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Microlocal analysis of global hyperbolic propagators on manifolds without boundary

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Declaration

I, Matteo Capoferri, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.

Matteo Capoferri

Abstract

The main goal of this thesis is to construct explicitly, modulo smooth terms, propagators for physically meaningful hyperbolic partial differential equations (PDEs) and systems of PDEs on closed manifolds without boundary, and to do this in a global (i.e. as a single oscillatory integral) and invariant (under changes of local coordinates and any gauge transformations that may be present) fashion. The crucial element in our approach is the use of complex-valued, as opposed to real-valued, phase functions — an idea proposed in the nineties by Laptev, Safarov and Vassiliev. It is known that one cannot achieve a construction global in time using a real-valued phase function due to obstructions brought about by caustics; however the use of a complex-valued one makes it possible to circumvent such obstructions. This is the subject of the first part of the thesis, where we study the global propagator for the wave equation on a closed Riemannian manifold of dimension $d \geq 2$ and the global propagator for the massless Dirac equation on a closed orientable Riemannian 3-manifold. Our results allow us to compute, as an application, the third local Weyl coefficient for the massless Dirac operator.

A natural way to obtain a system of PDEs on a manifold is to vary a suitably defined sesquilinear form. In the second part of the thesis, we study first order sesquilinear forms acting on sections of the trivial $\mathbb{C}^m$-bundle over a smooth d-manifold. Thanks to the interplay of techniques from analysis, geometry and topology, we achieve a classification of these forms up to $GL(m, \mathbb{C})$ gauge equivalence in the special case of $d = 4$ and $m = 2$.

Finally, in the last chapter we develop a Lorentzian analogue of the theory of elasticity. We analyse the resulting nonlinear field equations for general Lorentzian 4-manifolds, and provide explicit solutions for the Minkowski spacetime.

Impact statement

The 2010 International Review of Mathematical Sciences expressed the following concern:

"Despite progress since 2004, analysis in the UK is still under-represented compared to the rest of the world, with a notable shortage of home-grown talent; efforts to strengthen existing excellent groups in analysis of all sizes should accordingly be continued."

And it goes on saying:

"The part of geometry that needs most strengthening in the UK is the connection between geometric analysis and partial differential equations."

This thesis lies at the intersection between analysis, geometry and mathematical physics, as it deals with advances of different nature in the analysis of physically meaningful partial differential equations and systems of partial differential equations on manifolds. For this reason, it fully addresses the above concerns and contributes to what is identified as a research area that needs strengthening. The author hopes to stimulate further research at the crossroads of analysis and geometry.

The results of our research have been communicated to the mathematical research community by delivering numerous talks at national and international conferences and research seminars, as well as by writing research papers for peer reviewed publication.

Additional cross-contamination of diverse research areas has been encouraged by establishing research collaborations across different departments, universities and countries.

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Contents

Abstract **5**

Impact statement **7**

Acknowledgements **9**

1 Introduction **15**

2 The wave propagator **25**

2.1 Statement of the problem 25

2.2 Lagrangian manifolds and Hamiltonian flows 30

2.3 Main results 35

2.4 The Levi-Civita phase function 36

2.5 The global invariant symbol of the propagator 39

2.6 The amplitude-to-symbol operator 45

2.7 Invariant representation of the identity operator 52

2.8 The subprincipal symbol of the propagator 56

2.9 Small time expansion for the subprincipal symbol 62

2.10 Weyl coefficients 66

2.11 Explicit examples 71

2.11.1 The 2-sphere 71

2.11.2 The hyperbolic plane 76

2.12 Circumventing topological obstructions: geometric picture 77

3 The massless Dirac propagator **83**

3.1 Statement of the problem 83

3.2 Main results 89
3.3 Preliminary results for general first order systems 91
3.3.1 Positive and negative propagators: an abstract approach . . . 93
3.3.2 Construction of positive and negative propagators 95
3.3.3 The algorithm 99
3.4 Invariant description of pseudodifferential operators acting on scalar functions 103
3.5 Global propagator for the massless Dirac operator 107
3.5.1 Transport equations 109
3.5.2 Pseudodifferential operators $U^{\pm}(0)$ 111
3.6 Principal symbol of the global Dirac propagator 114
3.7 Explicit small time expansion of the symbol 117
3.7.1 Special framing 118
3.7.2 Small time expansion of the principal symbols 119
3.7.3 Small time expansion of the subprincipal symbols 120
3.7.4 Invariant reformulation 128
3.8 Spectral asymptotics 130
3.9 Examples 132
3.9.1 The case $M = \mathbb{S}^3$ 132
3.9.2 The case $M = \mathbb{S}^2 \times \mathbb{S}^1$ 135

