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Kernel Asymptotics of Exotic Second-Order Operators

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The Navier–Lamé operator of classical elasticity, $\mu\Delta\mathbf{v}+(\lambda+\mu)\nabla(\nabla\cdot\mathbf{v})$, is the simplest example of a linear differential operator whose second-order terms involve a coupling among the components of a vector-valued function. Similar operators on Riemannian manifolds arise in conformal geometry and in quantum gravity. (In the latter context they have come to be called "nonminimal", but "exotic" is proposed as a better term.) The heat kernel of such an operator has a short-time expansion in terms of geometrical invariants: $K(t,x,x) \approx (4\pi t)^{-d/2}\sum_{n\geq 0} t^n a_n(x)$; but the traditional methods of calculating a_n for nonexotic operators do not apply in this situation. For the special case of operators $a^2 d\delta + b^2\delta d$ on differential forms, the Hodge decomposition has been used to reduce the problem to that for the usual Laplacians on forms (which are not exotic). More general exotic operators can be handled, in principle, by the calculus of pseudodifferential operators. Indeed, all the integrations encountered can be carried out in closed form; these are Cauchy integrals over the spectral parameter, Gaussian integrals over the radial coordinate in Fourier space, and angular integrals over the unit sphere in Fourier space. Unfortunately, the numbers of terms in intermediate steps of the calculations are so great that computer assistance seems necessary. Progress is reported on the reduction of this complexity with the aid of both commercial computer algebra software and direct computer programming.

Physics, old and new. Let Ω be a region in $\mathbf{R}^3$, and $\mathbf{v}(t,\mathbf{x})\colon \mathbf{R}\times\Omega \to \mathbf{R}^3$ a vector field. Elastic waves in a solid are described by the *Navier equations*,

$$\begin{aligned}\frac{\partial^2\mathbf{v}}{\partial t^2} &= \mu\Delta\mathbf{v} + (\lambda+\mu)\nabla(\nabla\cdot\mathbf{v}) \\ &= (\lambda+2\mu)\nabla(\nabla\cdot\mathbf{v}) - \mu\nabla\times(\nabla\times\mathbf{v}),\end{aligned} \tag{1}$$

where the *Lamé constants*, λ and μ, characterize the material [7, 25]. This equation is distinguished from the other second-order PDEs of mathematical physics by the fact that its second-order terms are not merely the Laplacian, or even the Laplace–Beltrami operator of a nontrivial metric. Since both the independent and the dependent variable reside in $\mathbf{R}^3$, it is possible for them to be "tangled together" in the algebraic structure of the second-order derivative term. The result is an "exotic" differential operator.

Early in the twentieth century, Hermann Weyl investigated the asymptotic spectral behavior of this elastic operator [32–33, 2]. He found that for suitable boundary conditions, all the normal modes could be classified as either *longitudinal* waves, which can be constructed as the gradients of scalar functions ($\mathbf{v} = \nabla\phi$), or *transverse* waves, which satisfy the same divergence condition as electric fields ($\nabla \cdot \mathbf{v} = 0$). Thus the problem decomposes into two previously solved problems, the scalar and the electromagnetic one.

This observation is a special case of the *Hodge decomposition* in differential geometry. Vector fields on a Riemannian manifold are naturally identified with 1-forms. Let d be the operation of exterior differentiation, mapping k-forms into $(k+1)$-forms, and δ be the negative of its adjoint, mapping in the opposite direction. Then the Navier–Lamé operator (1) is of the form $B_1\delta d + B_2 d\delta$ for certain constants B_j, with $k = 1$. Longitudinal and transverse modes belong to the null-spaces of d and δ, respectively.

In recent years exotic operators of a similar sort have been encountered by physicists constructing quantum theories of gravity [3, 4, 30]. They are associated with so-called "ghost" degrees of freedom in theories where the gravitational field obeys fourth-order equations of motion. For example, Barth and Christensen [3] define an operator F by

$$Fv_\alpha = \Delta v_\alpha + \nabla^\beta(\nabla_\alpha v_\beta) - 2\eta\nabla_\alpha\nabla^\beta v_\beta\,, \tag{2}$$

where Δ is the (Bochner) Laplace–Beltrami operator and ∇ the covariant derivative relative to a semi-Riemannian metric on a four-dimensional manifold; η is a parameter formed out of the coupling constants of the gravitational theory. Commutation of derivatives in the middle term shows F to be a curved-space generalization of the Navier–Lamé operator (1), plus a zeroth-order term built out of the curvature tensor of the manifold. Operators of this type, acting on k-forms, have been called *generalized Ahlfors Laplacians* [6]. Some applications of them within differential geometry are cited in [21].

