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by

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# Derivatives of Spectral Function and Sobolev Norms of Eigenfunctions on a Closed Riemannian Manifold

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**Abstract**

Let $e(x,y,\lambda)$ (cf (1)) be the spectral function and $\chi_\lambda$ (cf (2)) the unit spectral projection operator, with respect to the Laplace-Beltrami operator on a closed Riemannian manifold $M$. We generalize the one-term asymptotic expansion of $e(x,x,\lambda)$ by Hörmander [3] to that of $\partial_x^\alpha \partial_y^\beta e(x,y,\lambda)|_{x=y}$ for any multi-indices $\alpha$, $\beta$ in a sufficiently small geodesic normal coordinate chart of $M$. Moreover, we extend the sharp $(L^2, L^p)\,(2 \leq p \leq \infty)$ estimates of $\chi_\lambda$ by Sogge [10] [11] to the sharp $(L^2$, Sobolev $L^p)$ estimates of $\chi_\lambda$.

## Contents



# 1 Introduction

Let $(M,\ g)$ be a smooth closed Riemannian manifold of dimension $n \geq 2$ and $\Delta$ the positive Laplace-Beltrami operator on $M$. Let $L^2(M)$ be the space of square integrable functions on $M$ with respect to the Riemannian density $dv(M) := \sqrt{\det\,(g_{ij})}\ dx =: \sqrt{\mathrm{g}(x)}\,dx$. Let $e_1(x)$, $e_2(x)$, $\cdots$ be a complete orthonormal basis in $L^2(M)$ for the eigenfunctions of $\Delta$ such that $0 \leq \lambda_1^2 \leq \lambda_2^2 \leq \cdots$

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for the corresponding eigenvalues, where $\lambda_j$ are nonnegative real numers. Also, let $\mathbf{e}_j$ denote the projection onto the 1-dimensional space $\mathbf{C}e_j$. Thus , an $L^2$ function $f$ can be written as

$$f = \sum_{j=0}^{\infty} \mathbf{e}_j(f),$$

where the partial sum converges in the $L^2$ norm. Let $\lambda$ be a positive real number $\geq 1$. We define the spectral function $e(x, y, \lambda)$ and the unit spectral projection operator (USPO) $\chi_\lambda$ as follows:

$$e(x, y, \lambda) := \sum_{\lambda_j \leq \lambda} e_j(x)\bar{e}_j(y) \ , \tag{1}$$

$$\chi_\lambda f := \sum_{\lambda_j \in [\lambda,\, \lambda+1]} \mathbf{e}_j(f) \ . \tag{2}$$

Since in (1) the definition of $e(x, y, \lambda)$ does not depend on the choice of the orthogonormal basis $\{e_j(x)\}_{j=1}^{\infty}$, without loss of generality from now on we assume that $e_j(x)$ $(1 \leq j < \infty)$ are real-valued functions on $M$ so that

$$e(x, y, \lambda) := \sum_{\lambda_j \leq \lambda} e_j(x)e_j(y) \ .$$

Approximating the fundamental solution of the wave equation precisely enough, Hörmander [3] [5] obtained a one-term asymptotic expansion of the spectral function $e(x, x, \lambda)$ as following:

$$e(x, x, \lambda) = C_n \, \lambda^n + \mathrm{O}(\lambda^{n-1}), \ \text{as } \lambda \to \infty, \tag{3}$$

where $C_n$ is equal to $(2\pi)^{-n}$ times the volume of the unit ball of $\mathbf{R}^n$. As a consequence Hörmander proved the uniform estimate of eigenfunctions for $x \in M$

$$\sum_{\lambda_j \in [\lambda,\, \lambda+1]} |e_j(x)|^2 \leq C \, \lambda^{n-1} \ , \tag{4}$$

which implies

$$||\chi_\lambda f||_\infty \leq C\lambda^{(n-1)/2}||f||_2 \ . \tag{5}$$

Here $||f||_r$ $(1 \leq r \leq \infty)$ means the $L^r$ norm of the function $f$ on $M$. Let $\delta(r)$ be the critical exponent $\max(n \cdot |1/r - 1/2| - 1/2,\ 0)$ for Bochner Riesz means of the Laplacian on $L^r(\mathbf{R}^n)$. With the help of the oscillatory integral theorems of Carleson-Sjölin [1] and Stein [13], Sogge showed in [10] and [11]

$$||\chi_\lambda f||_q \leq C\lambda^{\delta(q)}||f||_2, \ q = 2(n+1)/(n-1) \tag{6}$$

by using the Hadamard parametrix for $\Delta - (\lambda + i)^2$ and the wave operator $(\partial/\partial t)^2 + \Delta$ respectively. Interpolating (6) with (5) and the inequality

$$||\chi_\lambda f||_2 \leq ||f||_2 \tag{7}$$

from the orthogonal relation, Sogge proved the following

**Proposition 1.1.** (cf C. D. Sogge [10] and [11])

$$||\chi_\lambda f||_r \leq C\lambda^{\epsilon(r)}||f||_2, \ 2 \leq r \leq \infty, \tag{$\clubsuit$}$$

*where*

$$\epsilon(r) = \begin{cases} \frac{(n-1)(r-2)}{4r} & \text{if } 2 \leq r \leq \frac{2(n+1)}{n-1}, \\ \delta(r) & \text{if } \frac{2(n+1)}{n-1} \leq r \leq \infty. \end{cases}$$

*The estimate* ($\clubsuit$) *is sharp in the sense that the bounds cannot be replaced by* $\mathrm{o}(\lambda^{\epsilon(r)})$.

**Remark 1.1.** Sharpness of the bounds of estimates in this paper always has the similar meaning as above.

For a positive integer $m$, we set the following notations:

$$(2m-1)!! := (2m-1)(2m-3)\cdots 3\cdot 1,\ (-1)!! := 1\ .$$

We say $\alpha \equiv \beta \pmod 2$ for two multi-indices $\alpha, \beta \in \mathbf{Z}^n_+$ if and only if $\alpha_j \equiv \beta_j \pmod 2$ for $1 \le j \le n$. Let $\nabla$ be the Levi-Civita connection on $M$ and $|\nabla^k u|$ be the length of the $k$-covariant derivative of a smooth function $u$ on $M$. (cf Subsection 2.1) Let $B_n$ be the unit ball in $\mathbf{R}^n$ with center at 0. We firstly generalize Hörmander's asymptotic expansion (3) of the spectral function in the following

**Theorem 1.1.** *In a sufficiently small geodesic normal coordinate chart $(X\,,x)$ of $M$, for multi-indices $\alpha, \beta \in \mathbf{Z}^n_+$ the following estimates hold uniformly for $x \in X$ as $\lambda \to \infty$:*

$$\partial_x^\alpha \partial_y^\beta e(x,y,\lambda)|_{x=y} = \begin{cases} C_{n,\alpha,\beta}\,\lambda^{n+|\alpha+\beta|} + \mathrm{O}(\lambda^{n+|\alpha+\beta|-1}) & \text{if } \alpha \equiv \beta \pmod 2, \\ \mathrm{O}(\lambda^{n+|\alpha+\beta|-1}) & \text{otherwise,} \end{cases} \tag{8}$$

*where for multi-indices $\alpha, \beta$ such that $\alpha \equiv \beta \pmod 2$,*

$$C_{n,\alpha,\beta} = (2\pi)^{-n}\,(-1)^{(|\alpha|-|\beta|)/2} \int_{B_n} x^{\alpha+\beta}\,dx \tag{9}$$

$$= (-1)^{(|\alpha|-|\beta|)/2} \frac{\prod_{j=1}^n (\alpha_j+\beta_j-1)!!}{\pi^{n/2}\,2^{n+|\alpha+\beta|/2}\,\Gamma(\frac{|\alpha+\beta|+n}{2}+1)} \tag{10}$$

*In particular, if $\alpha = \beta$, then the following estimate holds uniformly for $x \in X$ as $\lambda \to \infty$:*

$$\sum_{\lambda_j \le \lambda} |\partial^\alpha e_j(x)|^2 = C_{n,\alpha}\lambda^{n+2|\alpha|} + \mathrm{O}(\lambda^{n+2|\alpha|-1}),\ \text{as } \lambda \to \infty\ , \tag{11}$$

*where $C_{n,\alpha} = C_{n,\alpha,\alpha} > 0$. Moreover, the following uniform estimate holds for $x \in M$ and it is sharp:*

$$\sum_{\lambda_j \in [\lambda,\, \lambda+1]} |\nabla^k e_j(x)|^2 \le C\,\lambda^{n+2k-1}\ . \tag{12}$$

**Remark 1.2.** More precisely speaking, Theorem 1.1 always holds for the geodesic coordinate $(X,x)$ satisfying the condition (25). (cf Subsection 2.2)

Using the notations in Definition 2.1, we generalize the sharp $L^\infty$ estimate 5 in the following

**Corollary 1.1.** *The following estimate holds and it is sharp:*

$$||\chi_\lambda f||_{C^k} \le C\,\lambda^{k+(n-1)/2}||f||_2\ .$$

As a consequence of Proposition 1.1 and Corollary 1.1, it is not hard for us to generalize the sharp $L^p$ estimate of $\chi_\lambda$ by Sogge to the sharp Sobolev $L^p$ estimate on $M$. (cf Definition 2.1 for Sobolev spaces $H^r_k$ and $C^k$ spaces on $M$)

**Theorem 1.2.** *Let $k$ be a nonnegative integer, $2 \le r \le \infty$ and $\epsilon(r)$ be the same as* Proposition 1.1. *Then the following estimate holds :*

$$||\chi_\lambda f||_{H^r_k} \le C\lambda^{\epsilon(r)+k}||f||_2\ . \tag{$\spadesuit$}$$

*Moreover the estimate ($\spadesuit$) is sharp. In particular, for a single eigenfunction $e_j(x)$ the following holds:*

$$||e_j||_{H^r_k} \le C\,\lambda_j^{\epsilon(r)+k}\ ,$$

*which in general can not be improved in the sense of* Example 1.1.

**Example 1.1.** Let $M^n$ be the unit n-sphere $S^n$ of the Euclidean space $\mathbf{R}^{n+1}$. Let $Z_m$ be the zonal harmonic function of degree $m$ with respect to the north pole and $Q_m$ the spherical harmonic defined by

$$Q_m(x) = (x_2 + ix_1)^m \ .$$

Then there exists a positive constant $C$ independent of $m$ such that the following inequalities hold:

$$||Z_m||_{H_k^r}/||Z_m||_2 \geq C\, m^{\epsilon(r)+k},\ 2(n+1)/(n-1) \leq r \leq \infty; \tag{13}$$

$$||Q_m||_{H_k^r}/||Q_m||_2 \geq C\, m^{\epsilon(r)+k},\ 2 \leq r \leq 2(n+1)/(n-1). \tag{14}$$

**Remark 1.3.** Let $N$ be a compact Riemannian manifold with smooth boundary $\partial N$. On $N$ we consider the Dirichlet Laplacian $\Delta_N$ with respect to the Dirichlet boundary value problem

$$\Delta_N u = f, \quad x \in N^\circ;\ u(x) = 0, \quad x \in \partial N.$$

Let $\{e_j^N(x)\}_{j=1}^\infty$ be the real normalized eigenfunctions of $\Delta_N$ such that

$$\Delta_N e_j^N(x) = \mu_j^2\, e_j^N(x),\ x \in N^\circ;\ e_j^N(x) = 0,\ x \in \partial N;$$

where $0 < \mu_1^2 \leq \mu_2^2 \leq \cdots$ are the eigenvalues of $\Delta_N$. Similarly to (2) we can also define the USPO $\chi_{N,\lambda}$ associated to $\Delta_N$. In particular, when $N$ is a bounded region in $\mathbf{R}^n$, by studying the heat kernel of $\Delta_N$, Ozawa [8] proved

$$\sum_{\mu_j \leq \lambda} \left| \frac{\partial e_j^N(x)}{\partial \nu} \right|^2 = C\lambda^{n+2} + \mathrm{O}(\lambda^{n+1}),\ \text{as } \lambda \to \infty, \tag{15}$$

for every $x \in \partial N$, where $\nu$ is the unit outward normal derivative at $x \in \partial N$. For the general Riemannian manifold $N$ with boundary $\partial N$, Grieser [2] and Sogge [12] proved that the estimate (5) holds for $\chi_{N,\lambda}$, by which Xiangjin Xu [15] used a clever maximum principle argument to show the estimate

$$||\chi_{N,\lambda} f||_{C^1(N)} \leq C\lambda^{(n+1)/2}||f||_{L^2(N)} \ . \tag{16}$$

The results of Ozawa and Xiangjin Xu stimulated the author to think of Theorem 1.2.