4 Classification of first order sesquilinar forms 137
4.1 Introduction 137
4.2 First order sesquilinear forms 140
4.3 Statement of the problem 142
4.3.1 General linear classification 142
4.3.2 Special linear classification 142
4.4 Main results 144
4.5 Invariant objects encoded within sesquilinear forms 145
4.5.1 Geometric objects 145
4.5.2 Topological objects 148
4.6 Transition from analysis to topology 150

4.6.1 Framings and their equivalence 150
4.6.2 Topological characterisation 153
4.6.3 Differential geometric characterisation 156
4.7 Proofs of main theorems 158
4.7.1 Proof of Theorem 4.6 158
4.7.2 Proof of Theorem 4.7 159
4.8 The 3-dimensional Riemannian case 160
4.8.1 Explicit examples 163
4.9 Sesquilinear forms vs linear operators 165
4.9.1 Four-dimensional case 166
4.9.2 Three-dimensional case 166
4.10 Applications 167

5 Lorentzian elasticity **169**
5.1 Introduction 169
5.2 Mathematical model 171
5.3 Nonlinear field equations 176
5.4 Displacements and rotations 179
5.5 Linearised field equations 183
5.6 Homogeneous diffeomorphisms 187
5.7 Special subgroups of the Poincaré group 189
5.8 Explicit massless solutions of nonlinear field equations 191
5.9 Explicit massive solutions of nonlinear field equations 196
5.10 Massless Dirac equation 199
5.11 Massive Dirac equation 201

Appendix A The wave propagator: complementary material **205**
A.1 The subprincipal symbol for the 2-sphere: Mathematica script 205

Appendix B The Dirac propagator: complementary material **215**
B.1 The Weitzenböck connection 215
B.2 Some techincal proofs 217
B.2.1 Proof of Theorem 3.23 217

B.2.2 Proof of Theorem 3.37 218
B.3 Third Weyl coefficient: an alternative derivation 220

Appendix C Classification of sesquilinear forms: complementary material 223

C.1 The concepts of principal and subprincipal symbol 223

Appendix D Lorentzian elasticity: notation and complementary material 227

D.1 Notation and conventions 227
D.1.1 Exterior calculus 227
D.1.2 Spinors 228
D.1.3 Spinor representation of 2-forms 229
D.2 Some results in linear algebra 230
D.2.1 Linear algebra involving a pair of quadratic forms 230
D.2.2 Nilpotent operators in a 2D symplectic space 231
D.3 Differential geometric characterisation of screw groups 232
D.4 Explicit formulae for our field equations 234

Bibliography 237

Chapter 1

Introduction

In this first Chapter we give a general overview of the type of problems addressed in this thesis and a preliminary description of the results obtained, postponing until subsequent chapters precise mathematical formulations and rigorous proofs. For the sake of keeping the Introduction light, we also postpone until subsequent chapters a more detailed literature review.

Let (M,g) be a closed Riemannian manifold of dimension $d \geq 2$. Let A be a self-adjoint elliptic[1] first-order linear (pseudo)differential operator acting on m-columns $u = (u_1, u_2, \dots, u_m)^T$ of complex-valued scalar functions over M. Consider the Cauchy problem

$$f|_{t=0} = f_0 \tag{1.0.1}$$

for the hyperbolic system

$$-\,i\,\frac{\partial f}{\partial t} + Af = 0. \tag{1.0.2}$$

Here f_0 is a column-function of the spatial variable $x \in M$, whereas f is a column-function of x and time t.

The *propagator* of the problem (1.0.1), (1.0.2) is the unitary operator

$$U(t) : f_0(x) \mapsto f(t,x) \tag{1.0.3}$$

[1] When $m = 1$, i.e. when we are dealing with a single PDE as opposed to a system, 'A is elliptic' means that the principal symbol $A_{\mathrm{prin}}(x,\xi)$ does not vanish on $T^*M \setminus \{0\}$. When $m \geq 2$, 'A is elliptic' means that the determinant of the principal symbol $\det A_{\mathrm{prin}}(x,\xi)$ does not vanish on $T^*M \setminus \{0\}$. When $m \geq 2$ and the operator is differential (as opposed to pseudodifferential) ellipticity is only possible when m is even. Further details will be provided in subsequent chapters.

solving (1.0.1)–(1.0.2), i.e. mapping initial data to solutions.

