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Geometric wave propagator on Riemannian manifolds

Matteo Capoferri, Michael Levitin, and Dmitri Vassiliev

We study the propagator of the wave equation on a closed Riemannian manifold M. We propose a geometric approach to the construction of the propagator as a single oscillatory integral global both in space and in time with a distinguished complex-valued phase function. This enables us to provide a global invariant definition of the full symbol of the propagator — a scalar function on the cotangent bundle — and an algorithm for the explicit calculation of its homogeneous components. The central part of the paper is devoted to the detailed analysis of the subprincipal symbol; in particular, we derive its explicit small time asymptotic expansion. We present a general geometric construction that allows one to visualise obstructions due to caustics and describe their circumvention with the use of a complex-valued phase function. We illustrate the general framework with explicit examples in dimension two.

1. Statement of the problem

Let (M, g) be a connected closed Riemannian manifold of dimension $d \geq 2$. We denote local coordinates on M by x^α, $\alpha = 1, \ldots, d$. The L^2 inner product on complex-valued functions is defined as

$$(u, v) := \int_M \overline{u(x)}\, v(x)\, \rho(x)\, \mathrm{d}x\,,$$

where

$$\rho(x) := \sqrt{\det g_{\mu\nu}(x)} \tag{1.1}$$

and $\mathrm{d}x = \mathrm{d}x^1 \ldots \mathrm{d}x^d$. The Laplace–Beltrami operator on scalar functions is

$$\Delta = \rho(x)^{-1} \frac{\partial}{\partial x^\mu}\, \rho(x)\, g^{\mu\nu}(x)\, \frac{\partial}{\partial x^\nu}\,. \tag{1.2}$$

Here and further on we adopt Einstein's summation convention over repeated indices.

It is well known that the operator (1.2) is non-positive and has discrete spectrum accumulating to $-\infty$. We adopt the following notation for the eigenvalues and normalised eigenfunctions of $-\Delta$,

$$-\Delta v_k = \lambda_k^2 v_k\,,$$

where eigenvalues are enumerated with account of their multiplicity as

$$0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_k \leq \ldots \to +\infty.$$

Consider the Cauchy problem for the wave equation

$$\left(\frac{\partial^2}{\partial t^2} - \Delta\right) f(t,x) = 0\,, \tag{1.3a}$$

$$f(0,x) = f_0(x), \qquad \frac{\partial f}{\partial t}(0,x) = f_1(x). \tag{1.3b}$$

Functional calculus allows one to write the solution of (1.3a), (1.3b) as

$$f = \cos\!\big(t\sqrt{-\Delta}\,\big)\, f_0 \,+\, \sin\!\big(t\sqrt{-\Delta}\,\big)\,(-\Delta)^{-1/2} f_1 \,+\, t\,(v_0\,,f_1)\,, \tag{1.4}$$

where

$$(-\Delta)^{-1/2} := \sum_{k=1}^{\infty} \frac{1}{\lambda_k}\,(v_k\,,\,\cdot\,)\,v_k$$

is the pseudoinverse of the operator $\sqrt{-\Delta}$ [Re, Chapter 2 Section 2].

The RHS of (1.4) contains three operators: $\cos\big(t\sqrt{-\Delta}\,\big)$, $\sin\big(t\sqrt{-\Delta}\,\big)$ and $(-\Delta)^{-1/2}$. The first two are Fourier Integral Operators (FIOs), whereas the third one is a pseudodifferential operator. Assuming one has a good description of the operator $(-\Delta)^{-1/2}$ — for which there is a well developed theory, see e.g. [Hö] — solving the Cauchy problem (1.3a), (1.3b) reduces to constructing the FIO

$$U(t) := \mathrm{e}^{-\mathrm{i}t\sqrt{-\Delta}} = \int u(t,x,y)\,(\,\cdot\,)\,\rho(y)\,\mathrm{d}y\,, \tag{1.5}$$

whose Schwartz kernel reads

$$u(t,x,y) := \sum_{k=0}^{\infty} \mathrm{e}^{-\mathrm{i}t\lambda_k}\, v_k(x)\,\overline{v_k(y)}\,. \tag{1.6}$$

The operator $U(t)$ is called the *wave propagator* (of the Laplacian) and is the (distributional) solution of

$$\left(-\mathrm{i}\,\frac{\partial}{\partial t} + \sqrt{-\Delta}\right) U(t) = 0\,, \tag{1.7a}$$

$$U(0) = \mathrm{Id}\,. \tag{1.7b}$$

The goal of this paper is to provide an explicit formula for the operator $U(t)$ modulo an integral operator with infinitely smooth integral kernel, written as a single invariantly defined oscillatory integral global in space and in time.

The study of solutions of hyperbolic partial differential equations on manifolds — and of the wave propagator in particular — is a well established subject, both within and outside microlocal analysis. As far as microlocal methods are concerned, rigorous descriptions of the singular structure of the propagator, as well as the construction of parametrices, can be found, for example, in [Ha], [Ri49, Ri60], [DuHö], [Hö, Vol. 3 & 4], [Tr], [Sh]. These publications rely on spectral-theoretic techniques, often combined with tools from the theory of local oscillatory integrals.

In this paper, we adopt a somewhat different *global* approach, which originates from the works of Laptev, Safarov and Vassiliev [LaSaVa] and Safarov and Vassiliev [SaVa]. They showed that it is possible to write the propagator for a fairly wide class of hyperbolic equations as *one* single Fourier integral operator, global both in space and in time, provided one uses a *complex-valued* phase function. This idea is not entirely new. For instance, constructions which look very similar at a formal level, albeit lacking mathematical rigour, have been for a long time appearing in solid state physics papers on electromagnetic wave propagation, obviously inspired by geometric optics. The mathematical formalisation of these ideas often appears under the name of 'Gaussian beams', see, e.g., [Ra]. In the realm of pure mathematics, FIOs with complex phase functions were considered, for example, by Melin and Sjöstrand [MeSj]. The fundamental difference between their approach and the one presented here lies in the fact that not only they have complex-valued phase functions, but, unlike [LaSaVa], [SaVa], they also work in a complexified phase space, which makes the analysis quite dissimilar.

Melin and Sjöstrand's techniques were later adopted by Zelditch in the construction of the wave group on real analytic manifolds, see, e.g., [Ze07] and [Ze14]. In his works, focussed on the study of nodal domains and nodal lines of complex eigenfunctions, the wave group appears as the composition of three Fourier integral operators. The general idea of his construction — up to technical details — goes as follows. Consider the complexification $M_{\mathbb{C}}$ of M and let

$$M_\tau := \{\zeta \in M_{\mathbb{C}} \,|\, \sqrt{\mathfrak{r}}(\zeta) \le \tau\}$$

be the Grauert tube of radius τ of M within $M_{\mathbb{C}}$, $\sqrt{\mathfrak{r}}$ denoting the Grauert tube function. Furthermore, let

$$\partial M_\tau := \{\zeta \in M_{\mathbb{C}} \,|\, \sqrt{\mathfrak{r}}(\zeta) = \tau\}.$$

Then the wave propagator $e^{-\mathrm{i}t\sqrt{-\Delta}} : L^2(M) \to L^2(M)$ is given by the composition of

(i) an operator $P^\tau : L^2(M) \to \mathcal{O}^{\frac{d-1}{4}}(\partial M_\tau) \subset L^2(\partial M_\tau)$, the analytic extension of the Poisson semigroup $\mathrm{e}^{\tau\sqrt{-\Delta}}$;

(ii) an operator T_{Φ^t} on $\mathcal{O}^{\frac{d-1}{4}}(\partial M_\tau)$,

$$T_{\Phi^t} f := f \circ \Phi^t,$$

realising the translation along the geodesic flow Φ^t;

(iii) the adjoint of P^τ, $(P^\tau)^* : \mathcal{O}^{\frac{d-1}{4}}(\partial M_\tau) \to L^2(M)$.

One needs, additionally, to incorporate a pseudodifferential operator S_t (multiplication by a symbol) in order to obtain, in the end, a unitary operator

$$(P^\tau)^* \circ S_t \circ T_{\Phi^t} \circ P^\tau : L^2(M) \to L^2(M).$$

Zelditch's approach consists, effectively, in writing the wave group $U(t)$ as the conjugation of the translation operator T_{Φ^t} by the (analytic extension of the) Poisson semigroup P^τ. For further details on the operator P^τ we refer the reader to [Bo], [Ze12], [Leb] and [St]. Despite some similarities in the idea of adopting a complex phase to achieve a representation global in time, our construction is overall quite different from Zelditch's one, as it will be clear later on.

The techniques from [LaSaVa], [SaVa] are rather abstract and do not account for any underlying geometry. This may be a reason why they have not been picked up by the wider mathematical community. There are only few subsequent publications using these methods as a fundamental tool. Laptev and Sigal [LaSi] constructed the propagator for the magnetic Schrödinger operator in flat Euclidean space for phase functions with purely quadratic imaginary part. Jakobson, Safarov and Strohmaier, when studying branching billiards on Riemannian manifolds with discontinuous metric in [JaSaSt], rely in their proofs on boundary layer oscillatory integrals with complex-valued phase function, in the spirit of [SaVa]. Furthermore, Safarov set his programme on global calculi on manifolds [Sa14, McSa] in the framework of [LaSaVa]. An extension of results from [SaVa] to first order systems of PDEs has been carried out by Chervova, Downes and Vassiliev [ChDoVa] in the process of computing two-term spectral asymptotics.

Laptev and Sigal's results mentioned above were improved and extended by Robert in [Rob], where he constructs explicitly the Schwartz kernel of the quantum propagator for the Schrödinger operator on $\mathbb{R}^d$ as a Fourier integral operator with quadratic complex-valued phase function and semiclassical subquadratic symbol. Robert adopts a distinguished phase function adapted to the Hamiltonian dynamics, which, however, does not coincide with a specialisation to the flat case of the Levi-Civita phase function used in the current paper.

The construction of [LaSaVa, SaVa] works, strictly speaking, for closed manifolds or compact manifolds with boundary. The compactness assumption, however, is not essential and can be removed with some effort. Results in this direction, although in a different setting and without the use of complex-valued phase functions, have been recently obtained by Coriasco and collaborators [CoSc, CoDoSc]. In the current paper, we will refrain from carrying out such an extension and we will stick to the case of closed manifolds.

The general properties and the singular structure of the integral kernel u of the wave propagator, see (1.6), are well understood. At the same time very little is known when it comes to explicit formulae. In particular, almost no information on the symbol of $U(t)$ can be found in the literature. With the exception of those cases where all eigenvalues and eigenfunctions are known, the only general result available to date is that the principal symbol is 1. In fact, we are unaware of any invariant definition of full symbol — or subprincipal symbol — for Fourier integral operators of the form (1.5). The goal of the current paper is to build upon [LaSaVa], developing their construction further for the case of Riemannian manifolds. The geometric nature of our construction will allow us to provide invariant definitions of full and g-subprincipal symbol of the wave propagator, analyse them, and give explicit formulae. Here 'g' is a reference to the Riemannian metric used in the construction of the phase function φ, leading up to the definition of the full symbol.

Our construction, although non-trivial, is quite natural and fully geometric in its building blocks. Among other things, we aim to show the potential of the method, which, due to the fact of being fully explicit, may find applications in pure and applied mathematics, as well as in other applied sciences. With this in mind, we will not pursue the standard microlocal approach involving half-densities, but, rather, we will adjust our theory to the case of operators acting on scalar functions.

One of the applications of our construction of the wave propagator is the calculation of higher Weyl coefficients, see Appendix B. For the Laplacian this can be done using a variety of alternative methods, the simplest being the heat kernel and the resolvent approaches. However, if one replaces the

Laplace–Beltrami operator by a first order system, whose spectrum is, in general, not semi-bounded, the heat kernel method can no longer be applied, at least in its original form. Furthermore, even resolvent techniques require major modification [AvSjVa]. In the future we plan to apply our approach to first order systems of partial differential equations on Riemannian manifolds for which we expect to compute additional (compared to what is known in the current literature) Weyl coefficients.

The paper is structured as follows.

In Section 2 we present a brief overview of the theory of global Lagrangian distributions and their relation to hyperbolic problems, as developed in [LaSaVa]. Section 3 contains a concise summary of the main results of the paper. In Section 4 we introduce a special phase function, the *Levi-Civita phase function*, which will later act as the key ingredient of our geometric analysis, and analyse its properties in detail. A global invariant definition of the full symbol of the wave propagator is formulated in Section 5, and an algorithm for the calculation of all its homogeneous components is provided. Some of the more technical material used in Section 5 has been moved to a separate Appendix A. In order to implement the algorithm presented in Section 5 one also needs to study invariant representations of the identity operator in the form of an oscillatory integral: this is the subject of Section 6. Section 7 is devoted to a detailed study of the g-subprincipal symbol of the wave propagator, culminating with Theorem 7.6 which gives an explicit formula for it. In Section 8 we provide an explicit small time asymptotic expansion for the g-subprincipal symbol. This allows us to recover, as a by-product, the third Weyl coefficient, see Appendix B. In Section 9 we apply our construction to two explicit examples in 2D: the sphere and the hyperbolic plane. Finally, in Section 10 we discuss in detail the issue of circumventing obstructions due to caustics.

2. Lagrangian manifolds and Hamiltonian flows

The theory of Fourier integral operators, beautifully set out in the seminal papers by Hörmander and Duistermaat [Hö71, DuHö], proved to be an extremely powerful tool in the analysis of partial differential equations and gave rise to several flourishing lines of research still active nowadays. As it is unrealistic to give a concise account of such a vast field of mathematical analysis, we refer the interested reader to the aforementioned papers and to the monographs by Duistermaat [Du], Trèves [Tr, Vol. 2] and Hörmander [Hö, Vol. 4] for a detailed exposition.

In this section we will briefly summarise the theory of global Fourier integral operators with complex-valued phase function as developed by Laptev, Safarov and Vassiliev [LaSaVa], in a formulation adapted to the current paper. Here and further on we adopt the notation $T'M := T^*M \setminus \{0\}$.

We call *Hamiltonian* any smooth function $h : T'M \to \mathbb{R}$ positively homogeneous in momentum of degree one, i.e. such that $h(x, \lambda\,\xi) = \lambda\, h(x,\xi)$ for every $\lambda > 0$. For any such Hamiltonian, we denote by $(x^*(t;y,\eta), \xi^*(t;y,\eta))$ the Hamiltonian flow, namely the (global) solution of Hamilton's equations

$$\begin{aligned} \dot{x}^*(t;y,\eta) &= h_\xi(x^*(t;y,\eta), \xi^*(t;y,\eta)), \\ \dot{\xi}^*(t;y,\eta) &= -h_x(x^*(t;y,\eta), \xi^*(t;y,\eta))\,, \end{aligned} \tag{2.1}$$

with initial condition $(x^*(0;y,\eta), \xi^*(0;y,\eta)) = (y,\eta)$. Observe that, as a consequence of (2.1), x^* and ξ^* are positively homogeneous in momentum of degree zero and one respectively. Further on, whenever x^* and ξ^* come without argument, $(t;y,\eta)$ is to be understood. This will be done for the sake of readability when there is no risk of confusion.

The Hamiltonian flow, in turn, defines a Lagrangian submanifold Λ_h of $T^*\mathbb{R} \times T'M \times T'M$ given by

$$\begin{aligned} \Lambda_h := \{(t, -h(y,\eta)), (x^*(t;y,\eta), \xi^*(t;y,\eta)), (y,-\eta) \mid \\ t \in \mathbb{R},\ (y,\eta) \in T'M\}. \end{aligned} \tag{2.2}$$

Indeed, a straightforward calculation shows that the canonical symplectic form ω on $T^*\mathbb{R} \times T'M \times T'M$ satisfies $\omega|_{\Lambda_h} = 0$.

We call *phase function* an infinitely smooth function

$$\varphi : \mathbb{R} \times M \times T'M \to \mathbb{C}$$

which is non-degenerate, positively homogeneous in momentum of degree one and such that $\operatorname{Im}\varphi \geq 0$. We say that a phase function φ *locally parameterises* the submanifold Λ_h if, in local coordinates x and y and in a neighbourhood of a given point of Λ_h, we have

$$\Lambda_h = \{(t, \varphi_t(t,x;y,\eta)), (x, \varphi_x(t,x;y,\eta)), (y, \varphi_y(t,x;y,\eta)) \mid (t,x;y,\eta) \in \mathfrak{C}_\varphi\},$$

where $\mathfrak{C}_\varphi := \{(t,x;y,\eta) \mid \varphi_\eta(t,x;y,\eta) = 0\}$.

The above definitions allow us to say what it means for a distribution (in the sense of distribution theory, see [Hö, Vol. 1]) to be associated with Λ_h. A distribution u is called a *Lagrangian distribution of order m associated with*

Λ_h if u can be represented locally, modulo C^∞, as the sum of oscillatory integrals of the form

$$\mathcal{I}_\varphi(a) = \int \mathrm{e}^{\mathrm{i}\,\varphi(t,x;y,\eta)}\, a(t,x;y,\eta)\, đ\eta$$

where φ is a phase function locally parameterising Λ_h and $a \in S^m_{\mathrm{ph}}(\mathbb{R} \times M \times T'M)$ is a polyhomogeneous function of order m. Here and further on

$$đ\eta = (2\pi)^{-d} \mathrm{d}\eta. \tag{2.3}$$

We recall that a polyhomogeneous function of order m is an infinitely smooth function

$$a : \mathbb{R} \times M \times T'M \to \mathbb{C}$$

admitting an asymptotic expansion in positively homogeneous components, i.e.

$$a(t,x;y,\eta) \sim \sum_{k=0}^{\infty} a_{m-k}(t,x;y,\eta), \tag{2.4}$$

where a_{m-k} is positively homogeneous in η of degree $m-k$. Here and in the following it is understood that whenever we write $S^m_{\mathrm{ph}}(E \times T'M)$ we mean polyhomogeneous functions of order m on $T'M$ depending smoothly on the variables in E.

In the theory of Fourier integral operators the function a is usually referred to as amplitude of the oscillatory integral. In the current paper we will call it *amplitude* and denote it by a Roman letter, e.g. $a(t,x;y,\eta)$, when it depends on the variable $x \in M$, whereas we will call it *symbol* and denote it by a fraktur letter, e.g. $\mathfrak{a}(t;y,\eta)$, when it is independent of the variable $x \in M$. In fact, as it will be explained in the following, one can always assume to be in the latter situation, modulo an infinitely smooth error in an appropriate sense.

It is a well known fact that with a real-valued phase function one can achieve the above mentioned parameterisation for a generic Lagrangian manifold only locally. Indeed, classical constructions involving global Fourier integral operators, see, for instance, [Hö71], [Tr, Vol. 2], always resort to (the sum of) local oscillatory integrals. This is due to obstructions of topological nature represented on the one hand by the non-triviality of a certain cohomology class in $H^1(\Lambda_h, \mathbb{Z})$ [Lee], known as the *Maslov class*, and on the other hand by the presence of caustics. In the case of a Lagrangian manifold generated by a homogeneous Hamiltonian flow the former obstruction is not present. The adoption of a complex-valued phase functions allows one to circumvent the latter and perform a construction which is inherently global.

To explain why this is the case, we first need to impose a restriction on the class of admissible phase functions. In particular, since our goal is to parameterise Lagrangian manifolds generated by a Hamiltonian, we need to impose compatibility conditions between our phase function and the Hamiltonian flow.

Definition 2.1 (Phase function of class $\mathcal{L}_h$). We say that a phase function $\varphi = \varphi(t, x; y, \eta)$ defined on $\mathbb{R} \times M \times T'M$ is *of class* $\mathcal{L}_h$ if it satisfies the conditions

(i) $\varphi|_{x=x^*} = 0$,

(ii) $\varphi_{x^\alpha}|_{x=x^*} = \xi^*_\alpha$,

(iii) $\det \varphi_{x^\alpha \eta_\beta}\big|_{x=x^*} \neq 0$,

(iv) $\operatorname{Im} \varphi \geq 0$.