Exotic second-order terms interfere with the standard methods of calculating asymptotic expansions of Green functions, effective Lagrangians, and so on. These are central tools of the quantum gravity theorists (and of mathematicians studying index theorems or inverse problems, and of physicists studying atomic nuclei or the thermodynamics of small grains of material). The general setting (restricted to the second-order case, however) is an operator

$$H = A^{\mu\nu}(x)\nabla_\mu\nabla_\nu + B^\mu(x)\nabla_\mu + C(x) \tag{3}$$

acting on sections of a vector bundle over a [semi-]Riemannian manifold M with metric tensor $g_{\mu\nu}$. (Here $x \in M$ is the independent variable, and the summation convention over repeated tensor indices is in force.) Locally each coefficient $A^{\mu\nu}$, B^μ, or C can be represented as a matrix (with respect to a local basis for the fiber space at x of the bundle). In nonexotic operators (which have come to be called "minimal" operators in the physics literature) $A^{\mu\nu}$ is proportional to $g^{\mu\nu}$ times the identity matrix, or $[A^{\mu\nu}]^a{}_b = \text{const.}\, g^{\mu\nu}\delta^a_b$. For the simplest exotic operators, such as (1) and (2), the bundle is the tangent (or cotangent) bundle of M, and

$$[A^{\mu\nu}]^\beta{}_\alpha = C_1\, g^{\mu\nu}\delta^\beta_\alpha + C_2\, \tfrac{1}{2}\big(g^{\mu\beta}\delta^\nu_\alpha + g^{\nu\beta}\delta^\mu_\alpha\big); \tag{4}$$

the last term "tangles" directions in the bundle with directions in the manifold, producing the distinctive "grad div" structure.

Three calculational methods. Let $K(t,x,y)$ be the integral kernel of the operator e^{-tH} — equivalently, the Green function solving the initial value problem for the "heat equation" $\partial\mathbf{v}/\partial t = -H\mathbf{v}$. (For greater precision, suppose that the differential expression H described earlier is formally self-adjoint, and understand H in the present discussion to be any self-adjoint realization of it.) It is well known that as $t\downarrow 0$ the diagonal value of the heat kernel has an asymptotic expansion of the form

$$K(t,x,x) \sim (4\pi t)^{-m/2}\sum_{n=0}^{\infty} t^n a_n(x). \tag{5}$$

This is true for exotic operators as well as minimal ones [22, 31]. (Here m is the dimension of the base manifold M. Note that K and a_n are matrix-valued (sections of the bundle of endomorphisms of the fiber bundle).) From (5) many other expansions of interest can be derived. (This "local" expansion merely scratches the surface of the geometrical information contained in the asymptotics of Green functions and spectra. Much more delicate analysis is needed to extract the effects of boundaries, closed geodesics, etc.; those matters are beyond the scope of this presentation.)

For nonexotic second-order operators, (5) has an off-diagonal generalization,

$$K(t,x,y) \sim e^{-d(x,y)^2/4t}(4\pi t)^{-m/2}\sum_{n=0}^{\infty} t^n a_n(x,y), \tag{6}$$

where d is the semi-Riemannian geodesic distance function. Substitution into the differential equation defining K then yields recursion relations that can be solved (laboriously) for the a_n [e.g., 28, 9]. (This process is known in the physics literature as the *Schwinger–DeWitt expansion*. In mathematics the series is associated with Hadamard and Minakshisundaram.) However, for fourth-order operators [26, 8] and exotic second-order operators such a simple factorization does not exist, and this classical method does not provide a recursive algorithm.

A second approach to finding the $a_n(x)$, or at least the integrals of their traces over M, is some variant of this: At each order n, a_n must be a linear combination of a finite list of allowable invariant objects built from the coefficient tensors in H, the curvature tensor, etc.; the problem is to determine its numerical coefficients. Certain relations among the coefficients can be deduced from general principles, such as how the heat kernel of an operator on a product manifold is related to the heat kernels of the factors. Other relations can be found by looking at special cases (e.g., spheres) for which the answer can be calculated easily. With luck one can compile enough information to fix the coefficients uniquely. This strategy was employed in the famous paper of McKean and Singer [27] and has been extensively developed by Peter Gilkey [e.g., 19]. Its great advantage is that, when it works, it provides results very efficiently, rendering pages of tedious algebraic calculations unnecessary, while providing some interesting geometrical insights. Its disadvantage is that it is not an algorithm; to push the method forward to a higher order or a more general class of operator, additional mathematical creativity is always required.

Gilkey and Branson [21] in this way found some important information about the integrated trace of the heat kernel of the natural exotic operators on differential forms on a compact Riemannian manifold without boundary. (On such a manifold (5) is uniformly valid and can be integrated, giving

$$\begin{aligned} \int_M \operatorname{tr} H(t,x,x)\,dx &\sim (4\pi t)^{-m/2} \sum_{n=0}^{\infty} t^n a_n(H) \\ &= \sum_{\nu}^{\infty} e^{-t\lambda_\nu} \equiv \operatorname{Tr} e^{-tH}, \end{aligned} \tag{7}$$

$$a_n(H) \equiv \int_M \operatorname{tr} a_n(x)\,dx, \tag{8}$$

where the λ_ν are the eigenvalues of H.) In the role of H consider

$$D = a^2 d\delta + b^2 \delta d \tag{9}$$

operating on k-forms ($C^\infty(\Lambda^k(M))$). If $a = b$, D is proportional to the *DeRham Laplacian* on forms,

$$\Delta_k = d\delta + \delta d \qquad \text{on } C^\infty(\Lambda^k), \tag{10}$$

which is a nonexotic operator. The $a_n(\Delta_j)$ for $0 \le j \le m$ may thus be regarded as "known". (In fact, $-\Delta_j$ differs only by a zeroth-order term — the *Weitzenböck endomorphism* — from the *Bochner Laplacian*, $\Delta \equiv g^{\mu\nu}\nabla_\mu\nabla_\nu$, and $a_n(x)$ for such an operator has been determined up through $n = 4$ [1]. Formulas for $a_0(\Delta_j)$ and $a_1(\Delta_j)$ are provided in Theorem 1.1 of [21].) As previously remarked, the Hodge decomposition cuts k-forms into "longitudinal" and "transverse" parts; D effectively acts on these two spaces separately, and hence a "telescoping" calculation [6, 21] expresses the trace of e^{-tD} in terms of the traces of $e^{-t\Delta_j}$ for $j \le k$, in a reminiscence of Weyl's classic treatment of the elasticity problem.