The propagator $U(t)$ can be formally constructed by resorting to functional calculus. In fact, by standard elliptic theory A has discrete spectrum accumulating to infinity and its eigenfunctions form an orthonormal basis in $L^2(M)$. Denoting by λ_k the eigenvalues of A and by v_k the corresponding orthonormalised eigenfunctions (counted with multiplicity), we have

$$U(t) = e^{-iAt} = \sum_k e^{-i\lambda_k t}\, v_k(x) \int_M \overline{v_k(y)}^T \,(\,\cdot\,)\; \rho(y)\,\mathrm{d}y. \tag{1.0.4}$$

Here $\rho(y) := \sqrt{\det g_{\alpha\beta}(y)}$ is the Riemannian density.

In order to construct the propagator (1.0.4) *precisely* one needs to know all the eigenvalues and eigenfunctions of the operator A, which is in general unrealistic to expect. In fact, barring some highly symmetric cases, even the spectrum of the Laplace–Beltrami operator on a generic closed manifold is not known explicitly.

An alternative approach to construct $U(t)$ is offered by microlocal analysis. Microlocal analysis is a technique generalising the Fourier transform. Assume one is working with a linear partial differential equation (PDE) (or a system of PDEs) with constant coefficients in Euclidean space; then, such a PDE can be fully examined by means of the Fourier transform. If one is, instead, working on manifolds and dealing with a PDE (or a system of PDEs) with variable coefficients the standard Fourier transform method does not work anymore. However, in the latter case one can still look for a solution in terms of suitably defined oscillatory integrals — a 'generalised version' of the Fourier transform — up to infinitely smooth contributions. The study of PDEs with variable coefficients was the main motivation that led to the development of microlocal analysis, whose foundations were laid by Lars Hörmander in his celebrated four-volume monograph [67].

Microlocal techniques allow one to construct the propagator (1.0.4) *approximately*, modulo an integral operator with infinitely smooth integral kernel: here $U(t)$ is written locally, in time and in space, as a composition of oscillatory integrals whose amplitudes and phase functions are obtained by solving certain ordinary (as opposed to partial) differential equations. The adjective 'microlocal' refers to the fact that one localises singularities of the Schwartz kernel of the operator $U(t)$ not only in the position variable (local coordinates x^α, $\alpha = 1, \dots, d$, on M) but also in the dual variable, momentum (coordinates ξ_α, $\alpha = 1, \ldots, d$, on $T_x^* M$). The latter effectively shows how the singularity looks in different directions.

The microlocal construction of the propagator (1.0.4) has been the subject of intensive research since the 1950s. In particular, a substantial part of Hörmander's monograph [67] is devoted to this matter.

There are, however, two fundamental problems with the classical construction.

(a) It is local in space: oscillatory integrals are written in local coordinates. As a result, the objects appearing in the oscillatory integral are *not* invariant under change of coordinates.

(b) It is local in time.

The latter issue, locality in time, is especially serious: it is to do with obstructions associated with caustics. In practice, constructing a propagator locally in time means that for large times one has to resort to compositions

$$U(t) = U(t - t_j) \circ U(t_j - t_{j-1}) \circ \cdots \circ U(t_2 - t_1) \circ U(t_1). \tag{1.0.5}$$

The propagator (1.0.4) is a special case of a Fourier integral operator (FIO): handling compositions of FIOs is a challenging task [115, Vol. 2]. Obtaining an explicit formula for the LHS of (1.0.5) by composing the operators on the RHS is impracticable.

The main goal of this thesis is to construct $U(t)$ explicitly (i.e up to solving ordinary differential equations) for a class of operators of physical interest, and to do so in a global (i.e. as a single oscillatory integral) and invariant (under changes of local coordinates and any gauge transformations that may be present) fashion, thus overcoming (a) and (b).

