

ON THE TRACE OF SCHRÖDINGER HEAT KERNELS AND REGULARITY OF POTENTIALS

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ABSTRACT. For the Schrödinger operator $-\Delta_g + V$ on a complete Riemannian manifold with real valued potential V of compact support, we establish a sharp equivalence between Sobolev regularity of V and the existence of finite-order asymptotic expansions as $t \rightarrow 0$ of the relative trace of the Schrödinger heat kernel. As an application, we generalize a result of Sà Barreto and Zworski [13], concerning the existence of resonances on compact metric perturbations of Euclidean space, to the case of bounded measurable potentials.

1. INTRODUCTION AND STATEMENT OF RESULTS

Consider a Schrödinger operator $P_V = -\Delta_g + V$ on a complete Riemannian manifold (M, g) of dimension n , with Δ_g the Laplace-Beltrami operator. We assume $V \in L_c^\infty(M)$ is real valued, where $L_c^\infty(M)$ denotes bounded measurable functions of compact support on M . We assume the Ricci curvature of (M, g) is bounded from below to ensure uniqueness of solutions to the heat equation; see [8]. Let e^{-tP_0} denote the heat semigroup on (M, g) , and e^{-tP_V} the heat semigroup for P_V , which can be constructed from e^{-tP_0} by iteration (e.g. see §2 of this paper).

For examples of (M, g) including compact manifolds [1], and Euclidean space [10], [7], it is well known that if $V \in C_c^\infty(M)$ then $e^{-tP_V} - e^{-tP_0}$ is of trace class for $t > 0$, and its trace admits a full asymptotic expansion as $t \rightarrow 0$

$$\mathrm{tr}(e^{-tP_V} - e^{-tP_0}) \sim (4\pi t)^{-\frac{n}{2}} \sum_{k=1}^{\infty} a_k t^k, \quad 0 < t \leq 1.$$

In this paper we prove a sharp equivalence between the existence of this expansion to finite order, and finite order Sobolev regularity of V . In order to ensure the above difference is of trace class when $n \geq 4$ we make an additional assumption (1.2) on (M, g) , but for $n \leq 3$ we prove that it is trace class using only uniqueness of solutions to the heat equation. Our main result is the following.

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Theorem 1.1. *Assume that (1.2) holds if $n \geq 4$. Suppose that $V \in L_c^\infty(M)$ is real valued, and that for a given integer $m \geq 0$ it holds that*

$$(1.1) \quad \operatorname{tr}(e^{-tP_V} - e^{-tP_0}) = (4\pi t)^{-\frac{n}{2}} \left(c_1 t + c_2 t^2 + \cdots + c_{m+1} t^{m+1} + r_{m+2}(t) t^{m+2} \right)$$

where $|r_{m+2}(t)| \leq C$ for $0 < t \leq 1$. Then $V \in H^m(M)$. Conversely, if $V \in L_c^\infty \cap H^m(M)$ then (1.1) holds with $r_{m+2}(t) \in C([0, 1])$, and in particular $\lim_{t \rightarrow 0^+} r_{m+2}(t)$ exists.

Here, $H^m(M)$ with $m \geq 0$ denotes the integer order Sobolev spaces on M , consisting of functions whose derivatives up to order m belong to $L^2(M)$. We consider only functions supported in a fixed compact set, so the norm on $H^m(M)$ can be defined using a finite collection of coordinate charts.

For $n \geq 4$, to show that $e^{-tP_V} - e^{-tP_0}$ is trace class we will assume trace class bounds for the heat kernel restricted on one side to a compact set. Let \mathcal{L}^1 denote the trace class operators on $L^2(M)$, which form an ideal in the algebra of bounded operators. If $\mathbb{1}_K$ denotes restriction of functions to K , then for $K \subset M$ compact we assume that

$$(1.2) \quad \|\mathbb{1}_K \circ e^{-tP_0}\|_{\mathcal{L}^1} \leq C_K t^{-\frac{n}{2}}, \quad 0 < t \leq 1.$$

This holds, for example, if the sectional curvatures of (M, g) are globally bounded above and below, and the injection radius is globally bounded below; see Lemma 1.3 below.

If M is compact, then e^{-tP_0} is itself of trace class, and by the theorem of Minakshisundaram-Pleijel [11], its trace admits a full asymptotic expansion as $t \rightarrow 0$, with trace coefficients expressed in terms of geometric invariants. For modern treatments of this result, see [5] and [12]. Thus, for M compact Theorem 1.1 states that $\operatorname{tr}(e^{-tP_V})$ admits an expansion

$$\operatorname{tr}(e^{-tP_V}) = (4\pi t)^{-\frac{n}{2}} \left(c_0 + c_1 t + c_2 t^2 + \cdots + c_{m+1} t^{m+1} + \mathcal{O}(t^{m+2}) \right), \quad 0 < t \leq 1,$$

precisely when $V \in H^m(\mathbb{R}^n)$. Throughout this paper we are interested only in the trace near $t = 0$, and henceforth in all statements we restrict to $t \in (0, 1]$.

Theorem 1.1 is closely related to a priori estimates that give bounds on the Sobolev norms of a real, smooth potential V in terms of the coefficients c_k . These bounds have been used to establish compactness in the C^∞ topology of isospectral families of smooth potentials on a compact Riemannian manifold, with some a priori bound assumed on V for dimensions $n \geq 4$. See for example [10], [3], and [9]. The novelty of Theorem 1.1 is to establish the regularity result analogous to these a priori bounds, for all finite orders of regularity. This requires in particular a careful analysis of the remainder terms in the heat trace expansion, for t in an interval and V of finite regularity, and not just of the coefficients c_k .

As an application of Theorem 1.1 we prove here the following result on existence of resonances for compact metric perturbations of the Laplacian.

We remark that there exist complex valued V with no resonances by [6], and that even when $V \in C_c^\infty$ the result is known only in dimension three.

Theorem 1.2. *Suppose that $M = \mathbb{R}^3$, and that $g^{ij}(x) = \delta^{ij}$ on the complement of some compact set. Suppose also that $V \in L_c^\infty(\mathbb{R}^3)$ is real valued. Then the operator $P_V = -\Delta_g + V$ has infinitely many scattering resonances, unless $V = 0$ and (M, g) is isometric to Euclidean space.*

Proof. This was proved in [13] in the case $V \in C_c^\infty(\mathbb{R}^3)$, and in [14] for $V \in L_c^\infty(\mathbb{R}^3)$ in the case $g^{ij}(x) = \delta^{ij}$ on all of \mathbb{R}^3 . We follow here the proof in [14], with the addition of a result from [13]. To start, assume that there are no resonances. Then the argument in [14, §2.3] shows that, since the scattering matrix is an entire function, the left hand side of (1.1) admits an asymptotic expansion with only terms of negative half-integral order. In particular, on \mathbb{R}^3 we have $\text{tr}(e^{-tP_V} - e^{-tP_0}) = c_0 t^{-\frac{1}{2}}$. By Theorem 1.1, this implies that $V \in C_c^\infty(\mathbb{R}^3)$. We may then apply the Theorem of [13] to see that $V = 0$, and (\mathbb{R}^3, g) is isometric to Euclidean space.

We thus assume there is at least one resonance. Note, by Theorem 1.1 with $m = 0$, that for some c_0

$$\text{tr}(e^{-tP_V} - e^{-tP_0}) = c_0 t^{-\frac{1}{2}} + \mathcal{O}(t^{\frac{1}{2}}).$$

If there were only finitely many resonances, then the argument of [14, §2.3] shows that

$$\lim_{t \rightarrow 0^+} \left(\text{tr}(e^{-tP_V} - e^{-tP_0}) - c_0 t^{-\frac{1}{2}} \right) \neq 0,$$

and hence there must in fact be infinitely many resonances. \square

We conclude this section with three results concerning the heat kernel e^{-tP_0} that will be used to obtain trace class bounds on $e^{-tP_V} - e^{-tP_0}$. A corollary of Lemma 1.3 is that (1.2) holds if the sectional curvatures are globally bounded above and below and there is a global lower bound on the injectivity radius. The first condition of the lemma holds in that case by [4], and the second by Bishop's volume comparison theorem [2].

Lemma 1.3. *Condition (1.2) holds if there is a constant C , and $x_0 \in M$, such that when $t \in (0, 1]$ and $R > 0$,*

$$H_0(t, x, y) \leq C t^{-\frac{n}{2}} e^{-\frac{d(x,y)^2}{Ct}}, \quad \mu(\{x : d(x, x_0) < 2R\}) \leq C e^{CR^2},$$

where μ is the Riemannian volume form for g .

