Sharp reflecting heat-kernel tensor bias on smooth manifolds with boundary

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Abstract

For uniform density on a smooth compact manifold with boundary, we compute the leading fractional-power bias of the reflecting heat-kernel Sinkhorn tensor. The coefficient depends on the first unmatched Neumann jet of the input and is universal across dimensions. The proof transfers the boundary Kuznecov law through the tensor's spectral multiplier. For ordinary smooth inputs, the strong bias has order $h^{7/4}$ and the next form bias has order $h^{5/2}$. A positive correction using a boundary trace probe attains the optimal form-comparable strong order $(h/\log(1/h))^{7/4}$ using polylogarithmic rank. We also give a matching rank lower bound on a flat cylinder. No correction commuting with the Neumann Laplacian gains the logarithmic factor.

1 Setting and results

The leading bias at uniform density is governed by the first unmatched normal derivative among the successive powers of the Neumann differential expression applied to the input. Theorem 1 gives the strong and quadratic-form asymptotics for every such order. The spectral input is the boundary Kuznecov law of Han, Hassell, Hezari and Zelditch. The contribution is its transfer through the reflecting Sinkhorn multiplier, including the necessary Taylor subtractions.

For inputs with a nonzero first normal derivative, Theorem 2 determines the optimal strong order among uniformly form-dominated positive corrections. The upper bound uses a finite-rank perturbation of a diagonal operator. The cylinder lower bound concerns perturbations of uniformly dominated commuting operators.

Let M be a connected, smooth compact Riemannian manifold of dimension d, with nonempty smooth boundary. Use its Riemannian volume and its induced boundary measure. Let $L = -\Delta_N/2$ be the Neumann Laplacian, nonnegative with orthonormal eigenfunctions ϕ_j and eigenvalues λ_j. Let $H_h = e^{-hL}$. At the uniform probability density, $q = \mathrm{vol}(M)^{-1/2}$. Since the Neumann semigroup fixes constants, the symmetric Sinkhorn scale is one. On the orthogonal complement of the constant define

$$T_h = hH_h(I - H_h^2)^{-1}, \qquad G = \tfrac{1}{2}L^{-1}.$$

Extend both operators by zero on constants. This is the intrinsic reflecting heat-kernel tensor in the normalization of [1, 2]. Write L_{int} for the differential expression $-\Delta/2$ without boundary conditions.

Set

$$f(s) = \frac{1}{2\sinh s} - \frac{1}{2s} = \sum_{j\ge 1} c_j s^{2j-1} \quad \text{near zero}, \qquad f_k(s) = f(s) - \sum_{1\le j\le k} c_j s^{2j-1}.$$

The empty sum is zero, and $c_1 = -1/12$. For a smooth mean-zero η suppose $\partial_\nu L_{\mathrm{int}}^j \eta = 0$ on the boundary for $0 \le j < \ell - 1$, where $\ell \ge 1$. Set $g = \partial_\nu L_{\mathrm{int}}^{\ell-1}\eta$.

Theorem 1. *For $k = \lfloor \ell/2 \rfloor$,*

$$h^{-2\ell-3/2} \left\| (T_h - G)\eta - \sum_{j=1}^{k} c_j h^{2j} L^{2j-1}\eta \right\|_2^2 \longrightarrow \frac{\sqrt{2}}{4\pi} \|g\|_{L^2(\partial M)}^2 \int_0^\infty f_k(s)^2 s^{-2\ell-1/2}\, ds.$$

For the quadratic form,

$$h^{-2\ell-1/2} \left[\langle \eta, (T_h - G)\eta \rangle - \sum_{j=1}^{\ell} c_j h^{2j} \langle \eta, L^{2j-1}\eta \rangle \right] \longrightarrow \frac{\sqrt{2}}{4\pi} \|g\|_{L^2(\partial M)}^2 \int_0^\infty f_\ell(s) s^{-2\ell-1/2}\, ds.$$

The powers in the second formula are interpreted as spectral quadratic forms. Both integrals are finite and nonzero. For $\ell = 1$ these are the $h^{7/4}$ strong bias and $h^{5/2}$ form remainder.