The main idea is to resolve the above issues by using a *complex-valued* phase function

$$\varphi(t, x; y, \eta), \qquad \varphi : \mathbb{R} \times M \times (T^*M \setminus \{0\}) \to \mathbb{C}, \qquad \operatorname{Im} \varphi \geq 0,$$

as opposed to a real-valued one. Quite remarkably, the propagator $U(t)$ can be written as a finite sum of invariantly defined oscillatory integrals, global *both* in space and in time, with complex-valued phase functions.

Our work builds upon earlier results by A. Laptev, Yu. Safarov and D. Vassiliev [77, 104] and advancements critically rely on the presence of a metric structure on M, which provides a solid 'skeleton' upon which our invariant construction rests.

We focus our analysis on two special cases:

(A) $d \geq 2$, $m = 1$ and $A = \sqrt{-\Delta}$. In this case, the operator $U(t)$ is the *wave propagator* (sometimes called 'wave group').

(B) $d = 3$, $m = 2$ and $A = W$, W being the massless Dirac operator.

In the case (A), the invariant global formula for the propagator reads

$$U(t) \overset{\mod \Psi^{-\infty}}{=} \frac{1}{(2\pi)^d} \int_{T^*M} e^{i\varphi(t,x;y,\eta)}\, \mathfrak{a}(t;y,\eta)\, \chi(t,x;y,\eta)\, w(t,x;y,\eta)\, (\,\cdot\,)\, \rho(y)\, dy\, d\eta, \tag{1.0.6}$$

where φ is a distinguished phase function determined by the geometry, $\chi(t,x;y,\eta)$ is a cut-off,

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

and ρ is the Riemannian density.

The scalar function

$$\mathfrak{a} : \mathbb{R} \times T^*M \setminus \{0\} \to \mathbb{C}$$

is the *symbol* of the operator (1.0.6). It admits an asymptotic expansion into components $\mathfrak{a}_{-k}$ positively homogeneous in η of degree $-k$,

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

and each homogeneous component is uniquely determined via an invariant algorithm.

We define the *full*, *principal* and *subprincipal* symbols of the wave propagator $U(t)$ to be the scalar functions $\mathfrak{a}$, $\mathfrak{a}_0$ and $\mathfrak{a}_{-1}$, respectively.

The concept of principal symbol of a Fourier integral operator is well established in microlocal analysis [67, 115], and applies both to operators acting on scalar functions and to operators acting on half-densities. The concept of subprincipal symbol, instead, was introduced by J. J. Duistermaat and L. Hörmander [52, Eqn. (5.2.8)], and it is defined only for pseudodifferential operators acting on half-densities. To our knowledge, for Fourier integral operators the notion of subprincipal symbol has never been defined.

The fundamental difference between pseudodifferential operators and Fourier integral operators is that in the latter singularities propagate, i.e. they do not possess the property of pseudolocality. It becomes possible to define, in an invariant fashion, the full and subprincipal symbols of the propagator because a) the propagator is a special case of a Fourier integral operator and b) we make use of the underlying geometric structure — Riemannian metric and associated Levi-Civita connection.

In the case (B) of the massless Dirac operator, we have a similar result, where now the propagator is written as the sum of two oscillatory integrals of type (1.0.6), one for each eigenvalue of the principal symbol of W. We can, in fact, say more: the two oscillatory integrals can be constructed in such a way that they approximate, modulo operators with infinitely smooth Schwartz kernel, the operators

$$U^+(t) := \sum_{\lambda_k>0} e^{-i\lambda_k t}\, v_k(x) \int_M \overline{v_k(y)}^T\, (\,\cdot\,)\ \rho(y)\,\mathrm{d}y \tag{1.0.7}$$

and

$$U^-(t) := \sum_{\lambda_k<0} e^{-i\lambda_k t}\, v_k(x) \int_M \overline{v_k(y)}^T\, (\,\cdot\,)\ \rho(y)\,\mathrm{d}y, \tag{1.0.8}$$

respectively. That is, not only our construction is geometric and global, but it allows one to maintain good control over the spectrum of the original operator W. As we did for the wave propagator, we can give an invariant notion of full, principal and subprincipal symbols of the massless Dirac propagator.