Proof. Let $w(x) = Cd(x, x_0)^2$, and write

$$\mathbb{1}_K e^{-tP_0} = \left(\mathbb{1}_K e^{-\frac{1}{2}tP_0} e^w \right) \left(e^{-w} e^{-\frac{1}{2}tP_0} \right)$$

The second factor has Hilbert-Schmidt norm given by the square root of

$$\int e^{-2w(x)} H_0\left(\frac{1}{2}t, x, y\right)^2 d\mu(y) d\mu(x) = \int e^{-2w(x)} H_0(t, x, x) d\mu(x).$$

This in turn is bounded by

$$Ct^{-\frac{n}{2}} \int e^{-2Cd(x,x_0)^2} d\mu(x) \leq Ct^{-\frac{n}{2}},$$

where the last inequality follows easily from the bound on $\mu(B(x_0, R))$. The first factor has Hilbert-Schmidt norm equal to the square root of

$$\int \mathbb{1}_K(x) H_0(\frac{1}{2}t, x, y)^2 e^{2Cd(y,x_0)^2} d\mu(y) d\mu(x).$$

For $t < \frac{1}{2}C^{-2}$, we use the triangle inequality to dominate this by

$$\begin{aligned} Ct^{-\frac{n}{2}} \int \mathbb{1}_K(x) e^{-8Cd(x,y)^2} e^{2Cd(y,x_0)^2} d\mu(y) d\mu(x) \\ \leq Ct^{-\frac{n}{2}} \left(\int \mathbb{1}_K(x) e^{8Cd(x,x_0)^2} d\mu(x) \right) \left(\int e^{-2Cd(y,x_0)^2} d\mu(y) \right) \\ \leq C_K t^{-\frac{n}{2}}, \end{aligned}$$

and together these imply (1.2) for sufficiently small t . For $\frac{1}{2}C^{-2} \leq t \leq 1$, (1.2) follows by the group property of the heat operator since \mathcal{L}^1 is an ideal. \square

In dimension $n \leq 3$, the following will suffice to obtain the needed trace-norm estimates. Here, $\|\cdot\|_{\mathcal{L}^2}$ is the Hilbert-Schmidt norm on operators.

Lemma 1.4. *Assume that (M, g) is complete, with global lower bounds on the Ricci curvature. If K is compact, then $\|\mathbb{1}_K \circ e^{-tP_0}\|_{\mathcal{L}^2} \leq C_K t^{-\frac{n}{4}}$.*

Proof. We calculate the Hilbert-Schmidt norm of the kernel H_0 of e^{-tP_0} with one variable restricted to K . Since $H_0 > 0$,

$$\|\mathbb{1}_K \circ e^{-tP_0}\|_{\mathcal{L}^2}^2 = \int \mathbb{1}_K(x) H_0(t, x, y)^2 d\mu(y) d\mu(x) = \int_K H_0(2t, x, x) d\mu(x).$$

This bounded by $\text{vol}(K) \sup_{x \in K} H_0(2t, x, x)$, and the result is a consequence of the following estimate, valid for compact subsets $K \subset M$,

$$\sup_{x \in K} H_0(t, x, x) \leq C_K t^{-\frac{n}{2}}.$$

This is known to hold if M is compact, hence for M as in the statement, by the following lemma. \square

Lemma 1.5. *Suppose that (\tilde{M}, \tilde{g}) is a compact Riemannian manifold that isometrically contains a neighborhood (U, g) of the compact subset $K \subset M$. Let \tilde{H}_0 be the heat kernel on (\tilde{M}, \tilde{g}) , and suppose $\chi \in C_c^\infty(U)$ equals 1 on a neighborhood of K . Then, if (M, g) is complete with global lower bounds on its Ricci curvature, the following holds*

$$\sup_{x \in M, y \in K} |H_0(t, x, y) - \chi(x) \tilde{H}_0(t, x, y)| \leq C_N t^N \quad \forall N, \quad t \in (0, 1].$$

Proof. For $y \in K$, we consider $\chi(x)\tilde{H}_0(t, x, y)$ as a function of $x \in U \subset M$. Then by the local heat kernel expansion (see e.g. [5, (23.64)-(23.65)])

$$\sup_{x \in U, y \in K} |(\partial_t - \Delta_g)\chi(x)\tilde{H}_0(t, x, y)| \leq C_N t^N \quad \forall N, \quad \text{if } t \in (0, 1].$$

Uniqueness of the heat kernel on (M, g) lets us write

$$\begin{aligned} H_0(t, x, y) - \chi(x)\tilde{H}_0(t, x, y) \\ = \int_0^t \int_M H_0(t-s, x, z)(\partial_s - \Delta_g)((\chi(z)\tilde{H}_0(s, z, y)) d\mu(z) ds. \end{aligned}$$

Since the heat semigroup has norm 1 on $L^\infty(M)$, the right hand side vanishes to infinite order at $t = 0$, uniformly over $y \in K$ and $x \in M$, leading to the desired estimate. \square

The outline of this paper is as follows. In §2 we express e^{-tP_V} as an iterative expansion, and use this, together with trace bounds for the localized heat kernel, to obtain an expansion for the trace of their difference. A key simplification is Corollary 2.1 where we reduce matters to the case of M compact by compact support of V . In §3, we reduce the proof of Theorem 1.1 to Theorems 3.1 and 3.2, the proofs of which are given in §4 and §5. A key tool in these sections is the small time expansion for the heat kernel of Δ_g near the diagonal, summarized in §2, and the resulting rule (2.4) for the product of heat kernels.

2. THE SCHRÖDINGER HEAT KERNEL

The proof of Theorem 1.1 relies on the following expansion for the Schrödinger heat kernel,

$$e^{-tP_V} = e^{-tP_0} + \sum_{k=1}^{\infty} W_k(t),$$

where

$$\begin{aligned} W_k(t) = (-1)^k \int_{0 < s_1 < \dots < s_k < t} e^{-(t-s_k)P_0} V e^{-(s_k-s_{k-1})P_0} V \dots \\ \times V e^{-(s_2-s_1)P_0} V e^{-s_1P_0} ds_1 \dots ds_k. \end{aligned}$$

The sum over k converges for $t > 0$ in the operator norm topology on $L^2(M)$, which follows since $\|W_k\|_{L^2 \rightarrow L^2} \leq t^k \|V\|_{L^\infty}^k / k!$. The latter bound follows since $\|e^{-tP_0}\|_{L^2 \rightarrow L^2} \leq 1$ for all $t \geq 0$, and since the region of integration over the s variables has measure $t^k / k!$.

We now estimate the trace norm of the operators $W_k(t)$. Let \mathcal{L}^2 denote the Hilbert-Schmidt operators on $L^2(M)$, and \mathcal{L}^1 the trace class operators. Recall that $\|ST\|_{\mathcal{L}^1} \leq \|S\|_{\mathcal{L}^2} \|T\|_{\mathcal{L}^2}$, and $\|ST\|_{\mathcal{L}^1} \leq \|S\|_{\mathcal{L}^1} \|T\|_{L^2 \rightarrow L^2}$.

Consider first the term $W_1(t)$, and $n \leq 3$. By Lemma 1.4 with $K = \text{supp}(V)$, we have

$$\|e^{-(t-s)P_0} V e^{-sP_0}\|_{\mathcal{L}^1} \leq C_{\text{supp}(V)}^2 \|V\|_{L^\infty} (t-s)^{-\frac{n}{4}} s^{-\frac{n}{4}}.$$

For $n \leq 3$ we can integrate this bound over $0 < s < t$ to obtain

$$\|W_1(t)\|_{\mathcal{L}^1} \leq C_{\text{supp}(V)}^2 \|V\|_{L^\infty} t^{1-\frac{n}{2}}, \quad n \leq 3.$$

Next consider $k \geq 2$, for $n \leq 3$. If $s_j - s_{j-1} > (2k)^{-1}t$ for some $k \geq j \geq 1$, then Lemma 1.4 and the group property yield the bound

$$\begin{aligned} \|Ve^{-(s_j-s_{j-1})P_0}V\|_{\mathcal{L}^1} &\leq C_{\text{supp}(V)} 2^{\frac{n}{2}} (s_j - s_{j-1})^{-\frac{n}{2}} \|V\|_{L^\infty}^2 \\ &\leq C_{\text{supp}(V)} (4k)^{\frac{n}{2}} t^{-\frac{n}{2}} \|V\|_{L^\infty}^2. \end{aligned}$$

Since the volume of integration over the s variables is $t^k/k!$, the integral over the region where $\max_j |s_j - s_{j-1}| > (2k)^{-1}t$ contributes to $W_k(t)$ a term with \mathcal{L}^1 norm at most $C_{\text{supp}(V)} (4k)^{\frac{n}{2}} (k!)^{-1} t^{k-\frac{n}{2}} \|V\|_{L^\infty}^k$.