The space of phase functions of class $\mathcal{L}_h$ is non-empty and path-connected [LaSaVa, Lemma 1.7].

We are now able to state the main result contained in [LaSaVa].

Theorem 2.2. *The Lagrangian submanifold Λ_h can be globally parameterised by a single phase function of class $\mathcal{L}_h$.*

Theorem 2.2 is crucial for the problem we want to study. In fact, take h to be the principal symbol of the pseudodifferential operator $\sqrt{-\Delta}$, namely

$$h(x, \xi) := \left(g^{\alpha\beta}(x)\, \xi_\alpha\, \xi_\beta\right)^{1/2}. \tag{2.5}$$

Then the flow (2.1) is (co)geodesic and the propagator for our hyperbolic PDE (1.7a) is a Fourier integral operator whose Schwartz kernel (1.6) is a Lagrangian distribution of order zero associated with the Lagrangian manifold Λ_h. As already noticed by Laptev, Safarov and Vassiliev in [LaSaVa], being able to globally parameterise Λ_h by a phase function of class $\mathcal{L}_h$ amounts to being able to write $u(t, x, y)$ as a single oscillatory integral, global both in space and in time.

This is not the only simplification brought about by this framework. Since the Maslov class of Λ_h is trivial, and so is the reduced Maslov class, one can canonically identify sections of the Keller–Maslov bundle with smooth functions on $T'M$. In particular, the principal symbol of the Fourier integral operator defined by our Lagrangian distribution is simply the component of the highest degree of homogeneity $\mathfrak{a}_m$ in the asymptotic expansion of the symbol. We stress the fact that $\mathfrak{a}_m$ is a smooth scalar function on $T'M$ — possibly depending on additional parameters — which is independent of the choice of the phase function φ. Components of lower degree of homogeneity will generally depend on the choice of the phase function.

The crucial condition that allows us to pass through caustics is (iii) in Definition 2.1. The degeneracy of

$$\varphi_{x^\alpha \eta_\beta}\big|_{x=x^*} \tag{2.6}$$

for real-valued phase functions in the presence of conjugate points is what causes the analytic machinery to break down. The introduction of an imaginary part in φ serves the purpose of ensuring that $\det \varphi_{x^\alpha \eta_\beta}\big|_{x=x^*} \neq 0$ for all times. This is more than just a technical requirement, though; the object (2.6) is actually capable of detecting information of topological nature about paths in Λ_h. This is reflected in the fact that, as it was firstly observed by Safarov and later formalised in [LaSaVa, SaVa], (2.6) is the core of a purely analytic definition of the Maslov index.

Consider the differential 1-form

$$\vartheta_\varphi = -\frac{1}{2\pi}\mathrm{d}\left[\arg\left(\det \varphi_{x^\alpha \eta_\beta}\big|_{x=x^*}\right)^2\right]. \tag{2.7}$$

Let $\gamma := \{(x^*(t;y,\eta), \xi^*(t;y,\eta)) \mid 0 \le t \le T\}$ be a T-periodic Hamiltonian trajectory such that $x^*_\eta(T;y,\eta) = 0$. Then the Maslov index of γ is defined by

$$\operatorname{ind}(\gamma) := \int_\gamma \vartheta_\varphi\,. \tag{2.8}$$

It is easy to see that $\operatorname{ind}(\gamma)$ does not depend on the choice of the phase function φ. In fact, the index $\operatorname{ind}(\gamma)$ is determined by the de Rham cohomology class of ϑ_φ and (2.8) is the differential counterpart under the standard isomorphism between Čech and de Rham cohomologies of the approach in terms of cocycles adopted in [Hö71]. See [SaVa, Section 1.5] for additional details.

3. Main results

We seek the Schwartz kernel (1.6) of the propagator (1.5) in the form

$$u(t,x,y) = \mathcal{I}_\varphi(\mathfrak{a}) + \mathcal{K}(t,x,y), \tag{3.1}$$

where $\mathcal{K}$ is an infinitely smooth kernel and

$$\mathcal{I}_\varphi(\mathfrak{a}) = \int_{T_y^*M} e^{i\varphi(t,x;y,\eta;\epsilon)}\, \mathfrak{a}(t;y,\eta;\epsilon)\, \chi(t,x;y,\eta)\, w(t,x;y,\eta;\epsilon)\, đ\eta \tag{3.2}$$

is a global oscillatory integral. Here φ is a particular phase function of class $\mathcal{L}_h$, with h given by (2.5), which will be introduced in Section 4. This phase function is completely determined by the metric and a positive parameter ϵ and will be called the Levi-Civita phase function. Rigorous definitions of the symbol $\mathfrak{a}$, cut-off χ and weight w appearing on the RHS of (3.2) will be provided in Section 5. Let us emphasise that the representation (3.2) will be global in time $t \in \mathbb{R}$ and in space $x, y \in M$.

Our main results are as follows.

1. We provide an invariant definition of the full symbol of the wave propagator as a scalar function $\mathfrak{a}(t;y,\eta;\epsilon)$,

$$\mathfrak{a} : \mathbb{R} \times T'M \times \mathbb{R}_+ \to \mathbb{C},$$

along with an explicit algorithm for the calculation of all its homogeneous components, see Section 5. Throughout the paper we use the notation $\mathbb{R}_+ := (0, +\infty)$.

2. We determine the symbol of the identity operator written as an invariant oscillatory integral, see Section 6.
3. We perform a detailed study of the g-subprincipal symbol of the propagator and provide a simplified algorithm for its calculation, see Section 7.
4. We write down a small time asymptotic formula for the g-subprincipal symbol of the propagator, see Theorem 8.1.
5. We apply our construction to maximally symmetric spaces of constant curvature in 2D, the standard 2-sphere and the hyperbolic plane, see Section 9.

6. Using our complex-valued phase function, we provide a geometric construction which allows us to visualise the analytical circumvention of obstructions due to caustics, see Theorem 10.2.

4. The Levi-Civita phase function

In this section we will introduce a distinguished phase function, the Levi-Civita phase function, providing motivation and basic properties.

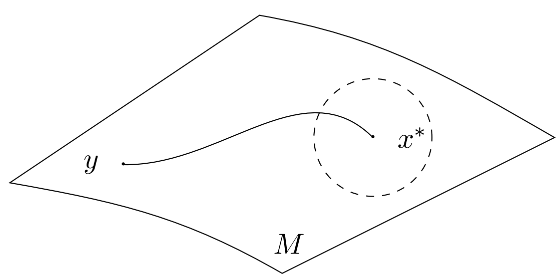
Definition 4.1 (Levi-Civita phase function). We call the *Levi-Civita phase function* the infinitely smooth function

$$\varphi : \mathbb{R} \times M \times T'M \times \mathbb{R}_+ \to \mathbb{C}$$

defined by

$$\varphi(t,x;y,\eta;\epsilon) := \int_\gamma \zeta \, \mathrm{d}z + \frac{\mathrm{i}\,\epsilon}{2}\, h(y,\eta)\ \mathrm{dist}^2(x,x^*(t;y,\eta)) \tag{4.1}$$

when x lies in a geodesic neighbourhood[1] of $x^*(t;y,\eta)$ and continued smoothly elsewhere in such a way that $\operatorname{Im}\varphi \geq 0$. The function dist is the Riemannian geodesic distance, the path of integration γ is the (unique) shortest geodesic connecting $x^*(t;y,\eta)$ to x, and ζ is the result of the parallel transport of $\xi^*(t;y,\eta)$ along γ.



The imaginary part of φ is pre-multiplied by a positive parameter ϵ in order to keep track of the effects of making φ complex-valued. The real-valued case can be recovered by setting $\epsilon = 0$.

[1] Here and further on by 'geodesic neighbourhood of z' we mean the image under the exponential map $\exp_z : T_zM \to M$ of a star-shaped neighbourhood $\mathcal{V}$ of $0 \in T_zM$ such that $\exp_z|_{\mathcal{V}}$ is a diffeomorphism.

It is straightforward to check that the Levi-Civita phase function φ is of class $\mathcal{L}_h$. Note that in geodesic normal coordinates x centred at $x^*(t;y,\eta)$ the function φ reads locally

$$\begin{aligned}\varphi(t,x;y,\eta;\epsilon) &= (x-x^*(t;y,\eta))^\alpha\,\xi^*_\alpha(t;y,\eta)\\ &\quad+\frac{\mathrm{i}\,\epsilon}{2}\,h(y,\eta)\,\delta_{\mu\nu}\,(x-x^*(t;y,\eta))^\mu(x-x^*(t;y,\eta))^\nu.\end{aligned}\tag{4.2}$$

Our phase function is invariantly defined and naturally dictated by the geometry of (M,g). Its construction relies on the use of the Levi-Civita connection associated with the Riemannian metric g, which justifies its name. From the analytic point of view, the adoption of the Levi-Civita phase function is particularly convenient in that it turns the Laplace-Beltrami operator into a partial differential operator with almost constant coefficients, up to curvature terms. In a sense, φ 'straightens out' the geometry of (M,g), thus bringing about considerable simplifications in the analysis. More precisely, the Levi-Civita phase function with $\epsilon=0$ has the following properties which a general phase function associated with the geodesic flow does not possess:

(i) $(\Delta\varphi)|_{x=x^*}=0$;

(ii) $(\varphi_{tt})|_{x=x^*}=0$;

(iii) the full symbol of the identity operator is 1, see Lemma 6.4.

Remark 4.2. The real-valued Levi–Civita phase function appears, in various forms, in [LaSaVa], [SaVa] and [McSa]. Note, however, that the geometric phase function used in the parametrix construction in [Ze09] and [CaHa] is not the same as (4.1) for $\epsilon=0$: the phase function appearing in [Ze09] and [CaHa] is *linear* in t, whereas ours is not. This is essentially due to the fact that the Levi-Civita phase function is constructed out of the cogeodesic flow.

Lemma 4.3. *We have*

$$\int_\gamma \zeta\,\mathrm{d}z=\langle\xi^*(t;y,\eta),\exp^{-1}_{x^*}(x)\rangle,$$

where exp *denotes the exponential map and* $\langle\,\cdot\,,\,\cdot\,\rangle$ *is the (pointwise) canonical pairing between cotangent and tangent bundles.*

Proof. Denoting by $P_{\gamma(s)}:T^*_{x^*(t;y,\eta)}M\to T^*_{\gamma(s)}M$ the one-parameter family of operators realising the parallel transport of covectors from $x^*(t;y,\eta)$ to

$\gamma(s)$ along $\gamma : [0,1] \to M$, we have

$$\begin{aligned}\int_\gamma \zeta \,\mathrm{d}z &= \int_0^1 \langle P_{\gamma(s)}(\xi^*(t;y,\eta)), \dot\gamma(s)\rangle \,\mathrm{d}s \\ &= \int_0^1 \langle \xi^*(t;y,\eta), \dot\gamma(0)\rangle \,\mathrm{d}s = \langle \xi^*(t;y,\eta), \exp_{x^*}^{-1}(x)\rangle,\end{aligned}$$

where the dot stands for the derivative with respect to the parameter s. At the second step we used the fact that

$$\begin{aligned}&\frac{d}{ds}\langle P_{\gamma(s)}(\xi^*(t;y,\eta)), \dot\gamma(s)\rangle \\ &\quad = \langle \nabla_{\dot\gamma(s)}\, P_{\gamma(s)}(\xi^*(t;y,\eta)), \dot\gamma(s)\rangle + \langle P_{\gamma(s)}(\xi^*(t;y,\eta)), \nabla_{\dot\gamma(s)}\dot\gamma(s)\rangle = 0.\end{aligned}$$

□

In view of Lemma 4.3, we can recast the Levi-Civita phase function (4.1) in the more explicit form

$$\begin{aligned}\varphi(t,x;y,\eta;\epsilon) := &-\frac{1}{2}\langle \xi^*, \operatorname{grad}_z[\operatorname{dist}^2(x,z)]\big|_{z=x^*}\rangle \\ &+ \frac{\mathrm{i}\,\epsilon}{2}\, h(y,\eta)\, \operatorname{dist}^2(x^*,x)\,,\end{aligned} \tag{4.3}$$

where the initial velocity $\exp_{x^*}^{-1}(x)$ is expressed in terms of the geodesic distance squared.

As briefly discussed in Section 2, the phase function is capable of detecting information of topological nature. In particular, a crucial role is played by the two-point tensor $\varphi_{x^\alpha\eta_\beta}$ and its determinant.

Theorem 4.4. *In any coordinate systems x and y, $\varphi_{x^\alpha\eta_\beta}$ along the flow is given by*

$$\varphi_{x^\alpha\eta_\beta}\big|_{x=x^*} = \frac{\partial \xi^*_\alpha}{\partial \eta_\beta} - \Gamma^\mu{}_{\alpha\nu}(x^*)\,\xi^*_\mu\,\frac{\partial x^{*\nu}}{\partial\eta_\beta} - \mathrm{i}\,\epsilon\, h(y,\eta)\, g_{\alpha\nu}(x^*)\,\frac{\partial x^{*\nu}}{\partial \eta_\beta}\,, \tag{4.4}$$

where $\Gamma^\mu{}_{\alpha\nu}$ are the Christoffel symbols.

Proof. Let us seek an expansion for the phase function φ in powers of $(x - x^*)$ up to second order. To this end, we need to obtain an analogous expansion for $\dot\gamma(0)$ first. Recall that $\gamma : [0,1] \to M$ is the shortest geodesic connecting x^* to x, hence satisfying

$$\gamma(0) = x^*, \qquad \gamma(1) = x.$$

Put

$$\gamma(s) = x^* + (x - x^*)\, s + z(s; x, x^*),$$

where z is a correction of order $O(\|x - x^*\|^2)$ such that $z(0) = 0$ and $z(1) = 0$. By requiring γ to satisfy the geodesic equation, we obtain

$$\ddot{z}(s) + \Gamma^\alpha{}_{\mu\nu}(\gamma(s))\, (x - x^*)^\mu\, (x - x^*)^\nu = 0 + O(\|x - x^*\|^3),$$

from which we get

$$z(s) = \frac{s(1-s)}{2}\, \Gamma^\alpha{}_{\mu\nu}(x^*)\, (x - x^*)^\mu\, (x - x^*)^\nu + O(\|x - x^*\|^3)$$

and, in turn,

$$\dot{\gamma}^\alpha(0) = (x - x^*)^\alpha + \frac{1}{2}\, \Gamma^\alpha{}_{\mu\nu}(x^*)\, (x - x^*)^\mu\, (x - x^*)^\nu + O(\|x - x^*\|^3).$$

It ensues that the Levi-Civita phase function admits the expansion

$$\begin{aligned}\varphi(t, x; y, \eta; \epsilon) = (x - x^*)^\alpha\, \xi^*_\alpha &+ \frac{1}{2}\, \Gamma^\alpha{}_{\mu\nu}(x^*)\, \xi^*_\alpha\, (x - x^*)^\mu\, (x - x^*)^\nu \\ &+ \frac{\mathrm{i}\,\epsilon\, h(y, \eta)}{2} g_{\mu\nu}(x^*)\, (x - x^*)^\mu\, (x - x^*)^\nu + O(\|x - x^*\|^3).\end{aligned}$$

Formula (4.4) now follows by direct differentiation. □

The explicit formula established in Theorem 4.4 is quite useful. In fact, it offers a direct way of investigating the properties of Λ_h and computing the Maslov index. We will come back to this later on.

5. The global invariant symbol of the propagator

In this section we will present an algorithm for the construction of a global invariant full symbol $\mathfrak{a}$ for the wave propagator.

In view of formulae (3.1) and (3.2), let us consider the Lagrangian distribution

$$\mathcal{I}_\varphi(\mathfrak{a}) = \int_{T^*_y M} e^{\mathrm{i}\varphi(t,x;y,\eta;\epsilon)}\, \mathfrak{a}(t; y, \eta; \epsilon)\, \chi(t, x; y, \eta)\, w(t, x; y, \eta; \epsilon)\, \text{đ}\eta\,, \tag{5.1}$$

where the quantities on the RHS are defined as follows.

- φ is the Levi-Civita phase function (4.3).
- $\mathfrak{a} \in S^0_{\mathrm{ph}}(\mathbb{R} \times T'M \times \mathbb{R}_+)$ is a polyhomogeneous symbol with asymptotic expansion

$$\mathfrak{a}(t; y, \eta; \epsilon) \sim \sum_{k=0}^{\infty} \mathfrak{a}_{-k}(t; y, \eta; \epsilon), \tag{5.2}$$

  where the $\mathfrak{a}_{-k} \in S^{-k}(\mathbb{R} \times T'M \times \mathbb{R}_+)$ are positively homogeneous in momentum of degree $-k$. They represent the unknowns of our construction.

- $\chi \in C^\infty(\mathbb{R} \times M \times T'M)$ is a cut-off satisfying the requirements
  (i) $\chi(t, x; y, \eta) = 0$ on $\{(t, x; y, \eta) \,|\, |h(y, \eta)| \le 1/2\}$;
  (ii) $\chi(t, x; y, \eta) = 1$ on the intersection of $\{(t, x; y, \eta) \,|\, |h(y, \eta)| \ge 1\}$ with some conical neighbourhood of $\{(t, x^*(t; y, \eta); y, \eta)\}$;
  (iii) $\chi(t, x; y, \alpha\, \eta) = \chi(t, x; y, \eta)$ for $\alpha \ge 1$ on $\{(t, x; y, \eta) \,|\, |h(y, \eta)| \ge 1\}$.
  The function χ serves the purpose of localising the domain of integration to a neighbourhood of orbits with initial conditions $(y, \eta) \in T'M$ and away from the zero section. Recall that the Hamiltonian h is positively homogeneous in η of degree 1. Further on, we will set $\chi \equiv 1$ while carrying out calculations. This will not affect the final result, as stationary phase arguments show that contributions to the oscillatory integral (5.1) only come from a neighbourhood of the set

$$\{(t, x; y, \eta) \mid x = x^*(t; y, \eta)\}$$

  on which $\varphi_\eta = 0$. Different choices of χ result in oscillatory integrals differing by infinitely smooth contributions.

- $w(t, x; y, \eta; \epsilon)$ is defined by

$$w(t, x; y, \eta; \epsilon) := [\rho(x)]^{-1/2}\, [\rho(y)]^{-1/2} \left[\det{}^2\big(\varphi_{x^\alpha \eta_\beta}(t, x; y, \eta; \epsilon)\big)\right]^{1/4} \tag{5.3}$$

  with $\rho = \sqrt{\det g_{\mu\nu}}$ as in (1.1). The branch of the complex root is chosen in such a way that

$$\arg \left[\det{}^2\big(\varphi_{x^\alpha \eta_\beta}(t, x; y, \eta; \epsilon)\big)\right]^{1/4}\Big|_{t=0} = 0.$$

  The existence of a smooth global branch whose argument turns to zero at $t = 0$ was established by [LaSaVa, Lemma 3.2]. The weight w is a (-1)-density in y and a scalar function in all other arguments.

It ensures that the oscillatory integral (5.1) is a scalar and that the principal symbol $\mathfrak{a}_0$ of the wave propagator does not depend on the choice of the phase function [SaVa, Theorem 2.7.11]. Thanks to condition (iii) in Definition 2.1 we can assume, without loss of generality, that w is non-zero whenever χ is non-zero.

Remark 5.1. The reason we write $\left[\det^2\left(\varphi_{x^\alpha \eta_\beta}\right)\right]^{1/4}$ in formula (5.3) rather than $\sqrt{\det \varphi_{x^\alpha \eta_\beta}}$ is that the coordinate systems x and y may be different: inversion of a single coordinate x^α changes the sign of $\det \varphi_{x^\alpha \eta_\beta}$ and so does inversion of a single coordinate y^β.

The general idea is to choose the phase function to be the Levi-Civita phase function, fixing it once and for all, and to seek a formula for the corresponding scalar symbol $\mathfrak{a}$. This is achieved by means of the following algorithm, which reduces the problem of solving partial differential equations to the much simpler problem of solving ordinary differential equations.