We will show in Section 3.3 that an analogous construction holds for general first order pseudodifferential operators A acting on m-columns of scalar fields, under the condition the eigenvalues of the principal symbol A_{prin} are simple. In this case, the operator $U(t)$ can be written, modulo an operator with infinitely smooth Schwartz kernel, as the sum of m oscillatory integrals of the form (1.0.6), one for each eigenvalue of A_{prin}. The sum of the oscillatory integrals corresponding to positive eigenvalues of A_{prin} approximate (1.0.7), whereas the oscillatory integrals corresponding to negative eigenvalues of A_{prin} approximate (1.0.8).

By setting $t = 0$, our definitions of principal and subprincipal symbols specialise to pseudodifferential operators. A natural question to ask is whether they are related to the standard ones when the latter are defined. The answer is affirmative, and a detailed examination of this issue is provided in Section 3.4. Crucially, in drawing a comparison one has to translate our results for operators acting on scalar functions into the more customary setting of operators acting on half-densities.

The construction of hyperbolic propagators — besides being of interest on its own and having the potential of finding applications in natural sciences — is a very powerful tool in the study of elliptic spectral problems. In fact, the hyperbolic problem (1.0.1), (1.0.2) is closely related to the elliptic eigenvalue problem

$$Av = \lambda v. \tag{1.0.9}$$

More precisely, if one constructs the hyperbolic propagator with sufficiently high accuracy (in terms of smoothness), then this allows one to write down asymptotic formulae for the corresponding elliptic spectral problem. These ideas go under the name of *wave method* and were first developed by B. Levitan [82] and V. G. Avakumovic [6] in the 1950s.

Define the *spectral function* to be

$$N(y,\lambda) := \sum_{0<\lambda_k<\lambda} \overline{v_k(y)}^T\, v_k(y). \tag{1.0.10}$$

It is well-known that, given a suitable mollifier μ, the function[2] $(N' * \mu)(y,\lambda)$ admits a complete asymptotic expansion in integer powers of λ:

$$(N' * \mu)(y,\lambda) = c_{d-1}(y)\,\lambda^{d-1} + c_{d-2}(y)\,\lambda^{d-2} + c_{d-3}(y)\,\lambda^{d-3} + \dots \quad \text{as} \quad \lambda \to +\infty. \tag{1.0.11}$$

In the above formulae $*$ stands for the convolution. The functions

$$c_j : M \to \mathbb{R}$$

are called *local Weyl coefficients* and one can show that they are independent of the choice of mollifier μ. As an application of our results on $U(t)$ we compute the third local Weyl coefficient for the massless Dirac operator, to our knowledge unknown to date.

Note that in the scalar case, e.g. for the Laplace–Beltrami operator, there are many alternative ways for dealing with spectral asymptotics, the simplest being the heat kernel and resolvent approaches. However, if one moves on to first order systems,

[2] Here the prime denotes the derivative with respect to λ.

whose spectrum is, in general, not semi-bounded, the heat method can no longer be applied, at least in its original form. Furthermore, even resolvent techniques require major modification [9]. For first order systems, the wave method provides a natural and effective way to compute higher order Weyl coefficients.

Although our main goal is the global analysis of hyperbolic propagators, this is not the only topic this thesis is concerned with. In the second part of this thesis we will present the outcome of two of the research projects undertaken on the side during the PhD: the problem of classifying sesquilinar forms generating first order systems (Chapter 4) and the development of a theory of elasticity in the Lorentzian setting (Chapter 5). If on the one hand the questions addressed in these Chapters are related to the main topic and, to some extent, motivated by it, on the other hand they can as well be considered as standalone units and read independently from the rest of the thesis.

For the sake of time, space and overall homogeneity of the material, we decided not to include in this thesis the results of two other research projects, dealing with

(i) the extension of the construction of global propagators to globally hyperbolic Lorentzian spacetimes and

(ii) the construction of Lorentzian metrics on noncommutative 4-manifolds.

The outcome of (i) has recently appeared in [32] and the outcome of (ii) will be provided in a forthcoming co-authored paper [15].

The main body of the thesis is structured into four Chapters, closely based upon the three co-authored papers [33], [34], [36] and the forthcoming [35]. Naturally, the thesis partially coincides both in content and in writing with [33], [34], [36] and [35].

In Chapter 2 we study the propagator of the wave equation on a closed Riemannian manifold M. We propose a geometric approach for 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 Chapter 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 topological obstructions and describe their circumvention with the use of a complex-valued phase function. The general framework is illustrated via explicit examples in dimension two.