If each $s_j - s_{j-1} \leq (2k)^{-1}t$, then $t - s_k + s_1 > \frac{1}{2}t$, hence either $t - s_k > \frac{1}{4}t$ or $s_1 > \frac{1}{4}t$. In the former case, using Lemma 1.4, L^2 boundedness of the heat kernel, and that \mathcal{L}^2 is an ideal, we get the bound

$$\begin{aligned} \|e^{-(t-s_k)P_0} V e^{-(s_k-s_{k-1})P_0} V \dots V e^{-(s_2-s_1)P_0} V e^{-s_1P_0}\|_{\mathcal{L}^1} \\ \leq C_{\text{supp}(V)} \|V\|_{L^\infty}^k t^{-\frac{n}{4}} s_1^{-\frac{n}{4}}. \end{aligned}$$

Since the total volume of integration over this range of (s_k, \dots, s_2) is less than $(2k)^{-(k-1)}t^{k-1}$, the contribution to $W_k(t)$ over this region has \mathcal{L}^1 norm bounded by

$$C_{\text{supp}(V)} \|V\|_{L^\infty}^k (2k)^{-(k-1)} t^{k-\frac{n}{2}}, \quad n \leq 3.$$

Similar consideration of $s_1 > \frac{1}{4}t$ leads to the same bound, and putting the above bounds together, using $k^k \geq k!$, we get

$$\|W_k(t)\|_{\mathcal{L}^1} \leq C_{\text{supp}(V)} \frac{k^{\frac{n}{2}}}{k!} \|V\|_{L^\infty}^k t^{k-\frac{n}{2}}, \quad n \leq 3.$$

The above argument fails if $n \geq 4$, so we assume (1.2) holds if $n \geq 4$. Consider $W_k(t)$. For each (s_k, \dots, s_1) in the region of integration, at least one of the terms $t - s_k$ or $s_j - s_{j-1}$ is greater than $t/(k+1)$. Applying assumption (1.2), where $K = \text{supp}(V)$, and the fact that \mathcal{L}^1 is an ideal, we conclude

$$\begin{aligned} \|e^{-(t-s_k)P_0} V e^{-(s_k-s_{k-1})P_0} V \dots V e^{-(s_2-s_1)P_0} V e^{-s_1P_0}\|_{\mathcal{L}^1} \\ \leq C_{\text{supp}(V)} \|V\|_{L^\infty}^k \left(\frac{t}{k+1}\right)^{-\frac{n}{2}} \end{aligned}$$

uniformly over the region of integration. Thus, we again get the bound

$$\|W_k(t)\|_{\mathcal{L}^1} \leq C_{\text{supp}(V)} \frac{k^{\frac{n}{2}}}{k!} \|V\|_{L^\infty}^k t^{k-\frac{n}{2}}.$$

In each case, the sum $\sum_{k=1}^{\infty} W_k(t)$ converges in \mathcal{L}^1 for $t > 0$, and bringing the trace into the sum we can write

$$\text{tr}(e^{-tP_V} - e^{-tP_0}) = \sum_{k=1}^{\infty} \text{tr}(W_k(t)).$$

Furthermore, by the above bounds on $\|W_k(t)\|_{\mathcal{L}^1}$,

$$\left| \operatorname{tr}(e^{-tP_V} - e^{-tP_0}) - \sum_{k=1}^m \operatorname{tr}(W_k(t)) \right| \leq C_{V,m} t^{m+1-\frac{n}{2}}, \quad t \in (0, 1].$$

For $V \in L_c^\infty(M)$ the term $\operatorname{tr}(W_1(t))$ has an expansion to all orders in t . To see this, write

$$\begin{aligned} \operatorname{tr}(W_1(t)) &= - \int_0^t \int_{M \times M} H_0(t-s, x, y) V(y) H_0(s, y, x) d\mu(x) d\mu(y) ds \\ &= -t \int_M H_0(t, y, y) V(y) d\mu(y), \end{aligned}$$

where we use the group property of the heat kernel. The expansion of $H_0(t, y, y)$, see (2.2) below, yields an expansion for $\operatorname{tr}(W_1(t))$ of the form on the right hand side of (1.1) for arbitrary positive integer m .

Generally, for all k the function $\operatorname{tr}(W_k(t))$ involves $H_0(t, x, y)$ only for $x, y \in \operatorname{supp}(V)$. This follows since, after using the composition rule, we can write $(-1)^k \operatorname{tr}(W_k(t))$, for $k \geq 2$ and $t > 0$, as

$$\begin{aligned} &\int_{0 < s_1 < \dots < s_k < t} \int_{M^k} H_0(t + s_1 - s_k, y_1, y_k) H_0(s_k - s_{k-1}, y_k, y_{k-1}) \cdots \\ &\quad \times H_0(s_2 - s_1, y_2, y_1) V(y_k) \cdots V(y_1) d\mu(y_1) \cdots d\mu(y_k) ds_1 \cdots ds_k. \end{aligned}$$

Let $\Lambda^{k-1} \subset \mathbb{R}^k$ be the $(k-1)$ -simplex, consisting of $\mathbf{r} = (r_1, \dots, r_k)$ with $r_j > 0$ for all j , and with $r_1 + \dots + r_k = 1$. Let $d\mathbf{r}$ be the measure on Λ^{k-1} induced by projection onto (r_2, \dots, r_k) , and let $\mathbf{y} = (y_1, \dots, y_k) \in M^k$. Then, by cyclicity of the integrand, we can write $(-1)^k \operatorname{tr}(W_k(t))$ as

$$(2.1) \quad \frac{t^k}{k} \int_{\Lambda^{k-1}} \int_{M^k} H_0(tr_k, y_1, y_k) H_0(tr_{k-1}, y_k, y_{k-1}) \cdots H_0(tr_1, y_2, y_1) \\ \times V(y_k) \cdots V(y_1) d\mu(\mathbf{y}) d\mathbf{r}.$$

We then have the following simple corollary of Lemma 1.5, which allows us to henceforth reduce matters to the case of M compact.

Corollary 2.1. *Suppose that (\tilde{M}, \tilde{g}) is a compact Riemannian manifold that isometrically contains a neighborhood of $\operatorname{supp}(V) \subset M$. Then Theorem 1.1 holds for V on (M, g) iff it holds for V on (\tilde{M}, \tilde{g}) .*

We now recall the construction of an asymptotic formula for $H_0(t, x, y)$ on compact M , for example as in [5, Chapter 23] and [12, §3.2]. Choose $c \leq 1$ such that the injectivity radius at each point in M is greater than c . Define $E(t, x, y)$ on $M \times M$ by

$$E(t, x, y) = (4\pi t)^{-\frac{n}{2}} e^{-\frac{d(x,y)^2}{4t}}.$$

This is a smooth function on $\{(0, \infty) \times M^2 : d(x, y) < c\}$. Then there are real valued $u_k(x, y) \in C^\infty(M^2)$, supported in $\{d(x, y) < c\}$, such that

$$(2.2) \quad H_0(t, x, y) = E(t, x, y) \sum_{k=0}^N t^k u_k(x, y) + w_N(t, x, y),$$

where

$$u_k(x, y) = u_k(y, x), \quad u_0(y, y) = 1,$$

and

$$(2.3) \quad |w_N(t, x, y)| \leq C_N t^{N+1-\frac{n}{2}} e^{-\frac{d(x,y)^2}{8t}}, \quad t \in (0, 1].$$

Note that $w_N \in C^\infty((0, \infty) \times M^2)$ since the other terms in (2.2) are.

As a corollary of (2.2)–(2.3), we have the following multiplicative relation, where $0 < v < 1$,

$$(2.4) \quad H_0(vt, x, y) H_0((1-v)t, x, y) = (4\pi t)^{-\frac{n}{2}} \left(H_0(v(1-v)t, x, y) + R(t, v, x, y) \right),$$

where $R(t, v, x, y) \in C^\infty((0, \infty) \times (0, 1) \times M^2)$, and for each N ,

$$(2.5) \quad R(t, v, x, y) = E(v(1-v)t, x, y) \sum_{k=0}^N \sum_{j=0}^{2k} t^k v^j r_{k,j}(x, y) + R_N(t, v, x, y),$$

where

$$(2.6) \quad r_{k,j}(x, y) = r_{k,j}(y, x), \quad r_{0,0}(x, y) = u_0(x, y)^2 - u_0(x, y),$$

and

$$(2.7) \quad |R_N(t, v, x, y)| \leq C_N t^{N+1} E(2v(1-v)t, x, y), \quad t \in (0, 1].$$

3. PRELIMINARY REDUCTIONS

By the results of §2, it suffices to establish the analogue of Theorem 1.1 where $\text{tr}(e^{-tP_V} - e^{-tP_0})$ is replaced by $\sum_{k=2}^\infty \text{tr}(W_k(t))$, on a compact Riemannian manifold (M, g) . In this section we reduce matters to the following two theorems.

Theorem 3.1. *If $V \in L_c^\infty \cap H^m(M)$ is real valued, then one can write*

$$\text{tr}(W_2(t)) = (4\pi t)^{-\frac{n}{2}} \left(c_{2,2} t^2 + \cdots + c_{2,2+m} t^{2+m} + \epsilon(t) t^{2+m} \right),$$

where $\lim_{t \rightarrow 0^+} \epsilon(t) = 0$.

Conversely, assume $V \in L_c^\infty \cap H^{m-1}(M)$ is real valued. If one can write

$$(3.1) \quad \text{tr}(W_2(t)) = (4\pi t)^{-\frac{n}{2}} \left(c_{2,2} t^2 + \cdots + c_{2,1+m} t^{1+m} + r_{2,2+m}(t) t^{2+m} \right),$$

where $|r_{2,2+m}(t)| \leq C$ for $0 < t \leq 1$, then necessarily $V \in H^m(M)$.