Step one. Set $\chi(t, x; y, \eta; \epsilon) = 1$ and apply the wave operator

$$\mathcal{P} := \partial_t^2 - \Delta_x \tag{5.4}$$

to (5.1). The result is an oscillatory integral

$$\mathcal{I}_\varphi(a) = \mathcal{P}\, \mathcal{I}_\varphi(\mathfrak{a}) \tag{5.5}$$

of the same form but with a different amplitude

$$\begin{aligned} &a(t, x; y, \eta; \epsilon) \\ &\quad = \mathrm{e}^{-\mathrm{i}\varphi(t,x;y,\eta;\epsilon)}\, [w(t, x; y, \eta; \epsilon)]^{-1}\, \mathcal{P}\left(\mathrm{e}^{\mathrm{i}\varphi(t,x;y,\eta;\epsilon)}\, \mathfrak{a}(t; y, \eta; \epsilon)\, w(t, x; y, \eta; \epsilon)\right). \end{aligned}$$

Observe that $a \in S^2_{\mathrm{ph}}(\mathbb{R} \times M \times T'M \times \mathbb{R}_+)$. The use of the full wave operator $\mathcal{P}$ as opposed to the half-wave operator $(-\mathrm{i}\,\partial_t + \sqrt{-\Delta})$ is justified by [SaVa, Theorem 3.2.1].

Step two. Construct a new oscillatory integral with x-independent amplitude $\mathfrak{b} = \mathfrak{b}(t; y, \eta; \epsilon)$, coinciding with (5.5) up to an infinitely smooth term:

$$\mathcal{I}_\varphi(\mathfrak{b}) \overset{\mathrm{mod}\ C^\infty}{=} \mathcal{I}_\varphi(a). \tag{5.6}$$

Such a procedure is called *reduction of the amplitude*. This can be done by means of special operators, as described below.

Put

$$L_\alpha := \left[(\varphi_{x\eta})^{-1}\right]_\alpha{}^\beta \frac{\partial}{\partial x^\beta} \tag{5.7}$$

and define

$$\mathfrak{S}_0 := (\,\cdot\,)|_{x=x^*}\ , \tag{5.8a}$$

$$\mathfrak{S}_{-k} := \mathfrak{S}_0 \left[\mathrm{i}\, w^{-1} \frac{\partial}{\partial \eta_\beta} w \left(1 + \sum_{1 \le |\boldsymbol{\alpha}| \le 2k-1} \frac{(-\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!\,(|\boldsymbol{\alpha}|+1)} L_{\boldsymbol{\alpha}} \right) L_\beta \right]^k . \tag{5.8b}$$

Bold Greek letters in (5.8b) denote multi-indices in $\mathbb{N}_0^d$, $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_d)$, $|\boldsymbol{\alpha}| = \sum_{j=1}^d \alpha_j$ and $(-\varphi_\eta)^{\boldsymbol{\alpha}} := (-1)^{|\boldsymbol{\alpha}|} (\varphi_{\eta_1})^{\alpha_1} \dots (\varphi_{\eta_d})^{\alpha_d}$. All differentiations are applied to the whole expression to the right of them. The operator (5.8b) is well defined because the differential operators L_α commute, see Lemma A.2 in Appendix A.

When applied to a homogeneous function, the operator $\mathfrak{S}_{-k}$ decreases the degree of homogeneity in η by k. Hence, denoting by $a \sim \sum_{j=0}^\infty a_{2-j}$ the asymptotic polyhomogeneous expansion of a, the homogeneous components of the symbol $\mathfrak{b}$ are

$$\mathfrak{b}_l := \sum_{2-j-k=l} \mathfrak{S}_{-k}\, a_{2-j}, \qquad l = 2, 1, 0, -1, \dots. \tag{5.9}$$

We call the operator $\mathfrak{S} \sim \sum_{k=0}^\infty \mathfrak{S}_{-k}$ the *amplitude-to-symbol operator*. It maps the x-dependent amplitude a to the x-independent symbol $\mathfrak{b}$. The construction of $\mathfrak{S}$ and the proof of the equality (5.6) are presented in Appendix A.

Step three. Impose the condition that our oscillatory integral (5.1) satisfies the wave equation, namely

$$\mathcal{P}\mathcal{I}_\varphi(\mathfrak{a}) \overset{\mathrm{mod}\ C^\infty}{=} \mathcal{I}_\varphi(\mathfrak{b}) = 0.$$

This is achieved by solving *transport equations* obtained by equating to zero the homogeneous components of the reduced amplitude $\mathfrak{b}$:

$$\mathfrak{b}_l = 0, \qquad l = 2, 1, 0, -1, \dots. \tag{5.10}$$

Note that the equation $\mathfrak{b}_2 = 0$ may be referred to as *eikonal equation*, see [SaVa, subsection 2.4.2] for details.

Formula (5.10) describes a hierarchy of ordinary differential equations in the variable t whose unknowns are the homogeneous components of the original amplitude $\mathfrak{a}$. Solving such equations iteratively produces an explicit formula for the symbol of the wave kernel. Initial conditions $\mathfrak{a}_{-k}(0; y, \eta; \epsilon)$ are established in such a way that at $t = 0$ our oscillatory integral (5.1) is, modulo C^∞, the integral kernel of the identity operator — see Section 6 for details.

Remark 5.2. One knows *a priori* that the leading homogeneous term in the expansion (5.2) is

$$\mathfrak{a}_0(t; y, \eta; \epsilon) = 1. \tag{5.11}$$

This is a consequence of the fact that the subprincipal symbol of the Laplace–Beltrami operator is zero, see [LaSaVa, Theorem 4.1] or [SaVa, Theorem 3.3.2]. Formula (5.11) holds for any choice of phase function due to the way (5.1) is designed.

Let us explain more precisely what we mean by saying that our construction is global in time. The issue with the standard construction is that, in the presence of caustics, one cannot parameterise globally the Lagrangian manifold generated by the Hamiltonian flow of the principal symbol by means of a single real-valued phase function. In our analytic framework, this means that the phase function may become degenerate when $x = x^*(t; y, \eta)$ and $x^*(t; y, \eta)$ is in the cut locus or conjugate locus of y. In turn, the weight w vanishes and the Fourier integral operator with integral kernel (5.1) ceases to be well-defined. The adoption of a complex-valued phase function allows us to circumvent these problems and construct a Fourier integral operator which is always well defined.

Note that the issue of 'local vs global' is *not* related to the use of the geodesic distance in the definition of our phase function. In fact, what appears in our construction is the geodesic distance between x and x^*. Now, non-smoothing contributions come from points x close to x^*, as these are the only stationary points for the phase in the support of the amplitude. As the injectivity radius is strictly positive, one can always choose a cut-off χ in such a way that the above points x are not in the cut locus or conjugate locus of x^*. What happens outside a small open neighbourhood of the geodesic flow gives an infinitely smoothing contribution.

We are now in a position to give the following definition.

Definition 5.3. We define the *symbol of the wave propagator* as the scalar function

$$\begin{gathered}\mathfrak{a} : \mathbb{R} \times T'M \times \mathbb{R}_+ \to \mathbb{C} \\ \mathfrak{a}(t; y, \eta; \epsilon) = 1 + \mathfrak{a}_{-1}(t; y, \eta; \epsilon) + \mathfrak{a}_{-2}(t; y, \eta; \epsilon) + \dots\end{gathered}$$

obtained through the above algorithm with the choice of the Levi-Civita phase function.

The above definition is invariant: $\mathfrak{a}$ depends only on φ which, in turn, arises from the geometry of (M, g) in a coordinate-free, covariant manner.

The algorithm provided in this section allows us to construct the wave propagator as a Fourier integral operator whose Schwartz kernel is a global Lagrangian distribution, namely, a single oscillatory integral global in space and in time, with invariantly defined symbol. In particular, it allows one to circumvent at an analytic level obstructions arising from caustics.

In Section 7 we will see the algorithm in action and perform a detailed analysis of the g-subprincipal symbol. In Section 9 we will apply our algorithm to two explicit examples.

Remark 5.4. The remainder terms in the asymptotic formulae provided in this paper are not uniform in time: they are only uniform over finite time intervals. This is to be expected when working with Fourier integral operators.

Remark 5.5 (Scalar functions vs half-densities). In microlocal analysis and spectral theory it is often convenient to work with operators acting on half-densities, as opposed to scalar functions. Our construction is easily adaptable to half-densities as follows.

- Replace the Laplacian on functions Δ with the corresponding operator on half-densities

$$\widetilde{\Delta} = \rho(x)^{1/2}\, \Delta\, \rho(x)^{-1/2}.$$

- Replace the weight w with

$$\widetilde{w} = \left[\det{}^2\left(\varphi_{x^\alpha \eta_\beta}\right)\right]^{1/4}.$$

  Note that $\widetilde{w}$ is now a $\frac{1}{2}$-density in x and a $-\frac{1}{2}$-density in y.

- Seek the integral kernel of the propagator as an oscillatory integral of the form
$$\widetilde{\mathcal{I}}_\varphi(\mathfrak{a}) = \int e^{i\varphi}\, \mathfrak{a}\, \widetilde{w}\, đ\eta\,.$$
Note that $\widetilde{\mathcal{I}}_\varphi(\mathfrak{a})$ is a half-density both in x and in y.
- Carry out the above algorithm.

It can be shown that we end up with the same full symbol of the wave propagator as when working with scalar functions.

Remark 5.6. By carrying out the integration in η in (5.1) for x sufficiently close to y one obtains the well-known Hadamard expansion, see, e.g., [Bé] and [Bä, Remark 2.5.5]. Our construction provides an explicit global version of the known local expansion.

6. Invariant representation of the identity operator

Step three of our algorithm described in Section 5 involves initial conditions determined by the symbol of the identity operator, which appears in our construction as a pseudodifferential operator written in the form

$$\int_{T'M} e^{i\varphi(0,x;y,\eta;\epsilon)}\, \mathfrak{s}(y,\eta;\epsilon)\, \chi(0,x;y,\eta)\, w(0,x;y,\eta;\epsilon)\ (\,\cdot\,)\, \rho(y)\, dy\, đ\eta$$

with the Levi-Civita phase function and some symbol $\mathfrak{s}$, cf. (5.1). Recall that χ is a cut-off and w is defined by formula (5.3). Note also that coordinate systems x and y may be different.

Invariant representation of pseudodifferential operators on manifolds is not a well studied subject. Existing literature comprises [McSa] and [DeLaSi], though invariant representations come there in slightly different forms. The aim of this section is to establish a few results in this direction for the identity operator.

Clearly, the principal symbol of the identity operator is

$$\mathfrak{s}_0(y,\eta) = 1, \tag{6.1}$$

irrespective of the choice of the phase function. In general, one would expect subleading homogeneous components of the symbol to depend on the phase function. This turns out not to be the case for $\mathfrak{s}_{-1}$, which is zero for any choice of phase function.

Theorem 6.1. *Let* $\phi \in C^\infty(M \times T'M; \mathbb{C})$ *be a positively homogeneous function (in momentum) of degree 1 satisfying the conditions*

(a) $\phi(x; y, \eta) = (x-y)^\alpha \, \eta_\alpha + O(\|x-y\|^2)\,,$

(b) $\operatorname{Im} \phi \geq 0.$

In stating condition (a) we use the same local coordinates for x and y.

Consider a pseudodifferential operator

$$(\mathfrak{I}_{\phi,\mathfrak{s}}\, f)(x) = \int_{T'M} \mathrm{e}^{\mathrm{i}\,\phi(x;y,\eta)}\, \mathfrak{s}(y,\eta)\, \chi(x;y,\eta)\, v(x;y,\eta)\, f(y)\, \mathrm{d}y\, \text{đ}\eta\,, \tag{6.2}$$

where $\mathfrak{s} \sim \sum_{k\in\mathbb{N}_0} \mathfrak{s}_{-k} \in S^0(T'M)$, χ *is a cut-off and*

$$v(x;y,\eta) = \rho(x)^{-1/2}\, \rho(y)^{1/2}\, [\det{}^2 \phi_{x\eta}]^{1/4}\,. \tag{6.3}$$

If $\mathfrak{I}_{\phi,\mathfrak{s}} - \mathrm{Id}$ *is an infinitely smoothing operator, then*

$$\mathfrak{s}_{-1}(y,\eta) = 0.$$

Remark 6.2. It is easy to see that the quantity defined by formula (6.3) is a scalar function $v : M \times T'M \to \mathbb{C}$. The branch of the complex root is chosen so that $v = 1$ on the diagonal $x = y$.

Proof of Theorem 6.1. Let us define the dual pseudodifferential operator $\mathfrak{I}'_{\phi,\mathfrak{s}}$ via the identity

$$\int_M [k(x)]\, [(\mathfrak{I}_{\phi,\mathfrak{s}}\, f)(x)]\, \rho(x)\, \mathrm{d}x = \int_M [(\mathfrak{I}'_{\phi,\mathfrak{s}}\, k)(y)]\, [f(y)]\, \rho(y)\, \mathrm{d}y\,,$$

where $f, k : M \to \mathbb{C}$ are smooth functions. The explicit formula for the pseudodifferential operator $\mathfrak{I}'_{\phi,\mathfrak{s}}$ reads

$$(\mathfrak{I}'_{\phi,\mathfrak{s}}\, k)(y) = \int_{M\times T'_y M} \mathrm{e}^{\mathrm{i}\,\phi(x;y,\eta)}\, \mathfrak{s}(y,\eta)\, \chi(x;y,\eta)\, u(x;y,\eta)\, k(x)\, \mathrm{d}x\, \text{đ}\eta\,,$$

where

$$u(x;y,\eta) = \rho(x)\, \rho(y)^{-1}\, v(x;y,\eta) = \rho(x)^{1/2}\, \rho(y)^{-1/2}\, [\det{}^2 \phi_{x\eta}]^{1/4}\,. \tag{6.4}$$

Of course, the condition that $\mathfrak{I}_{\phi,\mathfrak{s}} - \mathrm{Id}$ is an infinitely smoothing operator is equivalent to the condition that $\mathfrak{I}'_{\phi,\mathfrak{s}} - \mathrm{Id}$ is an infinitely smoothing operator.

Let us now fix an arbitrary point $P \in M$ and work in local coordinates y such that $y = 0$ at P. Furthermore, let us use the same local coordinates for x and for y. Consider the map

$$k \mapsto (\mathfrak{I}'_{\phi,s}\, k)(0). \tag{6.5}$$

The map (6.5) is a distribution, a continuous linear functional. We want the distribution (6.5) to approximate, modulo C^∞, the delta distribution, i.e. we want

$$\int e^{i\,\phi(x;0,\eta)}\,\mathfrak{s}(0,\eta)\,\chi(x;0,\eta)\,u(x;0,\eta)\,k(x)\,\mathrm{d}x\,\text{đ}\eta \;=k(0) \tag{6.6}$$

modulo a smooth functional. Substituting (6.4) into (6.6) we rewrite the latter as

$$\int e^{i\,\phi(x;0,\eta)}\,\mathfrak{s}(0,\eta)\,\chi(x;0,\eta)\,\kappa(x)\,\sqrt{\det\phi_{x\eta}}\,\mathrm{d}x\,\text{đ}\eta \;=\kappa(0)\,, \tag{6.7}$$

where $\kappa(x) = \rho(x)^{1/2}\,k(x)$ and the branch of the square root is chosen so that $\sqrt{\det\phi_{x\eta}} = 1$ at $x = 0$; see also Remark 5.1. Formula (6.7) is, in turn, equivalent to

$$\int e^{i\,\phi(x;0,\eta)}\,\mathfrak{s}(0,\eta)\,\chi(x;0,\eta)\,\sqrt{\det\phi_{x\eta}}\,\text{đ}\eta \;= \int e^{i\,x^\alpha\eta_\alpha}\,\text{đ}\eta\,. \tag{6.8}$$

The integrals in (6.8) are understood as distributions in the variable x and equality is understood as equality modulo a smooth distribution.

The complex exponential in (6.8) admits the expansion

$$e^{i\,\phi(x;0,\eta)} = e^{i\,x^\alpha\eta_\alpha}\left[1+\frac{i}{2}\,\phi_{x^\mu x^\nu}(0;0,\eta)\,x^\mu\,x^\nu + O(\|x\|^3)\right]. \tag{6.9}$$

Furthermore,

$$\sqrt{\det\phi_{x\eta}}\,(x;0,\eta) = 1+\frac{1}{2}\,\phi_{x^\alpha x^\beta\eta_\alpha}(0;0,\eta)\,x^\beta + O(\|x\|^2). \tag{6.10}$$

Substituting (6.9) and (6.10) into the LHS of (6.8) and integrating by parts we get

$$\int e^{i\,x^\gamma \eta_\gamma} \Big(1 + \mathfrak{s}_{-1}(0,\eta) - \frac{i}{2}\,\phi_{x^\mu x^\nu \eta_\mu \eta_\nu}(0;0,\eta) + \frac{i}{2}\,\phi_{x^\alpha x^\beta \eta_\alpha \eta_\beta}(0;0,\eta) + O(\|\eta\|^{-2})\Big)\, đ\eta = \int e^{i\,x^\gamma \eta_\gamma} \left(1 + \mathfrak{s}_{-1}(0,\eta) + O(\|\eta\|^{-2})\right) đ\eta\,,$$

from which we conclude that $\mathfrak{s}_{-1}(0,\eta) = 0$.

We have shown that $\mathfrak{s}_{-1}$ vanishes identically on the punctured cotangent fibre at the point $P \in M$. As the point P is arbitrary and $\mathfrak{s}_{-1}$ is a scalar function, we conclude that $\mathfrak{s}_{-1}(y,\eta) = 0$, $\forall (y,\eta) \in T'M$. □

Stronger results can be established for the Levi-Civita phase function.

Theorem 6.3. *The sub-subleading contribution to the symbol of the identity operator written as a pseudodifferential operator* (6.2) *with the Levi-Civita phase function* $\varphi(0,x;y,\eta;\epsilon)$ *is*

$$\mathfrak{s}_{-2}(y,\eta) = \frac{(d-1)\,(d-2)\,\epsilon^2}{8\,g^{\alpha\beta}(y)\,\eta_\alpha\eta_\beta}\,. \tag{6.11}$$

Proof. Let us fix a point $P \in M$ and argue as in the proof of Theorem 6.1, arriving at (6.8). Note that in this argument we did not specify the choice of a local coordinate system in a neighbourhood of the point P.

Let us choose geodesic normal coordinates centred at P. Then the explicit formula for the phase function appearing in (6.8) reads

$$\phi(x;0,\eta) = \varphi(0,x;0,\eta;\epsilon) = x^\alpha \eta_\alpha + \frac{i\,\epsilon}{2}\,\|\eta\|\,\|x\|^2\,,$$

where $\|\cdot\|$ stands for the Euclidean norm, see also (4.2).