Now we sketch the proof of Theorem 1.1. Firstly we make an observation that

$$\sum_{\lambda_j \leq \lambda} \partial^\alpha e_j(x) \partial^\beta e_j(x) = \partial_x^\alpha \partial_y^\beta e(x, y, \lambda)|_{x=y} \ . \tag{17}$$

We recall that the wave kernel $K(t, x, y) \in \mathscr{D}'(\mathbf{R} \times M \times M)$ is the Schwarz kernel of the wave operator $\cos(t\sqrt{\Delta})$ associated with the Laplace-Beltrami operator $\Delta$. For each $x, y \in M$, by (17.5.9) of [5] $K(t, x, y)$ is the Fourier transformation with respect to $\tau$ of the temperate measure $dm(x, y, \tau)$:

$$m(x, y, \tau) = \sqrt{\mathbf{g}(y)}\, (\operatorname{sgn} \tau)\, e(x, y, |\tau|) \ .$$

In Proposition 2.2 and Corollary 2.1 of Subsection 2.3, we obtain the detailed information of the singularities for $\partial_x^\alpha \partial_y^\beta K(t, x, y)|_{x=y}$ for $x$ in a sufficiently small geodesic coordinate $X$ of $M$ and $t$ in a small interval $(-c, c)$, where $c$ is a positive constant depending on the geometry of $M$. In particular, by Corollary 2.1 $t^{n+|\alpha+\beta|}\partial_x^\alpha \partial_y^\beta K(t, x, y)|_{x=y}$ is smooth in $[0, c) \times X$. Then in Subsection 2.4 we complete the proof of (11) with the help of a Tauberian lemma (cf Lemma 2.5). As long as the constant $C_{n,\alpha,\beta}$ is concerned, we firstly observe that it does not depend on the Riemannian manifold $M$ and then obtain its accurate value by the computation on the $n$-dimensional flat torus.

(cf Subsection 2.5) We can easily derive Corollary 1.1 from (11) and the detail is given in Lemma 2.7.

Then we state the outline of the proof of Theorem 1.2. We have only to consider $2 \leq r < \infty$ by Corollary 1.1. Making reduction by the elliptic regularity (cf Corollary 3.1) and the duality, we only need to show that the following estimates hold for $j = 0, 1, \cdots$ and they are sharp:

$$||\Delta^j \chi_\lambda f||_2 \leq C\lambda^{2j+\epsilon(r)}||f||_{r'}, \ ||\mathbf{grad}\, \Delta^j \chi_\lambda f||_2 \leq C\lambda^{2j+1+\epsilon(r)}||f||_{r'}, \ r' = r/(r-1). \tag{18}$$

Finally we can obtain the above estimates and their sharpness by Proposition 1.1 and direct computations. The detail will be given in Section 3.

As long as the organization of the rest of this paper is concerned, in Subsection 2.1 we set the notations related to the covariant derivatives, Sobolev spaces and the wave kernel on $M$. In Subsection 2.2 we give a quick review for the Hadamard parametrix of $\cos(t\sqrt{\Delta})$, which approximates the wave kernel $K(t, x, y)$ as well as we desire, and is the crucial tool to the proof of Theorem 1.1. In Section 4 we have some explicit calculations to check the validity of (13) and (14), in which the asymptotic property of the Jacobi polynomials is involved.

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# 2 Derivatives of spectral function

## 2.1 Sobolev spaces and the wave kernel

For $k$ a nonnegative integer and $u \in C^\infty(M)$, $\nabla^k u$ denotes the $k$th covariant derivative of $u$ (with the convention $\nabla^0 u = u$). As an example, the components of $\nabla u$ in local coordinates are given by $(\nabla u)_i = \partial_i u$, while the components of $\nabla^2 u$ in local coordinates are given by

$$(\nabla^2 u)_{ij} = \partial^2_{ij} u - \sum_k \Gamma^k_{ij} \partial_k u \ , \tag{19}$$

where $\Gamma^k_{ij}$ are the Christoffel symbols of the Levi-Civita connection $\nabla$ of $(M, g)$. We define the length $|\nabla^k u|$ of $\nabla^k u$ by

$$|\nabla^k u|^2 := \sum g^{i_1 j_1} \cdots g^{i_k j_k} (\nabla^k u)_{i_1 \cdots i_k} (\nabla^k u)_{j_1 \cdots j_k} \ ,$$

where $(g^{ij})$ denotes the inverse matrix of $(g_{ij})$ and the sum is taken for $1 \leq i_1, \cdots, i_k$, $j_1, \cdots, j_k \leq n$.

**Definition 2.1.** The Sobolev space $H^r_k(M)$ is the completion of $C^\infty(M)$ with respect to the norm

$$||u||_{H^r_k} := \left( \sum_{j=0}^k \int_M |\nabla^j u|^r dv(g) \right)^{1/r}, \ 1 \leq r < \infty \ ,$$

$$||u||_{H^r_k} := \sum_{j=0}^k \sup_{x \in M} |\nabla^j u(x)|, \qquad r = \infty \ .$$

Sometimes we also write $C^k, H^k$ instead of $H^\infty_k, H^2_k$.

The following result is well known.

**Proposition 2.1.** *$H_k^r(M)$ does not depend on the Riemannian metric. And $H^k(M)$ is a Hilbert space.*

**Lemma 2.1.** *Let $X$ be a relatively compact open set of $M$ and $x : X \to \mathbf{R}^n$ a diffeomorphism of $X$ into $\mathbf{R}^n$, that is, a chart on $M$. For $k$ a nonnegative integer and $u \in C^\infty(M)$,*

$$||u||_{C^k(X)} \le C \sum_{|\alpha|\le k} ||\partial^\alpha u||_{L^\infty(X)} \ ,$$

*where $\alpha = (\alpha_1, \cdots, \alpha_n)$ is a multi-index and $\partial^\alpha = (\partial/\partial x_1)^{\alpha_1} \cdots (\partial/\partial x_n)^{\alpha_n}$.*

**Proof.** By the similar computation to the equalities (19), we can see that the component $(\nabla^k u)_{i_1 \cdots i_k}$ of $\nabla^k u$ is equal to the main term $\partial_{i_1} \cdots \partial_{i_k} u$ plus the lower-order partial derivatives of $u$ with smooth coefficients coming from the Riemannian metric. Then the statement follows from that $X$ is relatively compact in $M$.

In the chart $X$ the Laplace-Beltrami operator takes the form

$$\Delta = -\sum \partial_j (g^{jk} \partial_k) + \sum b^j \partial_j \ ,$$

where $b^j = -\sum_k g^{jk} \partial_k (\log \sqrt{\mathrm{g}})$. Let $\mathscr{P}$ be the operator defined by $\Delta$ in $L^2(M)$ with $\mathscr{D}_{\mathscr{P}} = H^2(M)$. It is well known that $\mathscr{P}$ is a self-adjoint operator on $L^2(M)$ and that $\mathscr{P}$ has a discrete spectrum so that the spectral resolution of $\Delta$ in the beginning of Section 1 holds. Let $\cos(t\sqrt{\mathscr{P}})$ be the wave operator associated with $\mathscr{P}$ defined by

$$\cos(t\sqrt{\mathscr{P}}) = \int_0^\infty \cos(t\sqrt{\mu}) dE_\mu \ ,$$

where $E_\mu$ is the spectral family of $\mathscr{P}$. By the standard computations (cf Section 17.5 of [5]), the wave kernel $K(t,x,y) \in \mathscr{D}'(\mathbf{R} \times M \times M)$ of $\cos(t\sqrt{\mathscr{P}})$ is the Fourier transformation with respect to $\tau$ of the temperate measure $dm(x,y,\tau)$,

$$m(x,y,\tau) = \sqrt{\mathrm{g}(y)}\,(\mathrm{sgn}\ \tau)\, e(x,y,|\tau|)/2 \ . \tag{20}$$

We remark that $K(t,x,y) = \widehat{dm}(t)$ is an even function with respect to $t$.

## 2.2 The Hadamard parametrix of the wave operator

In this subsection we shall quickly review a remarkably simple and precise construction due to J. Hadamard, which gives the singularities of the wave kernel $K(t,x,y)$ with any desired precision.

Let the open subset $X$ (cf Lemma 2.1) of $M$ be sufficiently small so that for an arbitrary point $p \in X$ we can introduce the geodesic normal coordinates of $X$ which vanish at $p$ and satisfy the condition

$$\sum_k g_{jk}(x) x_k = \sum_k g_{jk}(0) x_k \ . \tag{21}$$

By Lemma 17.4.1 in [5], there exist unique smooth functions $u_0, \cdots, u_\nu$ with $u_0(0) = 1$ satisfying

$$2\nu u_\nu - h u_\nu + 2\langle x, \partial u/\partial x\rangle + 2\Delta u_{\nu-1} \ , \tag{22}$$

where $u_{-1} = 0$ and

$$h(x) = \sum_{j,k} g_{jk}(0) b^j(x) x_k = \sum_{j,k} g_{jk}(x) b^j(x) x_k \ . \tag{23}$$

It follows from Corollary C.5.2 of [5] that there is a neighborhood $\mathscr{V}$ of the zero section $\{0\} \times M$ of the tangent bundle $TM$, a neighborhood $\mathscr{W}$ of the diagonal in $M \times M$, and a well-defined diffeomorphism

$$\mathscr{V} \ni (\tilde{x}, y) \mapsto (\exp_y \tilde{x},\, y) \in \mathscr{W} \ ,$$

where $\exp_y$ is the exponential map at $y$ with $\exp_y 0 = y$ and $(d\,\exp_y)|_{\tilde{x}=0}$ equal to the identity. The metric tensor in the $\tilde{x}$ coordinates

$$\sum \tilde{g}^{jk}(\tilde{x}, y)\xi_j\xi_k = p(\exp_y \tilde{x},\, {}^t(d\,\exp_y)^{-1}(\tilde{x})\,\xi)$$

satisfies (21), where $p$ is the principal symbol of $\Delta$. If $(x, y) \in \mathscr{W}$ we have a well-defined Riemannian distance $s(x, y)$ which is realized by a unique geodesic between $x$ and $y$. We choose $\mathscr{V}$ such that $\{\tilde{x} : (\tilde{x}, y) \in \mathscr{V}\}$ is convex for every $y \in M$. Pulling the functions $u_\nu(\tilde{x}, y)$ defined by (22) back to $\mathscr{W}$ from $\mathscr{V}$, we obtain uniquely defined $U_\nu \in C^\infty(\mathscr{W})$. We remark that

$$U_0(x, x) = 1, \quad (x, x) \in \mathscr{W}. \tag{24}$$

Since $\mathscr{W}$ is open, we further choose the open set $X$ so small that $X \times X \subset \mathscr{W}$. We can choose $c > 0$ such that

$$X^c \times X^c \subset \mathscr{W}, \tag{25}$$

where

$$X^c = \{y \in M : \inf_{x \in X} s(x, y) < c\} \ .$$

As Lemma 17.4.2 of [5], with the notation (3.2.17) of [4] In $\mathbf{R}_t \times \mathbf{R}_x^n$ we define the homogeneous distributions $E_\nu$ $(k \in \mathbf{Z})$ of degree $2\nu + 1 - n$ with support in the forward light cone $\{(t, x) : t \geq |x|\}$ by

$$E_\nu = 2^{-2\nu-1}\pi^{(1-n)/2}\chi_+^{\nu+(1-n)/2}(t^2 - |x|^2), \ t > 0 \ . \tag{26}$$