Theorem 1. *With the definitions (7) [or (8)], (9), and (10), one has*

$$a_n(D) = b^{2n-m} a_n(\Delta_k) + \left(b^{2n-m} - a^{2n-m}\right) \sum_{j<k} (-1)^{k-j} a_n(\Delta_j). \tag{11}$$

An interesting broader class of exotic operators (including (2), for instance) comprises those of the form

$$H = a^2 d\delta + b^2 \delta d - E(x), \tag{12}$$

where E is a zeroth-order operator (a matrix-valued function). In [21], $a_0(H)$ and $a_1(H)$ were determined for such operators. (See [6] for an extension to manifolds with boundary.)

Theorem 2. *For the operator (12) on k-forms, one has (in terms of the quantities in Theorem 1)*

$$a_0(H) = a_0(D), \tag{13}$$

$$a_1(H) = a_1(D) + \frac{a_0(D)}{\binom{m}{k} \int_M 1\,dx} \int_M \operatorname{tr} E(x)\,dx. \tag{14}$$

(The integral in the denominator in (14) is simply the volume of M, which appears as a factor in $a_0(D)$.)

Proof: The only invariants eligible to appear in a_1 are the curvature scalar R (already contained in $a_1(D)$) and $\operatorname{tr} E$. (Any lingering doubts about this can be settled by examining the structure of the pseudodifferential calculation presented below.) Therefore, it suffices to determine the coefficient of the trace term by considering the case $E =$ identity operator. For that case we have in (7)

$$\operatorname{Tr} e^{-tH} = e^t \ \operatorname{Tr} e^{-tD}$$

and hence

$$a_0(H) + ta_1(H) + \cdots = a_0(D) + t[a_1(D) + a_0(D)] + \cdots. \tag{15}$$

For the identity we also have

$$\operatorname{tr} E = \dim \Lambda^k(M) = \binom{m}{k},$$

so the $O(t)$ part of (15) can be written in the generic form (14).

This argument does not generalize in any obvious way to give $a_n(H)$ for $n \geq 2$. (For example, $a_2(H)$ contains both $\operatorname{tr}(E^2)$ and $(\operatorname{tr} E)^2$ (not to mention terms bilinear in E and in curvature), and these are not separated by the identity operator.) Moreover, formulas for the global quantities $a_n(H)$ do not give complete information about the local quantities $a_n(x)$. For one thing, any exact divergence, such as $\Delta_0 R$, integrates to zero. For another, $[a_1(x)]^\alpha{}_\beta$ may contain both terms proportional to $[E(x)]^\alpha{}_\beta$ and terms proportional to $\operatorname{tr} E(x)\,\delta^\alpha_\beta$, and these are no longer independent after the trace is taken in (8) and (14). (Traces of the coefficient tensors of H do not appear in the untraced $a_n(x)$ for ordinary operators H, but if H is exotic, they do.)

A third way to calculate $a_n(x)$ is based on the calculus of pseudodifferential operators [31, 22, 18, 34, 30, 16, 23, 24]. It has broader validity than the two traditional methods; it offers in principle a complete solution of the problem for operators of the class (12). (For more general exotic (3) or higher-order operators, integrals may be encountered that cannot be evaluated in closed form.) Unfortunately, it is much less efficient than the other methods. An attack upon its computational complexity is the main subject of the present work.

The symbol. In the *intrinsic pseudodifferential calculus* [5, 34, 11, 16] each covariant derivative, ∇, in an operator such as (3) is represented by a Fourier (cotangent bundle) variable, $i\xi$. Thus the operator on $C^\infty(\Lambda^1)$

$$H_0 \equiv -\Delta - \frac{c}{2}\left(\nabla_\beta\nabla^\alpha + \nabla^\alpha\nabla_\beta\right) \qquad (\Delta \equiv g^{\mu\nu}\nabla_\mu\nabla_\nu) \tag{16}$$

has the intrinsic symbol

$$\mathrm{Sy}(H_0) = |\xi|^2 + c\,\xi \otimes \xi. \tag{17}$$

By definition, an *exotic* operator is one with *nonscalar principal symbol*; that is, the terms in the symbol of highest degree in ξ are not just a multiple of the identity matrix. We may think of H_0 as operating either on vector fields or on one-forms; to match up with physics literature, I shall consider vector fields. Then the coefficient tensor in (16) and (17) is

$$[A^{\mu\nu}]^\beta{}_\alpha = -g^{\mu\nu}\delta^\beta_\alpha - \frac{c}{2}\left(g^{\mu\beta}\delta^\nu_\alpha + g^{\nu\beta}\delta^\mu_\alpha\right). \tag{18}$$

Here all the indices are Greek, since they refer to the same vector bundle (or its dual); their place of origin in the symbol is momentarily preserved by the distinction between the beginning and middle of the alphabet.