Theorem 2. *If $0 \le C_h \le M_0 T_h$ uniformly in h, and a fixed smooth mean-zero η has $\partial_\nu \eta \not\equiv 0$, then*

$$\|(C_h - G)\eta\|_2 \gtrsim_{\eta, M_0} (h/\log(1/h))^{7/4}.$$

If C_h commutes with the spectral projections of L, the lower bound becomes $h^{7/4}$. There exist compact positive operators C_h with $cT_h \le C_h \le CT_h$ and

$$\|C_h - G\|_{H^r \cap 1^\perp \to L^2} \lesssim (h/\log(1/h))^{7/4}, \qquad r > d/2 + 3.$$

They are finite-rank perturbations of a diagonal operator. These Sobolev spaces impose no boundary condition.

Han, Hassell, Hezari and Zelditch [3, Theorem 6] already establish the boundary Kuznecov law used below. The result here uses that spectral law to resolve the tensor bias, its compatible jet hierarchy, and the constrained approximation rate. The interval companion [1] gives the fixed nonuniform density profile and weak Fisher coefficient in one dimension. Here the geometry may have arbitrary smooth boundary and curvature, with uniform density.

2 The boundary spectral measure

Write Γ for restriction to the boundary. For $g \in L^2(\partial M)$ let

$$b_j(g) = \int_{\partial M} g\, \phi_j, \qquad \mu_g = \sum_{\lambda_j > 0} |b_j(g)|^2 \delta_{\lambda_j}.$$

Two boundary heat estimates we use are

$$\|\Gamma H_t \Gamma^*\|_{L^2(\partial M) \to L^2(\partial M)} \lesssim t^{-1/2}, \quad \Gamma H_t \Gamma^* g = \sqrt{2/\pi}\, t^{-1/2} g + O_{L^2(\partial M)}(\|g\|_{C^1}).$$

Here g is C^1 in the second estimate. Recall their kernel explanation. At a boundary point use boundary normal coordinates with orthonormal tangent frame. In the parabolically scaled coordinates the leading Neumann heat kernel is the sum of the direct and reflected Gaussians [4, Appendix B, Theorem 41 and Claim 42]. At the boundary diagonal these two terms agree. Restricted to both boundary points the leading kernel is $2(2\pi t)^{-d/2}e^{-|y'|^2/(2t)}$ in tangential coordinates through that point. The Jacobian and the remainder after freezing the leading model have order $\sqrt{t}$ relative to the scaled kernel, with rapid decay in $y'/\sqrt{t}$. Integrating this bound and the C^1 variation of g gives an $O(1)$ remainder and leading factor $2(2\pi t)^{-1/2}$. Off the diagonal the contribution is rapidly small by the heat kernel bound on a smooth compact manifold [5]. The uniform operator bound follows by the Schur test from the same boundary integral estimate. In particular,

$$\mu_g([0,R]) \lesssim (1+R)^{1/2}\|g\|_2^2, \qquad R \geq 0,$$

by bounding the spectral projection by a constant times $H_{1/R}$ for large R.

For smooth g the boundary Kuznecov law of [3] gives

$$\mu_g([0,R]) \sim \frac{2\sqrt{2}}{\pi}\|g\|_2^2 R^{1/2}$$

if $g \neq 0$. One can also deduce this leading term from the boundary heat estimate by the positive-measure Laplace Tauberian theorem. Thus the rescaled measures $h^{1/2}\mu_g(d(s/h))$ converge vaguely on $(0,\infty)$ to $(\sqrt{2}/\pi)\|g\|_2^2 s^{-1/2}\,ds$. The cumulative upper bound supplies uniform integrability for any test function with absolute envelope $O(s^\alpha)$ near zero for $\alpha > -1/2$ and $O(s^{-\beta})$ at infinity for $\beta > 1/2$. This follows by dyadic decomposition at either end. For small frequencies below the fixed first positive eigenvalue the measures vanish. Thus the term $1+R$ in the cumulative envelope is harmless after rescaling.