The complex exponential in (6.8) admits the expansion

$$e^{i\,\phi(x;0,\eta)} = e^{i\,x^\alpha\eta_\alpha}\left[1 - \frac{\epsilon}{2}\,\|\eta\|\,\|x\|^2 + \frac{\epsilon^2}{8}\,\|\eta\|^2\,\|x\|^4 + O(\|x\|^6)\right]. \tag{6.12}$$

We have

$$(\phi_{x^\alpha \eta_\beta})(x;0,\eta) = \delta_\alpha{}^\beta + i\,\epsilon\,\delta_{\alpha\mu}\,\delta^{\beta\nu}\,\frac{\eta_\nu}{\|\eta\|}\,x^\mu\,. \tag{6.13}$$

It is well know that, given the identity matrix I and arbitrary small square matrix A of the same size, the expansion for $\det(I+A)$ reads

$$\det(I+A) = 1 + \operatorname{tr} A + \frac{1}{2}\big[(\operatorname{tr} A)^2 - \operatorname{tr}(A^2)\big] + O(\|A\|^3). \tag{6.14}$$

Formulae (6.13) and (6.14) imply

$$\sqrt{\det \phi_{x\eta}}\,(x;0,\eta) = 1 + \frac{\mathrm{i}\epsilon}{2\|\eta\|}\, x^\alpha \eta_\alpha + \frac{\epsilon^2}{8\|\eta\|^2}\,(x^\beta\eta_\beta)^2 + O(\|x\|^3). \tag{6.15}$$

Substituting (6.12) and (6.15) into the LHS of (6.8) and integrating by parts we get

$$\begin{aligned} &\int \mathrm{e}^{\mathrm{i}\,x^\gamma\eta_\gamma}\Big(1+\mathfrak{s}_{-2}(0,\eta) - \frac{\epsilon^2}{8}\left(\frac{\eta_\alpha\eta_\beta}{\|\eta\|^2}\right)_{\eta_\alpha\eta_\beta} + O(\|\eta\|^{-3})\Big)\,đ\eta \\ &\qquad = \int \mathrm{e}^{\mathrm{i}\,x^\gamma\eta_\gamma}\left(1+\mathfrak{s}_{-2}(0,\eta) - \frac{(d-1)\,(d-2)\,\epsilon^2}{8\|\eta\|^2} + O(\|\eta\|^{-3})\right)đ\eta\,, \end{aligned}$$

which gives us (6.11). □

The algorithm described in the proof of Theorem 6.3 allows one to calculate explicitly $\mathfrak{s}_{-3}, \mathfrak{s}_{-4}, \dots$ but the calculations become cumbersome. We list the resulting formulae for the special case $d = 2$:

$$\begin{aligned} \mathfrak{s}_{-3}(y,\eta) &= \frac{1}{2^3}\,\frac{\epsilon^3}{(g^{\alpha\beta}(y)\,\eta_\alpha\eta_\beta)^{3/2}}\,, & \mathfrak{s}_{-4}(y,\eta) &= 0\,,\\ \mathfrak{s}_{-5}(y,\eta) &= \frac{3^2\times 5}{2^6}\,\frac{\epsilon^5}{(g^{\alpha\beta}(y)\,\eta_\alpha\eta_\beta)^{5/2}}\,, & \mathfrak{s}_{-6}(y,\eta) &= 0\,,\\ \mathfrak{s}_{-7}(y,\eta) &= \frac{3^2\times 5^2\times 13}{2^{10}}\,\frac{\epsilon^7}{(g^{\alpha\beta}(y)\,\eta_\alpha\eta_\beta)^{7/2}}\,, & \mathfrak{s}_{-8}(y,\eta) &= 0\,,\\ \mathfrak{s}_{-9}(y,\eta) &= \frac{3^3\times 5^2\times 7^2\times 47}{2^6}\,\frac{\epsilon^9}{(g^{\alpha\beta}(y)\,\eta_\alpha\eta_\beta)^{9/2}}\,, & \mathfrak{s}_{-10}(y,\eta) &= 0\,. \end{aligned} \tag{6.16}$$

We have an even stronger result for the real-valued Levi-Civita phase function. The following theorem holds for Riemannian manifolds M of arbitrary dimension d.

Lemma 6.4. *The full symbol of the identity operator written as a pseudodifferential operator* (6.2) *with the real-valued Levi-Civita phase function* $\varphi(0,x;y,\eta;0)$ *is*

$$\mathfrak{s}(y,\eta) = 1. \tag{6.17}$$

Proof. Formula (6.17) is established by arguing as in the proof of Theorem 6.3. □

7. The g-subprincipal symbol of the propagator

Sometimes, for particular purposes (e.g. in spectral theory), one needs only a few leading homogeneous components of the full symbol $\mathfrak{a}$. In this section we will revisit and analyse further the construction of Section 5 for the special case of the g-subprincipal symbol.

Definition 7.1. We call the scalar function $\mathfrak{a}_{-1}(t;y,\eta;\epsilon)$ appearing in Definition 5.3 the *g-subprincipal symbol of the wave propagator.*

Acting with the wave operator (5.4) on the oscillatory integral

$$\int e^{i\,\varphi(t,x;y,\eta;\epsilon)}\,(1+\mathfrak{a}_{-1}(t;y,\eta;\epsilon))\;w(t,x;y,\eta;\epsilon)\,đ\eta, \tag{7.1}$$

one obtains a new oscillatory integral

$$\int e^{i\,\varphi(t,x;y,\eta;\epsilon)}\,a(t,x;y,\eta;\epsilon)\,w(t,x;y,\eta;\epsilon)\,đ\eta,$$

with

$$\begin{aligned} a = {} & (1+\mathfrak{a}_{-1})\,e^{-i\,\varphi}\,\left[\mathcal{P}\,(e^{i\,\varphi}\,w)\right]w^{-1} \\ & +(\mathfrak{a}_{-1})_{tt}+2\,(\mathfrak{a}_{-1})_t\left(i\,\varphi_t+w_t\,w^{-1}\right)\,. \end{aligned} \tag{7.2}$$

Here and in the following we drop the arguments for the sake of clarity.

Lemma 7.2. *The function*

$$b(t,x;y,\eta;\epsilon):=e^{-i\,\varphi}\,\left[\mathcal{P}\,(e^{i\,\varphi}\,w)\right]w^{-1}$$

decomposes as $b=b_2+b_1+b_0$, *where*

$$b_2=-\,(\varphi_t)^2+\|\nabla\varphi\|_g^2, \tag{7.3a}$$

$$b_1=i\,[\varphi_{tt}-\Delta\varphi+2\,(\ln\,w)_t\,\varphi_t-2\,\langle\nabla(\ln\,w),\nabla\varphi\rangle] \tag{7.3b}$$

$$b_0=w^{-1}\,[w_{tt}-\Delta w]\,, \tag{7.3c}$$

the b_k, $k=2,1,0$, *are positively homogeneous in* η *of degree* k, *and* ∇ *is the Levi-Civita connection acting in the variable* x.

Proof. The contribution to b from the Laplacian reads

$$-\mathrm{e}^{-\mathrm{i}\,\varphi}\,\Delta\left(\mathrm{e}^{\mathrm{i}\,\varphi}\,w\right)w^{-1} = -\mathrm{i}\,\Delta\varphi + \langle\nabla\varphi,\nabla\varphi\rangle - w^{-1}\Delta w - 2\mathrm{i}\,\langle\nabla\varphi,\nabla w\rangle w^{-1}. \tag{7.4}$$

On the other hand, the contribution from the second derivative in time is

$$\mathrm{e}^{-\mathrm{i}\,\varphi}\,\frac{\partial^2}{\partial t^2}\left(\mathrm{e}^{\mathrm{i}\,\varphi}\,w\right)w^{-1} = -\,(\varphi_t)^2 + \mathrm{i}\,\varphi_{tt} + 2\,\mathrm{i}\,\varphi_t\,w_t\,w^{-1} + w_{tt}\,w^{-1}\,. \tag{7.5}$$

Combining (7.4) and (7.5), and singling out terms with the same degree of homogeneity we arrive at (7.3a)–(7.3c). □

In terms of the homogeneous components of b, formula (7.2) reads

$$\begin{aligned} a = {} & b_2 \\ & + b_1 + b_2\,\mathfrak{a}_{-1} \\ & + b_0 + b_1\,\mathfrak{a}_{-1} + 2\,\mathrm{i}\,(\mathfrak{a}_{-1})_t\,\varphi_t \\ & + b_0\,\mathfrak{a}_{-1} + (\mathfrak{a}_{-1})_{tt} + 2\,\mathfrak{a}_{-1}\,w_t\,w^{-1}\,, \end{aligned} \tag{7.6}$$

where we arranged on different lines contributions of decreasing degree of homogeneity, from 2 to -1.

Before constructing the amplitude-to-symbol operator and writing down the transport equations, we need a few preparatory lemmata.

Lemma 7.3. *We have*

$$\varphi_t|_{x=x^*} = -h(y,\eta). \tag{7.7}$$

Proof. Differentiating in t both sides of (i) in Definition 2.1, one obtains

$$\begin{aligned} 0 &= \varphi_t|_{x=x^*} + \varphi_{x^\alpha}|_{x=x^*}\,\dot{x}^{*\alpha} \\ &= \varphi_t|_{x=x^*} + \xi^*_\alpha\,h_{\xi_\alpha}(x^*,\xi^*) \\ &= \varphi_t|_{x=x^*} + h(x^*,\xi^*)\,. \end{aligned}$$

In the second step condition (ii) from Definition 2.1 has been used, whereas the last step is a consequence of Euler's theorem on homogeneous functions. Formula (7.7) now follows from the fact that the Hamiltonian is preserved along the flow. □

Lemma 7.4. *The function* b_2 *defined by* (7.3a) *has a second order zero in* x *at* $x = x^*(t; y, \eta)$, *namely,*

$$b_2|_{x=x^*} = 0, \qquad \nabla b_2|_{x=x^*} = 0.$$

Proof. Rewriting b_2 as

$$b_2 = -(\varphi_t)^2 + h^2(x, \nabla\varphi),$$

one immediately concludes that b_2 vanishes along the flow by Lemma 7.3 and Definition 2.1, condition (ii).

Proving that the derivative vanishes as well is slightly trickier. We have

$$\nabla_\mu b_2 = -2\,\varphi_t\,\varphi_{tx^\mu} + 2\,h(x, \nabla\varphi)\,[h(x, \nabla\varphi)]_{x^\mu},$$

from which it ensues, by evaluating along the flow, that

$$\begin{aligned}\nabla_\mu b_2|_{x=x^*} &= \left(-2\,\varphi_t\,\varphi_{tx^\mu} + 2\,h(x, \nabla\varphi)\,[h(x, \nabla\varphi)]_{x^\mu}\right)\big|_{x=x^*}\\ &= 2\,h(y, \eta)\,\left(\varphi_{tx^\mu} + [h(x, \nabla\varphi)]_{x^\mu}\right)\big|_{x=x^*},\end{aligned}$$

where, once again, we used Lemma 7.3. The problem at hand is now down to showing that

$$\left(\varphi_{tx^\mu} + [h(x, \nabla\varphi)]_{x^\mu}\right)\big|_{x=x^*} = 0. \tag{7.8}$$

From the general properties of a phase function of class $\mathcal{L}_h$, one argues that, in an arbitrary coordinate system, φ can be represented as

$$\varphi = (x - x^*)^\alpha\,\xi^*_\alpha + \frac{1}{2}\,[H_\varphi]_{\mu\nu}\,(x - x^*)^\mu\,(x - x^*)^\nu + O(\|x - x^*\|^3), \tag{7.9}$$

with

$$[H_\varphi]_{\alpha\beta} := \varphi_{x^\alpha x^\beta}|_{x=x^*}\,.$$

Combining (7.9) with Hamilton's equations, we get

$$\varphi_{tx^\alpha}|_{x-x^*} = \dot{\xi}^*_\alpha - [H_\varphi]_{\alpha\mu}\,\dot{x}^{*\mu} = -h_{x^\alpha}(x^*, \xi^*) - [H_\varphi]_{\alpha\mu}\,h_{\xi_\mu}(x^*, \xi^*). \tag{7.10}$$

Moreover, we have

$$\begin{aligned}[h(x, \nabla\varphi)]_{x^\alpha}|_{x=x^*} =& h_{x^\alpha}(x^*, \xi^*) + h_{\xi_\mu}(x^*, \xi^*)\ \ \varphi_{x^\alpha x^\mu}|_{x=x^*}\\ =& h_{x^\alpha}(x^*, \xi^*) + [H_\varphi]_{\alpha\mu}\,h_{\xi_\mu}(x^*, \xi^*).\end{aligned} \tag{7.11}$$

Substitution of (7.10) and (7.11) into (7.8) concludes the proof. $\square$

Lemmata 7.3 and 7.4 are not specific to the Levi-Civita phase function: they remain true for any phase function of the class $\mathcal{L}_h$.

We are now in a position to analyse the transport equations. With the notation from Section 5, in view of formulae (5.9) and (7.6) we have

$$\mathfrak{b}_2 = \mathfrak{S}_0\, b_2\,, \tag{7.12a}$$

$$\mathfrak{b}_1 = \mathfrak{S}_{-1}\, b_2 + \mathfrak{S}_0\, b_1\,, \tag{7.12b}$$

$$\mathfrak{b}_0 = \mathfrak{S}_{-2}\, b_2 + \mathfrak{S}_{-1}\, b_1 + \mathfrak{S}_0\, b_0 - 2\,\mathrm{i}\, h\, (\mathfrak{a}_{-1})_t + \mathfrak{a}_{-1}\, \mathfrak{b}_1\,. \tag{7.12c}$$

Note that homogeneous components of the symbol $\mathfrak{a}_{-k}$ with degree of homogeneity less than -1, even if taken into account in (7.1), would not contribute to (7.12a)–(7.12c). Note also the appearance of the x-independent term $\mathfrak{a}_{-1}\,\mathfrak{b}_1$ on the RHS of (7.12c): it can be traced back to the fact that Lemma 7.4 implies

$$\mathfrak{S}_{-1}(b_2\, \mathfrak{a}_{-1}) = \mathfrak{a}_{-1}\mathfrak{S}_{-1} b_2.$$

The zeroth transport equation $\mathfrak{b}_2 = 0$ is clearly satisfied, due to Lemma 7.4.

Lemma 7.5. *The first transport equation (FTE) $\mathfrak{b}_1 = 0$ can be equivalently rewritten as*

$$(\varphi_{tt} - \Delta\varphi)\big|_{x=x^*} = 2\,h\,\frac{\mathrm{d}(\ln\, w^*)}{\mathrm{d}t} + \frac{1}{2}\,(x^*_{\eta_\alpha})^\gamma\,\left[[(\varphi_{x\eta})^{-1}]_\alpha{}^\beta\,(b_2)_{x^\beta x^\gamma}\right]\Big|_{x=x^*}\,, \tag{7.13}$$

where $w^*(t;y,\eta;\epsilon) = w(t, x^*(t;y,\eta); y,\eta;\epsilon)$.

Proof. Consider the operator $\mathfrak{S}_{-1}$ defined in (5.8b). When acting on a function with a second order zero along the flow, it can be simplified to read

$$\mathfrak{S}_{-1}\, b_2 = \mathrm{i}\,\frac{\partial(L_\beta\, b_2)}{\partial\eta_\beta}\bigg|_{x=x^*} - \frac{\mathrm{i}}{2}\,\left[\varphi_{\eta_\alpha\eta_\beta}\, L_\alpha L_\beta\, b_2\right]\big|_{x=x^*}\,. \tag{7.14}$$

Here we used the fact that $\mathfrak{S}_0\,\varphi_\eta = 0$. Using the notation $H_f := f_{xx}|_{x=x^*}$ and putting $\Phi_{x\eta} := \varphi_{x\eta}|_{x=x^*}$, we observe that

$$(\Phi_{x\eta})_\alpha{}^\beta = (\xi^*_{\eta_\beta})_\alpha - (H_\varphi)_{\alpha\mu}\,(x^*_{\eta_\beta})^\mu$$

and, consequently,

$$\begin{aligned}\varphi_{\eta_\alpha\eta_\beta}\Big|_{x=x^*} &= -(x^*_{\eta_\alpha})^\gamma\,(\xi^*_{\eta_\beta})_\gamma + (H_\varphi)_{\mu\nu}\,(x^*_{\eta_\alpha})^\mu (x^*_{\eta_\beta})^\nu \\ &= -(x^*_{\eta_\alpha})^\gamma \left[(\xi^*_{\eta_\beta})_\gamma - (H_\varphi)_{\gamma\nu}\,(x^*_{\eta_\beta})^\nu\right] \\ &= -(x^*_{\eta_\alpha})^\gamma\,(\Phi_{x\eta})_\gamma{}^\beta.\end{aligned}$$

Hence, recalling formula (5.7), we obtain

(7.15)
$$\begin{aligned}-\frac{\mathrm{i}}{2}\,\left[\varphi_{\eta_\alpha\eta_\beta}\,L_\alpha L_\beta\,b_2\right]\Big|_{x=x^*} &= \frac{\mathrm{i}}{2}(x^*_{\eta_\alpha})^\gamma\,(\Phi_{x\eta})_\gamma{}^\beta\,(\Phi^{-1}_{x\eta})_\alpha{}^\delta\,(\Phi^{-1}_{x\eta})_\beta{}^\rho\,(H_{b_2})_{\delta\rho} \\ &= \frac{\mathrm{i}}{2}(x^*_{\eta_\alpha})^\gamma\,\delta_\gamma{}^\rho\,(\Phi^{-1}_{x\eta})_\alpha{}^\delta\,(H_{b_2})_{\delta\rho} \\ &= \frac{\mathrm{i}}{2}(x^*_{\eta_\alpha})^\rho\,(\Phi^{-1}_{x\eta})_\alpha{}^\delta\,(H_{b_2})_{\delta\rho}\,.\end{aligned}$$

Furthermore, upon writing

$$b_2 = \frac{1}{2}(H_{b_2})_{\alpha\beta}\,(x-x^*)^\alpha\,(x-x^*)^\beta + O(\|x-x^*\|^3),$$

the first term in (7.14) becomes

$$\mathrm{i}\,\frac{\partial(L_\beta\,b_2)}{\partial\eta_\beta}\bigg|_{x=x^*} = -\mathrm{i}\,(x^*_{\eta_\alpha})^\gamma\,(\Phi^{-1}_{x\eta})_\alpha{}^\mu\,(H_{b_2})_{\mu\gamma}\,. \tag{7.16}$$

By substituting (7.15) and (7.16) into (7.14) we arrive at the last summand in the RHS of (7.13). As for the remaining terms, they correspond to $\mathfrak{S}_0\,b_1$ in (7.12b) and are obtained by evaluating (7.3b) along the flow and performing straightforward algebraic manipulations. □

It is possible to show directly, by means of a long and tedious, though non-trivial, computation that (7.13) is satisfied automatically, thus providing a direct proof that the principal symbol of the wave propagator is indeed 1. If one started with a generic term $\mathfrak{a}_0$ in (7.1), the FTE would be an ordinary differential equation allowing for the (unique) determination thereof. Lemma 7.5 gives us an explicit formula for the action of the wave operator on the Levi-Civita phase function.

Let us now move on to the second transport equation $\mathfrak{b}_0 = 0$, the one that allows for the determination of the g-subprincipal symbol $\mathfrak{a}_{-1}(t; y, \eta; \epsilon)$. For computing the g-subprincipal symbol, a simplified representation of the operators $\mathfrak{S}_{-1}$ and $\mathfrak{S}_{-2}$ may be used. Recall that for general k the operators $\mathfrak{S}_{-k}$ are defined by formulae (5.8a) and (5.8b). Put

$$\mathfrak{B}_{-1} := \mathrm{i}\, w^{-1} \frac{\partial}{\partial \eta_\alpha} w\, L_\alpha - \frac{\mathrm{i}}{2} \varphi_{\eta_\alpha \eta_\beta} L_\alpha L_\beta \,. \tag{7.17}$$

Then we have

$$\mathfrak{S}_{-1} = \mathfrak{S}_0 \,\mathfrak{B}_{-1}\,, \tag{7.18}$$

$$\mathfrak{S}_{-2} = \mathfrak{S}_0 \,\mathfrak{B}_{-1} \left[\mathrm{i}\, w^{-1} \frac{\partial}{\partial \eta_\beta} w \left(1 + \sum_{1 \le |\boldsymbol{\alpha}| \le 3} \frac{(-\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!(|\boldsymbol{\alpha}|+1)} L_{\boldsymbol{\alpha}} \right) L_\beta \right], \tag{7.19}$$

and these representations can now be used in formula (7.12c).

The last ingredient needed to write down the g-subprincipal symbol is the initial condition at $t = 0$, extensively discussed in Section 6. The Levi-Civita phase function evaluated at $t = 0$, $\varphi(0, x; y, \eta; \epsilon)$, clearly satisfies the assumptions (a) and (b) of Theorem 6.1, hence $\mathfrak{a}_{-1}|_{t=0} = 0$. Integrating in time, we arrive at the following theorem.