We consider the class of operators

$$H = b^2 H_0 + V(x). \tag{19}$$

(Here b^2 and c are constants, obeying sign constraints to be discussed presently, and V is a C^∞ endomorphism-valued function, called the *potential* in analogy with quantum mechanics.) Equivalently, H is of the form (12) with

$$-E^\beta{}_\alpha = V^\beta{}_\alpha - b^2\left(1 + \frac{c}{2}\right) R^\beta{}_\alpha \tag{20}$$

and

$$a^2 = b^2(c+1), \qquad c = \frac{a^2 - b^2}{b^2}\,. \tag{21}$$

The operator can be parametrized by a and b, to exploit the Hodge decomposition, or by b and c, so that c is the magnitude of the exotic term and b is merely a scale factor. (In [24], V is called X and c is called $-a$. The terms in (20) proportional to the Ricci tensor $R^\beta{}_\alpha$ are the Weitzenböck operator for $k = 1$ and a similar contribution from the desymmetrization of the exotic term in (16).)

From the second-order derivative terms one reads off the principal symbol of H as

$$\begin{aligned} +b^2(|\xi|^2 + c\,\xi\otimes\xi) &= b^2|\xi|^2 + (a^2 - b^2)\,\xi\otimes\xi \\ &= a^2 \mathrm{ext}_\xi \mathrm{int}_\xi + b^2 \mathrm{int}_\xi \mathrm{ext}_\xi\,, \end{aligned} \tag{22}$$

where int and ext are the operators of interior and exterior multiplication on forms. (Here $\xi \otimes \xi$ has the matrix

$$\xi^\beta \xi_\alpha$$

in a conventional local basis.) Under the assumption that the metric is positive definite and $b^2 > 0$, the condition that both eigenvalues be nonnegative, so that the heat kernel exists, is

$$c \geq -1, \quad \text{or} \quad a^2 \geq 0. \tag{23}$$

(If b^2 and a^2 are replaced by negative numbers, we have a heat operator e^{+tP}, which still corresponds to $c \geq -1$. The results of a calculation, which are basically combinatorial rather than analytic, can be formally continued to other cases, such as indefinite metric.) By convention, $b > 0$ and $a \geq 0$.

In the calculation a major role is played by the eigenvalues and eigenprojections of the matrix (22). They are

$$\lambda_1 = a^2|\xi|^2 = b^2(c+1)|\xi|^2, \qquad P_1 = \frac{\xi \otimes \xi}{|\xi|^2} \quad (\text{along } \xi), \tag{24a}$$

$$\lambda_2 = b^2|\xi|^2, \qquad P_2 = \frac{|\xi|^2 - \xi \otimes \xi}{|\xi|^2} \quad (\perp \text{ to } \xi). \tag{24b}$$

In the notation of [16] we have

$$b_0(\lambda) \equiv [\mathrm{Sy}(b^2 H_0) - \lambda]^{-1} = -\sum_{j=1}^{2} \frac{P_j}{\lambda - \lambda_j}\,. \tag{25}$$

The first step in calculating the heat kernel of H is to find the symbol of the resolvent operator, $(H - \lambda)^{-1}$, following [34] and [16]. For background reading on the resolvent symbol and the heat kernel, I highly recommend the expositions of Gilkey [17, 18, 20]. (They, however, deal with the *conventional* pseudodifferential calculus, where ξ is a literal Fourier variable corresponding to conventional partial differentiation. The basic formulas of that approach are simpler than those of the intrinsic formalism, but extra work is needed at the end to express the results in coordinate-independent geometrical form.) The series of conference reports [14–15] provides a brief introduction to and summary of [16].

THEOREM 3. *The intrinsic symbol of the resolvent parametrix of an elliptic linear differential operator has an asymptotic expansion*

$$Sy[(H-\lambda)^{-1}] \sim \sum_{s \geq 0} b_s(x, \xi, \lambda), \tag{26}$$

where b_0, as in (25), is the local resolvent of the principal symbol, and the higher b_s are given by an explicit formula [15, 16] involving very complicated index contractions and summations over multiindices. The formula for b_2 contains 40 terms for a generic operator, but only 5 in the present case (19):

$$\begin{aligned} b_2 = &- b_0 V b_0 \\ &- 4 b_0 A^{\alpha\mu} b_0 A^{\beta\nu} (\nabla_\mu \nabla_\nu I) b_0\, \xi_\alpha \xi_\beta \\ &- 2 b_0 A^{\alpha\mu} b_0 A^{\nu\rho} (\nabla_\mu \nabla_\nu \nabla_\rho \Phi^\beta) b_0\, \xi_\alpha \xi_\beta \\ &- 2 b_0 A^{\mu\nu} b_0 A^{\alpha\rho} (\nabla_\mu \nabla_\nu \nabla_\rho \Phi^\beta) b_0\, \xi_\alpha \xi_\beta \\ &- 8 b_0 A^{\alpha\mu} b_0 A^{\beta\nu} b_0 A^{\gamma\rho} (\nabla_{(\mu} \nabla_{\nu)} \nabla_\rho \Phi^\delta) b_0\, \xi_\alpha \xi_\beta \xi_\gamma \xi_\delta\,. \end{aligned} \tag{27}$$

