VACUUM EXPECTATION VALUE ASYMPTOTICS
FOR SECOND ORDER DIFFERENTIAL
OPERATORS ON MANIFOLDS WITH BOUNDARY

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Abstract. Let $M$ be a compact Riemannian manifold with smooth boundary. We study the vacuum expectation value of an operator $Q$ by studying $\text{Tr}_{L^2} Q e^{-tD}$, where $D$ is an operator of Laplace type on $M$, and where $Q$ is a second order operator with scalar leading symbol; we impose Dirichlet or modified Neumann boundary conditions.

§1 Introduction

Let $M$ be a compact smooth Riemannian manifold of dimension $m$ with smooth boundary $\partial M$. We say that a second order operator $D$ on the space of smooth sections $C^\infty(V)$ of a smooth vector bundle over $M$ has scalar leading symbol if the leading symbol is $h^{ij} I_V \xi_i \xi_j$ for some symmetric 2-tensor $h$. We say that $D$ is of Laplace type if $h^{ij}$ is the metric tensor on the cotangent bundle. Let $D$ be an operator of Laplace type. If the boundary of $M$ is non-empty, we impose Dirichlet or Neumann boundary conditions $B$ to define the operator $D_B$, see §4 for further details. Let $Q$ be an auxiliary second order partial differential operator on $V$ with scalar leading symbol; if the order of $Q$ is at most 1, then this hypothesis is satisfied trivially. As $t \downarrow 0$, there is an asymptotic expansion

$$(1.1) \text{Tr}_{L^2} (Q e^{-tD_B}) \sim \sum_{n=-2}^{\infty} a_n(Q, D, B) t^{(n-m)/2},$$

see Gilkey [8, Lemma 1.9.1] where a different numbering convention was used. The invariants $a_n(Q, D, B)$ are locally computable. We have $a_{-2}(Q, D, B) = 0$ and $a_{-1}(Q, D, B) = 0$ if $Q$ has order at most 1. If the boundary of $M$ is empty, the boundary condition $B$ plays no role and we drop it from the notation; in this case, if $n$ is odd, then $a_n(Q, D) = 0$.

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Our paper is motivated by several physical examples. First, consider a Euclidean quantum field theory with a propagator $D^{-1}$ depending on external fields. Typically, $D$ is a second order differential operator of Laplace type. In the one–loop approximation, the vacuum expectation value $<Q>$ of a second order differential operator is given by $<Q> = Tr_{L^2}(QD^{-1})$. By formal manipulations, this can be represented in the form

$$<Q> \sim \int_0^\infty dt \, Tr_{L^2}(Q e^{-tD}) \sim \int_0^\infty dt \sum_{n=-2}^\infty a_n(Q, D, B) t^{(n-m)/2}.$$  

These integrals are divergent at the lower limit and need to be regularized. This can be done by replacing 0 by 1/Λ in the limits of integration; Λ is called the ultraviolet cutoff parameter. The coefficients $a_n(Q, D, B)$ define the asymptotics of $<Q>$ as $\Lambda \to \infty$. The first $m$ terms are divergent and are essential for renormalization. The coefficients $a_n(Q, D, B)$ also define large mass asymptotics of $<Q>$ in the theory of a massive quantum field; for details see for example [1].

A second example is provided by quantum anomalies. In the Fujikawa approach [6], the anomaly $A$ is defined as $A = \lim_{\Lambda \to \infty} Tr(Q e^{-D/\Lambda^2})$, where $Q$ is the generator of an anomalous symmetry transformation, and $D$ is a regulator. Usually divergent terms may be absorbed in renormalization and one has that $A \sim a_{m-2}(Q, D, B)$. Other examples where these asymptotics arise naturally are the study of the anomaly for an arbitrary local symmetry transformation, and in the study of the vacuum expectation value of the stress-energy tensor.

In this paper, we will study the asymptotics $a_n(Q, D, B)$ in a general mathematical framework. In §2, we review the geometry of operators of Laplace type and derive some variational formulas. The operator $D$ determines the metric $g$, a connection $\nabla$ on $V$, and an endomorphism $E$ of $V$. Conversely, given these data, we can define an operator of Laplace type $D(g, \nabla, E)$: see Lemma 2.3 for details. Let $q_2$ be a symmetric 2-tensor and let $q_1$ be a 1-form valued endomorphism of $V$. We shall use $q_2$ to define a variation of the metric $g(\varepsilon) := g + \varepsilon q_2$ and we shall use $q_1$ to define a variation of the connection $\nabla(\varepsilon) := \nabla + \varepsilon q_1$. Let $Q_2 := \partial_\varepsilon D(g(\varepsilon), \nabla(\varepsilon), E)|_{\varepsilon=0}$ and let $Q_1 := \partial_\varepsilon D(g(\varepsilon), \nabla(\varepsilon), E)|_{\varepsilon=0}$. Let $Q$ be a second order operator with scalar leading symbol. We may decompose $Q = Q_2 + Q_1 + Q_0$ for $Q_0 \in \text{End}(V)$ and for $Q_2$ and $Q_1$ defined by suitably chosen $q_2$ and $q_1$. Since $a_n(Q, D) = \sum_i a_n(Q_i, D)$, it suffices to compute the $a_n(Q_i, D)$. In Lemma 2.4, we will study the operators $Q_2$ and $Q_1$ and show that $\partial_\varepsilon a_{n+2}(1, D(\varepsilon), B) = -a_n(\partial_\varepsilon D(\varepsilon), D(\varepsilon), B)$ for any 1-parameter family of operators of Laplace type and fixed boundary condition $B$. In §3 and §4 we use this variational formula and apply results of [2] and [5] to study the invariants $a_n(Q, D, B)$; in §3 we consider manifolds without boundary and in §4 we consider manifolds with boundary.

An operator $A$ is said to be of Dirac type if $A^2$ is of Laplace type. Branson and Gilkey [2] studied the asymptotics of $Tr_{L^2}(A e^{-tA^2})$ for an operator $A$ of Dirac type on a closed manifold. In §5, we use the results of §3 to rederive these results and to compute some additional terms in the asymptotic expansion. The numbering convention we shall use in this paper differs from that used in [2]; the invariants $a_n(A, A^2)$ of this paper were denoted by $a_{n-1}(A, A^2)$ in [2].