Theorem 7.6. *The global invariantly defined g-subprincipal symbol of the wave propagator is*

$$\mathfrak{a}_{-1}(t; y, \eta; \epsilon) = -\frac{\mathrm{i}}{2\,h} \int_0^t \left[\mathfrak{S}_{-2}\, b_2 + \mathfrak{S}_{-1}\, b_1 + \mathfrak{S}_0\, b_0 \right] (\tau; y, \eta; \epsilon)\, \mathrm{d}\tau \,. \tag{7.20}$$

The functions b_k, $k = 2, 1, 0$, are defined by (7.3a)–(7.3c), (4.3), (5.3), *while the operators $\mathfrak{S}_{-2}$, $\mathfrak{S}_{-1}$ and $\mathfrak{S}_0$ are given by* (7.17)–(7.19) *and* (5.7), (5.8a).

8. Small time expansion for the g-subprincipal symbol

The small time behaviour of the wave propagator carries important information about the spectral properties of the Laplace–Beltrami operator. Our geometric construction allows us to derive an explicit universal formula for the coefficient of the linear term in the expansion of the g-subprincipal symbol when t tends to zero. In Appendix B we will explain how this formula can be used to recover, in a straightforward manner, the third Weyl coefficient.

When time is sufficiently small we can use the real-valued Levi-Civita phase function, since condition (iii) in Definition 2.1 is automatically satisfied. Therefore, throughout this section we set $\epsilon = 0$.

Theorem 8.1. *The g-subprincipal symbol of the wave propagator admits the following expansion for small times:*

$$\mathfrak{a}_{-1}(t;y,\eta)=\frac{\mathrm{i}}{12\,h(y,\eta)}\,\mathcal{R}(y)\,t+O(t^2)\,, \tag{8.1}$$

where $\mathcal{R}$ is scalar curvature.

Proof. Let us fix an arbitrary point $y\in M$ and choose geodesic normal coordinates centred at y. As $\mathfrak{a}_{-1}$ is a scalar function, in order to prove the theorem it is sufficient to prove

$$\mathfrak{a}_{-1}(t;0,\eta)=\frac{\mathrm{i}}{12\,h(0,\eta)}\,\mathcal{R}(0)\,t+O(t^2) \tag{8.2}$$

in the chosen coordinate system.

As we are dealing with the case when t tends to zero, we can assume that x^* and x both lie in a geodesic neighbourhood of y. In what follows we use for x geodesic normal coordinates centred at y and perform a double Taylor expansion of the phase function in powers of t and x simultaneously. We shall also assume that t and $\|x\|$ are of the same order and write $O(\|x\|^n+|t|^n)$ as a shorthand for $O(\|x\|^p\,t^{n-p})$ for all $p\in\{0,1,\dots,n\}$.

It is well known that in geodesic normal coordinates centred at y we have

$$x^{*\alpha}=\frac{\eta^\alpha}{h}\,t\,, \tag{8.3}$$

where $\eta^\alpha=\delta^{\alpha\beta}\eta_\beta$. Substituting (8.3) into the first Hamilton's equation (2.1) we get

$$\begin{aligned}\xi^*_\alpha&=g_{\alpha\beta}(x^*)\,\eta^\beta\\&=\left[g_{\alpha\beta}\left(\frac{\eta}{h}\,t\right)\right]\eta^\beta\\&=\left(\delta_{\alpha\beta}-\frac{1}{3}\,R_{\alpha\mu\beta\nu}(0)\,\frac{\eta^\mu\eta^\nu}{h^2}\,t^2+O(t^3)\right)\eta^\beta\\&=\eta_\alpha+O(t^3).\end{aligned} \tag{8.4}$$

The simplifications in the above calculations are due to the properties of normal coordinates and the (anti)symmetries of the Riemann curvature tensor R. In fact, using the Gauss Lemma, one can show that the remainder in (8.4) is zero, i.e. $\xi^*_\alpha=\eta_\alpha$.

Arguing as in the proof of Theorem 4.4 and using formula (8.3), one concludes that the initial velocity of the (unique) geodesic connecting x^* to x is

$$\begin{aligned}\dot\gamma(0)^\alpha &= (x-x^*)^\alpha + \frac{1}{2}\,\Gamma^\alpha{}_{\beta\gamma}(x^*)\,(x-x^*)^\beta\,(x-x^*)^\gamma \\ &\quad + \frac{1}{2}\,(\partial_{x^\mu}\Gamma^\alpha{}_{\beta\gamma})(x^*)\,(x-x^*)^\mu\,(x-x^*)^\beta\,(x-x^*)^\gamma \\ &\quad + O(\|x-x^*\|^4) \\ &= x^\alpha - \frac{\eta^\alpha}{h}\,t + \frac{1}{2}(\partial_{x^\mu}\Gamma^\alpha{}_{\beta\gamma})(0)\,\frac{\eta^\mu}{h}\,t\,\left(x-\frac{\eta}{h}\,t\right)^\beta\left(x-\frac{\eta}{h}\,t\right)^\gamma \\ &\quad + \frac{1}{2}(\partial_{x^\mu}\Gamma^\alpha{}_{\beta\gamma})(0)\left(x-\frac{\eta}{h}\,t\right)^\mu\left(x-\frac{\eta}{h}\,t\right)^\beta\left(x-\frac{\eta}{h}\,t\right)^\gamma \\ &\quad + O(\|x\|^4+t^4) \\ &= x^\alpha - \frac{\eta^\alpha}{h}\,t - (\partial_{x^\mu}\Gamma^\alpha{}_{\beta\gamma})(0)\,\frac{\eta^\beta}{h}\,t\,x^\mu\,x^\gamma \\ &\quad + \frac{1}{2}(\partial_{x^\mu}\Gamma^\alpha{}_{\beta\gamma})(0)\,\frac{\eta^\beta\,\eta^\gamma}{h^2}\,t^2\,x^\mu \\ &\quad + \frac{1}{2}(\partial_{x^\mu}\Gamma^\alpha{}_{\beta\gamma})(0)\,x^\mu x^\beta x^\gamma + O(\|x\|^4+t^4) \\ &= x^\alpha - \frac{\eta^\alpha}{h}\,t + \frac{1}{3\,h}\,R^\alpha{}_{\gamma\beta\mu}(0)\,\eta^\beta\,t\,x^\gamma x^\mu \\ &\quad - \frac{1}{3}R^\alpha{}_{\beta\gamma\mu}(0)\,\frac{\eta^\beta\,\eta^\gamma}{h^2}\,t^2\,x^\mu + O(\|x\|^4+t^4)\,.\end{aligned} \tag{8.5}$$

Here at the last step we resorted to the identity

$$(\partial_{x^\mu}\Gamma^\alpha{}_{\beta\gamma})(0) = -\frac{1}{3}\,(R^\alpha{}_{\beta\gamma\mu}(0) + R^\alpha{}_{\gamma\beta\mu}(0)). \tag{8.6}$$

Lemma 4.3 and formulae (8.4), (8.5) imply that our real-valued Levi-Civita phase function admits the following Taylor expansion in powers of x and t:

$$\begin{aligned}\varphi(t,x;0,\eta) &= x^\alpha\,\eta_\alpha - t\,h + \frac{1}{3\,h}\,R^\alpha{}_\mu{}^\beta{}_\nu(0)\,\eta_\alpha\,\eta_\beta\,t\,x^\mu\,x^\nu \\ &\quad + O(\|x\|^4+t^4)\,.\end{aligned} \tag{8.7}$$

The next step is computing the homogeneous functions b_2, b_1 and b_0 defined by (7.3a)–(7.3c) at $t=0$.

Direct inspection tells us that

$$-(\varphi_t)^2\big|_{t=0} = -h^2 + \frac{2}{3}\,R^\alpha{}_\mu{}^\beta{}_\nu(0)\,\eta_\alpha\,\eta_\beta\,x^\mu\,x^\nu + O(\|x\|^3)$$

and

$$g^{\alpha\beta}(x)\,\varphi_{x^\alpha}\,\varphi_{x^\beta}\Big|_{t=0} = h^2 + \frac{1}{3}\,R^\alpha{}_\mu{}^\beta{}_\nu(0)\,\eta_\alpha\,\eta_\beta\,x^\mu\,x^\nu + O(\|x\|^3)\,.$$

Adding up the above two formulae, we get

$$b_2(0,x;0,\eta) = R^\alpha{}_\mu{}^\beta{}_\nu(0)\,\eta_\alpha\,\eta_\beta\,x^\mu\,x^\nu + O(\|x\|^3). \tag{8.8}$$

Let us now move on to b_1. Direct differentiation of (8.7) reveals that

$$\varphi_{tt}|_{t=0} = O(\|x\|^2), \quad \varphi_t|_{t=0} = -h + O(\|x\|^2)\,, \quad \varphi_{xx}|_{t=0} = O(\|x\|^2)\,. \tag{8.9}$$

Furthermore, we have

$$\begin{aligned}\varphi_{x^\rho\eta_\sigma} &= \delta_\rho{}^\sigma + t\,\frac{2}{3h}\left(R^\sigma{}_\rho{}^\beta{}_\nu(0)\,\eta_\beta + R^\alpha{}_\rho{}^\sigma{}_\nu(0)\,\eta_\alpha\right)x^\nu\\ &\quad + O(\|x\|^3+|t|^3)\end{aligned} \tag{8.10}$$

and, consequently,

$$\det\varphi_{x^\rho\eta_\sigma} = 1 - t\,\frac{2}{3h}\,\operatorname{Ric}^\alpha{}_\nu(0)\,\eta_\alpha\,x^\nu + O(\|x\|^3+|t|^3). \tag{8.11}$$

Plugging (8.11) into (5.3) and expanding the Riemannian density in normal geodesic coordinates, one eventually obtains

$$w = 1 + \frac{1}{12}\,\operatorname{Ric}_{\mu\nu}(0)\,x^\mu\,x^\nu - \frac{t}{3h}\,\operatorname{Ric}^\alpha{}_\nu(0)\,\eta_\alpha\,x^\nu + O(\|x\|^3+|t|^3). \tag{8.12}$$

Formulae (8.6), (8.7), (8.9) and (8.12) give us

$$\begin{aligned}-\mathrm{i}g^{\alpha\beta}(x)\,\nabla_\alpha\nabla_\beta\,\varphi\Big|_{t=0} &= -\mathrm{i}g^{\alpha\beta}(x)\left(-\Gamma^\gamma{}_{\alpha\beta}(x)\,\varphi_{x^\gamma}|_{t=0} + O(\|x\|^2)\right)\\ &= -\mathrm{i}\big(\delta^{\alpha\beta} + O(\|x\|^2)\big)\\ &\quad\times\big(\tfrac{1}{3}(R^\gamma{}_{\alpha\beta\mu}(0) + R^\gamma{}_{\beta\alpha\mu}(0))\,x^\mu\,\eta_\gamma + O(\|x\|^2)\big)\\ &= \frac{2\,\mathrm{i}}{3}\,\operatorname{Ric}^\gamma{}_\mu(0)\,\eta_\gamma\,x^\mu + O(\|x\|^2),\end{aligned} \tag{8.13}$$

$$2\,\mathrm{i}(\ln\,w)_t\,\varphi_t|_{t=0} = \frac{2\,\mathrm{i}}{3}\,\operatorname{Ric}^\alpha{}_\nu(0)\,\eta_\alpha\,x^\nu + O(\|x\|^2), \tag{8.14}$$

$$-2\,\mathrm{i}\,g^{\alpha\beta}(x)\,[\nabla_\alpha(\ln\,w)]\,\nabla_\beta\,\varphi\Big|_{t=0} = -\frac{\mathrm{i}}{3}\,\operatorname{Ric}^\alpha{}_\nu(0)\,\eta_\alpha\,x^\nu + O(\|x\|^2). \tag{8.15}$$

Substitution of (8.9) and (8.13)–(8.15) into (7.3b) yields

$$b_1(0,x;0,\eta) = \mathrm{i}\ \mathrm{Ric}^{\alpha}{}_{\mu}(0)\,\eta_\alpha\, x^\mu + O(\|x\|^2). \tag{8.16}$$

Finally, let us deal with b_0. Formula (8.12) implies that

$$\begin{aligned} w &= 1 + O(\|x\|^2 + t^2), & w_{tt} &= O(\|x\| + |t|), \\ w_x &= O(\|x\| + |t|), & w_{xx} &= \frac{1}{6}\,\mathrm{Ric}(0) + O(\|x\| + |t|). \end{aligned}$$

Substituting the above formulae into (7.3c), we get

$$b_0(0,x;0,\eta) = -\frac{1}{6}\,\mathcal{R}(0) + O(\|x\|). \tag{8.17}$$

Theorem 7.6 tells us that

$$\mathfrak{a}_{-1}(t;0,\eta) = -\frac{\mathrm{i}}{2\,h}\,[\mathfrak{S}_{-2}\,b_2 + \mathfrak{S}_{-1}\,b_1 + \mathfrak{S}_0\,b_0]|_{t=0}\,t + O(t^2)\,. \tag{8.18}$$

Recall that the $\mathfrak{S}_{-2}$, $\mathfrak{S}_{-1}$ and $\mathfrak{S}_0$ in the above formula are the amplitude-to-symbol operators.

Calculating the last term in the square brackets in (8.18) is easy. Namely, using (8.17), we get

$$[\mathfrak{S}_0\,b_0]|_{t=0} = b_0(0,0;0,\eta) = -\frac{1}{6}\,\mathcal{R}(0)\,. \tag{8.19}$$

Calculating the first two terms in the square brackets in (8.18) seems to be a challenging task because the formulae for the operators $\mathfrak{S}_{-2}$ and $\mathfrak{S}_{-1}$ are complicated. However, at $t=0$ and in chosen local coordinates our phase function reads

$$\varphi(0,x;0,\eta) = x^\alpha\,\eta_\alpha$$

and this leads to fundamental simplifications. Namely, at $t=0$ we have

$$[\mathfrak{S}_{-1}\,(\ \cdot\ )]|_{t=0} = \left[\mathrm{i}\,\frac{\partial}{\partial\eta_\alpha}\frac{\partial}{\partial x^\alpha}\,(\ \cdot\ )\right]\Big|_{t=0,\ x=0}\,, \tag{8.20}$$

$$[\mathfrak{S}_{-2}\,(\ \cdot\ )]|_{t=0} = \frac{1}{2}\left[\left(\mathrm{i}\,\frac{\partial}{\partial\eta_\alpha}\frac{\partial}{\partial x^\alpha}\right)^2(\ \cdot\ )\right]\Big|_{t=0,\ x=0}\,. \tag{8.21}$$

Substituting (8.8) and (8.16) into (8.20) and (8.21) respectively, we get

$$[\mathfrak{S}_{-2}\,b_2]|_{t=0} = \mathcal{R}(0)\,, \qquad [\mathfrak{S}_{-1}\,b_1]|_{t=0} = -\mathcal{R}(0)\,. \tag{8.22}$$

Formulae (8.18), (8.19) and (8.22) imply (8.2). □

9. Explicit examples

In this section we will apply our construction to the detailed analysis of two explicit examples.

9.1. The 2-sphere

The first example we will discuss is the 2-sphere. Clearly, for the 2-sphere one can construct the propagator via functional calculus, since eigenvalues and eigenfunctions are known explicitly. However, the 2-sphere is interesting as it represents, in a sense, the 'most singular' instance of a Riemannian manifold in terms of obstructions caused by caustics because the geodesic flow on the cosphere bundle is 2π-periodic. Furthermore, geodesics focus at $t = \pi k$, $k \in \mathbb{Z}$. As we will show, even in this simple example our method provides significant insight.

Let $\mathbb{S}^2$ be the standard 2-sphere embedded in Euclidean space $(\mathbb{E}^3, \delta_E := \mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2)$ via the map $\iota : \mathbb{S}^2 \to \mathbb{E}^3$, in such a way that the south pole is tangent to the plane $z = 0$ at the origin $O = (0, 0, 0)$. The sphere is endowed with the standard round metric $g := \iota^* \delta_E$.

Let us introduce coordinates on $\mathbb{S}^2$ minus the north pole by a stereographic projection onto the xy-plane,

$$\sigma : \mathbb{R}^2 \to \mathbb{S}^2 \setminus \begin{pmatrix} 0 \\ 0 \\ 2 \end{pmatrix}, \qquad \begin{pmatrix} u \\ v \end{pmatrix} \mapsto \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \frac{1}{1+K^2} \begin{pmatrix} u \\ v \\ 2K^2 \end{pmatrix}, \tag{9.1}$$

where $K := \frac{\sqrt{u^2+v^2}}{2}$. The metric in stereographic coordinates reads

$$g = \frac{1}{(1+K^2)^2} \left[\mathrm{d}u^2 + \mathrm{d}v^2 \right]. \tag{9.2}$$

Without loss of generality, we will set $y = (0, 0) \in \mathbb{R}^2$ in stereographic coordinates. Further on we denote by $z = (u, v)$ a generic point on the stereographic plane. Straightforward analysis shows that

$$z^*(t; \eta) = 2 \, \tan(t/2) \, \frac{\eta}{\|\eta\|}, \tag{9.3a}$$

$$\xi^*(t; \eta) = \cos^2(t/2) \, \eta, \tag{9.3b}$$

provide a solution to the Hamiltonian system (2.1) for the Hamiltonian (2.5) with initial conditions $z^*(0,\eta)=(0,0)$ and $\xi^*(0,\eta)=\eta=(\eta_1,\eta_2)$.

Our first goal is to compute the scalar part of the weight w^2 along the flow, i.e.

$$\frac{\rho(y)}{\rho(z)}\det\varphi_{z^\alpha\eta_\beta}\Big|_{z=z^*},$$

for the Levi-Civita phase function φ on the sphere associated with the metric g.

Lemma 9.1. *For the 2-sphere we have*

$$\frac{\rho(y)}{\rho(z)}\det\varphi_{z^\alpha\eta_\beta}\Big|_{z=z^*}=\cos(t)-\mathrm{i}\,\epsilon\,\sin(t). \tag{9.4}$$

Proof. A key ingredient in the computation of (9.4) is formula (4.4) from Theorem 4.4. As a first step, we need to compute the Christoffel symbols of g along the geodesic flow.

By means of (9.2) and (9.3), one obtains

$$\begin{aligned}
\Gamma^u{}_{uu}(u^*,v^*)&=-\frac{\sin(t)}{2}\frac{\eta_u}{\|\eta\|}, & \Gamma^u{}_{uv}(u^*,v^*)&=-\frac{\sin(t)}{2}\frac{\eta_v}{\|\eta\|},\\
\Gamma^u{}_{vv}(u^*,v^*)&=\frac{\sin(t)}{2}\frac{\eta_u}{\|\eta\|}, & \Gamma^v{}_{vv}(u^*,v^*)&=-\frac{\sin(t)}{2}\frac{\eta_v}{\|\eta\|},\\
\Gamma^v{}_{vu}(u^*,v^*)&=-\frac{\sin(t)}{2}\frac{\eta_u}{\|\eta\|}, & \Gamma^v{}_{uu}(u^*,v^*)&=\frac{\sin(t)}{2}\frac{\eta_v}{\|\eta\|}.
\end{aligned} \tag{9.5}$$

Substituting (9.2), (9.3) and (9.5) into (4.4), we get

$$\begin{aligned}
\varphi_{z^\alpha\eta_\beta}\big|_{z=z^*}&=\cos^2(t/2)\\
&\times\begin{pmatrix}
1-[1-\cos(t)+\mathrm{i}\,\epsilon\sin(t)]\dfrac{\eta_2^2}{\|\eta\|^2} & [1-\cos(t)+\mathrm{i}\,\epsilon\sin(t)]\dfrac{\eta_1\eta_2}{\|\eta\|^2}\\
[1-\cos(t)+\mathrm{i}\,\epsilon\sin(t)]\dfrac{\eta_1\eta_2}{\|\eta\|^2} & 1-[1-\cos(t)+\mathrm{i}\,\epsilon\sin(t)]\dfrac{\eta_1^2}{\|\eta\|^2}
\end{pmatrix},
\end{aligned}$$

from which it ensues that

$$\det\varphi_{z^\alpha\eta_\beta}\big|_{z=z^*}=\cos^4(t/2)\,[\cos(t)-\mathrm{i}\,\epsilon\sin(t)]\,.$$

Since $\rho(z^*(t;\eta))=\cos^4(t/2)$ and $\rho(y)=1$, this completes the proof. $\square$

Note that (9.4) is a scalar identity and, as such, independent of the choice of coordinates.