We have

$$(\partial^2/\partial t^2 - \sum \partial^2/\partial x_j^2)E_\nu = \nu E_{\nu-1}, \nu \neq 0; \ (\partial^2/\partial t^2 - \sum \partial^2/\partial x_j^2)E_0 = \delta_{0,0}; \tag{27}$$

$$-2\partial E_\nu/\partial x = x E_{\nu-1}, \ \nu \in \mathbf{Z} \ . \tag{28}$$

With some abuse of the notation we shall write $E_\nu(t, |x|)$ instead of $E_\nu(t, x)$ in what follows; when $t = 0$ this should be interpreted as the limit when $t \to +0$. Moreover it follows from the proof of Lemma 17.4.2 in [5] with the notation $(3.2.10)'$ of [4] that

$$\begin{aligned} &\partial_t(E_\nu(t, 0) - \check{E}_\nu(t, 0)) \\ &\quad = \begin{cases} 2^{-2\nu}\,\pi^{(1-n)/2}\,\underline{t}^{2\nu-n}/\Gamma(\nu + (1-n)/2), & \text{if n is even} \\ 2^{-2\nu-1}\,\pi^{(1-n)/2}\,|t|^{2\nu-n}/\Gamma(\nu + (1-n)/2), & \text{if } n \text{ is odd and } \ 2\nu > n \\ (-1)^k\,2^{-2\nu-k}\,\pi^{(1-n)/2}\,\delta^{(2k)}/(2k-1)!!, & \text{if } n = \text{odd and } n - 1 - 2\nu = 2k \geq 0, \end{cases} \end{aligned} \tag{29}$$

where $\check{E}_\nu$ is the reflection of $E_\nu$ with respect to the origin of $\mathbf{R}_t$. It follows from (21) and (27) (cf Proposition 17.4.3 in [5]) that we have in $(-\infty, c) \times X^c \times X$

$$\begin{aligned} (\partial^2/\partial t^2 \quad &+ \quad \Delta)\mathscr{E}(t, x, y) \\ &:= \quad (\partial^2/\partial t^2 + \Delta)\sum_0^N U_\nu(x, y)E_\nu(t, s(x, y)) \\ &= \quad \delta_{0,y}/\sqrt{g(y)} + (P(x, D)U_N(x, y))E_N(t, s(x, y)) \ . \end{aligned} \tag{30}$$

When $s(x,y) \le c$ the coefficients $U_j$ have been defined previously by integrating the equation (22) in geodesic coordinates, and when $s(x,y) > c$ their definition is irrelevant.

By the proof of Theorem 17.5.5 in [5], in $(-c,\ c) \times X^c \times X$, we have

$$K(t,x,y) - \partial_t(\mathscr{E}(t,x,y) - \check{\mathscr{E}}(t,x,y))\sqrt{\mathrm{g}(y)} \in C^{N-n-3} \tag{31}$$

and

$$\begin{aligned} \left|\partial^\alpha_{t,x,y}\left(K(t,x,y) - \partial_t(\mathscr{E}(t,x,y) - \check{\mathscr{E}}(t,x,y))\sqrt{\mathrm{g}(y)}\right)\right| &\le C|t|^{2N-n-|\alpha|}, \\ |\alpha| &\le N-n-3. \end{aligned} \tag{32}$$

By the definition of $E_\nu$ we know that $\mathscr{E}(t,x,y)$ has support in the forward light cone $\{t \ge s(x,y)\}$ and its reflection $\check{\mathscr{E}}(t,x,y))$ with respect to the origin of $\mathbf{R}_t$ has support in the backward light cone $\{t \le -s(x,y)\}$. Here all terms are continuous functions of $(x,y)$ with values in $\mathscr{D}'(\mathbf{R})$ by Lemma 17.4.2 in [5]. We shall apply (31) and (32) to investigating the singularities of the derivatives $\partial_x^\alpha \partial_y^\beta K(t,x,y)|_{x=y}$ of the wave kernel on the diagonal in the following subsection.

## 2.3 The derivatives of the wave kernel on the diagonal

Let $\alpha = (\alpha_1,\cdots,\alpha_n)$, $\beta = (\beta_1,\cdots,\beta_n) \in \mathbf{Z}_+^n$ be two multi-indices. In the coordinate chart $(X\times X,(x,y))$ of $M\times M$, we shall consider the singularities of $\partial_x^\alpha \partial_y^\beta K(t,x,y)|_{x=y}$. From now on, we let the positive integer $N$ in (31) be as large as we need. By (31), we know

$$\begin{aligned} \partial_x^\alpha \partial_y^\beta K(t,x,y)|_{x=y} &= \partial_x^\alpha \partial_y^\beta(\,\partial_t(\mathscr{E}(t,x,y) - \check{\mathscr{E}}(t,x,y))\sqrt{\mathrm{g}(y)}\,)|_{x=y} \\ &+ \ C^{N-n-|\alpha+\beta|-3}\,\text{term}\ . \end{aligned} \tag{33}$$

By the above equality we know that $\partial_x^\alpha \partial_y^\beta K(t,x,y)|_{x=y}$ is the sum of a continuous function of $(t,x) \in (-c,\ c)\times X$ and finite homogeneous distributions of $t$ with coefficients of smooth functions of $x \in X$. We call the distribution summand of $\partial_x^\alpha \partial_y^\beta K(t,x,y)|_{x=y}$ with the lowest homogeneous degree the *principal singular term* of $\partial_x^\alpha \partial_y^\beta K(t,x,y)|_{x=y}$. We observe that the principal singular term of $\partial_x^\alpha \partial_y^\beta K(t,x,y)|_{x=y}$ is equal to that of

$$\partial_x^\alpha \partial_y^\beta \left(\sqrt{\mathrm{g}(y)}\,U_0(x,y)\,\partial_t\left(E_0(t,s(x,y)) - \check{E}_0(t,s(x,y))\right)\right)_{x=y}. \tag{34}$$

In order to write out the above principal singular term explicitly, firstly we need the following

**Lemma 2.2.** *In the geodesic coordinate $X$ satisfying* (25)*, the Taylor expansion of the square distance function $s(x,y)^2$ is as follows :*

$$s(x,y)^2 = |x-y|^2 + \text{higher even order terms.}$$

*In particular, at a fixed point $(z,z) \in X\times X$*

$$\partial^\gamma_{x,y}\eta(z,z) = 0, \quad |\gamma| = \text{odd}; \tag{35}$$

$$\partial_{x_j}\eta(z,z) = \partial_{y_j}\eta(z,z) = 0,\ \partial^2_{x_jx_k}\eta(z,z) = \partial^2_{y_jy_k}\eta(z,z) = -\partial^2_{x_jy_k}\eta(z,z) = 2\delta_{jk}\ . \tag{36}$$

**Proof.** By [6] we know the square distance function $s(x,y)^2$ is a smooth on $X\times X$. Let $\eta(x,y) = s(x,y)^2$. Under the geodesic coordinates, the square distance function $\eta$ satisfies the following equalities:

(i) $\eta(0,0) = \eta(x,x) = 0$
(ii) $\eta(0,x) = \eta(0,-x) = |x|^2$
(iii) $\eta(x,y) = \eta(y,x)$

Let $\eta_k(x,y)$ be the $k$-th term of the Taylor expansion of $\eta$ with respect to $(0,0)$. By (i), $\eta_0 = 0$. By (ii) and (iii), $\eta_1(x,y) \equiv 0$. By (i)-(iii), the homogeneous quadratic polynomial $\eta_2(x,y)$ of $x$, $y$ satisfies the following equalities:

(a) $\eta_2(x,x) = 0$

(b) $\eta_2(0,x) = \eta_2(0,-x) = |x|^2$

(c) $\eta_2(x,y) = \eta_2(y,x)$

By (a),

$$\eta_2(x,y) = \sum_{j=1}^{n} \Big( \text{const } \times (x_j - y_j)^2 + \text{const } \times (x_j^2 - y_j^2) \Big) .$$

Then by (c), we can see

$$\eta_2(x,y) = \sum_{j=1}^{n} \text{const } \times (x_j - y_j)^2 ,$$

by which (ii) implies that $\eta_2(x,y) = |x-y|^2$.

Finally we have only to show that $\eta_{2k+1}(x,y) \equiv 0$ $(k \geq 1)$. By (i)-(iii), $\eta_{2k+1}$ satisfies (a), (c) and (b′) $\eta_{2k+1}(0,x) = \eta_{2k+1}(0,-x) = 0$.

By (b′) we can write the homogeneous polynomial $\eta_{2k+1}(x,y)$ of degree $2k+1$ as

$$\eta_{2k+1}(x,y) = \sum_{l=1}^{2k} \sum_{1 \leq i_1, \cdots, i_l; j_1, \cdots, j_{2k+1-l} \leq n} \theta^{i_1, \cdots, i_l}_{j_1, \cdots, j_{2k+1-l}}(x,y),$$

$$\begin{aligned} \theta^{i_1, \cdots, i_l}_{j_1, \cdots, j_{2k+1-l}}(x,y) &= \\ a^{i_1, \cdots, i_l}_{j_1, \cdots, j_{2k+1-l}} x_{i_1} \cdots x_{i_l} y_{j_1} \cdots y_{j_{2k+1-l}} &+ b^{i_1, \cdots, i_l}_{j_1, \cdots, j_{2k+1-l}} y_{i_1} \cdots y_{i_l} x_{j_1} \cdots x_{j_{2k+1-l}}. \end{aligned}$$

By (a),

$$a^{i_1, \cdots, i_l}_{j_1, \cdots, j_{2k+1-l}} + b^{i_1, \cdots, i_l}_{j_1, \cdots, j_{2k+1-l}} = 0 ;$$

by (c),

$$a^{i_1, \cdots, i_l}_{j_1, \cdots, j_{2k+1-l}} = b^{i_1, \cdots, i_l}_{j_1, \cdots, j_{2k+1-l}} .$$

By above equalities, we can see that all $a^{i_1, \cdots, i_l}_{j_1, \cdots, j_{2k+1-l}}$ and $b^{i_1, \cdots, i_l}_{j_1, \cdots, j_{2k+1-l}}$ vanish. That is, $\eta_{2k+1}(x,y) \equiv 0$. q.e.d.

We denote

$$E'_\nu(t,x) = \partial_t E_\nu(t,x), \ \check{E}'_\nu(t,x) = \partial_t \check{E}_\nu(t,x)$$

and then

$$-2\partial E'_\nu / \partial x = x E'_{\nu-1}, \ -2\partial \check{E}'_\nu / \partial x = x \check{E}'_{\nu-1} \tag{37}$$

hold. For simplicity of notations, we denote

$$F_\nu = F_\nu(t, s(x,y)) = E'_\nu(t, s(x,y)) - \check{E}'_\nu(t, s(x,y)) \tag{38}$$

in what follows. We compute $\partial_x^\alpha \partial_y^\beta F_\nu(t, s(x,y))|_{x=y}$ for some small $\alpha$, $\beta$ as follows.