§2 Geometry of operators of Laplace type

We adopt the following notational conventions. Greek indices $\mu, \nu$, etc. will range from 1 through $m = \text{dim}(M)$ and index local coordinate frames $\partial_\nu$ and $dx^\nu$
for the tangent and cotangent bundles $TM$ and $T^*M$. Roman indices $i$, $j$ will also range from 1 through $m$ and index local orthonormal frames $e_i$ and $e^i$ for $TM$ and $T^*M$. We shall suppress the bundle indices for tensors arising from $V$. We adopt the Einstein convention and sum over repeated indices. Let $D$ be an operator of Laplace type. This means that we can decompose $D$ locally in the form

\begin{equation}
D = -(g^{\mu\nu}I_V \partial_\nu \partial_\mu + a^\sigma \partial_\sigma + b)
\end{equation}

where $a$ and $b$ are local sections of $TM \otimes \text{End}(V)$ and $\text{End}(V)$ respectively. It is important to have a more invariant expression than that which is given in equation (2.1). Let $\Gamma$ be the Christoffel symbols of the Levi-Civita connection of the metric $g$ on $M$, let $\nabla$ be an auxiliary connection on $V$, and let $E \in C^\infty(\text{End}(V))$. Define:

\begin{equation}
D(g, \nabla, E) := -(\text{Tr}_g \nabla^2 + E)
= -g^{\mu\sigma}(I_V \partial_\mu \partial_\sigma + 2\omega_\mu \partial_\sigma - \Gamma_{\mu\sigma}^\nu I_V \partial_\nu + \partial_\mu \omega_\sigma + \omega_\mu \omega_\sigma - \Gamma_{\mu\sigma}^\nu \omega_\nu) - E.
\end{equation}

We compare equations (2.1) and (2.2) to prove the following Lemma.

**2.3 Lemma.** If $D$ is an operator of Laplace type, then there exists a unique connection $\nabla$ on $V$ and a unique endomorphism $E$ of $V$ so that $D = D(g, \nabla, E)$.

1. If $\omega$ is the connection 1-form of $\nabla$, then $\omega_\delta = g_{\nu\delta}(a^{\nu} + g^{\mu\sigma}\Gamma_{\mu\sigma}^\nu I_V)/2$.
2. We have $E = b - g^{\mu\nu}(\partial_\mu \omega_\nu + \omega_\nu \omega_\mu - \omega_\sigma \Gamma_{\mu\nu}^\sigma)$. Let $D = D(g, \nabla, E)$. We use the Levi-Civita connection of the metric $g$ and the connection $\nabla$ on $V$ to covariantly differentiate tensors of all types. We shall let ‘;' denote multiple covariant differentiation. Thus, for example, $Df = -(f;kk + Ef)$.

**2.4 Lemma.** Let $D = D(g, \nabla, E)$ be an operator of Laplace type. Let $q_2 = q_2, ij$ be a symmetric 2-tensor and let $q_1 = q_1, i$ be an endomorphism valued 1-tensor. Then

1. $Q_1f := \partial_i D(g, \nabla + \varepsilon q_1, E)|_{\varepsilon=0} = -2q_1, ij;i - q_1, i;i f$.
2. $Q_2f := \partial_i D(g + \varepsilon q_2, \nabla, E)|_{\varepsilon=0} = q_2, ij;i + (2q_2, ij;j - q_2, jj, ij)f/2$.
3. Let $D(g)$ be a smooth 1-parameter family of operators of Laplace type and fix $g$. Then $a_\mu(\partial_\mu D(g), D(g), B) = -\partial_\mu a_{\mu+2}(1, D(g), B)$.

**Proof.** Fix a point $x_0 \in M$; we may assume that $x_0$ is in the interior of $M$. Choose coordinates centered at $x_0$ and a local frame for $V$ so that $g_{\mu\nu}(x_0) = \delta_{\mu\nu}, \Gamma(x_0) = 0$, and so that $\omega(x_0) = 0$. We use equation (2.2) to compute:

\begin{align*}
\partial_\varepsilon D(g, \nabla + \varepsilon q_1, E)(x_0)|_{\varepsilon=0} &= -g^{\alpha\sigma}(2q_{1, \alpha, \sigma} + \partial_\sigma q_{1, \alpha})(x_0) \\
&= (-2q_{1, i, \varepsilon} - q_{1, i, i})(x_0),
\end{align*}

\begin{align*}
\partial_\varepsilon \{g + \varepsilon q_2\}^{\nu\sigma}(x_0)|_{\varepsilon=0} &= -\delta_{\nu\sigma}(x_0),
2\partial_\varepsilon \Gamma(g + \varepsilon q_2, \nu, \mu)(x_0)|_{\varepsilon=0} &= (q_{2, \mu, \nu, \sigma} + q_{2, \mu, \sigma, \nu} - q_{2, \nu, \sigma, \mu})(x_0),
\partial_\varepsilon D(g + \varepsilon q_2, \nabla, E)(x_0)|_{\varepsilon=0} &= (q_{2, \nu, \sigma} \partial_\sigma + \partial_\nu \omega_\sigma + \partial_\nu \Gamma(g + \varepsilon q_2, \mu, \nu, \sigma))(x_0)|_{\varepsilon=0}.
\end{align*}

The first two assertions now follow. We use [8, Lemma 1.9.3] to see that the asymptotic series of the variation is the variation of the asymptotic series. We
equate coefficients in the following two asymptotic expansions to complete the proof:

\[
\sum_n \partial_\theta a_n(1, D(\varrho), B) \epsilon^{(n-m)/2} \sim \partial_\theta \text{Tr} L^2(e^{-tD(\varrho)B}) \\
= \text{Tr} L^2(-t \partial_\theta D(\varrho) e^{-tD(\varrho)B}) \\
\sim -\sum_k a_k(\partial_\theta D(\varrho), D(\varrho), B) \epsilon^{(k+2-m)/2}. \quad \square
\]

To use Lemma 2.4, we shall need some variational formulas. Let \( R_{\mu\nu\sigma}^\delta \) be the curvature of the Levi-Civita connection with the sign convention that the Ricci tensor is given by \( \rho_{\mu\sigma} := R_{\mu\nu\sigma}^\nu \) and the scalar curvature is given by \( \tau := g^{\nu\sigma} \rho_{\nu\sigma} \). Let \( \Delta = \delta d \) be the curvature tensor of \( \nabla \).