Let $\epsilon = 0$, which corresponds to the adoption of a real-valued phase function. Direct inspection of (9.4) tells us that $\varphi_{z\eta}|_{z=z^*}$ becomes degenerate at $t = \frac{\pi}{2} + \pi k$, $k \in \mathbb{Z}$ and, consequently, w vanishes at these values of t.

If, on the other hand, $\epsilon > 0$, then w is non-zero for all values of t. This fact is the analytic counterpart of the circumvention of the obstruction caused by caustics.

The result of Lemma 9.1 can be used to compute the Maslov index. Let γ be the lift to the Lagrangian submanifold Λ_h of a great circle starting and ending at y and set, for simplicity, $\epsilon = 1$. Then by (2.7), (9.4) we get

$$\vartheta_\varphi = \frac{1}{\pi}\,\mathrm{d}t$$

and, in view of (2.8), we conclude that

$$\operatorname{ind}(\gamma) = \frac{1}{\pi}\int_0^{2\pi} \mathrm{d}t = 2\,.$$

Let us now move on to the calculation of the g-subprincipal symbol of the wave propagator. For the 2-sphere the geodesic distance between two arbitrary points can be computed explicitly via a closed formula. With the above notation, consider the auxiliary map

$$\tilde{\sigma} : \mathbb{R}^2 \to \mathbb{R}^3, \qquad (u,v) \mapsto \frac{1}{1+K^2}\begin{pmatrix} u \\ v \\ K^2 - 1\end{pmatrix},$$

which is nothing but the map (9.1) shifted by $(0,0,-1)$. Then the geodesic distance between (u,v) and (u',v') is given by

$$\operatorname{dist}((u,v),(u',v')) = \arccos\left[\,\tilde{\sigma}(u,v)\,\cdot\,\tilde{\sigma}(u',v')\,\right], \tag{9.6}$$

where the dot stands for the inner product in $\mathbb{E}^3$.

Formulae (9.6) and (2.1) yield an explicit representation for (4.3), which can be used to set up the algorithm described in Section 7.

For $\epsilon = 1$ the functions appearing on the RHS of (7.20) read

$$\mathfrak{S}_{-2}\, b_2 = \frac{1}{4}\left(-3 + 2\mathrm{e}^{2\,\mathrm{i}\,t} + \mathrm{e}^{4\,\mathrm{i}\,t}\right), \tag{9.7a}$$

$$\mathfrak{S}_{-1}\, b_1 = \frac{1}{6}\left(7 - 4\mathrm{e}^{2\,\mathrm{i}\,t} - 3\mathrm{e}^{4\,\mathrm{i}\,t}\right), \tag{9.7b}$$

$$\mathfrak{S}_0\, b_0 = \frac{1}{12}\left(-8 + \mathrm{e}^{2\,\mathrm{i}\,t}\right). \tag{9.7c}$$

Substitution of (9.7a)–(9.7c) into (7.20) yields a formula for the g-subprincipal symbol:

$$\mathfrak{a}_{-1}(t;y,\eta;1) = \frac{\mathrm{i}\,t}{8\,\|\eta\|} + \frac{2\mathrm{e}^{2\,\mathrm{i}\,t} + 3\mathrm{e}^{4\,\mathrm{i}\,t} - 5}{96\,\|\eta\|}.$$

For a general $\epsilon > 0$ the corresponding formulae are more complicated and the final expression for the g-subprincipal symbol reads

$$\mathfrak{a}_{-1}(t;y,\eta;\epsilon) = \frac{\mathrm{i}\,t}{8\,\|\eta\|} + \frac{\mathrm{i}\sin(2t) - 4\epsilon\sin^2(t) + 3\,\mathrm{i}\,\epsilon^2\sin(2t) + 6\epsilon^3\sin^2(t)}{48\,\|\eta\|\,(\cos(t) - \mathrm{i}\epsilon\sin(t))^2}. \tag{9.8}$$

Remark 9.2. For $t \neq \pi/2 + \pi k$, $k \in \mathbb{Z}$, the g-subprincipal symbol admits the following expansion in powers of ϵ:

$$\begin{aligned}\mathfrak{a}_{-1}(t;y,\eta;\epsilon) = \frac{\mathrm{i}\,t}{8\,\|\eta\|} + \frac{\mathrm{i}\,\tan(t)}{24\,\|\eta\|} - \frac{\epsilon\,\tan^2(t)}{6\,\|\eta\|} \\ + \mathrm{i}\sum_{k=2}^{\infty} \frac{(\mathrm{i}\,\epsilon)^k}{24\,\|\eta\|}\,(\tan(t))^{k-1}\left((3k+1)\tan^2(t) - 3\right).\end{aligned}$$

Note that for $\epsilon = 0$ the above formula turns to

$$\mathfrak{a}_{-1}(t;y,\eta;0) = \frac{\mathrm{i}}{24\,\|\eta\|}\,(3t + \tan(t)), \tag{9.9}$$

which is the g-subprincipal symbol of the propagator for the real-valued Levi-Civita phase function. Of course, formula (9.9) can only be used for $t \in (-\pi/2, \pi/2)$: topological obstructions prevent the use of the real-valued phase function for large t. It is easy to check that (9.9) agrees with (8.1), with $\mathcal{R}(y) = 2$.

Let us now run a test for our formula (9.8). To this end, let us shift the Laplacian by a quarter,

$$-\Delta \mapsto -\Delta + \frac{1}{4}. \tag{9.10}$$

Note that the eigenvalues of the operator $\sqrt{-\Delta+1/4}$ are half-integer, hence, the corresponding propagator $\widetilde{U}(t) := \mathrm{e}^{-\mathrm{i}t\sqrt{-\Delta+1/4}}$ is 2π-antiperiodic,

$$\widetilde{U}(t+2\pi) = -\widetilde{U}(t). \tag{9.11}$$

Going back to Lemma 7.2, we see that the shift of the Laplacian (9.10) does not affect b_2 and b_1, but shifts b_0 as

$$b_0 \mapsto b_0 + 1/4\,. \tag{9.12}$$

Theorem 7.6 and formula (9.12) tell us that the g-subprincipal symbol of the propagator transforms as

$$\mathfrak{a}_{-1}(t;y,\eta;0) \mapsto \mathfrak{a}_{-1}(t;y,\eta;0) - \frac{\mathrm{i}\,t}{8\|\eta\|}\,. \tag{9.13}$$

Applying the transformation (9.13) to formula (9.8), we see that the g-subprincipal symbol of the propagator becomes 2π-periodic. It remains only to reconcile the periodicity of the full symbol of the propagator with the antiperiodicity (9.11) of the propagator itself. This is to do with the Maslov index: formulae (5.3) and (9.4) tell us that the weight w picks up a change of sign as we traverse the periodic geodesic, a great circle.

It is known that constructing the wave propagator associated with the shifted Laplacian (9.10) is often easier and some formulae are available in the literature. For example, formulae for the wave kernel of shifted Laplacians on rank one symmetric spaces was computed in [BuOl]. See also [ChTa], [Sm, Section 3].

9.2. The hyperbolic plane

From a strictly rigorous point of view, our construction works for closed manifolds only. However, the compactness assumption is largely technical and can be relaxed, even though this generalisation is not absolutely straightforward. In the current paper we refrain from carrying out such an extension, but we discuss a non-compact example, formally applying our algorithm to the hyperbolic plane.

Adopting the hyperboloid model for the hyperbolic plane, we consider the upper sheet of the hyperboloid

$$\mathbb{H}^2 := \{(x,y,z) \in \mathbb{R}^3 \mid x^2+y^2-z^2=-1,\ z>0\}$$

endowed with metric $\delta_{\mathbb{H}} = \mathrm{d}x^2 + \mathrm{d}y^2 - \mathrm{d}z^2$. Projecting $\mathbb{H}^2$ onto $\mathbb{R}^2$ with coordinates (u, v), we obtain the induced metric

$$g = \frac{1}{1+u^2+v^2}\left[(1+v^2)\,\mathrm{d}u^2 - 2uv\,\mathrm{d}u\,\mathrm{d}v + (1+u^2)\,\mathrm{d}v^2\right].$$

The metric g is Riemannian, with constant Gaussian curvature equal to -1.

Setting, without loss of generality, $y = 0$ and denoting $z = (u, v)$, the cogeodesic flow is given by

$$\begin{aligned} z^*(t;\eta) &= \sinh(t)\,\frac{\eta}{\|\eta\|}\,, \\ \xi^*(t;\eta) &= \frac{1}{\cosh(t)}\,\eta\,. \end{aligned}$$

Unlike the sphere, the hyperbolic plane does not present caustics due to its negative curvature. Hence, there are no obstructions to a construction global in time with real-valued phase function. In particular, the Levi-Civita phase function with $\epsilon = 0$ can be used.

Arguing as for the 2-sphere, one gets for $\epsilon \geq 0$

$$\begin{aligned} \varphi_{z^\alpha \eta_\beta}\big|_{z=x^*} &= \frac{1}{\|\eta\|^2} \\ \times &\begin{pmatrix} \eta_1^2 \operatorname{sech}(t) + \eta_2^2(\cosh(t) + \mathrm{i}\,\epsilon\sinh(t)) & -\eta_1\eta_2 \tanh(t)(\sinh(t) + \mathrm{i}\,\epsilon\cosh(t)) \\ -\eta_1\eta_2 \tanh(t)(\sinh(t) + \mathrm{i}\,\epsilon\cosh(t)) & \eta_2^2 \operatorname{sech}(t) + \eta_1^2(\cosh(t) + \mathrm{i}\,\epsilon\sinh(t)) \end{pmatrix} \end{aligned}$$

and

$$\frac{\rho(y)}{\rho(x)}\det\,\varphi_{z^\alpha\eta_\beta}\bigg|_{z=z^*} = \cosh(t) + \mathrm{i}\,\epsilon\,\sinh(t).$$

Direct inspection immediately reveals that, as expected, $\varphi_{z\eta}|_{z=z^*}$ is non-degenerate for all times, even with $\epsilon = 0$.

Carrying out our algorithm for $\epsilon = 0$, we establish that the homogeneous components of the reduced amplitude read

$$\mathfrak{S}_{-2}\,a_2 = -\frac{2}{3}(2 + \cosh(2t))\operatorname{sech}^2(t)\,,$$

$$\mathfrak{S}_{-1}\,a_1 = \frac{2}{3}(2 + \cosh(2t))\operatorname{sech}^2(t)\,,$$

$$\mathfrak{S}_0\,a_0 = \frac{1}{12}(3 + \operatorname{sech}^2(t))\,.$$

Substitution of the above expressions into (7.20) yields a formula for the g-subprincipal symbol:

$$\mathfrak{a}_{-1}(t; y, \eta; 0) = -\frac{\mathrm{i}}{24\,\|\eta\|}\,(3t + \tanh(t))\,. \tag{9.16}$$

Note that formulae for the hyperbolic plane are very similar to those for the sphere, with trigonometric functions being replaced by their hyperbolic counterparts. This is consistent with the results in [Ta], see also [Ze12, Sec. 3.7.2]. Formula (9.16) is, of course, in agreement with (8.1), with $\mathcal{R}(y) = -2$.

Our explicit examples gave us the opportunity to illustrate, once again, the importance of formula (4.4): it allows one to extract topological information by means of a simple direct computation.

10. Circumventing the obstructions: a geometric picture

As discussed in the previous sections, the weight w defined by formula (5.3) is a crucial object in our mathematical construction in that it carries important information about Λ_h. It is possible, for instance, to compute the Maslov index purely in terms of w. The fact that, in general, a construction global in time is impossible using real-valued phase functions can be traced back to the degeneracy of w. In this section we will provide a geometric description of $\varphi_{x\eta}$, the key ingredient of w, along the flow.

Let us fix a point $y \in M$ and consider the one-parameter family of d-dimensional smooth submanifolds of the cotangent bundle defined by

$$\mathcal{T}_y(t) := \{(x^*(t; y, \eta), \xi^*(t; y, \eta)) \in T^*M \mid \eta \in T'_yM\}.$$

For every value of t, $\mathcal{T}_y(t)$ consists of all points of the cotangent bundle corresponding to the cogeodesic flow at time t for the initial position y and all possible momenta. The smoothness of $\mathcal{T}_y(t)$ follows, for example, from the preservation of the symplectic volume.

The manifolds $\mathcal{T}_y(t)$ are Lagrangian. In fact, $\mathcal{T}_y(0) = T'_yM = T^*_yM \setminus \{0\}$ is the punctured cotangent fibre at y, which is clearly Lagrangian, and the cogeodesic flow preserves the symplectic form.

In the following we will construct a family of metrics associated with the above submanifolds. In the rest of this section we will drop the arguments t and y in x^* and ξ^* whenever these arguments are fixed, writing simply $x^*(\eta)$ and $\xi^*(\eta)$.

In an arbitrary coordinate system a small increment $\delta\eta$ in momentum produces an increment in $x^*(\eta)$ given by

$$[x^*(\eta+\delta\eta)-x^*(\eta)]^\alpha = [x^*(\eta)]^\alpha_{\eta_\mu}\,\delta\eta_\mu + O(\|\delta\eta\|^2).$$

This allows us to define a bilinear form

$$Q^{\mu\nu}(\eta;t,y) := g_{\alpha\beta}(x^*(\eta))\,q^{\alpha\mu}(\eta;t,y)\,q^{\beta\nu}(\eta;t,y)\,, \tag{10.1}$$

where

$$q^{\alpha\mu}(\eta;t,y) := [x^*(\eta)]^\alpha_{\eta_\mu}\,. \tag{10.2}$$

We call Q *the position form.*

An analogous construction is possible for momentum $\xi^*(\eta)$, although extra care is needed due to the fact that $\xi^*(\eta)$ and $\xi^*(\eta+\delta\eta)$ live in different fibres of the bundle. Under the assumption that $\delta\eta$ is sufficiently small, let us parallel transport $\xi^*(\eta+\delta\eta)$ along the (unique) geodesic going from $x^*(\eta+\delta\eta)$ to $x^*(\eta)$, denoted by $\gamma:[0,1]\to M$. The parallel transport equation reads

$$\dot\gamma^\alpha(s)\,\nabla_\alpha\,\zeta(\gamma(s))_\beta = \dot\gamma^\alpha(s)\,[\partial_\alpha\zeta_\beta(\gamma(s)) - \Gamma^\rho{}_{\alpha\beta}(\gamma(s))\,\zeta_\rho(\gamma(s))] = 0\,, \tag{10.3}$$

where ζ denotes the image under parallel transport of $\xi^*(\eta+\delta\eta)$ along γ. It is not hard to check that the solution to (10.3) is given by

$$\zeta_\alpha(\gamma(s)) = \xi^*_\alpha(\eta+\delta\eta) + \Gamma^\rho{}_{\alpha\beta}(\gamma(s))\,\xi^*_\rho(\eta)\,s\,(\delta x^*)^\beta + O(\|\delta x^*\|^2)\,,$$

where $\delta x^* = x^*(\eta) - x^*(\eta+\delta\eta)$. Hence, we get

$$\begin{aligned}\zeta_\alpha(\gamma(1)) - \xi^*_\alpha(\eta) = &\left[(\xi^*_\alpha(\eta))_{\eta_\mu} - \Gamma^\rho{}_{\alpha\beta}(x^*(\eta))\,\xi^*_\rho(\eta)\,(x^*(\eta))^\beta_{\eta_\mu}\right]\,(\delta\eta)_\mu\\ &+ O(\|\delta\eta\|^2)\,.\end{aligned}$$

Put

$$p^{\alpha\mu}(\eta;t,y) := g^{\alpha\gamma}(x^*(\eta))\left[(\xi^*_\gamma(\eta))_{\eta_\mu} - \Gamma^\rho{}_{\gamma\beta}(x^*(\eta))\,\xi^*_\rho(\eta)\,(x^*(\eta))^\beta_{\eta_\mu}\right] \tag{10.4}$$

and define the bilinear form

$$P^{\mu\nu}(\eta;t,y) := g_{\alpha\beta}(x^*(\eta))\,p^{\alpha\mu}(\eta;t,y)\,p^{\beta\nu}(\eta;t,y)\,. \tag{10.5}$$

We call P *the momentum form.*

It is convenient, at this point, to redefine the position and momentum forms by lowering their indices using the metric g at the point y. Hence, further on we have $Q = Q_{\mu\nu}$ and $P = P_{\mu\nu}$. Clearly, by construction, we have

$$Q, P \in C^\infty(\mathcal{T}_y(t); \otimes_s^2 T^*\mathcal{T}_y(t)).$$

Our Q and P are natural candidates for metrics on $\mathcal{T}_y(t)$. This turns out not to be the case: P and Q are pseudometrics but not necessarily metrics. However, their sum is a metric.

Theorem 10.1. *Let a and b be positive parameters. Then the linear combination of the position and momentum forms*

$$ah^2 Q + bP \in C^\infty(\mathcal{T}_y(t); \otimes_s^2 T^*\mathcal{T}_y(t)) \tag{10.6}$$

is a metric.

The h in the above formula stands for $h(y, \eta)$. This factor has been introduced so that both terms have the same degree of homogeneity (zero) in η.

Proof. Our Q and P are symmetric and can be written as $Q = q^T g\, q$, $P = p^T g\, p$, which implies that they are non-negative. To prove that their linear combination $ah^2 Q + bP = ah^2 q^T g\, q + b\, p^T g\, p$ is a metric we only need show that it is non-degenerate. Choosing normal geodesic coordinates x centred at $x^*(t; y, \eta)$, it is easy to see that $v \in T_{(x^*(\eta), \xi^*(\eta))}\mathcal{T}_y(t)$ is in the null space of $ah^2 Q + bP$ if and only if $v^\flat$ satisfies

$$[x^*(\eta)]^\alpha_{\eta_\mu}\, v_\mu = 0 \qquad \text{and} \qquad [\xi^*_\alpha(\eta)]_{\eta_\mu}\, v_\mu = 0\,. \tag{10.7}$$

Since the Hamiltonian flow is non-degenerate, i.e. it preserves the tautological 1-form, the two conditions (10.7) cannot be simultaneously fulfilled unless $v = 0$. Therefore, $ah^2 Q + bP$ is non-degenerate. $\square$

The metric $ah^2 Q + bP$ is closely related to $\varphi_{x\eta}$ along the flow: condition (iii) in Definition 2.1 translates, in geometric terms, into the statement that the intersection of null spaces of Q and P is the zero subspace. The weight w becoming degenerate in the case of a real-valued phase function corresponds, in this geometric picture, to Q and P separately not being metrics. We will show this below for the case of the 2-sphere, as an explicit example.

Before moving to that, let us make the aforementioned relation between Q, P on the one hand and $\varphi_{x\eta}$ on the other mathematically precise.

Theorem 10.2. *We have*

$$\varphi_{x^\alpha \eta_\mu}\big|_{x=x^*} = g_{\alpha\beta}(x^*)\left[p^{\beta\mu} - \mathrm{i}\,\epsilon\, h\, q^{\beta\mu}\right]. \tag{10.8}$$

Proof of Theorem 10.2. The identity (10.8) is established by comparing (4.4) with (10.2) and (10.4). □

Example 10.3 (Position and momentum forms for $\mathbb{S}^2$). With the notation of Section 9, the quantities q and p defined by formulae (10.2) and (10.4) read

$$\begin{aligned} q^{\alpha\mu} &= \frac{2\,\tan(t/2)}{\|\eta\|^3}\begin{pmatrix} \eta_2^2 & -\eta_1\eta_2 \\ -\eta_1\eta_2 & \eta_1^2 \end{pmatrix}, \\ p^{\alpha\mu} &= \frac{1}{\cos^2(t/2)\,\|\eta\|^2}\begin{pmatrix} \eta_1^2+\eta_2^2\cos(t) & \eta_1\eta_2(1-\cos(t)) \\ \eta_1\eta_2(1-\cos(t)) & \eta_2^2+\eta_1^2\cos(t) \end{pmatrix}. \end{aligned}$$

Consequently, the position and momentum forms are given by

$$\begin{aligned} Q_{\mu\nu} &= \frac{\sin^2(t)}{\|\eta\|^4}\begin{pmatrix} \eta_2^2 & -\eta_1\,\eta_2 \\ -\eta_1\,\eta_2 & \eta_1^2 \end{pmatrix}, \\ P_{\mu\nu} &= \frac{1}{\|\eta\|^2}\begin{pmatrix} \eta_1^2+\eta_2^2\,\cos^2(t) & \eta_1\,\eta_2\,\sin^2(t) \\ \eta_1\,\eta_2\,\sin^2(t) & \eta_2^2+\eta_1^2\,\cos^2(t) \end{pmatrix}. \end{aligned}$$

We have $\det Q = 0$ and $\det P = \cos^2(t)$. This implies that P, which is associated with the real part of (4.4) via (10.8) and (10.5), becomes degenerate for $t = \pi/2$. However, for the full metric $h^2 Q + P$ we have in chosen local coordinates $h^2 Q_{\mu\nu} + P_{\mu\nu} = \delta_{\mu\nu}$, so that that the full metric $h^2 Q + P$ is non-degenerate for all $t \in \mathbb{R}$. This example is remarkable in that the metric (10.6) with $a = b = 1$ does not depend on t.