In Chapter 3 we study the propagator of the massless Dirac operator W on a closed Riemannian 3-manifold. The propagator naturally decomposes into two operators, the positive propagator and the negative propagator, associated with the positive and negative eigenvalues of W. We show that positive and negative propagators can be separately approximated by a single oscillatory integral, global in space and in time, in an invariant fashion, and provide an algorithm for their construction, taking into account gauge degrees of freedom. The adoption of distinguished complex-valued phase functions allows us to give a definition of full, principal and subprincipal symbols of our propagators, scalar matrix-functions on the cotangent bundle. In particular, we provide an explicit formula for the principal symbols and a small time expansion of principal and subprincipal symbols, in terms of geometric invariants (curvature of the Levi-Civita connection and torsion of the Weitzenböck connection). As an application of our results, we compute the third (local) Weyl coefficient of W. Along the way, we study invariant representations of pseudodifferential operators acting on scalar functions and prove general results about propagators of first order (pseudo)differential systems.

A natural way of obtaining a system of partial differential equations on a manifold is to vary a suitably defined sesquilinear form. In Chapter 4 we study a particular family of sesquilinar forms: Hermitian forms acting on sections of the trivial $\mathbb{C}^m$-bundle over a smooth d-dimensional manifold without boundary. More specifically, we are concerned with first order sesquilinear forms, namely, those generating first order systems. Our goal is to classify such forms up to $GL(m,\mathbb{C})$ gauge equivalence. We achieve this classification in the special case of $d = 4$ and $m = 2$ by means of geometric and topological invariants (e.g. Lorentzian metric, spin/spin^c structure, electromagnetic covector potential) naturally contained within the sesquilinear form — a purely analytic object. Essential to our approach is the interplay of techniques from analysis, geometry, and topology.

Finally, in Chapter 5 we propose a new mathematical model for a class of field theories in the Lorentzian setting – effectively, a (fully) Lorentzian theory of elasticity. We work on a 4-manifold equipped with Lorentzian metric g and consider a volume-preserving diffeomorphism which is the unknown quantity of our mathematical model. The diffeomorphism defines a second Lorentzian metric h, the pullback of g. Motivated by elasticity theory, we introduce a Lagrangian expressed algebraically (without differentiations) via our pair of metrics. The analysis of the resulting nonlinear field equations produces three main results. Firstly, we show that for Ricci-flat manifolds our linearised field equations are Maxwell's equations in the Lorenz gauge with exact current. Secondly, for Minkowski space we construct explicit massless solutions of our nonlinear field equations; these come in two distinct types, right-handed and left-handed. Thirdly, for Minkowski space we construct explicit massive solutions of our nonlinear field equations; these contain a positive parameter which has the geometric meaning of quantum mechanical mass and a real parameter which may be interpreted as electric charge. In constructing explicit solutions of nonlinear field equations we resort to group-theoretic ideas: we identify special 4-dimensional subgroups of the Poincaré group and seek diffeomorphisms compatible with their action, in a suitable sense.

Chapter 2

The wave propagator

2.1 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

$$\rho(x) := \sqrt{\det g_{\mu\nu}(x)} \tag{2.1.1}$$

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

$$\Delta = \rho(x)^{-1} \frac{\partial}{\partial x^\mu}\, \rho(x)\, g^{\mu\nu}(x)\, \frac{\partial}{\partial x^\nu}\,. \tag{2.1.2}$$

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

It is well known [101] that the operator (2.1.2) 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

$$\left(\frac{\partial^2}{\partial t^2} - \Delta\right) f(t,x) = 0\,, \tag{2.1.3a}$$

$$f(0,x) = f_0(x), \qquad \frac{\partial f}{\partial t}(0,x) = f_1(x). \tag{2.1.3b}$$

Functional calculus allows one to write the solution of (2.1.3a), (2.1.3b) as

$$f = \cos\!\big(t\sqrt{-\Delta}\,\big)\, f_0 \,+\, \sin\!\big(t\sqrt{-\Delta}\,\big)\,(-\Delta)^{-1/2} f_1 \,+\, t\,(v_0\,, f_1)\,, \tag{2.1.4}$$

where

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

is the pseudoinverse of the operator $\sqrt{-\Delta}$ [96, Chapter 2, Section 2].