2.5 Lemma. Let \( \nabla(\epsilon) := \nabla + \epsilon q_1 \) and \( q(\varrho) := \varrho + \rho q_2 \). Let \( \mathcal{F}_{ij} := (\partial_\epsilon|_{\epsilon=0} F)_{ij} \), \( R_{\mu\nu\sigma}^\delta := (\partial_\epsilon|_{\epsilon=0} R)_{\mu\nu\sigma}^\delta \), and let \( D := \partial_\epsilon|_{\epsilon=0} \Delta_0 \). Then

1. \( \mathcal{F}_{ij} = q_{1,ij} - q_{1,j;i} \) and \( \partial_\epsilon|_{\epsilon=0} (\nabla F)_{ij;k} = \mathcal{F}_{ij;k} + [q_{1,k}, \mathcal{F}_{ij}] \).
2. \( D f = q_{2,ij} f_{ij} + (2q_{2,ij;j} - q_{2,ij;i}) f_i/2. \)
3. \( \partial_\epsilon d \text{vol}|_{\epsilon=0} = q_{2,ii} d \text{vol}/2. \)
4. \( (\partial_\epsilon|_{\epsilon=0} R)^\mu_{\nu\sigma} = g^{\gamma\nu} (q_{2,\mu\gamma;\nu} + q_{2,\nu\gamma,\mu} - q_{2,\mu\nu;\gamma}/2). \)
5. \( R_{\mu\nu\sigma}^\delta = g^{\gamma\nu} (q_{2,\mu\rho;\gamma} + q_{2,\rho\gamma,\sigma} - q_{2,\mu\gamma;\rho} - q_{2,\sigma\gamma;\rho} - q_{2,\mu\sigma} R_{\rho\gamma}^\rho)^\delta. \)
6. \( \partial_\epsilon|_{\epsilon=0} \tau = -q_{2,ij} \rho_{ij} + R_{kik}. \)
7. \( \partial_\epsilon|_{\epsilon=0} |\rho|^2 = 2R_{kik}\rho_{ij} - 2q_{2,ij}\rho_{ik}\rho_{jk}. \)
8. \( \partial_\epsilon|_{\epsilon=0} |R|^2 = 2R_{ijkl} R_{ijkl} - 2q_{2,jn} R_{ijkl} R_{inkl}. \)

Proof. The assertion (1) is immediate from the definition. Assertion (2) follows from Lemma 2.4. Assertions (3) and (4) are straightforward calculations. Assertion (5) follows from assertion (4) and from the identity\(^1\):

\[ q_{2,\sigma\gamma;\mu} - q_{2,\sigma\gamma;ij} = -q_{2,\gamma\rho} R_{\mu\nu\sigma}^\rho - q_{2,\sigma\rho} R_{\mu\nu\gamma}^\rho. \]

Raising and lowering indices does not commute with varying the metric so we emphasize that the tensor \( R \) is the variation of a tensor of type \((3,1)\). The remaining assertions now follow. \( \square \)

\(^1\)We are grateful to Arkady Tseytlin who pointed out a sign error in this identity in the previous version of the paper.

§3 Manifolds without boundary

Lemma 2.4 reduces the computation of \( a_n(Q, D) \) to the special cases \( a_n(Q, D) \) for \( i = 0, 1, 2 \). Recall that \( a_n(Q, D) = 0 \) for odd \( a_{-2}(Q, D) = 0 \) if \( \text{ord}(Q) \leq 1 \). If \( P \) is a scalar invariant, let \( P[M] := \int_M P(x) d \text{vol}(x) \). Let \( \text{tr}_V \) be the fiber trace. We refer to Gilkey [7] for the proof of the following result:

3.1 Theorem. Let \( M \) be a compact Riemannian manifold without boundary, let \( D \) be an operator of Laplace type, and let \( Q_0 \in \text{End}(V) \). Then

1. \( a_0(Q_0, D) = (4\pi)^{-m/2} \text{tr}_V \{ Q_0 \} [M]. \)
3.2 Theorem. Let $D$ be a compact Riemannian manifold without boundary, let $D$ be an operator of Laplace type, and let $Q_1 = \partial_\tau D(g, \nabla + \varepsilon q_1, E)|_{\varepsilon=0}$. Then

1. $a_0(Q_1, D) = 0$.
2. $a_2(Q_1, D) = -(4\pi)^{-m/2}360^{-1} \text{tr}_V \{60F_{ij}F_{ij}\}[M]$.
3. $a_4(Q_1, D) = -(4\pi)^{-m/2}360^{-1} \text{tr}_V \{60E_{kk} + 60\tau E + 180E^2 + 12\tau_{kk} + 5\tau^2 - 2|\rho|^2 + 2|R|^2 + 30F_{ij}F_{ij}\}[M]$.
4. $a_6(Q_1, D) = (4\pi)^{-m/2} \text{tr}_V \{Q_0/7! (18\tau_{ij} + 28\tau_{ij}kk - 2\rho_{ij}kk\rho_{ij}kk - 4\rho_{jki}\rho_{jki}k + 9R_{ij}kkR_{ij}kk + 28\tau_{ijk}kk - 8\rho_{ij}kk\rho_{ij}kk + 24\rho_{jki}\rho_{jki}k + 12R_{ij}kkR_{ij}kk + 35/9\tau^3 - 14/3\tau R^2 + 208/9\rho_{ijk}\rho_{ijk}k - 64/3\rho_{ijkl}R_{ijkl}\}
\frac{16}{3}\rho_{jki}R_{jikl}R_{jiklp} - 80/9R_{ijkl}R_{ikljp} + 360^{-1} Q_0 \{8F_{ij}\kappa F_{ij}kk + 2F_{ij}\kappa F_{ij}kk + 6F_{ij}\kappa F_{ij}kk + 6F_{ij}F_{ij}kk - 12F_{ij}F_{ij}kk - 6R_{ijkl}F_{ijkl}F_{ijkl} - 4\rho_{jki}\rho_{jki}k + 5\tau F_{knn}F_{knn} + 6E_{ij},ijj + 30E_{ii}E_{ii} + 30E_{ii}E_{ii} + 30E_{ii}E_{ii} + 60E^5 + 12EF_{ij}F_{ij} + 6EF_{ij} + 12EF_{ij}E_{ij} + 10\tau E_{kk} + 4\rho_{jki}E_{ij} + 12\tau_{kk}E_{kk} - 6E_{ij}F_{ij} + 6F_{ij}E_{ij} + 30EE\kappa + 12E_{kk} + 5E^2 - 2E\rho_{jki}\rho_{jki} + 2E^2\kappa\}[M]$.