[Here a matrix multiplication is implied, and hence the fiber-bundle indices, including the last two indices in (18), are suppressed. I is the parallel transport operator in the tangent bundle, called τ^E in [16]. See (A.11–13) of [24]; their W will be 0 for us. $\Phi(x,y)$ is the tangent vector to the geodesic joining x and y (see [16], Remark 2.5). The important thing is that in the present case all the covariant derivatives of I and Φ, evaluated at $y=x$ as tacitly implied in (27), can be recursively calculated in terms of the Riemann tensor [9, 10, 12].] *More generally, a term in b_s has the form*

$$(\textit{coefficient})\, b_0 T_U b_0 T_{U-1} \cdots b_0 T_1 b_0\, \xi^{\otimes(2U-s)}, \tag{28}$$

where the T_u are tensors built out of A, V, Φ, and I and their covariant derivatives, with indices absorbing the ξ factors by contraction. (Each T is linear in (A,V).) U ranges from $U_0 \equiv -[-s/2] = \lceil s/2 \rceil$ to $2s$.

In particular, $1 \le U \le 4$ for $s=2$ (and in fact $U=4$ does not occur for our special operator), and $2 \le U \le 8$ for $s=4$. Note also that for our operator, the covariant derivatives of A vanish.

To obtain the diagonal value of the heat kernel we follow Widom [34], pp. 59–61.

Theorem 4. *In an orthonormal frame at x we have*

$$K(t,x,x) \sim \sum_{s=0}^{\infty} K_s(x), \tag{29}$$

$$K_s(x) = (2\pi)^{-m} \int_{\mathbf{R}^m} d^m\xi \left(\frac{-1}{2\pi i}\right) \int_\Gamma d\lambda\, e^{-t\lambda} b_s(x,\xi,\lambda), \tag{30}$$

where Γ surrounds λ_1 and λ_2 in the positive sense. K_s will be 0 for s odd. [In the contrary case, K_{2n} equals $(4\pi t)^{-m/2}\, t^n a_n$ in our earlier notation (5).] *Thus the contribution of the term (28) is*

$$\begin{aligned} t^{(s-m)/2}(\textit{coefficient})(-1)^U(2\pi)^{-m} \int d^m\eta \sum_{i_0=1}^{2} \cdots \sum_{i_U=1}^{2} P_{i_U} T_U \cdots T_1 P_{i_0} \\ \otimes\, \eta^{\otimes(2U-s)} \frac{1}{2\pi i} \int_\Gamma d\mu\, e^{-\mu} (\mu-\mu_1)^{-M_1} (\mu-\mu_2)^{-M_2}, \end{aligned} \tag{31}$$

where

$$M_j \equiv \textit{cardinality of } \{i_\iota : i_\iota = j\} \qquad (M_1 + M_2 = U+1), \tag{32}$$

$$\mu_1 \equiv a^2|\eta|^2, \qquad \mu_2 = b^2|\eta|^2. \tag{33}$$

To get to (31) one makes the substitutions

$$\eta = t^{1/2}\xi, \qquad \mu = t\lambda$$

and renames $t\Gamma$ as Γ. Whenever T_u equals A, another sum from 1 to 2 can be introduced into (31), corresponding to the two terms in (18); furthermore, P_2 splits into two terms

(24b), so the i sums are effectively over three values. This implies that each term in b_{2n} gives rise to a rather large number of terms in a_n — namely, $3^{U+1}2^{U-v}$, where v is the number of occurrences of the potential V in the term (28). Thus from (27) for b_2 we will get (in a_1) 9 terms involving V and $108 + 108 + 108 + 648 = 972$ other terms, which are all linear in the Ricci tensor. The number of terms in a_2 is over a million! These terms are highly redundant, in the senses that many of them are manifestly proportional, quite a few turn out to be zero, and they are all linear combinations of a small number of linearly independent objects. For example, a_1 must simplify to a sum of 5 terms, proportional to V, its transpose, its trace (times the identity), the Ricci tensor, and its trace (the curvature scalar R).

In what follows I shall demonstrate that all the integrations in (31) can be performed in closed form, so that in principle $a_n(x)$ has been expressed in terms of elementary functions (and local, polynomial functionals of the coefficient tensors). Furthermore, I shall show that modern computer technology makes practical the actual calculation of a_1 and probably a_2 by this method.

Integrals. In evaluating formula (31), one encounters three kinds of integrals:

1. *Cauchy integrals* over the spectral parameter, μ.
2. *Gaussian integrals* over the radial coordinate in Fourier space, $|\eta|$.
3. *Angular integrals* over the unit sphere in Fourier space.

LEMMA. *Define*

$$F_{M_1 M_2}(\mu_1, \mu_2) \equiv \frac{1}{2\pi i} \int_\Gamma f(\lambda)\, (\lambda - \mu_1)^{-M_1} (\lambda - \mu_2)^{-M_2}\, d\lambda, \tag{34}$$

where f, $\mu_1 \neq \mu_2$, and Γ satisfy the conditions for Cauchy's integral formula. Then if M_1 and M_2 are both positive integers,

$$\begin{aligned} F_{M_1 M_2}(\mu_1, \mu_2) = &\sum_{J=0}^{M_1-1} \frac{(-1)^J (M_2 + J - 1)!}{(M_2 - 1)!\,(M_1 - J - 1)!\,J!}\, f^{(M_1-1-J)}(\mu_1)(\mu_1 - \mu_2)^{-M_2-J} \\ &+ \sum_{J=0}^{M_2-1} \frac{(-1)^J (M_1 + J - 1)!}{(M_1 - 1)!\,(M_2 - J - 1)!\,J!}\, f^{(M_2-1-J)}(\mu_2)(\mu_2 - \mu_1)^{-M_1-J}. \end{aligned} \tag{35}$$