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Appendix A. The amplitude-to-symbol operator

In this appendix we will provide mathematical proofs and rigorous justification to the amplitude reduction algorithm described in Section 5, developing ideas outlined in [SaVa].

With the notation established throughout the paper, let $a \in S^m_{\mathrm{ph}}(\mathbb{R} \times M \times T'M)$ be a polyhomogeneous function of order m,

$$a \sim \sum_{k=0}^{\infty} a_{m-k} \,.$$

Consider the oscillatory integral

$$\mathcal{I}_\varphi(a) = \int_{T^*_y M} \mathrm{e}^{\mathrm{i}\varphi(t,x;y,\eta)}\, a(t,x;y,\eta)\, w(t,x;y,\eta)\, đ\eta \,, \tag{A.1}$$

where φ is any phase function of class $\mathcal{L}_h$. For the sake of clarity, we drop here the dependence of functions on extra parameters (e.g. ϵ).

It is a well known fact that, modulo an infinitely smooth contribution,

$$\mathcal{I}_\varphi(a) \overset{\operatorname{mod} C^\infty}{=} \int_{T^*_y M} \mathrm{e}^{\mathrm{i}\varphi(t,x;y,\eta)}\, \mathfrak{a}(t;y,\eta)\, w(t,x;y,\eta)\, đ\eta, \tag{A.2}$$

for some $\mathfrak{a} = \mathfrak{a}(t;y,\eta)$. We call the a in (A.1) *amplitude* and the $\mathfrak{a}$ in (A.2) *symbol.*

In this framework, one can construct an amplitude-to-symbol operator

$$\mathfrak{S} : a \mapsto \mathfrak{a}.$$

The aim of this appendix is to write down the operator $\mathfrak{S}$ explicitly.

Theorem A.1. *The amplitude-to-symbol operator* $\mathfrak{S}$ *reads*

$$\mathfrak{S} \sim \sum_{k=0}^{\infty} \mathfrak{S}_{-k}, \tag{A.3}$$

where

$$\mathfrak{S}_0 = (\,\cdot\,)|_{x=x^*}\,, \tag{A.4}$$

$$\mathfrak{S}_{-k} = \mathfrak{S}_0 \left[\mathrm{i}\, w^{-1} \frac{\partial}{\partial \eta_\beta}\, w \left(1 + \sum_{1 \le |\boldsymbol{\alpha}| \le 2k-1} \frac{(-\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!\,(|\boldsymbol{\alpha}|+1)}\, L_{\boldsymbol{\alpha}} \right) L_\beta \right]^k \tag{A.5}$$

with $L_\alpha := [(\varphi_{x\eta})^{-1}]_\alpha{}^\beta \dfrac{\partial}{\partial x^\beta}$.

We begin with two general comments regarding our phase function, which follow from the properties in Definition 2.1. Firstly, as already observed, $\varphi_\eta(t,x^*;y,\eta)=0$. Secondly, one can always assume that $\det(\varphi_{x^\alpha\eta_\beta})\ne 0$ on $\operatorname{supp} a$. If this is not the case, it is enough to multiply a by a smooth cut-off χ supported in a neighbourhood of

$$\mathfrak{C}=\{(t,x;y,\eta)\mid x=x^*(t;y,\eta)\}\subset\mathbb{R}\times M\times T'M$$

small enough. The oscillatory integrals $\mathcal{I}_\varphi(a)$ and $\mathcal{I}_\varphi(\chi\, a)$ differ by infinitely smooth contributions.

The idea of the proof, at times quite technical, goes as follows. Expand the amplitude a in power series in x about $x=x^*$. With the notation $a^*=a|_{x=x^*}$, we have

$$a=a^*+(x-x^*)^\alpha\, b_\alpha \tag{A.6}$$

for some covector $b=b(t,x;y,\eta)$. Plugging (A.6) into (A.1), we obtain

$$\begin{aligned}
\mathcal{I}_\varphi(a)&=\int_{T'_yM}e^{i\varphi}\,a^*\,w\,đ\eta+\int_{T'_yM}e^{i\varphi}\,(x-x^*)^\alpha\,b_\alpha\,w\,đ\eta\\
&=\int_{T'_yM}e^{i\varphi}\,a^*\,w\,đ\eta+\int_{T'_yM}e^{i\varphi}\,\varphi_{\eta_\alpha}\,\tilde b_\alpha\,w\,đ\eta\\
&=\int_{T'_yM}e^{i\varphi}\,a^*\,w\,đ\eta+\int_{T'_yM}\frac{1}{i}\left(\frac{\partial}{\partial\eta_\alpha}e^{i\varphi}\right)\tilde b_\alpha\,w\,đ\eta\\
&=\int_{T'_yM}e^{i\varphi}\,a^*\,w\,đ\eta+\int_{T'_yM}e^{i\varphi}\,i\,w^{-1}\left(\frac{\partial}{\partial\eta_\alpha}\tilde b_\alpha\,w\right)w\,đ\eta\,,
\end{aligned}\tag{A.7}$$

where the covector $\tilde b$ can be written down explicitly in terms of b and φ. It is easy to see that

$$i\,w^{-1}\left(\frac{\partial}{\partial\eta_\alpha}\tilde b_\alpha\,w\right)\in S^{m-1}_{\mathrm{ph}}(\mathbb{R}\times M\times T'M).$$

The first integral on the RHS of (A.7) has amplitude independent of x, whereas the second one has amplitude whose order is decreased by one. Repeating the above argument, we can recursively reduce the order and eventually obtain an oscillatory integral with x-independent amplitude

$$\mathfrak{a} \sim \sum_{k=0}^{\infty} \mathfrak{a}_{m-k}, \quad \mathfrak{a}_{m-k} \in S^{m-k}_{\mathrm{ph}}(\mathbb{R} \times T'M),$$

plus an oscillatory integral with amplitude in $S^{-\infty}(\mathbb{R} \times M \times T'M)$.

Note that the b and $\tilde{b}$ in the above argument are both covectors but in a different sense: b_α behaves as a covector under changes of local coordinates x, whereas $\tilde{b}_\alpha$ behaves as a covector under changes of local coordinates y.

The actual proof relies on a more sophisticated argument, which allows one to explicitly and constructively compute $\mathfrak{a}$. The whole idea, rooted in a version of the Malgrange preparation theorem, is to factor out φ_{η_α} rather than simply $(x - x^*)^\alpha$ in equation (A.6). Such factorisation will be eventually achieved in formula (A.23). A crucial point worth stressing is that the whole construction is global and covariant.

Before addressing the proof of Theorem A.1 we need to state and prove a preparatory lemma.

Lemma A.2. *The operators*

$$L_\alpha = (\varphi^{-1}_{x\eta})_\alpha{}^\gamma \frac{\partial}{\partial x^\gamma} \tag{A.8}$$

commute. Namely, for all $\alpha, \beta = 1, \dots, d$ *we have*

$$[L_\alpha, L_\beta] = 0. \tag{A.9}$$

Proof. We have

$$\begin{aligned} L_\alpha L_\beta - L_\beta L_\alpha &= (\varphi^{-1}_{x\eta})_\alpha{}^\mu \frac{\partial}{\partial x^\mu} (\varphi^{-1}_{x\eta})_\beta{}^\nu \frac{\partial}{\partial x^\nu} - (\varphi^{-1}_{x\eta})_\beta{}^\nu \frac{\partial}{\partial x^\nu} (\varphi^{-1}_{x\eta})_\alpha{}^\mu \frac{\partial}{\partial x^\mu} \\ &= \left((\varphi^{-1}_{x\eta})_\alpha{}^\mu [(\varphi^{-1}_{x\eta})_\beta{}^\nu]_{x^\mu}\right) \frac{\partial}{\partial x^\nu} - \left((\varphi^{-1}_{x\eta})_\beta{}^\nu [(\varphi^{-1}_{x\eta})_\alpha{}^\mu]_{x^\nu}\right) \frac{\partial}{\partial x^\mu} \\ &= \left((\varphi^{-1}_{x\eta})_\alpha{}^\nu [(\varphi^{-1}_{x\eta})_\beta{}^\mu]_{x^\nu} - (\varphi^{-1}_{x\eta})_\beta{}^\nu [(\varphi^{-1}_{x\eta})_\alpha{}^\mu]_{x^\nu}\right) \frac{\partial}{\partial x^\mu} \,. \end{aligned}$$

Contracting with $(\varphi_{x\eta})_\gamma{}^\alpha\,(\varphi_{x\eta})_\rho{}^\beta$, we get

$$
\begin{aligned}
&(\varphi_{x\eta})_\gamma{}^\alpha\,(\varphi_{x\eta})_\rho{}^\beta\,[L_\alpha, L_\beta]\\
&\qquad = \Big((\varphi_{x\eta})_\rho{}^\beta[(\varphi_{x\eta}^{-1})_\beta{}^\mu]_{x^\gamma} - (\varphi_{x\eta})_\gamma{}^\alpha\,[(\varphi_{x\eta}^{-1})_\alpha{}^\mu]_{x^\rho}\Big)\,\frac{\partial}{\partial x^\mu}\\
&\qquad = \Big(-[(\varphi_{x\eta})_\rho{}^\beta]_{x^\gamma}(\varphi_{x\eta}^{-1})_\beta{}^\mu + [(\varphi_{x\eta})_\gamma{}^\alpha]_{x^\rho}\,(\varphi_{x\eta}^{-1})_\alpha{}^\mu\Big)\,\frac{\partial}{\partial x^\mu}\\
&\qquad = \big(-\varphi_{x^\rho x^\gamma \eta_\beta}\,(\varphi_{x\eta}^{-1})_\beta{}^\mu + \varphi_{x^\gamma x^\rho \eta_\alpha}\,(\varphi_{x\eta}^{-1})_\alpha{}^\mu\big)\,\frac{\partial}{\partial x^\mu}\\
&\qquad = \big(-\varphi_{x^\rho x^\gamma \eta_\alpha}\,(\varphi_{x\eta}^{-1})_\alpha{}^\mu + \varphi_{x^\gamma x^\rho \eta_\alpha}\,(\varphi_{x\eta}^{-1})_\alpha{}^\mu\big)\,\frac{\partial}{\partial x^\mu}\\
&\qquad = 0.
\end{aligned}
\tag{A.10}
$$

Since $\varphi_{x\eta}$ is non-degenerate, (A.10) is equivalent to (A.9). □

We are now in a position to prove Theorem A.1.

Proof of Theorem A.1. The first step is to show that it is possible to write, modulo $O(\|x-x^*\|^\infty)$, the amplitude a as

$$
a(t,x;y,\eta) = a(t,x^*(t;y,\eta);y,\eta) + \varphi_{\eta_\alpha}(t,x;y,\eta)\,\tilde b_\alpha(t,x;y,\eta)
\tag{A.11}
$$

for some $\tilde b$.

In order to write down explicitly the $\tilde b$ appearing in formula (A.11), let us introduce the operators

$$
F_0 := 1,
\tag{A.12}
$$

$$
F_k := \sum_{|\boldsymbol\alpha|=k} \frac{(\varphi_\eta)^{\boldsymbol\alpha}}{\boldsymbol\alpha!} L_{\boldsymbol\alpha}\,,
\tag{A.13}
$$

where $\boldsymbol\alpha = (\alpha_1,\alpha_2,\dots,\alpha_d)\in\mathbb{N}_0^d$ is a multi-index, $\boldsymbol\alpha! = \alpha_1!\,\alpha_2!\cdots\alpha_d!\,$, $(\varphi_\eta)^{\boldsymbol\alpha} = (\varphi_{\eta_1})^{\alpha_1}(\varphi_{\eta_2})^{\alpha_2}\cdots(\varphi_{\eta_d})^{\alpha_d}$, $L_{\boldsymbol\alpha} = (L_1)^{\alpha_1}(L_2)^{\alpha_2}\cdots(L_d)^{\alpha_d}$. In view of Lemma A.2, F_k is well defined and the order of the L_α's is irrelevant. Note also that the coefficients $\frac{1}{\boldsymbol\alpha!}$ appearing in (A.13) are the ones from the algebraic multinomial expansion

$$
(z_1+\ldots+z_d)^k = k!\sum_{|\boldsymbol\alpha|=k}\frac{1}{\boldsymbol\alpha!}\,z^{\boldsymbol\alpha},
\tag{A.14}
$$

a generalisation of the binomial expansion.

Formulae (A.13) and (A.14) imply

$$(k+1)F_{k+1} = \sum_{\gamma=1}^{d} \varphi_{\eta_\gamma} F_k \, L_\gamma \, . \tag{A.15}$$

Furthermore, we have

$$\begin{aligned} F_1 \, F_k - k \, F_k &= \left(\sum_{\gamma=1}^{d} \varphi_{\eta_\gamma} \, L_\gamma \right) F_k - k \, F_k \\ &= \sum_{\gamma,\mu=1}^{d} \varphi_{\eta_\gamma} (\varphi_{x\eta}^{-1})_\gamma{}^\mu \sum_{|\boldsymbol{\alpha}|=k} \frac{[(\varphi_\eta)^{\boldsymbol{\alpha}}]_{x^\mu}}{\boldsymbol{\alpha}!} L_{\boldsymbol{\alpha}} \\ &\quad + \sum_{\gamma=1}^{d} \varphi_{\eta_\gamma} \sum_{|\boldsymbol{\alpha}|=k} \frac{(\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!} L_\gamma L_{\boldsymbol{\alpha}} - k \, F_k \\ &= k \, F_k + \sum_{\gamma=1}^{d} \varphi_{\eta_\gamma} \sum_{|\boldsymbol{\alpha}|=k} \frac{(\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!} L_{\boldsymbol{\alpha}} L_\gamma - k \, F_k \\ &= \sum_{\gamma=1}^{d} \varphi_{\eta_\gamma} F_k \, L_\gamma \, . \end{aligned} \tag{A.16}$$

Combining formulae (A.15) and (A.16), we arrive at a recurrent formula for our operators F_k :

$$(k+1)F_{k+1} = F_1 \, F_k - k \, F_k \, . \tag{A.17}$$

It turns out that the functions $(\varphi_\eta)^{\boldsymbol{\alpha}}$ with $|\boldsymbol{\alpha}| \ge k$ are eigenfunctions of the operators F_k. Namely, we have

$$F_k (\varphi_\eta)^{\boldsymbol{\alpha}} = \begin{cases} 0, & |\boldsymbol{\alpha}| < k, \\ \binom{|\boldsymbol{\alpha}|}{k} (\varphi_\eta)^{\boldsymbol{\alpha}}, & |\boldsymbol{\alpha}| \ge k. \end{cases} \tag{A.18}$$

Formula (A.18) can be proved by induction. It is clearly true for $k = 0$. Let us assume it is true for $k = n$. Let us prove it for $k = n + 1$. If $|\boldsymbol{\alpha}| < n$, then the required result immediately follows from formula (A.17) and the inductive assumption. If $|\boldsymbol{\alpha}| \ge n$, then formula (A.17) and the inductive assumption give us

$$\begin{aligned}F_{n+1}(\varphi_\eta)^{\boldsymbol{\alpha}} &= \frac{1}{n+1}\binom{|\boldsymbol{\alpha}|}{n}\left[F_1(\varphi_\eta)^{\boldsymbol{\alpha}} - n(\varphi_\eta)^{\boldsymbol{\alpha}}\right] \\ &= \frac{1}{n+1}\binom{|\boldsymbol{\alpha}|}{n}\left[|\boldsymbol{\alpha}|(\varphi_\eta)^{\boldsymbol{\alpha}} - n(\varphi_\eta)^{\boldsymbol{\alpha}}\right] \\ &= \frac{|\boldsymbol{\alpha}|-n}{n+1}\binom{|\boldsymbol{\alpha}|}{n}(\varphi_\eta)^{\boldsymbol{\alpha}} = \begin{cases} 0, & |\boldsymbol{\alpha}| = n, \\ \binom{|\boldsymbol{\alpha}|}{n+1}(\varphi_\eta)^{\boldsymbol{\alpha}}, & |\boldsymbol{\alpha}| > n,\end{cases}\end{aligned}$$

as required.

Formula (A.18) is, effectively, a generalised version of Euler's formula for homogeneous functions.

Given a multi-index $\boldsymbol{\alpha} \neq 0$, we have the elementary identity

$$0 = (1-1)^{|\boldsymbol{\alpha}|} = \sum_{k=0}^{|\boldsymbol{\alpha}|}(-1)^k\binom{|\boldsymbol{\alpha}|}{k} = 1 + \sum_{k=1}^{|\boldsymbol{\alpha}|}(-1)^k\binom{|\boldsymbol{\alpha}|}{k}.$$

The above identity and formula (A.18) imply

(A.19)

$$(\varphi_\eta)^{\boldsymbol{\alpha}} = -\left(\sum_{k=1}^{|\boldsymbol{\alpha}|}(-1)^k F_k\right)(\varphi_\eta)^{\boldsymbol{\alpha}} = -\left(\sum_{k=1}^{\infty}(-1)^k F_k\right)(\varphi_\eta)^{\boldsymbol{\alpha}}, \qquad \forall \boldsymbol{\alpha} \neq 0.$$

Consider now a function $a(t,x;y,\eta)$. It can be expanded into an asymptotic series in powers of $x-x^*$. Observe that φ_η can also be expanded into an asymptotic series in powers of $x-x^*$ and, furthermore, in view of Definition 2.1 this series can be inverted, giving an asymptotic expansion of $x-x^*$ in powers of φ_η. Consequently, the function $a(t,x;y,\eta)$ can be expanded into an asymptotic series in powers of φ_η. The coefficients of the latter expansion are determined using the fact that

$$\left[L_{\boldsymbol{\alpha}}(\varphi_\eta)^{\boldsymbol{\beta}}\right]\Big|_{x=x^*} = \begin{cases}\boldsymbol{\alpha}!, & \boldsymbol{\alpha} = \boldsymbol{\beta}, \\ 0, & \boldsymbol{\alpha} \neq \boldsymbol{\beta}.\end{cases}$$

This gives us

$$a \simeq \sum_{|\boldsymbol{\alpha}|\geq 0} \frac{(\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!}\left[L_{\boldsymbol{\alpha}} a\right]\big|_{x=x^*}. \tag{A.20}$$

The symbol $\simeq$ in (A.20) indicates that we are dealing with an asymptotic expansion. Namely, it means that for any $r \in \mathbb{N}_0$ we have

$$a - \sum_{0 \le |\boldsymbol{\alpha}| \le r} \frac{(\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!} \left[L_{\boldsymbol{\alpha}} a\right]\big|_{x=x^*} = O\big(\|x - x^*\|^{r+1}\big).$$

Formula (A.19) allows us to rewrite the asymptotic expansion (A.20) as

$$a \simeq a|_{x=x^*} - \sum_{k=1}^{\infty} (-1)^k F_k\, a. \tag{A.21}$$

The advantage of (A.21) over (A.20) is that the restriction operator $(\,\cdot\,)|_{x=x^*}$ appears only in one place, in the first term on the RHS of (A.21). Formula (A.21) is a generalisation of the formula

$$a(x) \simeq a(0) + x a'(x) - \frac{x^2}{2} a''(x) + \frac{x^3}{6} a'''(x) + \ldots \tag{A.22}$$

from the analysis of functions of one variable. Namely, formula (A.21) turns into (A.22) if we set $d = 1$ and choose a phase function φ linear in x.