With $\eta = s(x,y)^2, \ s = s(x,y)$, then

$$\partial_{x_j} F_\nu = -\frac{1}{4} \partial_{x_j} \eta F_{\nu-1}, \ \partial_{x_j} F_\nu|_{x=y} = 0.$$

By Lemma 2.2, (37) and above equality, we have

$$\partial^2_{x_j y_j} F_\nu = -\frac{1}{4}\partial^2_{x_j y_j}\eta F_{\nu-1} + \frac{1}{16}\partial_{x_j}\eta\partial_{y_j}\eta F_{\nu-2} \tag{39}$$

In particular,

$$\partial^2_{x_j y_j} F_\nu|_{x=y} = \frac{1}{2}F_{\nu-1}(t,0)\ .$$

We also have

$$\begin{aligned}
\partial^2_{x_j}\partial^2_{y_j}F_\nu &= (-1/4)F_{\nu-1}\partial^2_{x_j}\partial^2_{y_j}\eta \\
&+ (-1/4)^2 F_{\nu-2}\Big(2(\partial^2_{x_j y_j}\eta)^2 + 2(\partial^2_{x_j}\partial_{y_j}\eta\partial_{y_j}\eta + \partial^2_{y_j}\partial_{x_j}\eta\partial_{x_j}\eta) + \partial^2_{x_j}\eta\partial^2_{y_j}\eta\Big) \\
&+ (-1/4)^3 F_{\nu-3}\Big(4\partial^2_{x_j y_j}\eta\partial_{x_j}\eta\partial_{y_j}\eta + \partial^2_{x_j}\eta(\partial_{y_j}\eta)^2 + \partial^2_{y_j}\eta(\partial_{x_j}\eta)^2\Big) \\
&+ (-1/4)^4 F_{\nu-4}(\partial_{x_j}\eta)^2(\partial_{y_j}\eta)^2\ .
\end{aligned} \tag{40}$$

In particular,

$$\partial^2_{x_j}\partial^2_{y_j}F_\nu|_{x=y} = \frac{3}{4}F_{\nu-2}(t,0) - \frac{1}{4}\partial^2_{x_j}\partial^2_{y_j}\eta(x,x)F_{\nu-1}(t,0)\ .$$

In general we can prove the following

**Lemma 2.3.** *Let $\alpha$, $\beta \in \mathbf{Z}^n_+$ be two multi-indices and $(X,\ x)$ a geodesic normal coordinate chart of $M$ satisfying (25). Let $(t,\ x)$ be in $(-c,\ c)\times X$ and $\Gamma_{\alpha,\beta,m}$ be the set defined by*

$$\Gamma_{\alpha,\beta,m} = \{\{\gamma_j\}_1^m : \gamma_j \in \mathbf{Z}^{2n}_+,\ |\gamma_j| > 0,\ \sum_{j=1}^m \gamma_j = (\alpha,\beta)\}\ .$$

*Then we have the following equality:*

$$\partial^\alpha_x\partial^\beta_y F_\nu(t,s(x,y)) = \sum_{m=1}^{|\alpha+\beta|} Q_{\alpha,\beta,m}(x,y)F_{\nu-m}(t,s(x,y))\ , \tag{41}$$

*where*

$$Q_{\alpha,\beta,m}(x,y) = \sum_{\{\gamma_j\}_1^m\in\Gamma_{\alpha,\beta,m}} \Big(-\frac{1}{4}\Big)^m \times \text{const} \times \prod_{j=1}^m \partial^{\gamma_j}_{x,y}\eta \tag{42}$$

*and the* const *above is a positive integer depending on $\alpha$, $\beta$ and $\{\gamma_j\}_1^m$. Moreover,*

$$\partial^\alpha_x\partial^\beta_y F_\nu(t,s(x,y))|_{x=y} = \sum_{m=1}^{[|\alpha+\beta|/2]} Q_{\alpha,\beta,m}(x,x)F_{\nu-m}(t,0)\ , \tag{43}$$

*where $[a]$ is the maximal integer not exceeding the real number $a$. More detailedly speaking, we have the followings:*
(i) *Suppose $\alpha\equiv\beta$ (mod 2). Then*

$$\partial^\alpha_x\partial^\beta_y F_\nu(t,s(x,y))|_{x=y} = \sum_{m=1}^{|\alpha+\beta|/2} Q_{\alpha,\beta,m}(x,x)F_{\nu-m}(t,0)\ , \tag{44}$$

*where $q_{\alpha,\beta} = Q_{\alpha,\beta,|\alpha+\beta|/2}(x,x)$ is a positive (negative) constant depending only on $n$, $\alpha$, $\beta$ if and only if $|\alpha|-|\beta|$ can (cannot) be divided by 4. In particular, when $\alpha=\beta$, letting $Q_{\alpha,m}(x,y) = Q_{\alpha,\alpha,m}(x,y)$, we have the following equality*

$$\partial^\alpha_x\partial^\alpha_y F_\nu(t,s(x,y))|_{x=y} = \sum_{m=1}^{|\alpha|} Q_{\alpha,m}(x,x)F_{\nu-m}(t,0) \tag{45}$$

*and* $q_\alpha = Q_{\alpha,|\alpha|}(x,x)$ *is a positive constant depending only on* $\alpha$.
(ii) *Suppose that* $|\alpha+\beta|$ *is even and* $\alpha \equiv \beta \pmod 2$ *does not hold. Then* $Q_{\alpha,\beta,|\alpha+\beta|/2}(x,x) = 0$. *Hence*

$$\partial_x^\alpha \partial_y^\beta F_\nu(t, s(x,y))|_{x=y} = \sum_{m=1}^{|\alpha+\beta|/2-1} Q_{\alpha,\beta,m}(x,x) F_{\nu-m}(t,0). \tag{46}$$

(iii) *Suppose that* $|\alpha+\beta|$ *is odd. Then* $\partial_x^\alpha \partial_y^\beta F_\nu(t,s(x,y))|_{x=y} = 0$.

**Proof.** For simplicity, we write $F_\nu = F_\nu(t,s(x,y))$, $Q_{\alpha,\beta,m} = Q_{\alpha,\beta,m}(x,y)$ in what follows if there is no confusion. We shall firstly show (41) by induction with respect to the nonnegative integer $|\alpha+\beta|$. If $|\alpha+\beta| = 0$, 1, 2, the validity of (41) can be checked by the previous computation. Letting (41) hold for $\partial_x^\alpha \partial_y^\beta F_\nu$, we show that it also holds for $\partial_{x_j}\partial_x^\alpha\partial_y^\beta F_\nu$ as following and then complete the induction argument.

Let $\partial^{\tilde\alpha} = \partial_{x_j}\partial^\alpha$, $\partial^{\tilde\beta} = \partial^\beta$.

$$\begin{aligned}
\partial^{\tilde\alpha}\partial^{\tilde\beta} F_\nu &= \partial_{x_j} \sum_{m=1}^{|\alpha+\beta|} Q_{\alpha,\beta,m} F_{\nu-m} \\
&= \sum_{m=1}^{|\alpha+\beta|} \Big( \partial_{x_j} Q_{\alpha,\beta,m} F_{\nu-m} + (-1/4)\partial_{x_j}\eta\, Q_{\alpha,\beta,m} F_{\nu-m-1} \Big) \\
&= \sum_{\tilde m=1}^{|\tilde\alpha+\tilde\beta|} P_{\tilde\alpha,\tilde\beta,\tilde m} F_{\nu-\tilde m}\ ,
\end{aligned}$$

where $P_{\tilde\alpha,\tilde\beta,\tilde m}$ are as follows:

$$P_{\tilde\alpha,\tilde\beta,1} = \partial_{y_j} Q_{\alpha,\beta,1} = (-1/4)\, \partial_x^{\tilde\alpha}\partial_y^{\tilde\beta}\eta\ ;$$

$$P_{\tilde\alpha,\tilde\beta,|\tilde\alpha+\tilde\beta|} = (-1/4)\, \partial_{y_j}\eta\, Q_{\alpha,\beta,|\alpha+\beta|} = (-1/4)^{|\tilde\alpha+\tilde\beta|} \prod_{j=1}^{|\tilde\alpha+\tilde\beta|} \partial_{x,y}^{\gamma_j}\eta\ ;$$

$$\text{where}\ \ \{\gamma_j\}_1^{|\tilde\alpha+\tilde\beta|} \in \Gamma_{\tilde\alpha,\tilde\beta,|\tilde\alpha+\tilde\beta|} = \{\{\gamma_j\}_1^{|\tilde\alpha+\tilde\beta|}\}.$$

and if $2 \le \tilde m \le |\alpha+\beta|$, then by the induction assumption on the expression of $Q_{\alpha,\beta,m}$ the following holds:

$$\begin{aligned}
P_{\tilde\alpha,\tilde\beta,\tilde m} &= \partial_{x_j} Q_{\alpha,\beta,\tilde m} + (-1/4)\, \partial_{x_j}\eta\, Q_{\alpha,\beta,\tilde m-1} \\
&= \sum_{\{\gamma_j\}_1^{\tilde m} \in \Gamma_{\tilde\alpha,\tilde\beta,\tilde m}} \Big(-\frac{1}{4}\Big)^{\tilde m} \times \text{const} \times \prod_{j=1}^{\tilde m} \partial_{x,y}^{\gamma_j}\eta\,,
\end{aligned}$$

where the const is a positive integer depending on $\{\gamma_j\}_1^{\tilde m}$.

We observe that in the equality (42) the number of the multi-index $\gamma_j$ with length 1 is not less than $2m - |\alpha+\beta|$. In fact, if the number be $l$, then it follows from the inequality

$$l + 2(m-l) \le |\alpha+\beta|$$

implied by the definition of the set $\Gamma_{\alpha,\beta,m}$. Then by (36), we obtain the equalities (43). Now we are going to prove (i)-(iii).

(i) Let $R$ be the set of partial derivative operators defined by

$$R = \{\partial_{x_l}^2,\ \partial_{x_l y_l}^2,\ \partial_{y_l}^2\ :\ 1 \le l \le n\}$$

and $\Gamma_{\alpha,\beta}$ be the set defined by

$$\Gamma_{\alpha,\beta} = \{\{\gamma_j\}_1^{|\alpha+\beta|/2} : \ \gamma_j \in \mathbf{Z}_+^{2n},\ \partial_{x,y}^{\gamma_j} \in R,\ \sum_{j=1}^{|\alpha+\beta|/2} \gamma_j = (\alpha,\beta)\} \ .$$

Then by (36), we have the following equality:

$$Q_{\alpha,\beta,|\alpha+\beta|/2}(x,x) = \sum_{\{\gamma_j\}_1^{|\alpha+\beta|/2}\in\Gamma_{\alpha,\beta}} \left(-\frac{1}{4}\right)^{|\alpha+\beta|/2} \times \mathrm{const} \times \prod_{j=1}^{|\alpha+\beta|/2} \partial_{x,y}^{\gamma_j}\eta(x,x)\ ,$$

where the const is a positive integer depending on $\{\gamma_j\}_1^{|\alpha+\beta|/2}$. For any element $\{\gamma_j\}_1^{|\alpha|}$ from $\Gamma_{\alpha,\beta}$, let the numbers of $\gamma_j$ such that $\partial_{x,y}^{\gamma_j}$ takes the forms of

$$\partial_{x_l}^2,\ \partial_{x_l y_l}^2,\ \partial_{y_l}^2 \quad (1 \le l \le n)$$

be $a_l,\ b_l,\ c_l$ respectively. Then by the definition of $\Gamma_{\alpha,\beta}$

$$2a_l + b_l = \alpha_l, \quad 2c_l + b_l = \beta_l \ . \tag{47}$$

Let

$$a = \sum_{l=1}^n a_l,\ \ b = \sum_{l=1}^n b_l,\ \ c = \sum_{l=1}^n c_l \ .$$

Then

$$2a + b = |\alpha|, \quad 2c + b = |\beta|.$$

By (36) we have

$$\prod_{j=1}^{|\alpha+\beta|/2} \partial_{x,y}^{\gamma_j}\eta(x,x)(-1/4)^{|\alpha+\beta|/2} = 2^{a+c}\,(-2)^b(-1/4)^{|\alpha+\beta|/2} = 2^{-|\alpha+\beta|/2}(-1)^{(|\alpha|-|\beta|)/2}\ ,$$

from which (i) follows.

(ii) For the proof of $Q_{\alpha,\beta,|\alpha+\beta|/2} = 0$, we only need to show that for any $\{\gamma_j\}_1^{|\alpha+\beta|/2} \in \Gamma_{\alpha,\beta,|\alpha+\beta|/2}$, $\prod_{j=1}^{|\alpha+\beta|/2} \partial_{x,y}^{\gamma_j}\eta(x,x) = 0$. Otherwise, there exists a $\{\gamma_j\}_1^{|\alpha+\beta|/2} \in \Gamma_{\alpha,\beta,|\alpha+\beta|/2}$ such that $\{\partial_{x,y}^{\gamma_j}\}_1^{|\alpha+\beta|/2}$ belongs to $R$. Hence the equality (47) holds for $\{\gamma_j\}_1^{|\alpha+\beta|/2}$. It implies $\alpha \equiv \beta \pmod 2$. Contradiction!

(iii) Since $|\alpha+\beta|$ is odd, for any $\{\gamma_j\}_1^m \in \Gamma_{\alpha,\beta,m}$ $(1 \le m \le (|\alpha+\beta|-1)/2)$, there exists $\gamma_l$ such that $|\gamma_l|$ is odd. The statement follows from (35). q.e.d.