Proof. We use Lemma 2.4 and Theorem 3.1. Note that $\Delta_0(f) = -f_{kk}$ is independent of the connection $\nabla$ for $f \in C^\infty(M)$. We compute:

1. $\partial_\kappa \text{tr}_V \{60E_{kk}\}[\kappa = 0] = 60\partial_\kappa \text{tr}_V (E)_{kk}[\kappa = 0] = -60\partial_\kappa \Delta_0 \text{tr}_V (E) = 0$.
2. $\partial_\kappa \text{tr}_V (30F^2)[\kappa = 0] = \text{tr}_V (60F_{ij}F_{ij})$.
3. $\partial_\kappa \text{tr}_V (8F_{ij}F_{ij} + 6F_{ij}F_{ij} + 6F_{ij}F_{ij}kk)[\kappa = 0]$
   $\quad = \partial_\kappa \{\text{tr}_V (-4F_{ij}F_{ij}) + \text{tr}_V (6F_{ij}F_{ij})\}[\kappa = 0]$
   $\quad = \text{tr}_V (-8F_{ij}F_{ij} + 8F_{ij}q_{ij}F_{ij} + 8F_{ij}F_{ij}kk)$.
4. $\partial_\kappa \text{tr}_V (30E_{ii} + 30E_{ii}E + 30E_{ii}E)[\kappa = 0]$
   $\quad = \partial_\kappa \{\text{tr}_V (30E_{ii}E) + \text{tr}_V (30EE)_{ii}\}[\kappa = 0]$
   $\quad = \text{tr}_V (-60E_{kkq_{ij}k}E + 60E_{kkq_{ij}q_{ij}})$.

We conclude this section by studying $a_n(Q_2, D)$. The following result is a consequence of Lemmas 2.4, Lemma 2.5, and Theorem 3.1. We omit the formula for $a_4(Q_2, D)$ in the interests of brevity.
3.3 Theorem. Let $M$ be a compact Riemannian manifold without boundary, let $D$ be an operator of Laplace type on $C^\infty(V)$, and let $Q_2 = \partial_2 D(g + \varepsilon_2, \nabla, E)|_{\varepsilon = 0}$.

(1) $a_{-2}(Q_2, D) = -\frac{1}{2}Q_0(q_{2,ii}, D)$.

(2) $a_0(Q_2, D) = -\frac{1}{2}a_2(q_{2,ii}, D) - (4\pi)^{-m/2}6^{-1} \text{tr}_{V}\{\{-q_{2,ij}\rho_{ij} + R_{kiij}\}I_V\}|M|.$

(3) $a_2(Q_2, D) = -\frac{1}{2}a_4(q_{2,ii}, D) - (4\pi)^{-m/2}36^{-1}\{-D\text{tr}_V(60E + 12\tau I_V) + \text{tr}_V\{10(-q_{2,ij}\rho_{ij} + R_{kiij})\}I_V - 2(2R_{kiij}\rho_{ij} - 2q_{2,ij}\rho_{ij} + R_{kiij})I_V + 2(2R_{ijkl}R_{ijkl} - 2q_{2,ij}\rho_{ij} + R_{kiij})I_V + 60(-q_{2,ij}\rho_{ij} + R_{kiij})E - 60q_{2,ij}F_{ij}F_{ik}\}|M|.$

§4 Manifolds with boundary

We now suppose $M$ has smooth non-empty boundary $\partial M$. Near $\partial M$, let $e_i$ be a local orthonormal frame for $TM$ where we normalize the choice so that $e_m$ is the inward unit normal. We let indices $a, b, \ldots$ range from $1$ through $m - 1$ and index the resulting orthonormal frame for the tangent bundle $T(\partial M)$ of the boundary. Let $f \in C^\infty(V)$. Let $S$ be an endomorphism of $V$ defined on $\partial M$. The Neumann boundary operator is defined by $B^+_S f := (\nabla_m + S)f|_{\partial M}$ and the Dirichlet boundary operator is defined by $B^-_S f = f|_{\partial M}$; we set $S = 0$ with Dirichlet boundary conditions to have a uniform notation. Let $L_{ab} = (\nabla_e e_b, e_m)$ be the second fundamental form. Let $\cdot \cdot$ denote multiple covariant differentiation tangentially with respect to the Levi-Civita connection of the metric on the boundary and the connection $\nabla$ on $V$. The difference between $\cdot \cdot$ and $\cdot \cdot$ is given by the second fundamental form. For example, $E_a$ and $E_a$ agree since there are no tangential indices in $E$ to be differentiated while $E_{ab} = E_{ab} - L_{ab}E_m$. There are some new features here which are not present in the case of manifolds without boundary in the following formulas. The invariants $a_n(Q, D, B)$ are non-zero for odd $n$ and the normal derivatives of $Q_0$ enter. We still have $a_{-2}(Q, D, B) = 0$ if $\text{ord}(Q) \leq 1$.

4.1 Theorem. Let $M$ be a compact Riemannian manifold with smooth boundary, let $D$ be an operator of Laplace type and let $Q_0 \in \text{End}(V)$. Then

(1) $a_0(Q_0, D, B^+_S) = (4\pi)^{-m/2}\text{tr}_{V}\{Q_0\}|M|.$

(2) $a_1(Q_0, D, B^+_S) = \pm(4\pi)^{-m/2}3^{-1}\text{tr}_{V}\{Q_0\}|\partial M|.$

(3) $a_2(Q_0, D, B^+_S) = (4\pi)^{-m/2}6^{-1}\{\text{tr}_V\{Q_0(6E + \tau)\}\}|M| + \text{tr}_V\{Q_0(2L_{aa} + 12S) + (3^+, -3^-)Q_{0,m}\}|\partial M|.$

(4) $a_3(Q_0, D, B^+_S) = (4\pi)^{-m/2}38^{-1}\text{tr}\{Q_0(96^+, -96^-)E + (16^+, -16^-)\tau + (8^+, -8^-)R_{amam} + (13^+, -7^-)L_{aa}L_{bb} + (2^+, -10^-)L_{ab} + 96S_{aa} + 192S^2) + Q_{0,m}(6^+, 3^+)L_{aa} + 96S^2 + (24^+, -24^-)Q_{0,m}\}|\partial M|.$