If one of the integers is 0, the formula degenerates to

$$F_{M_1 0}(\mu_1, \mu_2) = \frac{f^{(M_1-1)}(\mu_1)}{(M_1 - 1)!}\,, \qquad F_{0 M_2}(\mu_1, \mu_2) = \frac{f^{(M_2-1)}(\mu_2)}{(M_2 - 1)!}\,. \tag{36}$$

PROOF: Cauchy's formula is

$$\frac{1}{2\pi i} \int_\Gamma \frac{g(\lambda)}{(\lambda - \zeta)^{n+1}}\, d\lambda = \frac{1}{n!}\, g^{(n)}(\zeta). \tag{37}$$

From this, (36) follows immediately. To get (35) we need to calculate

$$\left(\frac{d}{d\lambda}\right)^{M_1-1}\left[\frac{f(\lambda)}{(\lambda-\mu_2)^{M_2}}\right] = \sum_{J=0}^{M_1-1}\binom{M_1-1}{J} f^{(M_1-1-J)}(\lambda)\left[\frac{(M_2+J-1)!}{(M_2-1)!}(-1)^J(\lambda-\mu_2)^{-M_2-J}\right]$$

and the analogue with $1 \leftrightarrow 2$. Then (35) follows quickly.

In (31) we have a special case of the foregoing.

Theorem 5. *If $f(\lambda)=e^{-\lambda}$ and*

$$\mu_1 = a^2|\eta|^2, \qquad \mu_2 = b^2|\eta|^2, \qquad c \equiv \frac{a^2-b^2}{b^2} \neq 0, \tag{38}$$

then

$$\begin{aligned} F_{M_1M_2}(\mu_1,\mu_2) = &\sum_{J=0}^{M_1-1}\frac{(-1)^{M_1-1}(M_2+J-1)!}{(M_2-1)!\,(M_1-J-1)!\,J!}(b^2c)^{-M_2-J}|\eta|^{-2(M_2+J)}e^{-a^2|\eta|^2} \\ &-\sum_{J=0}^{M_2-1}\frac{(-1)^{M_2-M_1-J}(M_1+J-1)!}{(M_1-1)!\,(M_2-J-1)!\,J!}(b^2c)^{-M_1-J}|\eta|^{-2(M_1+J)}e^{-b^2|\eta|^2}, \end{aligned} \tag{39}$$

$$F_{M_10}(\mu_1,\mu_2) = \frac{(-1)^{M_1-1}}{(M_1-1)!}e^{-a^2|\eta|^2}, \qquad F_{0M_2}(\mu_1,\mu_2) = \frac{(-1)^{M_2-1}}{(M_2-1)!}e^{-b^2|\eta|^2}. \tag{40}$$

Contrary to appearance, the functions in (39) are guaranteed to be nonsingular as $\eta \to 0$.

Henceforth we shall write $F_{M_1M_2}(a,b)$ instead of $F_{M_1M_2}(\mu_1,\mu_2)$ and r in place of $|\eta|$.

Examples:

$$F_{11}(a,b) = \frac{e^{-a^2r^2}-e^{-b^2r^2}}{b^2cr^2}. \tag{41a}$$

$$F_{31}(a,b) = \frac{1}{2}\frac{e^{-a^2r^2}}{b^2cr^2} + \frac{e^{-a^2r^2}}{b^4c^2r^4} + \frac{e^{-a^2r^2}}{b^6c^3r^6} - \frac{e^{-b^2r^2}}{b^6c^3r^6}. \tag{41b}$$

We shall dispose of the angular integrals quickly, since a similar problem has been discussed in depth in the appendix of [8].

Theorem 6. *Consider an integral of the form*

$$\mathcal{I}_F \equiv \int_{\mathbf{R}^m} d^m\eta\, F(|\eta|)\,\eta^\alpha, \tag{42}$$

where α is a multiindex, corresponding to a string of tensor indices $\mu_1, \mu_2, \ldots, \mu_{|\alpha|}$ (unordered, but not necessarily distinct). $\mathcal{I}_F$ equals 0 unless all components of α are even. If $\alpha = 2\beta$, then

$$\mathcal{I}_F = \frac{I_F}{(2|\beta|-1)!!}\, g_{2\beta}\,, \tag{43}$$

where

$$I_F \equiv \int_{\mathbf{R}^m} d^m\eta\, F(|\eta|)\, {\eta_m}^{2|\beta|}, \tag{44}$$

and

$$g_{2\beta} \equiv g_{\mu_1\mu_2} g_{\mu_3\mu_4} \ldots + g_{\mu_1\mu_3} g_{\mu_2\mu_4} \ldots + \cdots \tag{45}$$

involves a sum over the $(2|\beta|-1)!!$ essentially distinct permutations of the indices. (As a factor in a scalar integrand, this tensor produces a contraction over all possible pairings of the indices in α.) Furthermore,

$$I_F = \pi^{m/2}\, \frac{2^{1-|\beta|}(2|\beta|-1)!!}{\Gamma(\frac{m}{2}+|\beta|)} \int_0^\infty r^{m+2|\beta|-1} F(r)\, dr. \tag{46}$$

(The numerical factors in (46) are the product of $\int_0^\pi \cos^{2|\beta|}\theta \sin^{m-2}\theta\, d\theta$ and the volume of the unit $(m-2)$-sphere.)