The RHS of (2.1.4) 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. [67] — solving the Cauchy problem (2.1.3a), (2.1.3b) reduces to constructing the FIO

$$U(t) := e^{-it\sqrt{-\Delta}} = \int u(t,x,y)\,(\,\cdot\,)\,\rho(y)\,\mathrm{d}y\,, \tag{2.1.5}$$

whose Schwartz kernel reads

$$u(t,x,y) := \sum_{k=0}^{\infty} e^{-it\lambda_k}\, v_k(x)\,\overline{v_k(y)}\,. \tag{2.1.6}$$

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

$$\left(-i\,\frac{\partial}{\partial t} + \sqrt{-\Delta}\right) U(t) = 0\,, \tag{2.1.7a}$$

$$U(0) = \mathrm{Id}\,. \tag{2.1.7b}$$

The goal of this Chapter 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 [62], [97, 98], [52], [67, Vol. 3 & 4], [115], [106]. These publications rely on spectral-theoretic techniques, often combined with tools from the theory of local oscillatory integrals.

In this thesis, we adopt a somewhat different *global* approach, which originates from the works of Laptev, Safarov and Vassiliev [77] and Safarov and Vassiliev [104]. 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., [95]. In the realm of pure mathematics, FIOs with complex phase functions were considered, for example, by Melin and Sjöstrand [89]. 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 [77], [104], 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., [118] and [121]. 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 $e^{-it\sqrt{-\Delta}} : L^2(M) \to L^2(M)$ 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 $e^{\tau\sqrt{-\Delta}}$;

(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 [26], [120], [80] and [109]. Despite some similarities in the idea of adopting a complex phase to achieve a representation global in time, our construction is overall very different from Zelditch's one, as it will be clear later on.

The techniques from [77], [104] 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 [78] constructed the propagator for the magnetic Schrödinger operator in flat Euclidean space for phase functions with purely quadratic imaginary part. Jakobson *et al*, when studying branching billiards on Riemannian manifolds with discontinuous metric in [71], rely in their proofs on boundary layer oscillatory integrals with complex-valued phase function, in the spirit of [104]. Furthermore, Safarov set his programme on global calculi on manifolds [103, 85] in the framework of [77]. An extension of results from [104] to first order systems of PDEs has been carried out by Chervova, Downes and Vassiliev [41] in the process of computing two-term spectral asymptotics.

Laptev and Sigal's results mentioned above were improved and extended by Robert in [99], 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, though, does not coincide with a specialisation to the flat case of the Levi-Civita phase function used in the current thesis.

Another approach to global FIOs is represented by Maslov's canonical operators. Maslov's construction — the *complex WKB method* — is somewhat different from ours in nature and purpose; we refer the reader to [84] for an expository overview.

The construction of [77, 104] 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 [46, 45]. In our thesis, 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 (2.1.6), 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 (2.1.5). The goal of the current Chapter is to build upon [77], developing further the construction therein for the case of Riemannian manifolds. The geometric nature of our construction will allow us to provide invariant definitions of full and subprincipal symbol of the wave propagator, analyse them, and give explicit formulae.

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 Section 2.10. In Chapter 3 we will apply our approach to (possibly non semi-bounded) first order systems of partial differential equations on Riemannian manifolds: this will enable us to compute additional (compared to what is known in the current literature) Weyl coefficients for the massless Dirac operator.

This Chapter is structured as follows.

In Section 2.2 we give a brief overview of the theory of global Lagrangian distributions and their relation to hyperbolic problems, as developed in [77]. Section 2.3 contains a concise summary of the main results of the Chapter. In Section 2.4 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 2.5, and an algorithm for the calculation of all its homogeneous components is provided. Some of the more technical material used in Section 2.5 has been postponed to Section 2.6. In order to implement the algorithm presented in Section 2.5 one also needs to study invariant representations of the identity operator in the form of an oscillatory integral: this is the subject of Section 2.7. Section 2.8 is devoted to a detailed study of the subprincipal symbol of the wave propagator, culminating with Theorem 2.24 which gives an explicit formula for it. In Section 2.9 we provide an explicit small time asymptotic expansion for the subprincipal symbol. This allows us to recover, as a by-product, the third Weyl coefficient, see Section 2.10. In Section 2.11 we apply our construction to two explicit examples in 2D: the sphere and the hyperbolic plane. Finally, in Section 2.12 we discuss the issue of circumventing topological obstructions.