Theorem 3.2. *If $V \in L_c^\infty \cap H^m(M)$ is real valued, then for $k \geq 2$ one can write*

$$\operatorname{tr}(W_k(t)) = (4\pi t)^{-\frac{n}{2}} \left(c_{k,k} t^k + \cdots + c_{k,k+m-1} t^{k+m-1} + r_{k,k+m}(t) t^{k+m} \right),$$

where for $0 \leq j \leq m$, and a constant C depending on k and m ,

$$|c_{k,k+j}| \leq C \|V\|_{L^\infty}^{k-2} \|V\|_{H^j}^2, \quad \sup_{0 < t \leq 1} |r_{k,k+m}(t)| \leq C \|V\|_{L^\infty}^{k-2} \|V\|_{H^m}^2.$$

That $V \in L_c^\infty \cap H^m(M)$ implies existence of the asymptotic expansion (1.1) of order $m+2$ follows easily from these two theorems: by the bound $\|W_k(t)\|_{\mathcal{L}^1} \leq C^k k^{\frac{n}{2}} t^{k-\frac{n}{2}}/k!$, we see that

$$(3.2) \quad \operatorname{tr} \sum_{k=m+3}^{\infty} W_k(t) \leq C t^{m+3-\frac{n}{2}}, \quad 0 < t \leq 1.$$

On the other hand, Theorems 3.1 and 3.2 show that, with $c_j = \sum_{k=2}^j c_{k,j}$,

$$\operatorname{tr} \sum_{k=2}^{m+2} W_k(t) = (4\pi t)^{-\frac{n}{2}} \left(c_2 t^2 + \cdots + c_{m+1} t^{m+1} + c_{m+2} t^{m+2} + \epsilon(t) t^{m+2} \right).$$

The other direction of Theorem 1.1, that existence of an asymptotic expansion implies regularity, is carried out by induction. Assume $m \geq 1$ and $V \in L_c^\infty \cap H^{m-1}(M)$, which trivially holds if $m = 1$ since $L_c^\infty(M) \subset L^2(M)$, and assume (1.1) holds. By (3.2) this implies that, with $|r_{m+2}(t)| \leq C$,

$$\operatorname{tr} \sum_{k=2}^{m+2} W_k(t) = (4\pi t)^{-\frac{n}{2}} \left(c_2 t^2 + \cdots + c_{m+1} t^{m+1} + r_{m+2}(t) t^{m+2} \right).$$

Since $V \in L_c^\infty \cap H^{m-1}(M)$, Theorem 3.2 shows that $\operatorname{tr} \sum_{k=3}^{m+2} W_k(t)$ has a similar expansion, with coefficients that are bounded in terms of the L^∞ and H^j norms of V with $j \leq m-1$. Hence the relation (3.1) holds, and we conclude $V \in H^m(M)$.

In proving Theorems 3.1 and 3.2, we will use a simple calculus lemma.

Lemma 3.3. *Suppose that $f \in C^\infty((0,1))$, and that for all $0 \leq j \leq m$*

$$\sup_{0 < t < 1} |f^{(j)}(t)| \leq C_j$$

for finite constants C_j . Then for $t \in (0,1)$ one has

$$f(t) = a_0 + a_1 t + \cdots + a_{m-1} t^{m-1} + r_m(t) t^m,$$

where $\sup_{0 < t < 1} |r_m(t)| < C_m/m!$, and $|a_j| \leq C_j/j!$.

The lemma is proved taking the Taylor expansion about $\epsilon > 0$, then letting $\epsilon \rightarrow 0^+$, using that $\lim_{\epsilon \rightarrow 0^+} f^{(j)}(\epsilon)$ exists if $0 \leq j \leq m-1$.

4. PROOF OF THEOREM 3.1

In this, and subsequent sections, we will assume M is compact. We reduce the proof of Theorem 3.1 to that of two propositions, which we then prove in this section. As in §2, we write $\text{tr}(W_2(t))$ as

$$\frac{1}{2} t^2 \int_0^1 \int_{M^2} H_0((1-v)t, y, z) H_0(vt, y, z) V(y) V(z) d\mu(y) d\mu(z) dv.$$

We now apply the relation (2.4). We show that the remainder R leads to a term that is better by one power of t than the main term, for V of a given Sobolev regularity.

Proposition 4.1. *If $V \in L_c^\infty \cap H^{m-1}(M)$, then one can write*

$$(4.1) \quad \int_0^1 \int_{M^2} R(t, v, y, z) V(y) V(z) d\mu(y) d\mu(z) dv \\ = a_1 t + \cdots + a_{m-1} t^{m-1} + r_m(t) t^m,$$

where, for fixed constants C_j , and $1 \leq j \leq m-1$,

$$|a_j| \leq C_j \|V\|_{H^{j-1}}^2, \quad \sup_{0 < t < 1} |r_m(t)| \leq C_m \|V\|_{H^{m-1}}^2.$$

A simple induction argument shows that Theorem 3.1 is a consequence of Proposition 4.1 and the following.

Proposition 4.2. *If $V \in L_c^\infty \cap H^m(M)$ is real valued, then one can write*

$$(4.2) \quad \int_0^1 \int_{M^2} H_0(v(1-v)t, y, z) V(y) V(z) d\mu(y) d\mu(z) dv \\ = a_0 + \cdots + a_m t^m + \epsilon(t) t^m,$$

where $\lim_{t \rightarrow 0^+} \epsilon(t) = 0$.

Conversely, assuming $V \in L_c^\infty \cap H^{m-1}(M)$ is real valued, if one has

$$(4.3) \quad \int_0^1 \int_{M^2} H_0(v(1-v)t, y, z) V(y) V(z) d\mu(y) d\mu(z) dv \\ = a_0 + \cdots + a_{m-1} t^{m-1} + r_m(t) t^m,$$

where $|r_m(t)| \leq C_m$ for $0 < t \leq 1$, then $V \in H^m(M)$, and hence (4.2) holds.

4.1. Proof of Proposition 4.2. Since M is compact, we can expand V in a basis of eigenfunctions $V = \sum_{j=1}^\infty b_j \phi_j$, where $-\Delta_g \phi_j = \rho_j \phi_j$, and $\rho_j \geq 0$. Since V is real-valued, the left hand side of (4.2) equals

$$\int_0^1 \sum_{j=1}^\infty e^{-v(1-v)t\rho_j} |b_j|^2 dv.$$

We use the equivalence

$$\|V\|_{H^m}^2 \approx \sum_{j=1}^\infty (1 + \rho_j^m) |b_j|^2.$$

Consider $m = 1$, and suppose that the expansion (4.3) holds, hence that

$$\int_0^1 \sum_{j=1}^{\infty} e^{-v(1-v)t\rho_j} |b_j|^2 dv = a_0 + r_1(t)t.$$

Letting $t \rightarrow 0$ gives $a_0 = \sum |b_j|^2 = \|V\|_{L^2}^2 < \infty$, so we can rewrite this as

$$\int_0^1 \sum_{j=1}^{\infty} \left(\frac{1 - e^{-v(1-v)t\rho_j}}{t} \right) |b_j|^2 dv \leq |r_1(t)|, \quad t \in (0, 1].$$

The integrand is positive, so applying Fatou's lemma as $t \rightarrow 0$ we get

$$\left(\int_0^1 v(1-v) dv \right) \sum_{j=1}^{\infty} \rho_j |b_j|^2 \leq C_1,$$

implying that $V \in H^1(M)$. Conversely, if $V \in H^1(M)$ we would get an expansion of the form (4.2) with $m = 1$ by dominated convergence.

To consider higher values of m , write

$$e^{-s} = \sum_{j=0}^{m-1} \frac{(-1)^j}{j!} s^j + e_m(s) \frac{(-1)^m}{m!} s^m.$$

Then

$$(4.4) \quad 0 \leq e_m(s) \leq 1 \quad \text{if } s \geq 0, \quad \lim_{s \rightarrow 0} e_m(s) = 1.$$

The proof of (4.2) for $V \in L^\infty \cap H^m(M)$ follows by dominated convergence.

Suppose then that $V \in L^\infty \cap H^{m-1}(M)$ for some $m \geq 1$, and that (4.3) holds. By induction, or comparison with (4.2), we must have

$$a_k = \left(\frac{(-1)^k}{k!} \int_0^1 v^k (1-v)^k dv \right) \sum_{j=1}^{\infty} \rho_j^k |b_j|^2, \quad 0 \leq k \leq m-1.$$

We can then expand

$$\begin{aligned} & \int_0^1 \sum_{j=1}^{\infty} e^{-v(1-v)t\rho_j} |b_j|^2 dv = \\ & \sum_{k=0}^{m-1} a_k t^k + \frac{(-1)^m}{m!} \left(\int_0^1 \sum_{j=1}^{\infty} e_m(v(1-v)t\rho_j) v^m (1-v)^m \rho_j^m |b_j|^2 dv \right) t^m. \end{aligned}$$

We thus must have uniform bounds for $t \in (0, 1]$

$$\int_0^1 \sum_{j=1}^{\infty} e_m(v(1-v)t\rho_j) v^m (1-v)^m \rho_j^m |b_j|^2 dv \leq m! C_m.$$

By Fatou's lemma and (4.4), we deduce that

$$\left(\int_0^1 v^m (1-v)^m dv \right) \sum_{j=1}^{\infty} \rho_j^m |b_j|^2 \leq m! C_m,$$

so necessarily $V \in H^m(M)$, completing the proof of Proposition 4.2. \square

4.2. Proof of Proposition 4.1. We use the expansion (2.5). By the Schur test and (2.7), we can bound

$$\left| \int_0^1 \int_{M^2} R_N(t, v, y, z) V(y) V(z) d\mu(y) d\mu(z) dv \right| \leq C_{N,\Omega} t^{N+1} \|V\|_{L^2}^2.$$

Taking $N = m$, it suffices to establish the expansion in (4.1) for each of the other terms in (2.5). Other than the term $k = 0$, this is handled by the following.