(5) $a_4(Q_0, D, B^+_S) = (4\pi)^{-m/2}36^{-1}\{\text{tr}_V\{Q_0(60E_{kk} + 120E^2 + 20F_{ij}F_{ij} + 12\tau_{kk} + 5\tau^2 - 2\rho^2 + 2R^2)\}\}|M| + \text{tr}\{Q_0(240^+, -120^-)E_{mm} + (42^+, -18^-)\tau_{mm} + 24L_{aa, bb} + 120E_{aa} + 20\tau L_{aa} + 4R_{amam}L_{bb} - 12R_{amam}L_{ab} + 4R_{abab}L_{ac} + 360(SE + ES) + 21^{-1}(280^+, 40^-)L_{aa}L_{bb}L_{cc} + (165^+, -264^-)L_{ab}L_{ab}L_{aa} + (224^+, 320^-)L_{ab}L_{bc}L_{ac} + 120S^2 + 144S_{aa}L_{bb} + 28SL_{ab} + 480S_{aa} + (180^+, -180^-)E + (30^+, -30^-)\}$
4.2 Theorem. Let $M$ be a compact Riemannian manifold with smooth boundary, let $D$ be an operator of Laplace type, and let $Q_1 = \partial_x D(g, \nabla + \varepsilon q_1, E)|_{\varepsilon=0}$. Then

(1) $a_{-1}(Q_1, D, B_S^\pm) = 0$.

(2) $a_0(Q_1, D, B_S^\pm) = -(4\pi)^{-m/2}6^{-1}\text{tr}_V((-12^+, 0^-)q_{1,m})[\partial M]$.

(3) $a_1(Q_1, D, B_S^\pm) = -(384)^{-1}(4\pi)^{-(m-1)/2}\text{tr}_V((-96^+, 0^-)q_{1,m}L_{aa} - 384S_{q_{1,m}})[\partial M]$.

(4) $a_2(Q_1, D, B_S^\pm) = -(4\pi)^{-m/2}360^{-1}\{\text{tr}_V(60F_{ij}F_{ij})[M]$

$+\text{tr}_V\{(-720^+, 0^-)q_{1,m}E + (-120^+, 0^-)q_{1,m}\tau + (-144^+, 0^-)q_{1,m}L_{aa}L_{bb} + (-48^+, 0^-)q_{1,m}L_{ab}L_{ab} - 960S_{q_{1,m}}L_{aa} - 1440S^2q_{1,m}][\partial M]\}$.

(5) $a_3(Q_1, D, B_S^\pm) = 5760^{-1}(4\pi)^{(m-1)/2}\text{tr}_V\{240F_{ab}F_{ab} - 720F_{am}F_{am}\}[\partial M]$.

(6) If the boundary of $M$ is totally geodesic, then

$$a_3(Q_1, D, B_S^\pm) = -5760^{-1}(4\pi)^{(m-1)/2}\text{tr}_V\{-1440E_{m}q_{1,m} + 1440(q_{1,m}E - E_{q_{1,m}})S + 240F_{ab}F_{ab} - 960\tau S_{q_{1,m}} - 240\rho_{mm}S_{q_{1,m}} + 180F_{am}F_{am} - 270\tau_{q_{1,m}} + 720S_{q_{1,m}} + 720S_{q_{1,m}} - 2880E(S_{q_{1,m}} + q_{1,m}S) - 5760q_{1,m}S^3\}[\partial M].$$

Proof. If $Q_0 = q_1IV$ for $q_0 \in C^\infty(M)$ is a scalar operator, then Theorem 4.1 follows from Branson and Gilkey [2]. If $Q_0$ is not a scalar operator, we must worry about the lack of commutativity; the only point at which this enters is in the coefficient of $\text{tr}_V(Q_0SE)$ and $\text{tr}_V(Q_0ES)$. We express

$$a_4(Q_0, D, B_S) = (4\pi)^{-m/2}360^{-1}\text{tr}_V(C_1Q_0SE + C_2Q_0ES)[\partial M] + \text{other terms};$$

the sum $C_1 + C_2 = 720$ is determined by the scalar case. If $D$, $Q_0$, and $S$ are real, then $\text{Tr}_{L^2}(Q_0e^{-1D})$ is real; this shows that $C_1$ and $C_2$ are real. If $Q_0$, $D$, and $S$ are self-adjoint, $\text{Tr}_{L^2}(Q_0e^{-1D})$ is real so $\text{tr}_V(Q_0(C_1SE + C_2ES))[\partial M]$ is real; this now shows $C_1 = C_2$ and completes the proof of Theorem 4.1.

To keep boundary conditions constant, let $S(\varepsilon) := S - \varepsilon q_{1,m}$ so $\partial_\varepsilon S|_{\varepsilon=0} = -q_{1,m}$. Assertions (1)-(5) of Theorem 4.2 now follow directly from Lemma 2.4, from Lemma 2.5, and from Theorem 4.1. In [5], we showed that

$$a_5(1, D, B_S^\pm) = \pm 5760^{-1}(4\pi)^{(m-1)/2}\text{tr}_V\{360E_{mm} + 1440E_{m}S$

$+ 720E^2 + 240E_{aa} + 240\tau E + 120F_{ab}F_{ab} + 48\tau_{ii} + 20\tau^2 - 8\rho^2$

$+ 8\rho^2 - 120\rho_{mm}E - 20\rho_{mm}\tau + 480\tau S^2 + (90^+, -360^-)F_{am}F_{am}$

$+ 12\tau_{mm} + 24\rho_{mm}aa + 15\rho_{mm:mm} + 270\tau_{mm}S + 120\rho_{mm}S^2 + 960S_{mm}S$

$+ 600S_{mm}S_{mm} + 16R_{ammb}\rho_{ab} - 17\rho_{mm}\rho_{mm} - 10R_{ammb}R_{ammb} + 2880ES^2$

$+ 1440S^4\} + [\partial M]$.