We turn to the final step of integration: Theorems 5 and 6 reduce (31) to integrals of the form

$$\int_0^\infty r^{m-1+2U-s}\, F_{M_1M_2}(r)\, dr. \tag{47}$$

All such integrals can be evaluated by the formula

$$\int_0^\infty e^{-qr^2} r^p\, dr = \frac{1}{2}\, q^{-(p+1)/2}\, \Gamma\!\left(\frac{p+1}{2}\right) \tag{48}$$

(found by the substitution $z = qr^2$). However, there is a subtlety here. Although the complete integral (47) converges, the individual terms may diverge at $r = 0$; this shows up in poles of the Γ function. This problem can be handled by "dimensional regularization": The integral is an analytic function of m, hence obtainable by analytic continuation of the formula for it provided by (48) from values of m so large that the term integrals converge; that formula will have a removable singularity. As p approaches the desired value in each term, the poles of the Γ functions must cancel, and the finite remainder can be extracted at the cost of some tedious algebra. In practice, one can evaluate the integrals formally by (48), treating m as a continuous variable, and then take the limit as m approaches an integer.

Examples: (The arguments a, b of $F_{M_1M_2}$ are suppressed.)

$$\int_0^\infty r^{m-1} F_{20}(r)\, dr = -\frac{1}{2}\, a^{-m}\Gamma\!\left(\frac{m}{2}\right). \tag{49a}$$

$$\int_0^\infty r^{m-1} F_{11}(r)\,dr = \frac{1}{2b^2c}\left(a^{2-m} - b^{2-m}\right)\Gamma\left(\frac{m}{2} - 1\right). \tag{49b}$$

When $m = 2$, the second of these formulas requires taking a limit:

$$\int_0^\infty r\,F_{11}(r)\,dr = \frac{1}{b^2c}(\ln b - \ln a). \tag{50}$$

Gusynin et al. [24] evaluated the Cauchy, and the resulting radial, integrals in terms of hypergeometric functions. In this way they succeeded in calculating a_0 and a_1 by hand. From the foregoing it is clear that all hypergeometric functions appearing in their results can be expressed in elementary functions, perhaps at the cost of less compact formulas.

The leading term. In contrast to the usual case, for an exotic operator even a_0 is nontrivial. Evaluating (31) with (28) collapsed to b_0, one gets

$$\begin{aligned} a_0(x) &= b^{-m} + \frac{a^{-m} - b^{-m}}{m} \\ &= \frac{1}{b^m m}\left[m - 1 + (c+1)^{-m/2}\right]. \end{aligned} \tag{51}$$

(An identity matrix is implicit here.) When $a = b$ (or $c = 0$) this reduces to the well known "minimal" result, $a_0 = b^{-m}$ (that is, $K_0 = (4\pi b^2 t)^{-m/2}$). When we trace (51) and integrate it over the manifold, we get

$$a_0(H) = \left[mb^{-m} + a^{-m} - b^{-m}\right]\int_M 1\,dx, \tag{52}$$

in accordance with Theorems 1 and 2.

Computerization. In pursuit of a_1 and a_2 a sequence of computer programs has been written. I have found, here as elsewhere [13], that "homegrown" programs are most effective in generating the large number of terms in asymptotic calculations, but that commercial, general-purpose computer algebra programs [35, 29] are essential for combining like terms and simplifying the output.

1. To implement the result of [16], I wrote a program in C to list the terms in each order, b_s, of the resolvent symbol. This program prints the values of the multiindices characterizing each term (28) and calculates the numerical coefficient. This program is quite general: for example, it could be used to generate the terms in the resolvent of a fourth-order nonexotic operator [23], and it is applicable to the conventional as well as the intrinsic pseudodifferential calculus.

2. That program acts as the basic engine in another program that lists the terms in the heat kernel of H (see (31) and following discussion). The new program, implemented as a subroutine of the other one and constantly revised as the need arises, calculates the new numerical factors accumulated in (31), (43), and (46) and outputs each term in a form suitable as input for *MathTensor*. (It is here that the structure of *tensor contraction*, described verbally in [16] and glossed over in Theorem 3, must be concretely implemented.)

3. A *Mathematica* package was written to evaluate the Cauchy and radial integrals, following (34), (39), (40), (47), and (48).

4. An additional *Mathematica* input file is needed to define for *MathTensor* the various tensors appearing in the T_u of (31), to simplify Γ functions, etc. For large $|\beta|$, creating the expression (45) is itself a nontrivial programming task, and digesting it the most time-consuming part of the later computation.

5. *Mathematica/MathTensor* is used interactively to work the various contributions to a_n into a usable final form.