3 Transferring the law to the tensor

Green's formula gives, for smooth η,

$$\lambda_j\langle\phi_j,\eta\rangle = \langle\phi_j, L_{\mathrm{int}}\eta\rangle + \tfrac{1}{2}b_j(\partial_\nu\eta).$$

Applying this repeatedly under the stated compatibility conditions yields

$$\langle\phi_j,\eta\rangle = \lambda_j^{-\ell}\big[\langle\phi_j, L_{\mathrm{int}}^{\ell}\eta\rangle + \tfrac{1}{2}b_j(g)\big].$$

The interior coefficients here are square summable. In particular the domain conditions for each strong Taylor term hold: $2j-1 \leq \ell-1$ for $j \leq \lfloor \ell/2 \rfloor$. For each form term the spectral moment is finite by the cumulative boundary upper bound and $2j-1 \leq 2\ell-1$.

The remainder strong multiplier is $hf_k(h\lambda_j)$. The boundary coefficient part of its squared norm is

$$\frac{1}{4}h^{2\ell+2}\int_0^\infty f_k(s)^2 s^{-2\ell}\,\mu_g(d(s/h)).$$

The weights satisfy the required endpoint envelopes: the first unsuppressed Taylor order is at least ℓ, while the maximum power of the large-s polynomial is at most $\ell-1$. The leading constant follows from rescaled boundary measure convergence. The interior term is $O(h^{\ell+1})$ in norm, since $s^{-\ell}f_k(s)$ is bounded. The cross term is therefore negligible on the indicated squared-norm scale. In the form calculation the same expression uses $h^{2\ell+1}f_\ell(s)s^{-2\ell}/4$ in place of the squared weight. The first unsuppressed Taylor order is $2\ell+1$ and the last subtracted one is $2\ell-1$, yielding the

required envelopes at both ends. The weighted square of the interior coefficients is $O(h^{2\ell+1})$ using boundedness of $s^{-2\ell} f_\ell(s)$. Use Cauchy–Schwarz with the absolute weight for the cross term. This proves the form limit.

The strong integral is strictly positive from its nonzero multiplier. For the weak integral put $z = 1/2 - 2\ell$. The Mellin transform of $1/(2\sinh s)$ for $\operatorname{Re} z > 1$ is $\Gamma(z)(1 - 2^{-z})\zeta(z)$ by its odd exponential series. Continue it by subtracting $1/(2s)$ and the Taylor terms through degree $2\ell - 1$ on $(0, 1)$. At the indicated z, each of these subtracted powers is integrable against s^{z-1} on $(1, \infty)$. Its continued pole term equals minus that latter integral. Thus the fully subtracted integral in the theorem is exactly $\Gamma(z)(1 - 2^{-z})\zeta(z)$. It is nonzero, since at a negative noninteger half-integer the gamma function is finite and nonzero, and the zeta functional equation gives no zero there.

4 An optimal positive correction

The eigenvalues of T_h are $t_h(\lambda) = h/(2\sinh(h\lambda))$ off constants. For $C_h \le M_0 T_h$, form Cauchy–Schwarz gives

$$\|P_{>R} C_h \eta\|_2 \lesssim_\eta \sqrt{h}\, e^{-hR/2}$$

when $hR \ge 1$, where $P_{>R}$ is the projection onto eigenvalues of L above R. Here $T_h \le G$ bounds the other factor independently of h. Green's formula and the boundary spectral law imply $\|P_{>R} G\eta\|_2 \asymp_\eta R^{-7/4}$ when $\partial_\nu \eta \not\equiv 0$. Indeed its weighted boundary tail norm squared has order $R^{-7/2}$, whereas its interior tail norm is $O(R^{-2})$. Take R a large constant times $h^{-1}\log(1/h)$ and subtract the exponentially small C_h tail. If C_h commutes with the spectral projections, on every eigenspace above $R \asymp h^{-1}$ with a large fixed factor one has $C_h \le M_0 t_h(\lambda) I \le (4\lambda)^{-1} I$. Thus the tail error is at least half the G tail, and the stronger lower bound follows.