The variation of the terms other than $E$ gives rise to the expressions listed in Theorem 4.2 (5,6). The remainder term $E$ is given below. It vanishes if the boundary is totally geodesic and involves 40 undetermined coefficients.

$$E = \sum_{i} d_i^L L_{aa}E_m + d_i^L L_{ab}R_{ammb} + d_i^L L_{aa}S_{ab} + d_i^L L_{ab}S_{ab} + d_i^L L_{aa}S_{ab} + d_i^L L_{ab}S_{ab} + d_i^L L_{aa}S_{ab} + d_i^L L_{ab}S_{ab} + d_i^L L_{aa}S_{ab} + d_i^L L_{ab}S_{ab}.$$

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The second assertion is immediate, the third follows from Lemma 2.5.

4.4 Theorem. Proof.

To study \(a_n(Q_2, D, B^+_{S})\) we need some additional formulas.

4.3 Lemma.

(1) Let \(g(q) := g + q g_2, N := \partial_q|_{q=0} e_m(q), \) and \(L_{\alpha\beta} := \partial_q|_{q=0} L_{\alpha\beta}. \) Then
   a. \(N = -q_{2, am} e_a - q_{2, mm} e_m / 2. \)
   b. \(L_{ab} = (q_{2, am} b + q_{2, bm} a - q_{2, ab} m - q_{2, mm} L_{ab}) / 2. \)

(2) \(q_{2, am, c} = q_{2, am, c} - L_{aa} q_{2, mm} + L_{ab} q_{2, ab}. \)

(3) \(R_{ki k} = q_{2, k i k} - q_{2, i j k}. \)

Proof. Let \(1 \leq \alpha, \beta \leq m - 1. \) Let \(y = (y^\alpha)\) be local coordinates on the boundary \(\partial M\) centered at \(y_0. \) We suppose \(g_{\alpha\beta}(y_0) = \delta_{\alpha\beta} + O(|y|^2). \) Introduce coordinates \(x = (y, x^m)\) so the curves \(t \mapsto (y, t)\) are unit speed geodesics perpendicular to the boundary. Then \(y_m = 1 \) and \(y_m = 0; \) \(\partial_m\) is the inward geodesic normal vector field for \(g. \) Let \(N(q)\) be the inward geodesic normal vector field for the metric \(g(q).\) Expand \(N(q)(y_0) = \partial_m + \theta^m \partial_m + c^\beta \partial_\beta + O(|y|^2). \) We prove the first assertion by solving the equations

\[0 = g(q)(N(q), \partial_q)(y_0) = g(e^\alpha + q_{2, am})(y_0) + O(|y|^2)\]
\[1 = g(q)(N(q), N(q))(y_0) = 1 + \theta(2e^m + g_{2, mm})(y_0) + O(|y|^2)\]

to see \(e^\alpha(y_0) = -q_{2, ma}(y_0)\) and \(e^m(y_0) = -q_{2, mm}/2. \) We use Lemma 2.5 to compute the variation of the Christoffel symbols and complete the proof by computing:

\[L_{\alpha\beta} = \Gamma(\beta)(\alpha, \beta, \partial_q)\]
\[L_{\alpha\beta}(y_0) = (\hat{\Gamma}_{\alpha\beta}^m - q_{2, mm} L_{\alpha\beta}/2)(y_0).\]

The second assertion is immediate, the third follows from Lemma 2.5. □

Dirichlet boundary conditions are unchanged by a variation of the metric \(g.\) The following result follows from Lemma 2.4, Theorem 4.1, and Lemma 4.3. We omit the formula for \(a_2\) in the interests of brevity.

4.4 Theorem. Let \(M\) be a compact Riemannian manifold with smooth boundary, let \(D\) be an operator of Laplace type, and let \(Q_2 := \partial_{\varepsilon}|_{\varepsilon=0} D(g + \varepsilon q_2, \nabla, E). \) Then

(1) \(a_{-2}(Q_2, D, B^-) = -(4\pi)^{-m/2} \text{tr}_V \{q_{2, ii}/2\}[M].\)
(2) \( a_{-1}(Q_2, D, B^-) = (4\pi)^{-m/2}4^{1-1}\text{tr}_V\{q_{2,aa}/2\}[\partial M] \).

(3) \( a_0(Q_2, D, B^-) = (4\pi)^{-m/2}4^{-1}\{\text{tr}_V\{q_{2,ii}(6E + \tau)/2 - q_{2,ij}\rho_{ij} + R_{kiik}\}\}[M] + \text{tr}_V\{q_{2,aa}L_{aa} + 2L_{aa} - 2q_{2,ab}L_{ab}\}[\partial M] \).

(4) \( a_1(Q_2, D, B^-) = (4\pi)^{-m/2}4^{1-1}\text{tr}_V\{q_{2,aa}(96E + 16\tau + 8R_{amam}
+ 7L_{aa}L_{bb} - 10L_{ab}L_{ab}/2 + 16(-q_{2,ij}\rho_{ij} + R_{ikik})
+ 8(R_{amam} - q_{2,ab}R_{abmn} + 2R_{amaN}) + 7(2L_{aa}L_{bb} - 2q_{2,ab}L_{ab}L_{cc})
- 10(2L_{ab}L_{ab} - 2q_{2,ac}L_{ab}L_{eb})\}[\partial M] \).

(5) Suppose for simplicity that the metric \( g \) is flat, i.e., that \( R_{ijkl} = 0 \). Then
\( a_2(Q_2, D, B^-) = (4\pi)^{-m/2}360^{-1}\{-D\text{tr}_V\{60E\} + \text{tr}_V\{60R_{ijij}E\}
+ 30q_{2,ii}E_{ik} + 90q_{2,ii}E^{2} + 15q_{2,ii}Q^{2}\}\}[M] \).

We now study Neumann boundary conditions. The situation is quite different as Neumann boundary conditions are not invariant under general perturbations of the metric; if \( q_{am} \neq 0 \) on \( \partial M \), \( B^{\pm}_S(\varphi) \) will involve tangential derivatives regardless of how \( S \) is varied. Thus Lemma 2.4 is not directly applicable. Nevertheless, we can still compute the first three terms in the asymptotic expansion.

4.5 Theorem. Let \( M \) be a compact Riemannian manifold with smooth boundary, let \( D \) be an operator of Laplace type, and let \( Q_2 := \partial_z D(g + \varepsilon q_2, \nabla, E)\) at \( \varepsilon = 0 \). Then

(1) \( a_{-2}(Q_2, D, B^+_S) = -(4\pi)^{-m/2}\text{tr}_V\{q_{2,ii}/2\}[M] \).