**Proposition 2.2.** (i) *Suppose $\alpha \equiv \beta \pmod 2$. Then the principal singular term of $\partial_x^\alpha \partial_y^\beta K(t,x,y)|_{x=y}$ is*

$$q_{\alpha,\beta}\,\sqrt{\mathbf{g}(x)}\,F_{-|\alpha+\beta|/2}(t,0)$$

*for $(t,x) \in (-c,\,c) \times X$. Moreover,*

$$\left(\partial_x^\alpha \partial_y^\beta K(t,x,y) - \partial_x^\alpha \partial_y^\beta \sum_{0\le 2\nu<|\alpha+\beta|+n} F_\nu(t,s(x,y))U_\nu(x,y)\sqrt{\mathbf{g}(y)}\right)_{x=y}$$

*is in $C^\infty((-c,\,c)\times X)$ if $n$ is even, and in $C^\infty((-c,\,c)\times X)$ after division by $|t|$ if $n$ is odd. All derivatives are bounded in $(-c,\,c)\times X$.*

(ii) *Suppose that $|\alpha+\beta|$ is even and $\alpha \equiv \beta \pmod 2$ does not hold. Then for $(t,x) \in (-c,\,c) \times X$*

*the principal singular term of* $\partial_x^\alpha \partial_y^\beta K(t,x,y)|_{x=y}$ *is* $F_{1-|\alpha+\beta|/2}(t,0)$ *times a smooth function of* $x$. *Moreover,*

$$\left(\partial_x^\alpha \partial_y^\beta K(t,x,y) - \partial_x^\alpha \partial_y^\beta \sum_{0\le 2\nu<|\alpha+\beta|+n-2} F_\nu(t,s(x,y))U_\nu(x,y)\sqrt{\mathrm{g}(y)}\right)_{x=y}$$

*is in* $C^\infty((-c,\,c)\times X)$ *if* $n$ *is even, and in* $C^\infty((-c,\,c)\times X)$ *after division by* $|t|$ *if* $n$ *is odd. All derivatives are bounded in* $(-c,\,c)\times X$.

(iii) *Suppose that* $|\alpha+\beta|$ *is odd. Then there exists a nonnegative integer* $r(\alpha,\beta) = (|\alpha+\beta|-1)/2$ or $(|\alpha+\beta|-3)/2$, *which will be determined in the proof afterward, such that for* $(t,x)\in(-c,\,c)\times X$ *the principal singular term of* $\partial_x^\alpha \partial_y^\beta K(t,x,y)|_{x=y}$ *is* $F_{-r(\alpha,\beta)}(t,0)$ *times a smooth function of* $x$. *Moreover,*

$$\left(\partial_x^\alpha \partial_y^\beta K(t,x,y) - \partial_x^\alpha \partial_y^\beta \sum_{0\le 2\nu<n+2r(\alpha,\beta)} F_\nu(t,s(x,y))U_\nu(x,y)\sqrt{\mathrm{g}(y)}\right)_{x=y}$$

*is in* $C^\infty((-c,\,c)\times X)$ *if* $n$ *is even, and in* $C^\infty((-c,\,c)\times X)$ *after division by* $|t|$ *if* $n$ *is odd. All derivatives are bounded in* $(-c,\,c)\times X$.

**Proof.** (i) The first statement directly follows from the equalities (24), (34) and (44). Let $R(t,x)$ be the function in the second statement. Then

$$\begin{aligned} R(t,x) &= \left(\partial_x^\alpha \partial_y^\beta K(t,x,y) - \partial_x^\alpha \partial_y^\beta\left(\,\partial_t(\mathscr{E}(t,x,y)-\check{\mathscr{E}}(t,x,y))\sqrt{\mathrm{g}(y)}\,\right)\right)_{x=y} \\ &+ \partial_x^\alpha \partial_y^\beta \sum_{|\alpha+\beta|+n\le 2\nu\le 2N} \left(F_\nu(t,s(x,y))U_\nu(x,y)\sqrt{\mathrm{g}(y)}\right)_{x=y}. \end{aligned} \tag{48}$$

The first term in the right hand side (RHS) of (48) is in $C^{N-n-|\alpha+\beta|-3}((-c,\,c)\times X)$ by (33). Since it is even in $t$, its quotient by $|t|$ is in $C^{N-n-|\alpha+\beta|-4}((-c,\,c)\times X)$. As a similar result of the first statement, the principal singular term of the summand

$$\partial_x^\alpha \partial_y^\beta\left(F_\nu(t,s(x,y)))U_\nu(x,y)\sqrt{\mathrm{g}(y)}\right)_{x=y},\ \ |\alpha+\beta|+n\le 2\nu\le 2N,$$

of the second term in the RHS of (48) is a smooth function of $x$ times $F_{\nu-|\alpha+\beta|/2}(t,0)$ $(2\nu\ge n+|\alpha+\beta|)$, which by (29) is in $C^\infty((-c,\,c)\times X)$ if $n$ is even, and in $C^\infty((-c,\,c)\times X)$ after division by $|t|$ if $n$ is odd. The same result holds for the second term of the RHS of (48). Letting $N\to\infty$, we complete the proof of (i).

(ii) The first statement directly follows from the equalities (24), (34) and (46). The other part can be proved similarly as above.

(iii) By the equality (34) and (iii) of Lemma 2.3, the principal singular term of $\partial_x^\alpha \partial_y^\beta K(t,x,y)|_{x=y}$ equals that of

$$\sum_{\gamma<(\alpha,\beta)}\left(\partial_{x,y}^\gamma F_0(t,s(x,y))\partial_{x,y}^{(\alpha,\beta)-\gamma}\left(\sqrt{\mathrm{g}(y)}U_0(x,y)\right)\right)_{x=y}.$$

If there exists a $\gamma=(\gamma^1,\gamma^2)<(\alpha,\beta)$ such that $|\gamma|=|\alpha+\beta|-1$ and $\gamma^1\equiv\gamma^2 \pmod 2$, by (i) the principal singular term of above sum is $F_{-(|\alpha+\beta|-1)/2}(t,0)$ times a smooth function of $x$, which implies $r(\alpha,\beta)=(|\alpha+\beta|-1)/2$. Otherwise, by (ii) the principal singular term of above sum is $F_{-(|\alpha+\beta|-3)/2}(t,0)$ times a smooth function of $x$, which implies $r(\alpha,\beta)=(|\alpha+\beta|-3)/2$. Hence the first statement holds. The left part can be showed similarly as (i).

**Corollary 2.1.** *Assume the notations in* Proposition 2.2. *Let* $(t,\,x)$ *be in* $(-c,\,c)\times X$ *and* $\alpha,\,\beta$ *be multi-indices in* $\mathbf{Z}_+^n$. *Let*

$$L(\alpha,\beta)=\begin{cases} 1-|\alpha+\beta|/2 & \text{if } \alpha\equiv\beta \pmod 2 \\ 1-r(\alpha,\beta) & \text{if } |\alpha+\beta|=\text{odd} \\ 2-|\alpha+\beta|/2 & \text{otherwise} \end{cases}$$

*If $n$ is even, $\partial_x^\alpha \partial_y^\beta K(t,x,y)|_{x=y}$ equals the principal singular term plus*

$$\sum_{L(\alpha,\beta)}^{(n-2)/2} F_\nu(t,0) \times \text{ a smooth function of } x + \text{ a smooth function.}$$

*If $n$ is odd, $\partial_x^\alpha \partial_y^\beta K(t,x,y)|_{x=y}$ equals the principal singular term plus*

$$\sum_{L(\alpha,\beta)}^{(n-1)/2} F_\nu(t,0) \times \text{a smooth function of } x + |t| \times \text{a smooth function} .$$

*In particular, $t^{|\alpha+\beta|+n}\partial_x^\alpha \partial_y^\beta K(t,x,y)|_{x=y}$ is a smooth function in $([0,c)\times X)$.*

**Proof.** By the definition of $F_\nu$, we can see that if $2\nu \geq n$, then $F_\nu(t,0)$ is a smooth function when $n$ is even and it is $|t|$ times a smooth function when $n$ is odd. By this fact, (29), Proposition 2.2 and Lemma 2.3 the proof is completed.

## 2.4 Proof of Theorem 1.1 — I The Tauberian method

Except the precise computation of the constant $C_{n,\alpha,\beta}$ in (9), in this subsection we shall prove Theorem 1.1 and Corollary 1.1. Firstly we need two lemmas on a rude estimate of derivatives of spectral function and on the Tauberian method respectively.

**Lemma 2.4.** (Theorem 17.5.3 in [5]) *Let $X$ be a geodesic normal coordinate of $M$. For a multi-index $\gamma \in \mathbf{Z}_+^{2n}$, there exists a constant $C$ depending on $\gamma$ such that*

$$|\partial_{x,y}^\gamma e(x,y,\lambda)| \leq C(1+\lambda)^{n+|\gamma|}$$

*for $(x,y)$ in $X\times X$.*

By Section 17.5 in [5] there exists an even positive function $\phi$ in $\mathscr{S}(\mathbf{R})$ such that

$$\int_{\mathbf{R}} \phi(\tau)d\tau = 1, \quad \operatorname{supp}\hat{\phi} \subset (-1,1) .$$

For a positive number $\epsilon$, let $\phi_\epsilon(\tau) := \phi(\tau/\epsilon)/\epsilon$.

**Lemma 2.5.** *Let $\iota$ be a nonnegative number and $\kappa$ in $[0,\iota]$. Let $a$ be a positive number and $a_0$, $a_1$ be two real numbers $\geq a$. Let $v$ be a function of locally bounded variation such that $v(0)=0$ and either one of (49) and (50) holds:*

$$\begin{aligned} |dv(\tau)| &\leq M_0(|\tau|+a_0)^\iota d\tau && (49)\\ v \text{ is increasing and satisfies } |dv*\phi_a(\tau)| &\leq M_0(|\tau|+a_0)^\iota && (50)\end{aligned}$$

*Let $u$ be an increasing temperate function with $u(0)=0$ such that*

$$|(du-dv)*\phi_a(\tau)| \leq M_1(|\tau|+a_1)^\kappa, \ \tau\in\mathbf{R} . \tag{51}$$

*Then*

$$|u(\tau)-v(\tau)| \leq C\Big(M_0\, a(|\tau|+a_0)^\iota + M_1(|\tau|+a)(|\tau|+a_1)^\kappa\Big) \tag{52}$$

*where $C$ only depends on $\iota$ and $\kappa$.*

**Proof.** The statement for the case (49) is just Lemma 17.5.6 in [5]. Note that in the proof of Lemma 17.5.6 in [5], the assumption (49) are only used to deduce the following inequalities:

$$|dv*\phi_a(\tau)| \leq CM_0(|\tau|+a_0)^\iota, \quad |v(\tau)-v*\phi_a(\tau)| \leq CaM_0(|\tau|+a_0)^\iota .$$

Suppose that $v$ satisfies (50). To prove the statement, we only need to show the second one of above two inequalities. Choose $c_0 > 0$ so that $\phi > c_0$ in $(-1/2,\, 1/2)$. Since $v$ is increasing,

$$c_0 a^{-1} \int_{\tau-a/2}^{\tau+a/2} dv \le dv * \phi_a \le M_0(1+|\tau|)^\iota \ .$$

Dividing $(0,\, s)$ into $\le [s]+1$ intervals of length $\le 1$, we obtain from the above inequality that

$$c_0|v(\tau) - v(\tau - as)| \le a(|s|+1)M_0(|\tau| + a_0 + a|s|)^\iota \ .$$

Multiplication by $\phi(s)$ and integration yields $|v(\tau) - v * \phi_a(\tau)| \le CaM_0(|\tau| + a_0)^\iota$. q.e.d.

**Lemma 2.6.** *Let $\alpha \in \mathbf{Z}_+^n$ be a multi-index and $(X,\, x)$ be a geodesic normal coordinate chart of $M$ satisfying (25). Then there exists a positive number $C_{n,\alpha}$ only dependent on $n$ and $\alpha$ such that (11) holds. Moreover the estimate (12) holds uniformly for $x \in M$ and it is sharp.*

**Proof.** By the equality (29) and Example 7.1.17 of [4], there exists a positive constant $D_{n,\nu}$ such that $F_\nu(t, 0)$ $(2\nu < n)$ is the Fourier transform of

$$\frac{d}{d\tau}\Big(D_{n,\nu}(\operatorname{sgn}\tau)|\tau|^{n-2\nu}\Big) \ . \tag{53}$$

Let $c$ be the constant in (25) and $C_{n,\alpha} = 2q_\alpha \times D_{n,-|\alpha|}$. We shall apply Lemma 2.5 with $a = 1/c$ and

$$\begin{aligned} u(\tau) &= (1/2)\sqrt{\mathbf{g}(x)}\,(\operatorname{sgn}\tau) \sum_{\lambda_j \le |\tau|} |\partial^\alpha e_j(x)|^2 = (1/2)\sqrt{\mathbf{g}(x)}\,(\operatorname{sgn}\tau)\, \partial_x^\alpha \partial_y^\alpha e(x, y, |\tau|)|_{x=y} \\ v(\tau) &= C_{n,\alpha}\sqrt{\mathbf{g}(x)}\operatorname{sgn}\tau\, |\tau|^{n+2|\alpha|}/2 \ . \end{aligned}$$

We use the following Claim to connect $u(\tau)$ with the wave kernel $K(t, x, y)$.

