \delta_x(y)$.

Then

(a) *$K = \sum_{j=0}^\infty (-1)^j K_1 * R^{j*}$ converges in $C^\infty([0,\infty) \times \Omega \times \Omega)$ and $K \in \Psi^{-1}_{H,Dir}(\Omega)$.*

(b) *K satisfies the heat equation and the Dirichlet boundary value.*

(c) *$K_1 * R^{N*} \in \Psi^{-1-N/2}(\Omega)$ and the series is an asymptotic series in $1/2$-powers of t.*

5.37. The concrete case. We use geodesic normal coordinates, so that locally near the boundary we have $x = (x', x_n)$ with $x' \in \partial\Omega$, $x_n \geq 0$ such that ∂_{x_n} is orthogonal to $T\partial\Omega$ and of length 1. The metric in this neighborhood is of the form

$$g(x) = \begin{pmatrix} * & 0 \\ 0 & 1 \end{pmatrix}.$$

With the notation $X' = \frac{x'-y'}{\sqrt{t}}$, $\xi_n = \frac{x_n}{\sqrt{t}}$, $\eta_n = \frac{y_n}{\sqrt{t}}$. Then the starting value for the iteration is

$$K_1(t,x,y) = (4\pi t)^{-n/2} e^{-|X'|^2_{g(y)}/4} \Big(e^{(\xi_n - \eta_n)^2/4} - e^{(\xi_n+\eta_n)^2/4}. \Big) \tag{1}$$

Clearly $K_1 \in \Psi^{-1}_{H,\mathrm{Dir}}$. Moreover, a computation using Proposition 5.20 and 5.35(c) shows that $\Phi^{\mathrm{int}}_0((\partial_t - \Delta)K_1) = 0$ and $\Phi^{\mathrm{bd}}_0((\partial_t - \Delta)K_1) = 0$, so that $(\partial_t - \Delta)K_1 \in \Psi^{-1/2}$ by the exactness of the sequence 5.35(1).

Hence K_1 satisfies the assumptions of Proposition 5.36.

5.38. The expansion (Pleijel 1954). Let us have a look at the expansion

$$\int_\Omega K(t,x,x)\, dS \sim t^{-n/2}(\alpha_0 + \alpha_1 t^{1/2} + \ldots).$$

For the leading terms it suffices to study K_1. For $x = y$ we obtain

$$K_1(t,x,x) = (4\pi t)^{-n/2} \cdot 1 \cdot (1 - e^{-\xi_n^2}).$$

This shows that (in the notation of Theorem 5.27)

$$K_1(t,x,x) = t^{-n/2}(A(t,x) + B(t,x))$$

with

$$A(t,x) \equiv (4\pi)^{-n/2} \text{ and } B(t,x) = -(4\pi)^{-n/2} e^{-x_n^2/t}.$$

The contribution from A to the expansion is the same as in the boundaryless case, namely

$$\int_\Omega A(t,x,x)\,dS = \int_\Omega (4\pi)^{-n/2} dS = (4\pi)^{-n/2}\mathrm{vol}\,\Omega.$$

For B we have

$$\begin{aligned}\int_\Omega B(t,x,x)dS &= -\int_{\partial\Omega} (4\pi)^{-n/2}\,dS' \int_0^\infty e^{(x_n'/\sqrt{t})^2}\,dx_n \\ &= -(4\pi)^{-n/2}\mathrm{vol}\,(\partial\Omega)\cdot\sqrt{t}\int_0^\infty e^{-u^2}\,du = -(4\pi)^{-n/2}\mathrm{vol}\,(\partial\Omega)\cdot\sqrt{t}\sqrt{\pi}/2 \\ &= -(4\pi)^{-(n-1)/2}\frac{\mathrm{vol}\,(\partial\Omega)}{4}\cdot\sqrt{t}\end{aligned}$$

5.39. Remark. For the Neumann problem one obtains almost the same formula; there the sign of the second coefficient is + instead of −.

5.d. **The formula of McKean and Singer.** As before let (Ω, g) be a smooth Riemannian manifold with boundary.

5.40. Theorem. McKean&Singer 1967 *The trace of the heat kernel has the expansion*

$$\mathrm{Tr}(e^{t\Delta_{Dir}}) = (4\pi t)^{-n/2}\Big(vol\,\Omega - \sqrt{t}\sqrt{4\pi}\frac{vol\,\partial\Omega}{4} - \frac{t}{6}\int_\Omega K\,dS + \frac{t}{6}\int_{\partial\Omega} J\,dS' + O(t^{3/2})\Big)$$

Here, K is the scalar curvature of Ω and J is the mean curvature, defined below, and dS' is the surface measure on $\partial\Omega$ introduced by the restriction of the metric.

5.41. Definition. Let $R_{k,i,j,m}$ be the components of the Riemann curvature tensor associated with g. The Ricci tensor has the components

$$\mathrm{Ric}_{ij} = \sum_{km} g^{km} R_{kijm},$$

and the scalar curvature is

$$K = -\,\mathrm{tr}\,\mathrm{Ric} = -\sum_{ij} g^{ij} R_{ij}.$$

The mean curvature of a hypersurface (in our case the boundary of the manifold is given by $H = \frac{1}{n-1}(\kappa_1 + \dots \kappa_{n-1})$, where κ_j are the principal curvatures of the hypersurface.

Idea of the proof. The proof of the theorem by McKean and Singer is a lengthy computation. In principle, we can apply the above iteration starting from the approximation of the heat kernel given in 5.37(1). Then the contribution to the factor $t^{-n/2+1}$ is given by the boundary contribution from the term $K_1 * R$, where $R = (\partial_t - \Delta)K_1$ and from the interior contribution of $K_1 * R * R$. This is essentially what McKean and Singer do; for the case without boundary, however, they start with a better approximation and therefore only have to do one iteration. ◁

Following up on work by Polterovich [7], Weingart [11] showed the following formula for the case without boundary:

5.42. Theorem. *Let (Ω, g) be a smooth closed Riemannian manifold. Then the heat coefficients are given by the formula:*

$$a_k(x) = \sum_{l=0}^{k}\Big(-\frac{1}{4}\Big)^l\binom{k+n/2}{k-l}\Big(\frac{(-1)^{k+l}}{(k+l)!}\Delta_y^{k+l}\Big(\frac{1}{l!}\mathrm{dist}^{2l}(x,y)\Big)_{y=x}\Big).$$