For an upper construction let A_h be diagonal, equal to G at $0 < \lambda \le 1/h$ and to T_h above. It is uniformly form-comparable to T_h. Set $N = h^{-1}\log(1/h)$, let $\mathbf{1}_{\mathrm{mid}}$ select $1/h < \lambda \le N$, and define the boundary-to-volume operator

$$V_h = \tfrac{1}{2}\mathbf{1}_{\mathrm{mid}}(L)(G - T_h)L^{-1}\Gamma^*.$$

Its range is in a finite-dimensional spectral subspace. The boundary spectral upper bound and dyadic summation give

$$\|V_h\|_{L^2(\partial M)\to L^2(M)} \lesssim h^{7/4}, \qquad \|T_h^{-1/2} V_h\| \lesssim h^{3/4}.$$

In fact $G - T_h \le G$ on the selected band, so the sum of squared coefficients is bounded by the integral of $C\lambda^{-4}$ against μ_g there. For the second estimate, $T_h \ge h H_h$ and $e^{hN/2} = h^{-1/2}$.

Let $\tau = h^{1/8}$ and define the volume-to-boundary probe

$$W_\tau = \frac{\Gamma(H_\tau - H_{4\tau})}{\sqrt{2/\pi}\sqrt{\tau}}.$$

It annihilates constants. For $g = \partial_\nu \eta$, Green's formula gives

$$\partial_t \Gamma H_t \eta = -\Gamma H_t L_{\mathrm{int}} \eta - \tfrac{1}{2}\Gamma H_t \Gamma^* g.$$

Integrate between τ and 4τ. The boundary heat estimate and the Markov bound on $H_t L_{\mathrm{int}}\eta$ give

$$\|W_\tau \eta - g\|_{L^2(\partial M)} \lesssim \sqrt{\tau}\, \|\eta\|_{H^r}.$$

The trace estimate $\|\Gamma H_\tau\| \lesssim \tau^{-1/4}$ comes from the boundary heat norm at time 2τ by multiplying by its adjoint. Likewise $H_h^{-1/2}$ can be composed with the probe adjoint by leaving heat time at least $\tau/2$. It follows that

$$\|W_\tau\| \lesssim \tau^{-3/4}, \qquad \|W_\tau T_h^{-1/2}\| \lesssim h^{-1/2}\tau^{-3/4}.$$

All inverse-square-root expressions here are on $1^\perp$, with bounded extensions as shown.

Define $C_h = A_h + V_h W_\tau + W_\tau^* V_h^*$. The perturbation is selfadjoint and finite rank, and its relative form bound is $O(h^{1/4}\tau^{-3/4}) = o(1)$. Thus it gives positivity, compactness and two-sided form comparison. By Green's formula the intermediate-frequency error $G - A_h$ equals $V_h g$ up to $O(h^2\|L_{\mathrm{int}}\eta\|_2)$. The probe replaces g to the order just proved. The high tail $\lambda > N$ of this error is bounded by $CN^{-7/4}\|\eta\|_{H^r}$ by the boundary spectral upper bound and the square summable interior term. The low part already matches G.

It remains to bound the reciprocal correction. For a dyadic band $[R, 2R]$, $\|\Gamma \mathbf{1}_{[R,2R]}(L)\| \lesssim R^{1/4}$ by the cumulative boundary upper bound. The interior contribution to $V_h^*\eta$ on this band is bounded by $CR^{-11/4}\|L_{\mathrm{int}}\eta\|_2$: Green's formula gives one λ^{-1}, and V_h^* contributes two more. The boundary contribution is bounded by $CR^{-5/2}\|g\|_2$, with two factors of the boundary restriction norm. Summing over $R \geq 1/h$ gives $\|V_h^*\eta\| \lesssim h^{5/2}\|\eta\|_{H^r}$. Hence the reciprocal term has error $O(\tau^{-3/4}h^{5/2}\|\eta\|_{H^r})$, smaller than the desired rate. The other errors are $O(h^2)$, $O(h^{7/4}\sqrt{\tau})$, and $O(N^{-7/4})$ times the input norm. This proves the matching construction.