Since b in (19) enters each category of terms only as a scale factor, it is convenient to set $b = 1$ in the calculation; the appropriate power of b is easily restored at the end. The results are most elegantly stated as rational functions in c and

$$\tilde{a} \equiv a/b = \sqrt{c+1}\,. \tag{53}$$

With this technology, the calculation of the terms in a_1 involving the potential V is fairly simple. We have

$$\begin{aligned} a_1^{(V)}(x)^\beta{}_\alpha = {} & \frac{\tilde{a}^m[c(2-m)+4] - c(m+2) - 4}{b^m \tilde{a}^m c\, m(m^2-4)} [V_\alpha{}^\beta + V^\mu{}_\mu \delta_\alpha^\beta] \\ & + \frac{-\tilde{a}^m[c(m^3-2m^2-3m+6)+4(m+1)] + 3c(m+2) + 4(m+1)}{b^m \tilde{a}^m c\, m(m^2-4)} V^\beta{}_\alpha\,. \end{aligned} \tag{54}$$

(Even if H is formally self-adjoint, forcing V to be Hermitian, V may still be a complex matrix; hence V and its transpose are independent objects.) Taking the trace yields

$$a_1^{(V)}(x)^\mu{}_\mu = -\frac{m-1+\tilde{a}^{-m}}{b^m m} V^\mu{}_\mu \tag{55}$$

in agreement with [21] (cf. (14) and (51)).

The curvature terms in a_1 proved to be much more involved, and the computation was barely finished in time for this conference. I find

$$\begin{aligned} a_1^{(R)}(x)^\beta{}_\alpha = {} & \frac{\begin{array}{c}\tilde{a}^m[3c^2(m-2)+c(m^3-m^2-24)-24] \\ +\,c^2(m^2+5m+6)+c(m^2+8m+24)+24\end{array}}{6b^{m-2}\tilde{a}^m c\, m(m^2-4)} R\delta_\alpha^\beta \\ & + \frac{\begin{array}{c}\tilde{a}^m[3c^2(m^3-2m^2-2m+4)+2c(-5m^2+14m+12)+24m] \\ -\,2c^2(m^2+5m+6)-2c(m^2+14m+12)-24m\end{array}}{6b^{m-2}\tilde{a}^m c\, m(m^2-4)} R^\beta{}_\alpha\,. \end{aligned} \tag{56}$$

The trace is

$$a_1^{(R)}(x)^\mu{}_\mu = \frac{\tilde{a}^m[3c(m-1)+m^2-m-6]+c(m+3)+m+6}{6b^{m-2}\tilde{a}^m m} R. \tag{57}$$

However, the result is much simpler for the operator $D = a^2 d\delta + b^2 \delta d$ defined in (9) (the operator that is simplest and most natural from the point of view of the geometer, as opposed to the Fourier analyst). From (20), (54), and (56) one finds

$$\begin{aligned} a_1^{(D)}(x)^\beta{}_\alpha = {} & \frac{\tilde{a}^m(m-3)+c+1}{6b^{m-2}\tilde{a}^m(m-2)}\, R\delta^\beta_\alpha \\ & + \frac{\tilde{a}^m(-3m+7)-c-1}{3b^{m-2}\tilde{a}^m(m-2)}\, R^\beta{}_\alpha\,. \end{aligned} \tag{58}$$

Its trace is

$$a_1^{(D)}(x)^\mu{}_\mu = \tfrac{1}{6} b^{2-m}[m-7+\tilde{a}^{-m}(c+1)]\, R, \tag{59}$$

which is the prediction of Theorem 1.

Main Theorem. [Formulas (51), (54), (56), and (58) are the main results. The notation is defined in (5), (16), and (19). Results (51) and (54) agree with [24], where a different but related method was employed; comparison of (56) with [24] has not yet been completed.]

After debugging, the *Mathematica* calculation of (56) requires two days of operation of a Sun 3/60 workstation. (Direct calculation of (57) is about 5 times faster. The execution time of the preparatory C program is negligible.) An attack on a_2, therefore, will require either a supercomputer or a more efficient algorithm. Experience gained in this computation indicates several ways in which greater efficiency can be achieved. In particular, the many terms that turn out to be zero tend to take more time (individually!) to compute than do the interesting terms; it is possible to state general principles for discarding some such terms a priori.

Concluding remarks. This work has provided valuable experience in the use of symbolic computation on problems of this nature. Efficiency is strongly dependent on the organization of the calculation, in ways that are not always obvious at the start. The result, and the hoped-for future calculation of a_2, have applications in quantum gravity, and one may hope that they will be useful in continuum mechanics or pure geometry as well. The algebraic structure of the formulas is of some interest in its own right: the complicated dependence on the dimension m, the exotic coupling constant c, and the trace and transpose of the potential V are quite different from the second-order nonexotic case. The relative simplicity of (58) gives some hope of finding an insight into the nature of $a_n(x)$ for general n, generalizing Theorem 1. The most satisfactory outcome of a massive computer calculation often is a qualitative discovery that renders the calculation itself unnecessary in hindsight; that has not yet happened here, but one may hope, and keep looking.

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permutations needed to construct $g_{2\beta}$. V. P. Gusynin proved in [23–24] that the intrinsic pseudodifferential calculus can indeed be used to get concrete results. He also caught an error in [21] before publication. I have learned an immense amount from P. B. Gilkey in public and private communications, and I am grateful to him and T. P. Branson for generously including me as a coauthor of [21]. I thank the organizers of this Colloquium for the opportunity to communicate this research.

Bulletin. Since the Colloquium, T. P. Branson, P. B. Gilkey, and A. Pierzchalski have announced a calculation of $a_2(H)$ for $k = 1$ by functorial methods, extending Theorems 1 and 2.

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