**Claim 1** The Fourier transform of

$$\frac{d}{d\tau}\Big(\sqrt{\mathbf{g}(y)}\,(\operatorname{sgn}\tau)\, \partial_x^\alpha \partial_y^\beta e(x, y, |\tau|)/2\Big)$$

with respect to $\tau$ can be written by

$$\partial_x^\alpha \partial_y^\beta K(t, x, y) + \sum_{\gamma<\beta} P_\gamma(y) \partial_x^\gamma \partial_y^\beta K(t, x, y),$$

where $P_\gamma(x)$ $(\gamma < \alpha)$ are smooth functions of $x$ depending on the metric $g$ of $M$. In particular, $\widehat{du}(t)$ equals

$$\Big(\partial_x^\alpha \partial_y^\alpha K(t, x, y) + \sum_{\gamma<\alpha} P_\gamma(y) \partial_x^\gamma \partial_y^\alpha K(t, x, y)\Big)_{x=y} \ .$$

*Proof of Claim 1*: We argue by induction with respect to the nonnegative integer $|\alpha+\beta|$. The case of $\alpha = \beta = 0$ follows from (20). We denote the Fourier transform of $w(\tau)$ by $\mathbf{F}[w](t)$. Since

$$\begin{aligned} &\mathbf{F}[(d/d\tau)\sqrt{\mathbf{g}(y)}\,(\operatorname{sgn}\tau)\, \partial_{y_j} \partial_x^\alpha \partial_y^\beta e(x, y, |\tau|)/2](t) \\ = \ &\partial_{y_j} \mathbf{F}[(d/d\tau)\sqrt{\mathbf{g}(y)}\,(\operatorname{sgn}\tau)\, \partial_x^\alpha \partial_y^\beta e(x, y, |\tau|)/2](t) \\ - \ &\partial_{y_j} \log(\sqrt{\mathbf{g}(y)}\,)\, \mathbf{F}[(d/d\tau)\sqrt{\mathbf{g}(y)}\,(\operatorname{sgn}\tau)\, \partial_x^\alpha \partial_y^\beta e(x, y, |\tau|)/2](t) \ , \end{aligned}$$

the left part of the induction argument can be completed by direct computation.

By Claim 1, (53), Proposition 2.2 and Corollary 2.1, when $t$ in $(-c,\, c)$, the principal singular term of $\widehat{du}$ equals that of $\partial_x^\alpha \partial_y^\alpha K(t, x, y)|_{x=y}$, which is the Fourier transform of $dv$; the other singular terms are Fourier transforms of $|t|^{n+2|\alpha|-2j-1}$ times smooth functions of $x$ for $0 < j \le |\alpha|+(n-1)/2$. Hence $(du-dv)*\phi_a$ is the sum of the regularizations of these functions and a bounded function, so by the choice of $a = 1/c$ and easy computations from

$$(du-dv)*\phi_a(\tau) = \mathbf{F}^{-1}[(\widehat{du}-\widehat{dv})\,\widehat{\phi_a}](\tau), \quad \operatorname{supp}\widehat{\phi_a} \subset (-c,\, c)\ ,$$

(51) holds with $\kappa = \max(n+2|\alpha|-3,\, 0)$ and (49) holds with $\iota = n+2|\alpha|-1$. Therefore by the (49) case of Lemma 2.5, we obtain

$$|u(\lambda)-v(\lambda)| \le C\lambda^{n+2|\alpha|-1} \quad (\lambda \ge 1). \tag{54}$$

The estimate (12) follows from the compactness of $M$ and the similar argument in the proof of Lemma 2.1. q.e.d.

Corollary 1.1 follows from (12) and the following

**Lemma 2.7.** *The following uniform estimates*

$$\sum_{\lambda_j\in[\lambda,\,\lambda+1]} |\nabla^k e_j(x)|^2 \le C\lambda^{n-1+2k}, \ x \in M, \ k = 0, 1, \cdots, \tag{55}$$

*are equivalent to the* $(L^2, C^k)$ *estimates for the USPO* $\chi_\lambda$:

$$||\chi_\lambda f||_{C^k} \le C\lambda^{k+(n-1)/2}||f||_2\ , k = 0, 1, \cdots, \tag{56}$$

**Proof.** Let the estimate (55) hold. By Lemma 2.1 in order to prove (56), we have only to show

$$||\partial^\alpha \chi_\lambda f||_{L^\infty(X)} \le C\lambda^{|\alpha|+(n-1)/2}||f||_2$$

for any multi-index $\alpha$. Without loss of generality, we assume that $f$ is a real-valued function on on $M$ in what follows. Since

$$\chi_\lambda f(x) = \int_M \sum_{\lambda_j\in[\lambda,\,\lambda+1]} e_j(x)e_j(y)f(y)dv(M)\ ,$$

for any $x \in X$, by the Cauchy-Schwarz inequality and (55) we have

$$\begin{aligned} |\partial_x^\alpha \chi_\lambda f(x)|^2 \ &\le \ \sum_{\lambda_j\in[\lambda,\,\lambda+1]} |\partial_x^\alpha e_j(x)|^2 \sum_{\lambda_j\in[\lambda,\,\lambda+1]} \left(\int_M e_j(y)f(y)dv(M)\right)^2 \\ &\le \ C\lambda^{n-1+2|\alpha|}||f||_2^2\ . \end{aligned}$$

Let the estimate (56) hold. Take a point $x \in M$ and without loss of generality we let $x$ belong to the coordinate chart $X$. In order to prove (55), we have only to show

$$\sum_{\lambda_j\in[\lambda,\,\lambda+1]} |\partial^\alpha e_j(x)|^2 \le C\,\lambda^{n-1+2|\alpha|} \tag{$\sharp$}$$

for any multi-index $\alpha$. The estimate (56) implies

$$|\partial^\alpha \chi_\lambda f\,(x)| = |\sum_{\lambda_j\in[\lambda,\,\lambda+1]} \int_M \partial^\alpha e_j(x)\, e_j(y)f(y)dv(M)| \le C\,\lambda^{(n-1)/2+|\alpha|}||f||_2\ .$$

Letting $f(\cdot) = \displaystyle\sum_{\lambda_j\in[\lambda,\,\lambda+1]} \partial^\alpha e_j(x)\, e_j(\cdot)$ in the above inequality, we obtain the inequality ($\sharp$). q.e.d.

Let $Z(x,\tau)=\dfrac{1}{2}\sqrt{\mathrm{g}(x)}\,\mathrm{sgn}\,\tau\,\partial_x^\alpha\partial_y^\beta e(x,y,|\tau|)|_{x=y}$ $((x,y)\in X\times X)$. Since

$$\partial_x^\alpha\partial_y^\beta e(x,y,\lambda)=\sum_{\lambda_j\le\lambda}\partial_x^\alpha e_j(x)\partial_y^\beta e_j(y)\ ,$$

letting $\alpha=\beta$ above and applying Lemma 2.4, we obtain

$$\sum_{\lambda_j\le\lambda}|\partial^\alpha e_j(x)|^2\le C(1+\lambda)^{n+2|\alpha|}\ ,$$

by which and the Cauchy inequality, we can see the total variation of $Z(x,\cdot)$ on $[0,\,\lambda]$ does not exceed

$$\begin{aligned}\sum_{\lambda_j\le\lambda}|\partial^\alpha e_j(x)\partial^\beta e_j(x)| &\le \Big(\sum_{\lambda_j\le\lambda}|\partial^\alpha e_j(x)|^2\Big)^{1/2}\Big(\sum_{\lambda_j\le\lambda}|\partial^\beta e_j(x)|^2\Big)^{1/2}\\ &\le C(1+\lambda)^{n+|\alpha+\beta|}\ .\end{aligned}$$

Then $Z(x,\cdot)$ has bounded variation locally so that by the Jordan decomposition $Z(x,\tau)=Z_+(x,\tau)-Z_-(x,\tau)$, where if $\tau\ge 0$, then $Z_+(x,\tau)$, $Z_-(x,\tau)$ are the positive variation and the negative variation of $Z(x,\cdot)$ on $[0,\,\tau]$ respectively; and if $\tau<0$, then $Z_\pm(x,\tau):=-Z_\pm(x,-\tau)$. Then $Z(x,\cdot)=Z_+(x,\cdot)-Z_-(x,\cdot)$ holds on $\mathbf{R}$. Let

$$G(x,\tau):=\mathrm{sgn}\,\tau\sum_{\lambda_j\le|\tau|}|\partial^\alpha e_j(x)\partial^\beta e_j(x)|\ . \tag{57}$$

Sometimes for simplicity we just write $Z(x,\tau)=Z(\tau)$, $G(\tau)=G(x,\tau)$ and $Z_\pm(x,\tau)=Z_\pm(\tau)$ if there is no confusion. Then $Z_\pm(\tau)$ and $G(\tau)$ are increasing temperate functions satisfying $Z_\pm(0)=G(0)=0$ and the following

**Lemma 2.8.** *Let $\psi$ be an even positive function in $\mathscr{S}(\mathbf{R})$. Then*

$$dG*\psi(\tau)\le C\,(1+|\lambda|)^{n+|\alpha+\beta|-1}\ . \tag{58}$$

*In particular,*

$$dZ_\pm*\psi(\tau)\le dG*\psi(\tau)\le C\,(1+|\lambda|)^{n+|\alpha+\beta|-1}\ . \tag{59}$$

**Proof.** The inequality $dZ_\pm*\psi(\tau)\le dG*\psi(\tau)$ in (59) follows from

$$Z_+(\tau)+Z_-(\tau)\le G(\tau),\quad \tau\in[0,\,\infty)\ .$$

Similarly to Section 4.1 in [4], the convolution of the rapidly decreasing function $\psi$ and the temperate distribution $dG$ is defined by $dG*\psi(\tau)=dG(\psi(\tau-\cdot))$. By the definition (57) of $G$, we have

$$\begin{aligned}dG(\psi(\tau-\cdot)) &= \langle\sum_{\lambda_j>0}|\partial^\alpha e_j(x)\partial^\beta e_j(x)|(\delta_{\lambda_j}+\delta_{-\lambda_j})\,,\,\psi(\tau-\cdot)\rangle\\ &= \sum_{\lambda_j>0}|\partial^\alpha e_j(x)\partial^\beta e_j(x)|\Big(\psi(\tau+\lambda_j)+\psi(\tau-\lambda_j)\Big)\ .\end{aligned}$$

Hence $dG*\psi(\tau)$ is an even function so that we only need to prove (58) for nonnegative $\tau$.