5 Size of the correction space

The correction can be realized with a polylogarithmic rank. On the boundary let P_B^∂ be its intrinsic Laplace spectral projection through frequency B, with

$$B = (\log(1/h))^{7/[4(r-3/2)]}.$$

Replace $V_h W_\tau$ by $V_h P_B^\partial W_\tau$ and the other term by its adjoint. The trace theorem and the boundary spectral Sobolev norm give

$$\|(I - P_B^\partial)\partial_\nu \eta\|_2 \leq CB^{-(r-3/2)}\|\eta\|_{H^r}.$$

After applying V_h, this costs at most the target rate. Orthogonal projection does not increase the earlier form bounds or the reciprocal estimate. The resulting correction has rank at most $2 \operatorname{rank} P_B^\partial = O(B^{d-1})$ by the ordinary boundary Weyl bound. For $d = 1$, the boundary space has finite dimension.

Theorem 3. *On the flat cylinder $M = [0,1] \times \mathbb{T}^{d-1}$, $d \geq 2$, this rank order is necessary among finite-rank perturbations of uniformly dominated spectral operators. More precisely, suppose A_h commutes with the spectral projections of L, $0 \leq A_h \leq M_0 T_h$ uniformly, and C_h has the strong upper rate in Theorem 2 for a given $r > d/2 + 3$. Then*

$$\operatorname{rank}(C_h - A_h) \gtrsim (\log(1/h))^{7(d-1)/[4(r-3/2)]}.$$

The implicit constant can depend on the constant in the strong upper estimate and on M_0.

To prove it, choose a smooth function ξ supported near the left edge of the half-line with $\xi'(0) \neq 0$, smooth up to that edge. For a large parameter B_*, consider the tangents

$$B_*^{1/2-r}\xi(B_* x)e^{2\pi i k\cdot y}, \qquad B_* \leq |k| \leq 2B_*,$$

or their real span. The tangential frequencies are nonzero, so the tangents have mean zero. Their span has dimension $\asymp B_*^{d-1}$. The H^r norm of a linear combination is bounded by a constant times the coefficient ℓ^2 norm. For instance extend ξ smoothly and compactly to the line and use the Fourier Sobolev norm on the product of the line and the torus, then restrict. The normal scaling $B_*^{1/2-r}$ compensates for the derivative weights B_*^r and the support width.

Uniformly for normal cosine frequency $n \gg B_*$, the coefficient of each tangent on its tangential frequency is a nonzero constant times $B_*^{3/2-r} n^{-2}$, with relative error $O((B_*/n)^2)$. This is obtained by two integrations by parts for the endpoint derivative and two more for the third derivative and the integral remainder. Take n in a band of fixed proportional width above a sufficiently large multiple of $h^{-1/2}$. On this band the fixed upper bound for A_h in the spectral eigenspaces implies a norm error at least half the G contribution, as in the commuting lower bound. Equivalently, take an eigenvalue tail containing this band, so any mixing within an eigenspace does not affect the estimate. The modes from distinct tangential frequencies are orthogonal in the G tail, and the eigenvalues of G there have order n^{-2} when B_* is polylogarithmic. Thus every such linear combination has $(A_h - G)$ tail norm bounded below by a constant times $h^{7/4} B_*^{3/2-r}$ times its coefficient norm.

If the corrective rank is below the dimension of this span, some nonzero vector in it belongs to the kernel of $C_h - A_h$, so the same lower bound applies to $C_h - G$. Taking B_* a sufficiently small fixed multiple of $(\log(1/h))^{7/[4(r-3/2)]}$ contradicts the assumed upper constant. This proves the rank lower bound.

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