At this point it is worth discussing what happens under changes of local coordinates x. Examination of formula (A.8) shows that the operators L_α map scalar functions to scalar functions, i.e. the map $a \mapsto L_\alpha a$ is invariant under changes of local coordinates x; note that the index α does not play a role in this argument as it lives at a different point, y, and in a different coordinate system. As the operators F_k are expressed in terms of the L_α, the operator $\sum_{k=1}^{\infty} (-1)^k F_k$ appearing on the RHS of formula (A.21) also maps scalar functions to scalar functions.

Using formulae (A.15) and (A.12), (A.13), we can rewrite (A.21) as

$$\begin{aligned}
a &\simeq a^* - \sum_{\gamma=1}^{d} \varphi_{\eta_\gamma} \sum_{k=1}^{\infty} \frac{(-1)^k}{k}\, F_{k-1}\, L_\gamma\, a \\
&= a^* - \sum_{\gamma=1}^{d} \varphi_{\eta_\gamma} \sum_{k=1}^{\infty} \frac{(-1)^k}{k} \sum_{|\boldsymbol{\alpha}|=k-1} \frac{(\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!}\, L_{\boldsymbol{\alpha}}\, L_\gamma\, a \\
&= a^* + \sum_{\gamma=1}^{d} \varphi_{\eta_\gamma} \sum_{|\boldsymbol{\alpha}| \ge 0} \frac{(-\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!\,(|\boldsymbol{\alpha}|+1)}\, L_{\boldsymbol{\alpha}}\, L_\gamma\, a\,,
\end{aligned} \tag{A.23}$$

where $a^* = a|_{x=x^*}$. Thus, we have represented our amplitude in the form (A.11) with

$$\tilde{b}_\gamma \simeq \sum_{|\boldsymbol{\alpha}|\ge 0} \frac{(-\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!\,(|\boldsymbol{\alpha}|+1)}\, L_{\boldsymbol{\alpha}}\, L_\gamma\, a\,. \tag{A.24}$$

Combining (A.1) with (A.11) and (A.24) and by using the identity

$$\varphi_{\eta_\gamma} \mathrm{e}^{\mathrm{i}\,\varphi} = \frac{1}{\mathrm{i}} \frac{\partial}{\partial \eta_\gamma}\, \mathrm{e}^{\mathrm{i}\varphi}$$

we get, upon integration by parts,

$$\mathcal{I}_\varphi(a) = \int_{T_y^*M} \mathrm{e}^{\mathrm{i}\varphi} \left[a^* + \mathrm{i}\, w^{-1} \frac{\partial}{\partial \eta_\gamma} \left(w \sum_{|\boldsymbol{\alpha}|\ge 0} \frac{(-\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!\,(|\boldsymbol{\alpha}|+1)}\, L_{\boldsymbol{\alpha}} \right) L_\gamma\, a \right] w\, đ\eta\,.$$

Note that a^* no longer depends on x and the second contribution to the amplitude is now of order $m-1$. Recursive repetition of this procedure yields (A.3)–(A.5). The cut-off on the possible values of $|\boldsymbol{\alpha}|$ in (A.5) follows from incorporating the information that $\varphi_\eta|_{x=x^*} = 0$. $\square$

Appendix B. Weyl coefficients

Let

$$N(y;\lambda) := \sum_{\lambda_k<\lambda} |v_k(y)|^2$$

be the local counting function. When integrated over the manifold, $N(y;\lambda)$ turns into the usual (global) counting function

$$N(\lambda) := \sum_{\lambda_k<\lambda} 1 = \int_M N(y;\lambda)\, \rho(y)\, \mathrm{d}y\,.$$

Let $\hat{\mu} : \mathbb{R} \to \mathbb{C}$ be a smooth function such that $\hat{\mu}(t) = 1$ in some neighbourhood of the origin and the support of $\hat{\mu}$ is sufficiently small. Here 'sufficiently small' means that $\operatorname{supp}\hat{\mu} \subset (-T_0, T_0)$, where T_0 is the infimum of the lengths of all possible loops. A loop is defined as follows. Suppose that we have a Hamiltonian trajectory $(x(t;y,\eta), \xi(t;y,\eta))$ and a real number $T>0$ such that $x(T;y,\eta) = y$. We say in this case that we have a loop of length T originating from the point $y \in M$.

We denote by

$$\mathcal{F}[f](t)=\hat{f}(t)=\int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}t\lambda}\, f(\lambda)\,\mathrm{d}\lambda$$

the one-dimensional Fourier transform and by

$$\mathcal{F}^{-1}[\hat{f}](\lambda)=f(\lambda)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}t\lambda}\, \hat{f}(t)\,\mathrm{d}t$$

its inverse. Accordingly, we denote $\mu:=\mathcal{F}^{-1}[\hat{\mu}]$.

Further on we will deal with the mollified counting function $(N*\mu)(y,\lambda)$ rather than the original discontinuous counting function $N(y,\lambda)$. Here the star stands for convolution in the variable λ. More specifically, we will deal with the derivative, in the variable λ, of the mollified counting function. The derivative will be indicated by a prime.

It is known [AvFaVa, ChDoVa, DuGu, Iv80, Iv84, Iv98, SaVa] that the function $(N'*\mu)(y,\lambda)$ admits an asymptotic expansion in integer powers of λ as $\lambda\to+\infty$:

$$(N'*\mu)(y,\lambda)=c_{d-1}(y)\,\lambda^{d-1}+c_{d-2}(y)\,\lambda^{d-2}+c_{d-3}(y)\,\lambda^{d-3}+\dots. \tag{B.1}$$

Definition B.1. We call the coefficients $c_k(y)$ appearing in formula (B.1) *local Weyl coefficients*.

Note that our definition of Weyl coefficients does not depend on the choice of mollifier μ.

Integrating (B.1) in λ and using the fact that $(N'*\mu)(y,\lambda)$ decays faster than any power of λ as $\lambda\to-\infty$, we get

$$\begin{aligned}(N*\mu)(y,\lambda)=\frac{c_{d-1}(y)}{d}\,\lambda^{d}+\frac{c_{d-2}(y)}{d-1}\,\lambda^{d-1}+\dots+c_0(y)\,\lambda+\\ c_{-1}(y)\,\ln\lambda+b-c_{-2}(y)\,\lambda^{-1}-\frac{c_{-3}(y)}{2}\,\lambda^{-2}-\dots\quad\text{as}\quad\lambda\to+\infty,\end{aligned} \tag{B.2}$$

where b is some constant. Our Definition B.1 is somewhat non-standard as it is customary to call the coefficients

$$\frac{c_{d-1}(y)}{d},\ \frac{c_{d-2}(y)}{d-1},\ \dots$$

appearing in the asymptotic expansion (B.2) Weyl coefficients rather than those in the asymptotic expansion (B.1). However, for the purposes of this paper we will stick with Definition B.1. This is the definition that was used in [AvSjVa].

A separate question is whether one can get rid of the mollifier in (B.2). It is known [Sa89, SaVa] that under appropriate geometric conditions on loops we do indeed have

$$N(y,\lambda) = \frac{c_{d-1}(y)}{d}\lambda^d + \frac{c_{d-2}(y)}{d-1}\lambda^{d-1} + o(\lambda^{d-1}) \quad \text{as} \quad \lambda \to +\infty.$$

We do not discuss unmollified spectral asymptotics in the current paper.

The aim of this appendix is show that the small time expansion for the g-subprincipal symbol of the propagator (Theorem 8.1) allows us to recover in a straightforward manner the first three Weyl coefficients — see also [Lev], [Ava] and [Hö68] — and that our result agrees with those obtained by the heat kernel method.

We have

$$(N' * \mu)(y,\lambda) \;=\; \mathcal{F}^{-1}\left[\mathcal{F}\left[(N' * \mu)\right]\right](y,\lambda) \;=\; \mathcal{F}^{-1}\left[u(t,y,y)\,\hat{\mu}(t)\right], \tag{B.3}$$

where u is the Schwartz kernel (1.6) of the propagator (1.5). At each point of the manifold the quantity $u(t,y,y)$ is a distribution in the variable t and the construction presented in the main text of the papers allows us to write down this distribution explicitly, modulo a smooth function. Hence, formula (B.3) opens the way to the calculation of Weyl coefficients.

Theorem B.2. *The first three Weyl coefficients are*

$$c_{d-1}(y) = \frac{S_{d-1}}{(2\pi)^d}\,, \tag{B.4}$$

$$c_{d-2}(y) = 0\,, \tag{B.5}$$

$$c_{d-3}(y) = \frac{d-2}{12}\,\mathcal{R}(y)\,c_{d-1}(y)\,, \tag{B.6}$$

where

$$S_{d-1} = \frac{2\pi^{d/2}}{\Gamma(\frac{d}{2})} \tag{B.7}$$

is the Riemannian volume of the $(d-1)$*-dimensional unit sphere,* $\mathcal{R}$ *is scalar curvature and* Γ *is the gamma function.*

Proof. Our task is to substitute (3.1), (3.2) into $\mathcal{F}^{-1}\left[u(t,y,y)\,\hat{\mu}(t)\right]$ and expand the resulting quantity in powers of λ as $\lambda \to +\infty$. The smooth term $\mathcal{K}$

from (3.1) does not affect the asymptotic expansion, so the problem reduces to the analysis of an explicit integral in $d+1$ variables depending on the parameter λ. In what follows we fix a point on the manifold and drop the y in our intermediate calculations. As in the proof of Theorem 6.3, we work in geodesic normal coordinates centred at our chosen point.

The construction presented in the main text of the paper tells us that the only singularity of the distribution $u(t,y,y)\,\hat{\mu}(t)$ is at $t=0$. Hence, in what follows, we can assume that the support of $\hat{\mu}$ is arbitrarily small. In particular, this allows us to use the real-valued ($\epsilon=0$) Levi-Civita phase function.

We have

$$\mathfrak{a}_0(t,\eta)=1 \tag{B.8}$$

and, by Theorem 8.1,

$$\mathfrak{a}_{-1}(t,\eta)=\frac{\mathrm{i}}{12\,\|\eta\|}\,\mathcal{R}\,t+O(t^2)\,. \tag{B.9}$$

The lower order terms $\mathfrak{a}_{-2},\mathfrak{a}_{-3},\dots$ in the expansion (5.2) do not affect the first three Weyl coefficients and neither does the remainder term in (B.9), so further on we assume that the full symbol of the propagator reads

$$\mathfrak{a}(t,\eta)=1+\frac{\mathrm{i}}{12\,\|\eta\|}\,\mathcal{R}\,t\,. \tag{B.10}$$

Using formula (8.7) with $x=y$ we get

$$\varphi(t,\eta)=-\|\eta\|\,t+O(t^4)\,. \tag{B.11}$$

Replacing $\mathrm{e}^{\mathrm{i}\,\varphi(t,\eta)}$ by $\mathrm{e}^{-\mathrm{i}\,\|\eta\|\,t}$ in the oscillatory integral (3.2) does not affect the first three Weyl coefficients: this fact is established by using (B.11) and expanding $\mathrm{e}^{O(t^4)}$ into a power series, with account of the fact that this O-term is positively homogeneous in η of degree one (a similar argument was used in the proofs of Theorems 6.1 and 6.3). Hence, further on we assume that

$$\mathrm{e}^{\mathrm{i}\varphi(t,\eta)}=\mathrm{e}^{-\mathrm{i}\|\eta\|t}\,. \tag{B.12}$$

Using formula (8.10) with $x=y$ we get

$$\varphi_{x^\alpha\eta_\beta}(t,\eta)=\delta_\alpha{}^\beta+O(t^3)\,. \tag{B.13}$$

Substitution of (B.13) into (5.3) gives us

$$w(t,\eta)=1+O(t^3)\,. \tag{B.14}$$

The remainder term in (B.14) does not affect the first three Weyl coefficients, so further on we assume that

$$w(t,\eta)=1\,. \tag{B.15}$$

Substituting (B.10), (B.12) and (B.15) into (3.2), we conclude that formula (B.3) can now be rewritten as

$$(N'*\mu)(y,\lambda)= \frac{1}{2\pi}\int_{\mathbb{R}^{d+1}}\left(1+\frac{\mathrm{i}}{12\,\|\eta\|}\,\mathcal{R}\,t\right)\mathrm{e}^{\mathrm{i}(\lambda-\|\eta\|)t}\,\hat{\mu}(t)\,\chi(\|\eta\|)\,đ\eta\,\mathrm{d}t\;+O(\lambda^{d-4}). \tag{B.16}$$

Here $\chi\in C^\infty(\mathbb{R})$ is a cut-off such that $\chi(r)=0$ for $r\le 1/2$ and $\chi(r)=1$ for $r\ge 1$.

Switching to spherical coordinates in $\mathbb{R}^d$, we rewrite (B.16) as

$$(N'*\mu)(y,\lambda)= \frac{S_{d-1}}{(2\pi)^{d+1}}\int_{\mathbb{R}^2}\left(r^{d-1}+\frac{\mathrm{i}}{12}\,\mathcal{R}\,r^{d-2}\,t\right)\mathrm{e}^{\mathrm{i}(\lambda-r)t}\,\hat{\mu}(t)\,\chi(r)\,\mathrm{d}r\,\mathrm{d}t\;+\;O(\lambda^{d-4}). \tag{B.17}$$

Here r is the radial coordinate and the extra factor $(2\pi)^d$ in the denominator came from (2.3).

Observe that

$$t\,\mathrm{e}^{\mathrm{i}(\lambda-r)t}=\mathrm{i}\frac{\partial}{\partial r}\mathrm{e}^{\mathrm{i}(\lambda-r)t}\,,$$

so integrating by parts in (B.17) we simplify this formula to read

$$(N'*\mu)(y,\lambda)=\frac{S_{d-1}}{(2\pi)^{d+1}}\int_{\mathbb{R}^2}r^{d-1}\,\mathrm{e}^{\mathrm{i}(\lambda-r)t}\,\hat{\mu}(t)\,\chi(r)\,\mathrm{d}r\,\mathrm{d}t\;+\;O(\lambda^{d-4}) \tag{B.18}$$

for $d=2$ and

$$(N'*\mu)(y,\lambda)= \frac{S_{d-1}}{(2\pi)^{d+1}}\int_{\mathbb{R}^2}\left(r^{d-1}+\frac{d-2}{12}\,\mathcal{R}\,r^{d-3}\right)\mathrm{e}^{\mathrm{i}(\lambda-r)t}\,\hat{\mu}(t)\,\chi(r)\,\mathrm{d}r\,\mathrm{d}t\;+O(\lambda^{d-4}) \tag{B.19}$$

for $d\ge 3$.

It remains only to drop the cut-off χ in formulae (B.18) and (B.19) as this does not affect the asymptotics when $\lambda \to +\infty$ and to make use of the formula

$$\frac{1}{2\pi} \int_{\mathbb{R}^2} r^m \, \mathrm{e}^{\mathrm{i}(\lambda - r)t} \, \hat{\mu}(t) \, \mathrm{d}r \, \mathrm{d}t = \lambda^m,$$

which holds for $m = 0, 1, 2, \ldots$.

We see that formulae (B.18) and (B.19) give us (B.4)–(B.6). $\square$

As a final step, let us show that Theorem B.2 agrees with the classical heat kernel expansion. To this end, let us introduce the (local) heat trace

$$Z(y,t) := \int_{-\infty}^{+\infty} \mathrm{e}^{-t\lambda^2} \, N'(y,\lambda) \, \mathrm{d}\lambda \, = \int_0^{+\infty} \mathrm{e}^{-t\lambda^2} \, N'(y,\lambda) \, \mathrm{d}\lambda \, + \, \frac{1}{\mathrm{Vol}(M,g)} \, . \tag{B.20}$$

If we now replace $N'(y,\lambda)$ in formula (B.20) with its mollified version $(N' * \mu)(y,\lambda)$ this gives an error, but this error can be easily estimated:

$$Z(y,t) = \int_0^{+\infty} \mathrm{e}^{-t\lambda^2} \, (N' * \mu)(y,\lambda) \, \mathrm{d}\lambda \, + \, O(1) \quad \text{as} \quad t \to 0^+. \tag{B.21}$$

Substituting (B.1) and (B.4)–(B.6) into (B.21), we get

$$Z(y,t) = c_{d-1}(y) \int_0^{+\infty} \mathrm{e}^{-t\lambda^2} \, \lambda^{d-1} \, \mathrm{d}\lambda \, + \, O(1) \quad \text{as} \quad t \to 0^+ \tag{B.22}$$

for $d = 2$,

$$Z(y,t) = \int_0^{+\infty} \mathrm{e}^{-t\lambda^2} \left(c_{d-1}(y) \, \lambda^{d-1} + c_{d-3}(y) \, \lambda^{d-3} \right) \mathrm{d}\lambda \, + \, O(|\ln t|) \quad \text{as} \quad t \to 0^+ \tag{B.23}$$

for $d = 3$, and

$$Z(y,t) = \int_0^{+\infty} \mathrm{e}^{-t\lambda^2} \left(c_{d-1}(y) \, \lambda^{d-1} + c_{d-3}(y) \, \lambda^{d-3} \right) \mathrm{d}\lambda \, + \, O\big(t^{(3-d)/2}\big) \quad \text{as} \quad t \to 0^+ \tag{B.24}$$

for $d \geq 4$.

We have

$$\int_0^{+\infty} \mathrm{e}^{-z^2}\, z^{d-1}\, \mathrm{d}z \;=\; \frac{\Gamma(\frac{d}{2})}{2}\,. \tag{B.25}$$

We also have

$$\int_0^{+\infty} \mathrm{e}^{-z^2}\, z^{d-3}\, \mathrm{d}z \;=\; \frac{\Gamma(\frac{d}{2}-1)}{2} \;=\; \frac{\Gamma(\frac{d}{2})}{d-2} \tag{B.26}$$

for $d \ge 3$.

Using (B.4)–(B.7), (B.25) and (B.26) we can rewrite formulae (B.22)–(B.24) as a single formula

$$Z(y,t) = \begin{cases} (4\pi t)^{-d/2} + O(1) \quad \text{for} \quad d=2, \\ (4\pi t)^{-d/2}\left(1+\frac{1}{6}\,\mathcal{R}(y)\,t\right) + O(|\ln t|) \quad \text{for} \quad d=3, \\ (4\pi t)^{-d/2}\left(1+\frac{1}{6}\,\mathcal{R}(y)\,t\right) + O\big(t^{(3-d)/2}\big) \quad \text{for} \quad d\ge 4 \end{cases} \tag{B.27}$$

as $t \to 0^+$.

It is known [MiPl], [BeGaMa, Ch. III, E.IV.], [Ros, Section 3.3], that for all $d \ge 2$ the heat trace admits the expansion

$$Z(y,t) = (4\pi t)^{-d/2}\left(1+\frac{1}{6}\,\mathcal{R}(y)\,t\right) + O\big(t^{(4-d)/2}\big) \quad \text{as} \quad t\to 0^+. \tag{B.28}$$

We see that our result (B.27) agrees with the classical formula (B.28).

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Department of Mathematics, University College London
Gower Street, London WC1E 6BT, UK
Current address:
Department of Mathematics, Heriot-Watt University
Edinburgh EH14 4AS, UK
E-mail address: m.capoferri@hw.ac.uk

Department of Mathematics and Statistics, University of Reading
Pepper Lane, Whiteknights, Reading RG6 6AX, UK
E-mail address: M.Levitin@reading.ac.uk

Department of Mathematics, University College London
Gower Street, London WC1E 6BT, UK
E-mail address: D.Vassiliev@ucl.ac.uk

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