Lemma 4.3. *Suppose that $V \in L^\infty \cap H^{m-1}(M)$, M compact, and that $r(x, y) \in C^\infty(M^2)$ is supported in $d(x, y) < c$. Then, one can write*

$$\begin{aligned} \int_0^1 \int_{M^2} E(v(1-v)t, x, y) r(x, y) V(y) V(x) d\mu(y) d\mu(x) dv \\ = a_0 + a_1 t + \cdots + a_{m-2} t^{m-2} + r_{m-1}(t) t^{m-1}, \end{aligned}$$

where, for constants C_j ,

$$|a_j| \leq C_j \|V\|_{H^j}^2, \quad \sup_{0 < t < 1} |r_{m-1}(t)| \leq C_{m-1} \|V\|_{H^{m-1}}^2.$$

Proof. For any $\delta > 0$, the kernel $E(v(1-v)t, x, y)$ is smooth over $v \in [0, 1]$ and $t \geq 0$ for $d(x, y) > \delta$, hence we can use a partition of unity to reduce to the case that V is supported in a local coordinate neighborhood, over which we fix an orthonormal frame on $T(M)$. Write $y = \exp_x(z)$, $z \in \mathbb{R}^n \equiv T_x(M)$ via the frame. We absorb the Jacobian factors $D\mu(y)/Dz$ and $D\mu(x)/Dx$ into the smooth function $r(x, z)$, supported in $|z| < c$, and consider

$$(4.5) \quad \int_0^1 \int_{\mathbb{R}^{2n}} (4\pi v(1-v)t)^{-\frac{n}{2}} e^{-\frac{|z|^2}{4v(1-v)t}} r(x, z) V(\exp_x(z)) V(x) dz dx dv.$$

Applying ∂_t to the integrand in (4.5) is equivalent, after integrating by parts in z , to applying $v(1-v)\Delta_z$ to $r(x, z)V(\exp_x(z))$. Using the following lemma and integrating by parts in x , we can convert half of the z -derivatives falling on $V(\exp_x(z))$ into x -derivatives acting on either $r(x, z)$ or the other factor $V(x)$.

Lemma 4.4. *Given a local coordinate chart, and orthonormal frame on $T(M)$ over the chart, then for $z \in \mathbb{R}^n$ with $|z| < c$, there are smooth first order differential operators $A_j(x, z, \partial_x)$ and $B_j(x, z, \partial_z)$, so that*

$$\partial_{z_j} V(\exp_x(z)) = A_j(x, z, \partial_x) V(\exp_x(z)),$$

$$\partial_{x_j} V(\exp_x(z)) = B_j(x, z, \partial_z) V(\exp_x(z)).$$

This lets us express the j -th derivative with respect to t of (4.5) as a sum

$$\begin{aligned} \sum_{|\alpha|, |\beta| \leq j} \int_0^1 \int_{\mathbb{R}^{2n}} (4\pi v(1-v)t)^{-\frac{n}{2}} e^{-\frac{|z|^2}{4v(1-v)t}} r_{\alpha, \beta}(v, x, z) \\ \times \partial_z^\alpha V(\exp_x(z)) \partial_x^\beta V(x) dz dx dv \end{aligned}$$

where $r_{\alpha,\beta}(v, x, z)$ is a smooth function supported in $|z| < c$. Changing variables back to $(x, y) \in M \times M$, we apply the Schur test to $E(v(1-v)t, x, y)$ to bound this by $\|V\|_{H^j}^2$, with bounds uniform in t . The result now follows by Lemma 3.3. \square

To handle the remaining term $k = 0$, we will use that

$$|r_{0,0}(x, \exp_x(z))| \leq C|z|^2.$$

To see this, note that $r_{0,0}(x, x) = 0$ and $r_{0,0}(x, y) = r_{0,0}(y, x)$ by (2.6), which together imply that $\nabla_y r_{0,0}(x, y)|_{y=x} = 0$. Taking a Taylor expansion of $r_{0,0}(x, \exp_x(z))$ about $z = 0$ thus reduces matters to showing that, when $V \in L^\infty \cap H^{m-1}(M)$,

$$\begin{aligned} \int_0^1 \int_M \int_{\mathbb{R}^n} (4\pi v(1-v)t)^{-\frac{n}{2}} \langle A(x)z, z \rangle e^{-\frac{|z|^2}{4v(1-v)t}} \\ \times r(x, z) V(\exp_x(z)) V(x) dz d\mu(x) dv \\ = a_1 t + \cdots + a_{m-1} t^{m-1} + r_m(t) t^m \end{aligned}$$

with coefficients a_j satisfying the bounds of Proposition 4.1. Here $r(x, z)$ is assumed smooth and supported in $|z| < c$, and $A(x)$ is a smooth, symmetric matrix valued function of $x \in M$. We use the identity (see Lemma 5.3 below)

$$\langle A(x)z, z \rangle e^{-\frac{|z|^2}{4s}} = s \operatorname{tr}(A(x)) e^{-\frac{|z|^2}{4s}} + 4s^2 \langle A(x) \partial_z, \partial_z \rangle e^{-\frac{|z|^2}{4s}}.$$

With $s = v(1-v)t$, the first term on the right is handled by Lemma 4.3. For the second term, we integrate by parts as above to distribute one derivative on each of the two factors of V , and apply Lemma 4.3 with $m-1$ replaced by $m-2$. \square

5. PROOF OF THEOREM 3.2

We will use the following version of the Gagliardo-Nirenberg inequalities. Recall that we assume (M, g) is a compact Riemannian manifold.

Lemma 5.1. *Suppose that $m_j \leq m$, and $\sum_{j=1}^k m_j = 2m$. Then*

$$\left\| \prod_{j=1}^k |\nabla^{m_j} u_j| \right\|_{L^1} \leq C \left(\sum_{j=1}^k \|u_j\|_{L^\infty} \right)^{k-2} \left(\sum_{j=1}^k \|u_j\|_{H^m} \right)^2.$$

Proof. By a partition of unity we can work with smooth cutoffs of u_j in local coordinates, with the standard gradient ∇ , and with the Sobolev space $H^m(\mathbb{R}^n)$. We apply the following bound, see [15, (3.17)], where we assume $u \in L^\infty \cap H^m$,

$$\|\nabla^{m_j} u_j\|_{L^{\frac{2m}{m_j}}} \leq C \|u_j\|_{L^\infty}^{1-\frac{m_j}{m}} \|\nabla^m u_j\|_{L^2}^{\frac{m_j}{m}}$$

and use Hölder's inequality after taking the product over j . \square

Recall the formula (2.1). For any $\delta > 0$, the kernel $H_0(t, y, z)$ belongs to $C^\infty(\mathbb{R}_+ \times M \times M)$ on the set $d(y, z) > \delta$, with uniform bounds over $t \in (0, 1]$, and all derivatives vanish to infinite order at $t = 0$. Hence, as in the proof of Lemma 4.3, for a small $c > 0$ to be chosen, we may restrict to the case that $V(y)$ is supported in the set $U = \{y : d(y, x_0) < c\}$ for some point x_0 . From the expansion (2.2), it suffices to show that when $f(t)$ takes the form

$$\int_{\Lambda^{k-1} \times M^k} (4\pi t)^{-\frac{n(k-1)}{2}} \left(\prod_{j=1}^k r_j^{-\frac{n}{2}} \right) e^{-\frac{1}{4t} (r_k^{-1} d^2(y_1, y_k) + r_{k-1}^{-1} d^2(y_k, y_{k-1}) + \cdots + r_1^{-1} d^2(y_2, y_1))} \\ \times V_k(y_k) \cdots V_1(y_1) \phi(\mathbf{y}) d\mu(\mathbf{y}) d\mathbf{r},$$

where $\mathbf{y} = (y_1, \dots, y_k)$, and $\phi(\mathbf{y}) \in C_c^\infty(U^k)$, then if each $V_j \in L_c^\infty \cap H^m(M)$ we can write

$$f(t) = a_0 + a_1 t + \cdots + a_{m-1} t^{m-1} + r_m(t) t^m,$$

with bounds on $|a_j|$ and $\|r_m\|_{L^\infty}$ as in the statement of Theorem 3.2.

We fix local coordinates on U to identify y_1 with $x \in \mathbb{R}^n$, and fix an orthonormal frame over U . For each $x \in U$, and c sufficiently small, this induces exponential coordinates $e_x(u) \equiv \exp_x(u)$ on U , based at x . We then set $y_j = e_x(u_j)$ for $2 \leq j \leq k$, so that (x, u_2, \dots, u_k) are coordinates on the support of $\phi(\mathbf{y})$.