(2) \( a_{-1}(Q_2, D, B^+_S) = -(4\pi)^{-(m-1)/2}4^{-1}\text{tr}_V\{q_{2,aa}/2\}[\partial M] \).

(3) \( a_0(Q_2, D, B^+_S) = -(4\pi)^{-m/2}4^{-1}\text{tr}_V\{q_{2,ii}(6E + \tau)/2 - q_{2,ij}\rho_{ij}\}[M]
- (4\pi)^{-m/2}4^{-1}\text{tr}_V\{q_{2,aa}L_{aa} - q_{2,ab}L_{ab} - 6q_{2,mm}S + 6q_{2,aa}\}[\partial M] \).

Proof. Define ord\( (q_{2,ij}) = 0 \), ord\( (E) = 2 \), ord\( (R_{ijkl}) = 2 \), ord\( (F) = 2 \), ord\( (L) = 1 \), and ord\( (S) = 1 \). Increase the order by 1 for each explicit covariant derivative which is present. Dimensional analysis then shows the interior integrands in the formula for \( a_n(Q_2, D, B) \) are homogeneous of order \( n + 2 \) while the boundary integrands are homogeneous of degree \( n + 1 \). We use H. Weyl’s theorem to write a spanning set for the set of invariants and express:

(4.6) \( a_{-2}(Q_2, D, B^+_S) = -(4\pi)^{-m/2}\text{tr}_V\{b_1q_{2,ii}/2\}[M] \)

(4.7) \( a_{-1}(Q_2, D, B^+_S) = -(4\pi)^{-(m-1)/2}4^{-1}\text{tr}_V\{c_1q_{2,aa}/2 + c_2q_{2,mm}\}[\partial M] \).

(4.8) \( a_0(Q_2, D, B^+_S) = -(4\pi)^{-m/2}6^{-1}\{\text{tr}_V\{q_{2,ii}(6b_2E + b_3\tau)/2
- b_1q_{2,ij}\rho_{ij}\}\}[M] + \text{tr}_V\{c_3q_{2,aa}L_{bb} + c_4q_{2,ab}L_{ab} + c_5q_{2,mm}L_{aa}
+ c_6q_{2,mm}S + c_7q_{2,aa}S + c_8q_{2,mm}S + c_9q_{2,aa,m}\}[\partial M] \)
Product formulas then show the constants are independent of the dimension \( m \); these invariants form a basis for the integral invariants and are uniquely determined for \( m \) large. A word of explanation for the formula in equation (4.8) is in order. We can integrate by parts to replace the interior integrals \( q_{2,i;j} \) and \( q_{2,ii;jj} \) by boundary integrals of \( q_{2,m;m;m} \), \( q_{2,aa;m} \), and \( q_{2,aa;m} \). Since \( q_{2,aa;m}(\partial M) = 0 \), we use Lemma 4.3 to omit the variable \( q_{2,am,a} \). If we take \( \partial M \) empty, the boundary condition plays no role and \( R_{kiik}[M] = 0 \) (see equation (4.10) below). We use Theorem 3.3 to see \( b_1 = b_2 = b_3 = b_4 = 1 \); this completes the proof of assertion (1) and the first part of assertion (2).

We use Lemma 2.4 and Theorem 4.1 to see:

\[
a_0(q_2, D, B_S^+) = (4\pi)^{-(m-1)/2} \partial M \left\{ \text{tr}_V(q_{2,li}(6E + \tau)/2 - q_{2,ij}\rho_{ij} + R_{kiik}[M] + \text{tr}_V(q_{2,aa}(L_{bb} + 6S) - 2q_{2,ab}L_{ab} + 2L_{aa} - 6q_{2,mm}S}[\partial M] \right\}
\]

We have that

\[
\begin{align*}
R_{kiik}[M] &= (q_{2,ki;ki} - q_{2,ii;kk})[M] = (-q_{2,am,a} + q_{2,aa;m})[\partial M] \\
&= (L_{aa}q_{2,mm} - L_{ab}q_{2,ab} + q_{2,aa;m})[\partial M] \\
2L_{aa}[\partial M] &= (2q_{2,am;a} - q_{2,aa;m} - q_{2,mm}L_{aa})[\partial M] \\
&= (-3L_{aa}q_{2,mm} + 2L_{ab}q_{2,ab} - q_{2,aa;m})[\partial M].
\end{align*}
\]

We use equation (4.10) to compare equations (4.8) and (4.9). This shows

\[
c_3 = 1, \ c_4 = -1, \ c_5 = -2, \ c_6 = -6, \ c_7 = 6, \ c_8 = 0, \ c_9 = 0. \quad \Box
\]

\section{5 Operators of Dirac Type}

In this section, we study the invariants \( a_n(HA, A^2) \), where \( M \) is a closed manifold, \( A \) is an operator of Dirac type, and \( H \) is a smooth endomorphism; we refer to Branson and Gilkey [4] for a discussion of the case of manifolds with boundary. We begin with a technical result:

\subsection{5.1 Lemma}

Let \( A = \gamma^\nu \partial_\nu - \psi \) be an operator of Dirac type and let \( D = A^2 \) be the associated operator of Laplace type. Let \( D = D(g, \nabla, E) \) and let \( H \in C^\infty \operatorname{End}(V) \).

\begin{enumerate}
\item \( \omega_\mu = g_{\mu\nu}(\gamma^\nu \partial_\nu \gamma^\rho + \psi \gamma^\rho + \gamma^\rho \psi + g^{\rho\sigma} \Gamma_{\gamma^\rho} \gamma^\sigma)/2 \).
\item Let \( \phi := \psi + \gamma^\nu \omega_\nu \). Then \( A = \gamma^\nu \nabla_\nu - \phi \), and \( \phi \) is invariantly defined.
\item \( \gamma_{ij} + \gamma_{ji} = 0 \).
\item \( E = -\psi^2 + \gamma^\nu \partial_\nu \psi - g^{\rho\sigma}(\partial_\nu \omega_\nu + \omega_\nu \omega_\mu - \omega_\mu \Gamma_{\gamma^\nu} \gamma^\sigma) = -\gamma_1 F_{ij} + \gamma_4 \phi_{ij} - \phi^2 \).
\item Let \( q_{1,i} := -H \gamma_i/2 \), and \( Q_0 := -H \phi - H_1 \gamma_i/2 \), then \( HA = Q_1 + Q_0 \).
\end{enumerate}
Proof. We compute

\[
D = A^2 = (\gamma^\nu \partial_\nu - \psi)(\gamma^\mu \partial_\mu - \psi)
\]

\[
= \gamma^\nu \gamma^\mu \partial_\nu \partial_\mu + (\gamma^\nu \partial_\nu \gamma^\mu - \gamma^\mu \psi - \psi \gamma^\mu) \partial_\mu + \psi^2 - \gamma^\mu \partial_\mu \psi,
\]

\[
a^\mu = -\gamma^\nu \partial_\nu \gamma^\mu + \gamma^\mu \psi + \psi \gamma^\mu, \quad \text{and} \quad b = -\psi^2 + \gamma^\mu \partial_\mu \psi.
\]

Assertion (1) and the first assertion of (4) follows from Lemma 2.3. We prove

We choose a system of coordinates and a local frame so that \( \Gamma(x_0) = 0 \) and so that \( \omega(x_0) = 0 \).