Let $k$ be a nonnegative integer. Then by (12) showed in Lemma 2.6 and the Cauchy inequality we have

$$\sum_{k<\lambda_j\le k+1}|\partial^\alpha e_j(x)\partial^\beta e_j(x)|\le C(1+k)^{n+|\alpha+\beta|-1}\ . \tag{60}$$

For $\lambda_j>0$, there exists a unique integer $k\ge 0$ such that $\lambda_j\in(k,\,k+1]$ and

$$\psi(\tau+\lambda_j)+\psi(\tau-\lambda_j)\le C(2+|\tau-k|)^{-(n+|\alpha+\beta|+1)}\ ,$$

where $C$ is a positive constant only depending on $\psi$ and $n+|\alpha+\beta|$. By (60) and the above inequality, we obtain

$$\begin{aligned} dG(\psi(\tau-\cdot)) &\le C\sum_{k=0}^{\infty}(2+|\tau-k|)^{-(n+|\alpha+\beta|+1)}(1+k)^{n+|\alpha+\beta|-1} \\ &= \sum_{k=0}^{[\tau]}+\sum_{[\tau]+1}^{\infty} = S_1+S_2\ . \end{aligned}$$

We estimate $S_2$ as follows:

$$S_2 \le \sum_{j=1}^{\infty}(j+1)^{-(n+|\alpha+\beta|+1)}(1+j+\tau)^{n+|\alpha+\beta|-1} \le C(1+\tau)^{n+|\alpha+\beta|-1}\ .$$

We observe

$$S_1 \le \int_0^{\tau+1}(2+\tau-x)^{-(n+|\alpha+\beta|+1)}(1+x)^{n+|\alpha+\beta|-1} =: S_3\ .$$

Then $S_3 \le C(1+\tau)^{n+|\alpha+\beta|-1}$ follows from the following

**Claim 2** Let $a$, $b$ be positive integers such that $a \ge 2$. Then there exists a positive constant $C$ only depending on $a$, $b$ such that

$$\int_0^{\tau+1}(2+\tau-x)^{a}x^{b}\,dx \le C(1+\tau)^{b}\ .$$

*Proof of Claim 1* Using integration by part, we have

$$\int_0^{\tau+1}(2+\tau-x)^{a}x^{b}\,dx = \frac{1}{a-1}(\tau+1)^{b} - \frac{b}{a-1}\int_0^{\tau+1}(2+\tau-x)^{1-a}x^{b-1}\,dx\ .$$

Since $a \ge 2$,

$$\begin{aligned} \int_0^{\tau+1}(2+\tau-x)^{1-a}x^{b-1}\,dx &\le \int_0^{\tau+1}(2+\tau-x)^{-1/2}x^{b-1}\,dx \\ &\le (1+\tau)^{b-1/2}\int_0^{1}(1-y)^{-1/2}y^{b}\,dy \\ &= B(1/2\,,\,b+1)(1+\tau)^{b-1/2}\ . \end{aligned}$$

Combining the above two inequalities, we complete the proof of Claim 2 and (58). q.e.d.

Proof of Theorem 1.1 We shall discuss three cases as in Lemma 2.3. In the proof we shall use the notations in the proof of Lemma 2.6.

(i) Suppose $\alpha \equiv \beta \pmod 2$. Let $C_{n,\alpha,\beta} = 2q_{\alpha,\beta}\times D_{n,-|\alpha+\beta|}$. We shall apply the (50) case of Lemma 2.5 with $a = 1/c$ and

$$\begin{aligned} u(\tau) &= Z_+(\tau) \\ v(\tau) &= Z_-(\tau)+\frac{1}{2}C_{n,\alpha,\beta}\sqrt{\mathrm{g}(x)}\,\mathrm{sgn}\,\tau\,|\tau|^{n+|\alpha+\beta|}\ . \end{aligned}$$

Then by Lemma 2.8, the condition 50 holds for $\iota = n+|\alpha+\beta|-1$. Since

$$(Z_+-Z_-)(\tau) = Z(\tau) = \frac{1}{2}\sqrt{\mathrm{g}(x)}\,\mathrm{sgn}\,\tau\,\partial_x^{\alpha}\partial_y^{\beta}e(x,y,|\tau|)|_{x=y}\ ,$$

by the similar proof as Lemma 2.6, we can show that (51) holds for $\kappa = \max(n+|\alpha+\beta|-3,\,0)$. Therefore by the (50) case of Lemma 2.5, we obtain that for $\lambda \ge 1$ the following inequality holds:

$$C\lambda^{n+|\alpha+\beta|-1} \ge |u(\lambda)-v(\lambda)| = \frac{1}{2}\sqrt{\mathrm{g}(x)}\,\times\,|\partial_x^{\alpha}\partial_y^{\beta}e(x,y,|\tau|)|_{x=y}-C_{n,\alpha,\beta}\lambda^{n+|\alpha+\beta|}|\ .$$

(ii) Suppose that $|\alpha+\beta| =$ even and $\alpha \equiv \beta \pmod 2$ does not hold. We shall apply the (50) case of Lemma 2.5 with $a = 1/c$ and

$$u(\tau) = Z_+(\tau), \quad v(\tau) = Z_-(\tau) \ .$$

Then by Lemma 2.8, the condition (50) holds for $\iota = n + |\alpha+\beta| - 1$. By By Claim 1, (53), Proposition 2.2 and Corollary 2.1, when $t$ in $(-c, c)$, the principal singular term of $\widehat{du - dv}$ equals that of $\partial_x^\alpha \partial_y^\beta K(t, x, y)|_{x=y}$, which is the Fourier transform of

$$\frac{d}{d\tau} \operatorname{sgn} \tau \, |\tau|^{n+|\alpha+\beta|-2} \times \text{ a smooth function of } x \ ,$$

the other singular terms are Fourier transforms of $|t|^{n+|\alpha+\beta|-2j-3}$ times smooth functions of $x$ for $0 < j \le (n + |\alpha+\beta| - 3)/2$. Similarly as the proof of Lemma 2.6, we can show (51) holds with $\kappa = n + |\alpha+\beta| - 3$. Therefore by the (50) case of Lemma 2.5, we obtain for $\lambda \ge 1$

$$C\lambda^{n+|\alpha+\beta|-1} \ge |u(\lambda) - v(\lambda)| = \frac{1}{2}\sqrt{\mathbf{g}(x)} \times |\partial_x^\alpha \partial_y^\beta e(x, y, \lambda)|_{x=y}| \ .$$

(iii) Suppose that $|\alpha+\beta|$ is odd. We also apply the (50) case of Lemma 2.5 with $a = 1/c$ and

$$u(\tau) = Z_+(\tau), \quad v(\tau) = Z_-(\tau) \ .$$

Then by Lemma 2.8, the condition (50) holds for $\iota = n + |\alpha+\beta| - 1$. By Claim 1, (53), Proposition 2.2 and Corollary 2.1, when $t$ in $(-c, c)$, the principal singular term of $\widehat{du - dv}$ equals that of $\partial_x^\alpha \partial_y^\beta K(t, x, y)|_{x=y}$, which is the Fourier transform of

$$\frac{d}{d\tau} \operatorname{sgn} \tau \, |\tau|^{n+2r(\alpha,\beta)} \times \text{ a smooth function of } x \ ,$$

the other singular terms are Fourier transforms of $|t|^{n+2r(\alpha,\beta)-2j-1}$ times smooth functions of $x$ for $0 < j \le \big(n + 2r(\alpha, \beta) - 1\big)/2$. Similarly as the proof of Lemma 2.6, we can show (51) holds with $\kappa = n + 2r(\alpha,\beta) - 1 \le n + |\alpha+\beta| - 2$. Therefore by the (50) case of Lemma 2.5, we obtain for $\lambda \ge 1$

$$C\lambda^{n+|\alpha+\beta|-1} \ge |u(\lambda) - v(\lambda)| = \frac{1}{2}\sqrt{\mathbf{g}(x)} \times |\partial_x^\alpha \partial_y^\beta e(x, y, \lambda)|_{x=y}| \ .$$

We shall put off the computation of the constant $C_{n,\alpha,\beta}$ ($\alpha \equiv \beta \pmod 2$) to the following

### 2.5 Proof of Theorem 1.1 — II The constant $C_{n,\alpha,\beta}$

We remark that $C_{n,\alpha,\beta}$ does not depend on the Riemannian manifold $M$. Although it may be possible to find the precise value of $C_{n,\alpha,\beta}$ by refining the analysis in the proof of Lemma 2.3, we prefer another approach by considering the $n$-dimensional flat torus in the following

**Example 2.1.** Let $T^n = \mathbf{R}^n/(2\pi\mathbf{Z})^n$ be the standard $n$-dimensional torus with the flat metric induced from $\mathbf{R}^n$. Let $\mathbf{k} = (k_1, \cdots, k_n)$ denote a lattice point in $\mathbf{Z}^n$ and $|\mathbf{k}|^2 := \sum_1^n k_j^2$. Let $\theta = (\theta_1, \cdots, \theta_n)$ denote a point in $[0, 2\pi)^n$ and $\mathbf{k}\cdot\theta := \sum_1^n k_j\theta_j$. Then the eigenvalues of the positive Laplacian on $T^n$ are $|\mathbf{k}|^2$ ($\mathbf{k} \in \mathbf{Z}^n$), the corresponding $L^2$-normalized eigenfunctions are $\exp(i\mathbf{k}\cdot\theta)/(2\pi)^{n/2}$ ($\mathbf{k} \in \mathbf{Z}^n$), and the spectral function

$$e(\theta, \theta', \lambda) = (2\pi)^{-n} \sum_{|\mathbf{k}| \le \lambda} \exp\big(i\,\mathbf{k}(\theta - \theta')\big) \ .$$

By simple computation, we obtain

$$\partial_\theta^\alpha \partial_{\theta'}^\beta e(\theta, \theta', \lambda)|_{\theta=\theta'} = \begin{cases} (2\pi)^{-n}(-1)^{(|\alpha|-|\beta|)/2} \sum_{|\mathbf{k}|\le\lambda} \mathbf{k}^{\alpha+\beta} & \text{if } \alpha \equiv \beta \\ 0 & \text{otherwise} \end{cases} \tag{61}$$

Let $D$ be a bounded domain in $\mathbf{R}^n$ such that any line pararrel to any coordinate axes meets $D$ in a bounded number of straight-line segment. Let $D$ be completely contained in a hyper-rectangle

$$D' = \{x : a_j \le x_j \le b_j,\ b_j - a_j > 1\ (1 \le j \le n)\}\ .$$

**Proposition 2.3.** (Theorem 1.1.7 in [7]) *Let $f(x)$ in $D'$ be nonnegative, continuous and monotonic in each variable. If $|f(x)| \le F$ in $D'$, then*

$$\left| \sum_{\mathbf{k}\in D} f(\mathbf{k}) - \int_D f(x)\, dx \right| \le F|D'| \sum_1^n \frac{1}{b_j - a_j}\ .$$

By Proposition 2.3 the estimate

$$\sum_{|\mathbf{k}|\le\lambda} \mathbf{k}^{\alpha+\beta} = \lambda^{n+|\alpha+\beta|} \int_{B_n} x^{\alpha+\beta}\, dx + \mathrm{O}(\lambda^{n+|\alpha+\beta|-1}) \text{ as } \lambda\to\infty,\ \alpha\equiv\beta \ (\mathrm{mod}\ 2), \tag{62}$$

holds. In fact, we can apply Proposition 2.3 with

$$f(x) = x^{\alpha+\beta},\ D = \{x\in\mathbf{R}^n : |x|\le\lambda\}\cap[0,\,\infty)^n,\ D' = [0,\,\lambda]^n\ .$$

We complete the proof of (9) and (10) in Theorem 1.1 by (61), (62) and the following integral equality:

$$\int_{B_n} x^{\alpha+\beta}\, dx = \frac{\pi^{n/2}}{2^{|\alpha+\beta|/2}\,\Gamma(\frac{|\alpha+\beta|+n}{2}+1)} \prod_{j=1}^n (\alpha_j+\beta_j-1)!!,\quad \alpha\equiv\beta\ (\mathrm{mod}\ 2). \tag{63}$$

# 3 Sobolev norms of eigenfunctions

In this section we shall prove Theorem 1.2. Firstly we cite a well known elliptic estimates as following

**Proposition 3.1.** *Let $u$ be a smooth function on $M$, $1\le r<\infty$ and $k$ a positive integer. Then the followings hold*:

$$||u||_{H^r_{2k}} \le C\sum_{j=0}^k ||\Delta^j u||_r,\ ||u||_{H^r_{2k+1}} \le C\sum_{j=0}^k ||\Delta^j u||_{H^r_1}, \tag{64}$$

*where the constant $C$ only depends on the metric $g$ of $M$ and $k$.*

Let $u$ be a real valued smooth function on the Riemannian manifold $M$. The gradient $\mathbf{grad}\, u$ of $u$ is defined to be the dual vector field of one form $du = \nabla u$ by

$$g(\mathbf{grad}\, u,\, V) = du(V)$$

for arbitrary smooth vector field $V$ on $M$. In the coordinate chart $(X, x)$

$$|\mathbf{grad}\, u| = |\nabla u| = \sum g^{jk}\partial_j u \partial_k u\ , \tag{65}$$

we define the $L^p$ $(1\le p<\infty)$ norm of $\mathbf{grad}\, u$ as

$$||\mathbf{grad}\, u||_p = \Big(\int_M |\mathbf{grad}\, u(x)|^p\ dv(M)\, dx\Big)^{1/p}\ .$$