After absorbing $d\mu(\mathbf{y})/d\mathbf{u} dx$ into ϕ , we express $f(t)$ as

$$\int_{\Lambda^{k-1}} (4\pi t)^{-\frac{n(k-1)}{2}} \left(\prod_{j=1}^k r_j^{-\frac{n}{2}} \right) \int_{\mathbb{R}^{nk}} e^{-\frac{1}{4t} D(x, \mathbf{r}, \mathbf{u})} \\ \times V_k(e_x(u_k)) \cdots V_2(e_x(u_2)) V_1(x) \phi(x, \mathbf{u}) d\mathbf{u} dx d\mathbf{r}.$$

Here, $\text{supp}(\phi) \subset \{|u_j| < 2c\}$ for all j , $\mathbf{u} = (u_2, \dots, u_k)$, and

$$D(x, \mathbf{r}, \mathbf{u}) = r_k^{-1} |u_k|^2 + r_{k-1}^{-1} d^2(e_x(u_k), e_x(u_{k-1})) + \cdots \\ + r_2^{-1} d^2(e_x(u_3), e_x(u_2)) + r_1^{-1} |u_2|^2.$$

For $u, v \in \mathbb{R}^n$ with $|u|, |v| < 2c$, and some $C < \infty$,

$$C^{-1} |u - v|^2 \leq d^2(e_x(u), e_x(v)) \leq C |u - v|^2.$$

Consequently, by the analysis of [14, (3.12)], we have uniform bounds over $\mathbf{r} \in \Lambda^{k-1}$,

$$(5.1) \quad (4\pi t)^{-\frac{n(k-1)}{2}} \left(\prod_{j=1}^k r_j^{-\frac{n}{2}} \right) \int_{\mathbb{R}^{n(k-1)}} \sup_{x \in M} e^{-\frac{1}{4t} D(x, \mathbf{r}, \mathbf{u})} d\mathbf{u} \leq C.$$

Hence,

$$(5.2) \quad |f(t)| \leq C \sup_{\mathbf{u}} \int |V_k(e_x(u_k)) \cdots V_2(e_x(u_2)) V_1(x) \phi(x, \mathbf{u})| dx.$$

Taking c smaller if necessary, the map $x \rightarrow e_x(u)$ is a diffeomorphism for $|u| < 2c$, and so by Hölder's inequality we have bounds

$$|f(t)| \leq C \prod_{j=1}^k \|V_j\|_{L^{p_j}} \quad \text{if} \quad \sum_{j=1}^k p_j^{-1} = 1.$$

This establishes the case $m = 0$ of Theorem 3.2, taking $p_1 = p_2 = 2$, and $p_j = \infty$ for $j \geq 3$.

To consider derivatives of $f(t)$, we observe that the symmetric function $d^2(e_x(u), e_x(v))$ vanishes to second order at $u = v$, and hence

$$d^2(e_x(u), e_x(v)) = \sum_{i,j=1}^n q_{ij}(x, u, v)(u^i - v^i)(u^j - v^j),$$

with $q_{ij}(x, u, v)$ symmetric in ij , and depending smoothly on $x, u, v \in U$. Furthermore, $q_{ij}(x, 0, 0) = \delta_{ij}$, since $d^2(e_x(u), e_x(0)) = |u|^2$. Taking the Taylor expansion of $q_{ij}(x, u, v)$ in u and v lets us write

$$(5.3) \quad d^2(e_x(u), e_x(v)) = |u - v|^2 + \sum_{1 \leq |\alpha+\beta| < N} u^\alpha v^\beta Q_{\alpha\beta, x}(u - v) \\ + \sum_{|\alpha+\beta|=N} u^\alpha v^\beta R_{\alpha\beta, x}(u, v),$$

where $Q_{\alpha\beta, x}$ are quadratic forms in $u - v$ that depend smoothly on x , and $R_{\alpha\beta, x}(u, v)$ is smooth in (x, u, v) and satisfies $R_{\alpha\beta, x}(u, v) \leq C_{\alpha\beta}|u - v|^2$.

For $\mathbf{r} \in \Lambda^{k-1}$, let $Q_{\mathbf{r}}(\mathbf{u})$ denote the quadratic form on $\mathbb{R}^{n(k-1)}$,

$$Q_{\mathbf{r}}(\mathbf{u}) = r_k^{-1}|u_k|^2 + r_{k-1}^{-1}|u_k - u_{k-1}|^2 + \cdots + r_2^{-1}|u_3 - u_2|^2 + r_1^{-1}|u_2|^2.$$

Then, for all $\mathbf{r} \in \Lambda^{k-1}$ and x, \mathbf{u} in the support of $\phi(x, \mathbf{u})$, for c sufficiently small,

$$\frac{1}{2}Q_{\mathbf{r}}(\mathbf{u}) \leq D(x, \mathbf{r}, \mathbf{u}) \leq 2Q_{\mathbf{r}}(\mathbf{u}).$$

Also, by the above we can write:

$$(5.4) \quad D(x, \mathbf{r}, \mathbf{u}) = Q_{\mathbf{r}}(\mathbf{u}) + \sum_{1 \leq |\alpha| < N} \mathbf{u}^\alpha Q_{\alpha, \mathbf{r}, x}(\mathbf{u}) + \sum_{|\alpha|=N} \mathbf{u}^\alpha R_{\alpha, \mathbf{r}, x}(\mathbf{u})$$

where $Q_{\alpha, \mathbf{r}, x}(\mathbf{u})$ are quadratic forms, the $R_{\alpha, \mathbf{r}, x}(\mathbf{u})$ are smooth functions, and where, with constants $C_{\alpha, \beta}$ uniform over $\mathbf{r} \in \Lambda^{k-1}$ and $x, \mathbf{u} \in U$,

$$(5.5) \quad |\partial_x^\beta Q_{\alpha, \mathbf{r}, x}(\mathbf{u})| \leq C_{\alpha, \beta} Q_{\mathbf{r}}(\mathbf{u}), \quad |\partial_x^\beta R_{\alpha, \mathbf{r}, x}(\mathbf{u})| \leq C_{\alpha, \beta} Q_{\mathbf{r}}(\mathbf{u}).$$

The key point to the bounds (5.5) is that, although the various quadratic forms have singular behavior in \mathbf{r} , for $1 < j < k$ the terms $Q_{\alpha\beta, x}(u_{j+1} - u_j)$ and $R_{\alpha\beta, x}(u_{j+1} - u_j)$ in (5.3), which multiply against r_j^{-1} , are dominated, as are their derivatives in x , by the corresponding term $|u_{j+1} - u_j|^2$ in $Q_{\mathbf{r}}(\mathbf{u})$.

We next note the bound, uniformly over $\mathbf{r} \in \Lambda^{k-1}$,

$$(5.6) \quad (4\pi t)^{-\frac{n(k-1)}{2}} \left(\prod_{j=1}^k r_j^{-\frac{n}{2}} \right) \int_{\mathbb{R}^{n(k-1)}} |\mathbf{u}^\alpha| Q_{\mathbf{r}}(\mathbf{u})^j e^{-\frac{1}{4t} Q_{\mathbf{r}}(\mathbf{u})} d\mathbf{u} \leq C_{j,\alpha} t^{j+\frac{1}{2}|\alpha|},$$

which is a simple variation on (5.1), and the fact that $Q_{\mathbf{r}}(\mathbf{u}) \geq c|\mathbf{u}|^2$ for $\mathbf{r} \in \Lambda^{k-1}$. Since the estimate (5.6) involves only absolute bounds, it also holds when the term $Q_{\mathbf{r}}(\mathbf{u})^j$ is replaced by a j -fold product of quadratic forms $Q_{\alpha_i, \mathbf{r}, x}(\mathbf{u})$ from (5.4).

Consequently, if we expand $\exp(-(D(x, \mathbf{r}, \mathbf{u}) - Q_{\mathbf{r}}(\mathbf{u}))/4t)$ as a power series, then for any given N we can write $f(t)$, modulo $\mathcal{O}(t^N)$, as

$$\int_{\Lambda^{k-1}} (4\pi t)^{-\frac{n(k-1)}{2}} \left(\prod_{j=1}^k r_j^{-\frac{n}{2}} \right) \int_{\mathbb{R}^{nk}} \sum_{|\alpha_1+\dots+\alpha_L| \leq 2N} \mathbf{u}^{\alpha_1+\dots+\alpha_L} \prod_{i=1}^L \left(\frac{Q_{\alpha_i, \mathbf{r}, x}(\mathbf{u})}{4t} \right) \\ \times e^{-\frac{1}{4t} Q_{\mathbf{r}}(\mathbf{u})} V_k(e_x(u_k)) \cdots V_2(e_x(u_2)) V_1(x) \phi_\alpha(x, \mathbf{u}) d\mathbf{u} dx d\mathbf{r}.$$

The term $\mathbf{u}^{\alpha_1+\dots+\alpha_L}$ will be absorbed into $\phi_\alpha(x, \mathbf{u})$, and estimates we prove will be uniform over $\mathbf{r} \in \Lambda^{k-1}$, so it suffices to prove the following