Then at \( x_0 \), we have:

\[
D = (\gamma^\nu \partial_\nu - \phi)(\gamma^\mu \partial_\mu - \phi)
\]

\[
= (\gamma^\nu \gamma^\mu + \gamma^\mu \gamma^\nu)/2\gamma^\nu \partial_\mu + (\gamma^\mu \gamma^\nu \partial_\mu - \phi \gamma^\nu - \gamma^\nu \phi) \partial_\mu
\]

\[
- \gamma^\nu \partial_\mu \gamma^\nu \Omega_{\mu\nu}/2 + \phi^2
\]

\[
= -g^\nu\mu \partial_\nu \partial_\mu - E.
\]

We equate coefficients to derive the second part of assertion (4). Choose a coordinate system centered at \( x_0 \) so \( \gamma_{\mu
u} = \delta_{\mu\nu} + O(|x|^2) \). We use \([3, \text{Lemma 1.2}]\) to see that we can choose a local frame for \( V \) so \( \partial_\mu \gamma^\nu(x_0) = 0 \). Then we have that \( \omega_\mu(x_0) = (\gamma_\mu \gamma_\nu)(x_0)/2 \). We prove assertion (3) by computing at \( x_0 \):

\[
2(\gamma_{\nu\mu} + \gamma_{\mu\nu}) = [\psi \gamma_\mu + \gamma_\mu \psi, \gamma_\nu] + [\psi \gamma_\nu + \gamma_\nu \psi, \gamma_\mu]
\]

\[
= \psi \gamma_\mu \gamma_\nu + \gamma_\mu \psi \gamma_\nu - \gamma_\nu \psi \gamma_\mu - \gamma_\mu \psi \gamma_\nu
\]

\[
+ \psi \gamma_\nu \gamma_\mu + \gamma_\nu \psi \gamma_\mu - \gamma_\mu \psi \gamma_\nu - \gamma_\mu \gamma_\nu \psi
\]

\[
= \psi \delta_{\mu\nu} - \delta_{\mu\nu} \psi = 0.
\]

If we set \( q_{1,i} = -H \gamma_i/2 \), then \( Q_1 = H\gamma_i \partial_\nu + H_i \gamma_i/2 \) by Lemma 2.4 since \( \gamma_{i;i} = 0 \). We must therefore take \( Q_0 = -H \phi - H_i \gamma_i/2 \). \( \square \)

The following theorem now follows from Theorem 3.1, Theorem 3.2, and from Lemma 5.1.

5.2 Theorem. Let \( A = \gamma_\nu \partial_\nu - \psi \) be an operator of Dirac type on \( C^\infty(V) \) over a closed manifold \( M \). Adopt the notation of Lemma 5.1.

(1) \( a_0(HA, A^2) = (4\pi)^{-m/2} \text{tr}_V \{Q_0\}[M] \).

(2) \( a_2(HA, A^2) = (4\pi)^{-m/26 - 1} \text{tr}_V \{Q_0(\tau + 6E) - F_{ij} F_{ij}\}[M] \).

(3) \( a_4(HA, A^2) = (4\pi)^{-m/2360 - 1} \text{tr}_V \{Q_0(60E_{kk} + 60\tau E + 180 E^2 + 12 \tau_{kk} + 5 \tau^2 - 2 |\rho|^2 + 2 |R|^2 + 30 F_{ij} F_{ij} + 8 F_{ijkl} F_{ijkl} + 8 F_{ijk} q_{1,k} F_{ij}
\]

\[-8 F_{ijk} F_{ij} q_{1,k} - 4 F_{ijkl} F_{ik} q_{1,k} - 4 F_{ijkl} q_{1,k} F_{ik} + 4 F_{ijkl} F_{ik} q_{1,k}
\]

\[+36 F_{ijk} F_{k} F_{i,j} + 12 R_{ijk} F_{ij} F_{kn} + 8 \rho_{ijk} F_{jn} F_{kn} - 10 \tau F_{kn} F_{kn}
\]

\[+60 E_{k} q_{1,k} E - 60 E_{k} E q_{1,k} - 30 E F_{ij} F_{ij} - 30 E F_{ij} F_{ij}\}[M] \).
5.3 Remark. The first two authors [3, Theorem 2.7] computed $a_0$ and $a_2$ for $f$ scalar and showed that

$$a_0(fA, A^2) = - (4\pi)^{-m/2} \text{tr}_V (f\phi)[M]$$
$$a_2(fA, A^2) = - (4\pi)^{-m/2} 6^{-1} \text{tr}_V \{f(\phi \tau + 6\phi E - F_{ij}\gamma_i)\}[M].$$

For scalar $f$, $\text{Tr}_{L^2}(f\gamma_i e^{-tA^2}) = \text{Tr}_{L^2}(Afe^{-tA^2} - fAe^{-tA^2}) = 0$ so $a_n(f\gamma_i, A^2) = 0$ for all $n$ and we may replace $Q_0$ by $-\dot{\phi}$ in performing our computations. It then follows that Theorem 5.2 (1) agrees with equation (5.4). We see Theorem 5.2 (2) agrees with equation (5.5) by using Lemma 2.5 and integrating by parts:

$$- \text{tr}_V (F_{ij}F_{ij})[M] = \text{tr}_V ((f\gamma_j)_i - (f\gamma_i)_j)F_{ij}[M]/2$$
$$= - \text{tr}_V (f\gamma_jF_{ij})[M] = \text{tr}_V (f\gamma_iF_{ij})[M].$$

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