Then

$$||u||_{H^p_1} \approx ||u||_p + ||\mathbf{grad}\, u||_p\ ,$$

where $f\approx g$ means that there exists a positive constant $C$ depending only on the metric $g$ of $M$ such that $g/C \le f \le Cg$. By Proposition 3.1, we have the following

**Corollary 3.1.** *Let $u$ be a smooth function on $M$, $1 \le r < \infty$ and $k$ a positive integer. Then the following relations hold*:

$$||u||_{H^r_{2k}} \approx \sum_{j=0}^{k} ||\Delta^j u||_r, \ ||u||_{H^r_{2k+1}} \approx \sum_{j=0}^{k} (||\Delta^j u||_r + ||\mathbf{grad}\, \Delta^j u||_r), \tag{66}$$

*where $f \approx g$ means that there exists a positive constant $C$ depending on $k$, $r$ and the metric $g$ of $M$ such that $g/C \le f \le Cg$.*

Proof of Theorem 1.2: By Corollary 1.1 we can let $2 \le r < \infty$. By Corollary 3.1, we have only to prove the following estimates hold for $j = 0, 1, \cdots$:

$$||\Delta^j \chi_\lambda f||_r \le C\lambda^{2j+\epsilon(r)} ||f||_2, \ ||\mathbf{grad}\, \Delta^j \chi_\lambda f||_r \le C\lambda^{2j+1+\epsilon(r)} ||f||_2,$$

and they are sharp. By the duality, we need only to prove the estimates

$$||\Delta^j \chi_\lambda f||_2 \le C\lambda^{2j+\epsilon(r)} ||f||_{r'}, \ ||\mathbf{grad}\, \Delta^j \chi_\lambda f||_2 \le C\lambda^{2j+1+\epsilon(r)} ||f||_{r'} \tag{67}$$

hold for $r' = r/(r-1)$ and they are sharp. The dual version of Proposition 1.1 says that the following estimate holds and it is sharp:

$$||\chi_\lambda f||_2 \le C\lambda^{\epsilon(r)} ||f||_{r'} \ . \tag{68}$$

The proof is completed by the following relations:

$$||\Delta^j \chi_\lambda f||_2 \approx \lambda^{2j} ||\chi_\lambda f||_2, \ ||\mathbf{grad}\, \Delta^j \chi_\lambda f||_2 \approx \lambda^{2j+1} ||\chi_\lambda f||_2 \ . \tag{69}$$

The first relations follows from

$$\Delta \chi_\lambda f = \sum_{|\lambda - \lambda_j| \le 1} \lambda_j^2 \, \mathbf{e_j}(f) \ .$$

The second one can be deduced from the equality

$$\int_M \mathbf{grad}\, e_j(x) \cdot \mathbf{grad}\, e_k(x) dv(M) = \delta_{jk} \lambda_j^2$$

derived by the Green's formula. q.e.d.

# 4 Spherical harmonics

In this section, we do some computations on spherical harmonics $Q_m$, $Z_m$ in Example 1.1 to prove (13) and (14). With respect to the positive Laplacian on $S^n$, both $Q_m$ and $Z_m$ are eigenfunctions of eigenvalue $m(m+n-1)$.

Proof of (14) By (66) we only need to show that $k = 0$ case and the following estimate hold:

$$||\mathbf{grad}\, Q_m||_r / ||Q_m||_2 \ge C m^{\epsilon(r)+1} \quad (2 \le r \le 2(n+1)/(n-1)) \ . \tag{70}$$

The $k = 0$ case of (14) follows directly from the following integral estimate:

$$\int_{S^n} (\zeta_1^2 + \zeta_2^2)^a \, d\sigma_n(\zeta) = 2^{2-n} \pi^{(n+1)/2} \Gamma(a+1) / \Gamma\Big(\frac{n+2a+1}{2}\Big) \approx a^{1-n} \ , \ a \ge 1, \tag{71}$$

where $d\sigma_n(\zeta)$ is the area measure on $S^n$. Let

$$V = (\zeta_1^2 + \zeta_2^2)^{-1/2} \, (\zeta_2 \partial / \partial \zeta_1 - \zeta_1 \partial / \partial \zeta_2) \ ,$$

which is a vector field of unit length defined almost everywhere on $S^n$. Since $|VQ_m(\zeta)| = m(\zeta_1^2 + \zeta_2^2)^{(m-1)/2}$ and $|\mathbf{grad}\, Q_m| \geq |VQ_m|$ hold almost everywhere on $S^n$, by (71) we obtain (70). q.e.d.

Before the proof of (13) we need some preparations on the Bessel function and the Jacobi polynomials. In this section we let $\alpha$, $\beta$ be nonnegative real numbers. As (1.71.1) in [14] the Bessel function $J_\alpha(z)$ of the first kind of order $\alpha$ is defined to be

$$J_\alpha(z) = \sum_{\nu=0}^{\infty} \frac{(-1)^\nu (z/2)^{\alpha+2\nu}}{\nu!\Gamma(\nu+\alpha+1)} \ . \tag{72}$$

As in Sections 2.4.1, 4.1 of [14] the Jacobi polynomials $P_m^{(\alpha,\beta)}(x)$ are defined to be orthogonal on $[-1, 1]$ with the weight function $(1-x)^\alpha(1+x)^\beta$. The normalization of $P_m^{(\alpha,\beta)}(x)$ is made by

$$P_m^{(\alpha,\beta)}(1) = \frac{(m+\alpha)(m+\alpha-1)\cdots(m+\alpha-m+1)}{m!} \ .$$

Since the zonal function $Z_m$ only depends on the geodesic distance from the north pole $\mathbf{1}$. As [12] we define the function ${}^bZ_m$ on $[-1, 1]$ by $Z_m(\zeta) = {}^bZ_m(\langle\zeta, \mathbf{1}\rangle)$. We also write ${}^bZ_m(x) = {}^bZ_m(\cos\,\theta)$, where $x = \cos\,\theta$ and $\theta \in [0, \pi]$ is the angle between $\zeta$ and $\mathbf{1}$. By (2.1) in [12],

$$\begin{aligned} {}^bZ_m &= c_m\, P_m^{(n-2)/2,\,(n-2)/2}, & (73)\\ \text{where } c_m &= \Big(\frac{2m}{n-1}+1\Big)\frac{\Gamma(n/2)\Gamma(n+m-1)}{\Gamma(n-1)\Gamma(n/2+m)} \approx m^{n/2} \ . & (74) \end{aligned}$$

**Lemma 4.1.** (cf Theorem 8.1.1 in [14]) *Let $\alpha$, $\beta$ be nonnegative real numbers. Then*

$$\lim_{m\to\infty} m^{-\alpha} P_m^{(\alpha,\beta)}(\cos\frac{z}{m}) = (z/2)^{-\alpha}\, J_\alpha(z) \ .$$

*This formula holds uniformly in every bounded region of the complex $z$-plane.*

**Lemma 4.2.** *Let $\alpha$, $\beta$ be nonnegative real numbers. Then*

$$\lim_{m\to\infty} m^{-\alpha-1}\frac{d}{d\theta} P_m^{(\alpha,\beta)}(\cos\theta)|_{\theta=\frac{z}{m}} = -(z/2)^{1-\alpha}\, J_\alpha(z) \ .$$

*This formula holds uniformly in every bounded region of the complex $z$-plane.*

**Proof.** By (4.21.2) in [14],

$$P_m^{(\alpha,\beta)}(x) = \sum_{\nu=0}^{m} \frac{1}{\nu!(m-\nu)!}\frac{\Gamma(m+\alpha+\beta+\nu+1)}{\Gamma(m+\alpha+\beta+1)}\frac{\Gamma(m+\alpha+1)}{\Gamma(\nu+\alpha+1)}\Big(\frac{x-1}{2}\Big)^\nu \ .$$

Since $\frac{d}{d\theta}P_m^{(\alpha,\beta)}(\cos\theta) = \frac{d}{dx}P_m^{(\alpha,\beta)}(x)|_{x=\cos\theta}\,(-\sin\theta)$,

$$\begin{aligned} \frac{d}{d\theta}P_m^{(\alpha,\beta)}(\cos\theta)|_{\theta=\frac{z}{m}} = &\sum_{\nu=0}^{m-1} \frac{1}{(\nu+1)!(m-\nu-1)!}\frac{\Gamma(m+\alpha+\beta+\nu+2)}{\Gamma(m+\alpha+\beta+1)} \\ &\times\frac{\Gamma(m+\alpha+1)}{\Gamma(\nu+\alpha+2)}\frac{\nu+1}{2}\Big(-\sin^2\frac{z}{2m}\Big)\Big(-\sin\frac{z}{m}\Big) \ . \end{aligned}$$

Letting $z$ and $\nu$ be fixed and $m \to \infty$, we have for the $\nu$-term of the above sum the following asymptotic expression:

$$\begin{aligned} &\frac{1}{(\nu+1)!(m-\nu-1)!}\frac{\Gamma(m+\alpha+\beta+\nu+2)}{\Gamma(m+\alpha+\beta+1)}\frac{\Gamma(m+\alpha+1)}{\Gamma(\nu+\alpha+2)}\frac{\nu+1}{2}\times \\ &\Big(-\sin^2\frac{z}{2m}\Big)\Big(-\sin\frac{z}{m}\Big) \cong \frac{m^{\alpha+1}}{2\Gamma(\alpha+\nu+2)\nu!}\Big(\frac{-z^2}{4}\Big)^\nu\cdot(-z), \end{aligned}$$

where $f(m) \cong g(m)$ means $\lim_{m\to\infty} \frac{f(m)}{g(m)} = 1$ or $f(m) \equiv g(m)$. As $m$ is large enough and $z$ is in a bounded region of complex $z$-plane we have

$$\begin{aligned}
& m^{-1-\alpha} \left| \frac{d}{d\theta} P_m^{(\alpha,\beta)}(\cos\theta)|_{\theta=\frac{z}{m}} \right| \\
\leq\ & C \sum_{\nu=0}^{m-1} \frac{m^{-1-\alpha}}{(m-\nu-1)!} \frac{\Gamma(m+\alpha+\beta+\nu+2)}{\Gamma(m+\alpha+\beta+1)} \frac{\Gamma(m+\alpha+1)}{2^{2\nu} m^{2\nu+1}} \\
\leq\ & C \sum_{\nu=0}^{m-1} \frac{m^{-1-\alpha}}{m!} m^{\nu+1} (2m+\alpha+\beta)^{\nu+1} \frac{\Gamma(m+\alpha+1)}{(2m)^{\nu+1} m^{\nu}} \frac{2}{2^{\nu}} \\
=\ & \mathrm{O}\left( \sum_{\nu=0}^{m-1} \frac{1}{2^{\nu}} \right) = \mathrm{O}(1)\ .
\end{aligned}$$

Hence we can pass to the limit under the summation sign for $m^{-\alpha-1} \frac{d}{d\theta} P_m^{(\alpha,\beta)}(\cos\theta)|_{\theta=\frac{z}{m}}$ and complete the proof.

Proof of (13) Since $J_\alpha(z) \approx z^\alpha$ as $z \to 0$, by (73), (74) and Lemmas 4.1, 4.2 we have two precise estimates for a small constant $d > 0$:

$$ {}^{b}Z_m(\cos\theta) \approx m^{n-1}\ (0 \leq \theta \leq \frac{d}{m}) \tag{75}$$

$$ \frac{d}{d\theta}\, {}^{b}Z_m(\cos\theta) \approx -m^{n+1}\theta\ (0 \leq \theta \leq \frac{d}{m}) \tag{76}$$

Since it is well known that $||Z_m||_\infty = ||Z_m||_2^2 \approx m^{n-1}$, the $r = \infty$ case of (13) follows from (75) and (76). To show the left part for $r < \infty$, by (66) we only need to show the following two estimates:

$$||Z_m||_r / ||Z_m||_2 \geq C\, m^{\epsilon(r)},\ ||\frac{\partial}{\partial\theta} Z_m||_r / ||Z_m|| \geq C\, m^{\epsilon(r)+1}\ ,$$

which also follow from (75) and (76) by restricting the integrals of the numerators on the domain $\{0 \leq \theta \leq \frac{d}{m}\}$ of $S^n$.

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