Lemma 5.2. *Suppose that $g(t)$ takes the form*

$$(5.7) \quad g(t) = (4\pi t)^{-\frac{n(k-1)}{2}} \left(\prod_{j=1}^k r_j^{-\frac{n}{2}} \right) \int_{\mathbb{R}^{nk}} \prod_{i=1}^L \left(\frac{Q_{\alpha_i, \mathbf{r}, x}(\mathbf{u})}{4t} \right) e^{-\frac{1}{4t} Q_{\mathbf{r}}(\mathbf{u})} \\ \times V_k(e_x(u_k)) \cdots V_2(e_x(u_2)) V_1(x) \phi(x, \mathbf{u}) d\mathbf{u} dx$$

where $V_j \in L^\infty \cap H^m(M)$, and $Q_{\alpha_i, \mathbf{r}, x}(\mathbf{u})$ satisfies (5.5). Then for $t \in (0, 1]$,

$$(5.8) \quad g(t) = a_0 + a_1 t + \cdots + a_{m-1} t^{m-1} + r_m(t) t^m,$$

where

$$|a_i| \leq C_{k,m} \left(\sum_{j=1}^k \|V_j\|_{L^\infty} \right)^2 \left(\sum_{j=1}^k \|V_j\|_{H^i} \right)^{k-2}, \\ \sup_{t \in (0,1]} |r_m(t)| \leq C_{k,m} \left(\sum_{j=1}^k \|V_j\|_{L^\infty} \right)^2 \left(\sum_{j=1}^k \|V_j\|_{H^m} \right)^{k-2}.$$

In what follows, given a matrix B on $\mathbb{R}^{n(k-1)}$ we define the quadratic form $B(\mathbf{u}) = (B\mathbf{u}) \cdot \mathbf{u}$, and given a quadratic form $B(\mathbf{u})$ let B denote the symmetric matrix that determines it. It is useful to introduce the following notation comparing matrices, via their quadratic forms, to $Q_{\mathbf{r}}$ or $Q_{\mathbf{r}}^{-1}$.

Definition 5.1. Given a family of matrices $B_{\mathbf{r}, x}$ on $\mathbb{R}^{n(k-1)}$, depending on parameters $\mathbf{r} \in \Lambda^{k-1}$ and $x \in U$, we write $B_{\mathbf{r}, x} \lesssim Q_{\mathbf{r}}$ if there is a constant C such that the associated family of quadratic forms satisfies

$$|B_{\mathbf{r}, x}(\mathbf{u})| \leq C Q_{\mathbf{r}}(\mathbf{u}) \quad \text{for all } \mathbf{r} \in \Lambda^{k-1}, x \in U.$$

We then express (5.5) as $\partial_x^\beta Q_{\alpha, \mathbf{r}, x} \lesssim Q_{\mathbf{r}}$ and $\partial_x^\beta R_{\alpha, \mathbf{r}, x} \lesssim Q_{\mathbf{r}}$, for all β . The following is an immediate consequence of the definition, where $Q_{\mathbf{r}}^{-1/2}$ is the positive definite square root of $Q_{\mathbf{r}}^{-1}$,

$$(5.9) \quad A_{\mathbf{r}, x} \lesssim Q_{\mathbf{r}} \Leftrightarrow Q_{\mathbf{r}}^{-1/2} A_{\mathbf{r}, x} Q_{\mathbf{r}}^{-1/2} \lesssim I \Leftrightarrow Q_{\mathbf{r}}^{-1} A_{\mathbf{r}, x} Q_{\mathbf{r}}^{-1} \lesssim Q_{\mathbf{r}}^{-1}.$$

Lemma 5.3. *Suppose that B is a symmetric matrix on $\mathbb{R}^{n(k-1)}$, and $B(\mathbf{u})$ is the corresponding quadratic form in \mathbf{u} . Then*

$$B(\mathbf{u})e^{-\frac{1}{4t}Q_{\mathbf{r}}(\mathbf{u})} = \left(4t^2 B'_{\mathbf{r}}(\partial_{\mathbf{u}}) + 2t \operatorname{tr}(Q_{\mathbf{r}}^{-1}B)\right)e^{-\frac{1}{4t}Q_{\mathbf{r}}(\mathbf{u})}$$

where $B'_{\mathbf{r}} = Q_{\mathbf{r}}^{-1}BQ_{\mathbf{r}}^{-1}$, with $Q_{\mathbf{r}}$ the symmetric matrix associated to $Q_{\mathbf{r}}(\mathbf{u})$.

Proof. Given a quadratic form $Q(v)$ with symmetric matrix Q we have

$$\partial_{v_i} \partial_{v_j} e^{-\frac{1}{4t}Q(v)} = \left(\frac{(Qv)_i(Qv)_j}{4t^2} - \frac{Q_{ij}}{2t}\right)e^{-\frac{1}{4t}Q(v)},$$

and hence for symmetric matrix A

$$A(\partial_v)e^{-\frac{1}{4t}Q(v)} = \left(\frac{A(Qv)}{4t^2} - \frac{\operatorname{tr}(AQ)}{2t}\right)e^{-\frac{1}{4t}Q(v)}.$$

The statement of the lemma follows by taking $A = Q_{\mathbf{r}}^{-1}BQ_{\mathbf{r}}^{-1}$. \square

Proof of Lemma 5.2. We now turn to the proof that (5.8) holds for the expression (5.7). The bounds on a_j and $r_m(t)$ will follow from the proof. We divide consideration into cases.

- $m = 0$, $L \geq 0$. This follows exactly as for the estimate (5.2) above, using (5.6) instead of (5.1).
- $L = 0$, $m \geq 1$. We need to establish (5.8) for $g(t)$ of the form

$$g(t) = \left(\prod_{j=1}^k r_j^{-\frac{n}{2}}\right) \int_{\mathbb{R}^{nk}} (4\pi t)^{-\frac{n(k-1)}{2}} e^{-\frac{1}{4t}Q_{\mathbf{r}}(\mathbf{u})} \\ \times V_k(e_x(u_k)) \cdots V_2(e_x(u_2)) V_1(x) \phi(x, \mathbf{u}) \, d\mathbf{u} \, dx.$$

We proceed by induction on m , and assume the result holds at regularity $V_j \in H^{m-1}$. We will show that when $t \in (0, 1]$ and $V_j \in L_c^\infty \cap H^m(M)$ we can write

$$g'(t) = a_1 + a_2 t + \cdots + a_{m-1} t^{m-2} + t^{m-1} r(t).$$

This implies $g(t)$ is continuous on $0 \leq t \leq 1$, and the expansion for $g(t)$ follows by integration.

The following identity is a simple consequence of Lemma 5.3,

$$\partial_t e^{-\frac{1}{4t}Q_{\mathbf{r}}(\mathbf{u})} = \left(Q_{\mathbf{r}}^{-1}(\partial_{\mathbf{u}}) + \frac{n(k-1)}{2t}\right)e^{-\frac{1}{4t}Q_{\mathbf{r}}(\mathbf{u})}.$$

We apply this to the integrand for $g(t)$, and after integration by parts we see that $g'(t)$ equals the following:

$$\begin{aligned} & \left(\prod_{j=1}^k r_j^{-\frac{n}{2}} \right) \int_{\mathbb{R}^{nk}} (4\pi t)^{-\frac{n(k-1)}{2}} e^{-\frac{1}{4t} Q_{\mathbf{r}}(\mathbf{u})} \\ & \quad \times Q_{\mathbf{r}}^{-1}(\partial_{\mathbf{u}}) \left(V_k(e_x(u_k)) \cdots V_2(e_x(u_2)) V_1(x) \phi(x, \mathbf{u}) \right) d\mathbf{u} dx \end{aligned}$$

The coefficients of $Q_{\mathbf{r}}^{-1}$ are bounded by a fixed constant, uniformly over $\mathbf{r} \in \Lambda^{k-1}$, so we can replace $Q_{\mathbf{r}}^{-1}(\partial_{\mathbf{u}})$ by a component of $\partial_{u_i} \partial_{u_j}$ for some i, j . If $i \neq j$, at most one derivative falls on a given $V_j(e_x(u_j))$, leading to a k -fold product of V_j 's of regularity H^{m-1} . The desired expansion for $g'(t)$ follows from the induction hypothesis for regularity $m-1$.

When $i = j$, we need consider a term like

$$\begin{aligned} & \left(\prod_{j=1}^k r_j^{-\frac{n}{2}} \right) \int_{\mathbb{R}^{nk}} (4\pi t)^{-\frac{n(k-1)}{2}} e^{-\frac{1}{4t} Q_{\mathbf{r}}(\mathbf{u})} \\ & \quad \times \left(\partial_{u_k}^2 V_k(e_x(u_k)) \right) \cdots V_2(e_x(u_2)) V_1(x) \phi(x, \mathbf{u}) d\mathbf{u} dx. \end{aligned}$$

To handle this, we use Lemma 4.4 and integration by parts to convert one factor of ∂_{u_k} into ∂_x acting on a factor V_j for $j \neq k$, and proceed as for the case $i \neq j$.

• $L \geq 1$, $m \geq 0$. We proceed by induction on L , and assume (5.8) holds for a term of the form (5.7) with an $L-1$ fold product, for all integers $m \geq 0$. We note that, by (5.5) and (5.9), the function

$$\psi_{\mathbf{r},L}(x) = \frac{1}{2} \operatorname{tr}(Q_{\mathbf{r}}^{-1} Q_{\mathbf{r},\alpha_L,x}) = \frac{1}{2} \operatorname{tr}(Q_{\mathbf{r}}^{-1/2} Q_{\mathbf{r},\alpha_L,x} Q_{\mathbf{r}}^{-1/2})$$

is a smooth function of x , with $|\partial_x^\alpha \psi_{\mathbf{r},L}|$ uniformly bounded over $\mathbf{r} \in \Lambda^{k-1}$ and $x \in U$, for all α .

Considering the expression (5.7), we use Lemma 5.3 to write

$$\frac{Q_{\mathbf{r},\alpha_L,x}(\mathbf{u})}{4t} e^{-\frac{1}{4t} Q_{\mathbf{r}}(\mathbf{u})} = \left(t B_{\mathbf{r},\alpha_L,x}(\partial_{\mathbf{u}}) + \psi_{\mathbf{r},L}(x) \right) e^{-\frac{1}{4t} Q_{\mathbf{r}}(\mathbf{u})}$$

where $B_{\mathbf{r},\alpha_L,x} = Q_{\mathbf{r}}^{-1} Q_{\mathbf{r},\alpha_L,x} Q_{\mathbf{r}}^{-1}$, hence $B_{\mathbf{r},\alpha_L,x} \lesssim Q_{\mathbf{r}}^{-1}$ by (5.9). The smooth function $\psi_{\mathbf{r},L}(x)$ can be absorbed into $\phi_{\mathbf{r}}(x, \mathbf{u})$, which will denote a function in $C_c^\infty(U^k)$ with C_c^∞ bounds in (x, \mathbf{u}) that are uniform over \mathbf{r} . This term then leads to an $L-1$ fold product which is handled by the induction hypothesis.

We then need consider the commutators, for $1 \leq i < L$,

$$\left[Q_{\mathbf{r},\alpha_i,x}(\mathbf{u}), B_{\mathbf{r},\alpha_L,x}(\partial_{\mathbf{u}}) \right] = -4 \mathbf{u} \cdot Q_{\mathbf{r},\alpha_i,x} B_{\mathbf{r},\alpha_L,x} \partial_{\mathbf{u}} - 2 \operatorname{tr}(Q_{\mathbf{r},\alpha_i,x} B_{\mathbf{r},\alpha_L,x}).$$

The trace term is a smooth, bounded function of x , uniformly over $r \in \Lambda^{k-1}$, since $B_{\mathbf{r},\alpha_L,x} \lesssim Q_{\mathbf{r}}^{-1}$ and $Q_{\mathbf{r},\alpha_i,x} \lesssim Q_{\mathbf{r}}$, and thus can be harmlessly absorbed

into $\phi_{\mathbf{r}}(x, \mathbf{u})$. We also note the following,

$$\left[Q_{\mathbf{r}, \alpha_j, x}(\mathbf{u}), \mathbf{u} \cdot Q_{\mathbf{r}, \alpha_i, x} B_{\mathbf{r}, \alpha_L, x} \partial_{\mathbf{u}} \right] = -2 \mathbf{u} \cdot Q_{\mathbf{r}, \alpha_i, x} B_{\mathbf{r}, \alpha_L, x} Q_{\mathbf{r}, \alpha_j, x} \mathbf{u}.$$

The matrix $Q_{\mathbf{r}, \alpha_i, x} B_{\mathbf{r}, \alpha_L, x} Q_{\mathbf{r}, \alpha_j, x}$ is not necessarily symmetric, but the commutator involves only the symmetric part of this matrix. Additionally,

$$|\mathbf{u} \cdot Q_{\mathbf{r}, \alpha_i, x} B_{\mathbf{r}, \alpha_L, x} Q_{\mathbf{r}, \alpha_j, x} \mathbf{u}| \leq C Q_{\mathbf{r}}(\mathbf{u}),$$

and so the quadratic form behaves exactly like a term $Q_{\mathbf{r}, \alpha_j, x}(\mathbf{u})$. Also,

$$\left[\mathbf{u} \cdot Q_{\mathbf{r}, \alpha_i, x} B_{\mathbf{r}, \alpha_L, x} \partial_{\mathbf{u}}, B_{\mathbf{r}, \alpha_j, x}(\partial_{\mathbf{u}}) \right] = -2 \partial_{\mathbf{u}} \cdot B_{\mathbf{r}, \alpha_j, x} Q_{\mathbf{r}, \alpha_i, x} B_{\mathbf{r}, \alpha_L, x} \partial_{\mathbf{u}},$$

and the symmetric part of $B_{\mathbf{r}, \alpha_j, x} Q_{\mathbf{r}, \alpha_i, x} B_{\mathbf{r}, \alpha_L, x}$ is dominated by $Q_{\mathbf{r}}^{-1}$. Thus, for the purposes of estimates, the operator $\mathbf{u} \cdot Q_{\mathbf{r}, \alpha_i, x} B_{\mathbf{r}, \alpha_L, x} \partial_{\mathbf{u}}$ commutes with both $Q_{\mathbf{r}, \alpha_j, x}(\mathbf{u})$ and $B_{\mathbf{r}, \alpha_j, x}(\partial_{\mathbf{u}})$. Finally,

$$\mathbf{u} \cdot Q_{\mathbf{r}, \alpha_i, x} B_{\mathbf{r}, \alpha_L, x} \partial_{\mathbf{u}} e^{-\frac{Q_{\mathbf{r}}(\mathbf{u})}{4t}} = -\frac{(\mathbf{u} \cdot Q_{\mathbf{r}, \alpha_i, x} B_{\mathbf{r}, \alpha_L, x} Q_{\mathbf{r}} \mathbf{u})}{2t} e^{-\frac{Q_{\mathbf{r}}(\mathbf{u})}{4t}},$$

which behaves the same as multiplying by the factor $Q_{\mathbf{r}, \alpha_i, x}(\mathbf{u})/4t$.

The end result is that we can write, up to inconsequential modifications of the $Q_{\mathbf{r}, \alpha_i, x}$,

$$\begin{aligned} \prod_{i=1}^L \left(\frac{Q_{\mathbf{r}, \alpha_i, x}(\mathbf{u})}{4t} \right) e^{-\frac{1}{4t} Q_{\mathbf{r}}(\mathbf{u})} &= t B_{\mathbf{r}, \alpha_L, x}(\partial_{\mathbf{u}}) \prod_{i=1}^{L-1} \left(\frac{Q_{\mathbf{r}, \alpha_i, x}(\mathbf{u})}{4t} \right) e^{-\frac{1}{4t} Q_{\mathbf{r}}(\mathbf{u})} \\ &\quad + \phi_{\mathbf{r}}(\mathbf{u}, x) \prod_{i=1}^{L-1} \left(\frac{Q_{\mathbf{r}, \alpha_i, x}(\mathbf{u})}{4t} \right) e^{-\frac{1}{4t} Q_{\mathbf{r}}(\mathbf{u})}. \end{aligned}$$

We apply this identity to the integrand of (5.7). The second term on the right hand side (which is more precisely a sum of such terms) is handled by the induction hypothesis in L , so we continue with just the first term on the right. We integrate by parts in \mathbf{u} to move the $B_{\mathbf{r}, \alpha_L, x}(\partial_{\mathbf{u}})$ to act on $V(e_x(u_k)) \cdots V(e_x(u_2)) V(x) \phi_{\mathbf{r}}(x, \mathbf{u})$. At this point, the only estimate we use on $B_{\mathbf{r}, \alpha_L, x}$ is that it is a bounded matrix, together with all derivatives in x , which follows since $B_{\mathbf{r}, \alpha_L, x} \lesssim Q_{\mathbf{r}}^{-1} \lesssim I$, similarly for its derivatives in x . Thus, the coefficients of $B_{\mathbf{r}, \alpha_L, x}$ can be absorbed into $\phi_{\mathbf{r}}(x, \mathbf{u})$, leading to the term

$$\begin{aligned} t (4\pi t)^{-\frac{n(k-1)}{2}} \left(\prod_{j=1}^k r_j^{-\frac{n}{2}} \right) \int_{\mathbb{R}^{nk}} \prod_{i=1}^{L-1} \left(\frac{Q_{\mathbf{r}, \alpha_i, x}(\mathbf{u})}{4t} \right) e^{-\frac{1}{4t} Q_{\mathbf{r}}(\mathbf{u})} \\ \times \partial_{\mathbf{u}}^2 \left(V(e_x(u_k)) \cdots V(e_x(u_2)) V(x) \phi_{\mathbf{r}}(x, \mathbf{u}) \right) d\mathbf{u} dx. \end{aligned}$$

This is handled as above, using Lemma 4.4 and the result for $m-1$ and $L-1$. The only difference is that when we convert a factor of ∂_{u_k} into ∂_x , in addition to acting on the other factors of V_j the operator ∂_x can also act on the $Q_{\mathbf{r}, \alpha_i, x}$, which is harmless by (5.5). \square

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