2.2 Lagrangian manifolds and Hamiltonian flows

The theory of Fourier integral operators, beautifully set out in the seminal papers by Hörmander and Duistermaat [66, 52], 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 [50], Trèves [115, Vol. 2] and Hörmander [67, 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 [77], in a formulation adapted to our purposes. 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

$$\dot{x}^*(t; y, \eta) = h_\xi(x^*(t; y, \eta), \xi^*(t; y, \eta)), \qquad \dot{\xi}^*(t; y, \eta) = -h_x(x^*(t; y, \eta), \xi^*(t; y, \eta))\,, \tag{2.2.1}$$

with initial condition $(x^*(0; y, \eta), \xi^*(0; y, \eta)) = (y, \eta)$. Observe that, as a consequence of (2.2.1), 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

$$\Lambda_h := \{(t, -h(y, \eta)), (x^*(t; y, \eta), \xi^*(t; y, \eta)), (y, -\eta) \mid t \in \mathbb{R},\ (y, \eta) \in T'M\}. \tag{2.2.2}$$

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 and positively homogeneous in momentum of degree one. 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 [67, 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 as the sum of oscillatory integrals of the form

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

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

$$đ\eta = (2\pi)^{-d} \mathrm{d}\eta. \tag{2.2.3}$$

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.

$$a(t,x;y,\eta) \sim \sum_{k=0}^{\infty} a_{m-k}(t,x;y,\eta), \tag{2.2.4}$$

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 this thesis, 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, [66], [115, 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 $H^1(\Lambda_h, \mathbb{Z})$ [81], 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 [77, Lemmata 1.4 and 1.7].

We are now able to state the main result contained in [77].

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

$$h(x, \xi) := \left(g^{\alpha\beta}(x)\, \xi_\alpha\, \xi_\beta\right)^{1/2}. \tag{2.2.5}$$

Then the flow (2.2.1) is (co)geodesic and the propagator for our hyperbolic PDE (2.1.7a) is a Fourier integral operator whose Schwartz kernel (2.1.6) is a Lagrangian distribution of order zero associated with the Lagrangian manifold Λ_h. As already noticed by Laptev, Safarov and Vassiliev in [77], 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 [77], 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

$$\varphi_{x^\alpha\eta_\beta}\big|_{x=x^*} \tag{2.2.6}$$

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 (2.2.6) 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 [77, 104], (2.2.6) is the core of a purely analytic definition of the Maslov index.

Consider the differential 1-form

$$\vartheta_\varphi = -\frac{1}{2\pi}\mathrm{d}\left[\arg\left(\det\varphi_{x^\alpha\eta_\beta}\big|_{x=x^*}\right)^2\right]. \tag{2.2.7}$$

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

$$\operatorname{ind}(\gamma) := \int_\gamma \vartheta_\varphi\,. \tag{2.2.8}$$

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 (2.2.8) is the differential counterpart under the standard isomorphism between Čech and de Rham cohomologies of the approach in terms of cocycles adopted in [66]. See [104, Section 1.5] for additional details.

2.3 Main results

We seek the Schwartz kernel (2.1.6) of the propagator (2.1.5) in the form

$$u(t,x,y) = \mathcal{I}_\varphi(\mathfrak{a}) + \mathcal{K}(t,x,y), \tag{2.3.1}$$

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

$$\mathcal{I}_\varphi(\mathfrak{a}) = \int_{T_y^*M} e^{i\varphi(t,x;y,\eta;\epsilon)}\, \mathfrak{a}(t;y,\eta;\epsilon)\, \chi(t,x;y,\eta)\, w(t,x;y,\eta;\epsilon)\, \text{đ}\eta \tag{2.3.2}$$

is a global oscillatory integral. Here φ is a particular phase function of class $\mathcal{L}_h$, with h given by (2.2.5), which will be introduced in Section 2.4. 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 (2.3.2) will be provided in Section 2.5. Let us emphasise that the representation (2.3.2) will be global in time $t \in \mathbb{R}$ and in space $x, y \in M$.

The main results of Chapter 2 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 2.5.

2. We determine the symbol of the identity operator written as an invariant oscillatory integral, see Section 2.7.

3. We perform a detailed study of the subprincipal symbol of the propagator and provide a simplified algorithm for its calculation, see Section 2.8 and Theorem 2.24 therein.

4. We write down a small time asymptotic formula for the subprincipal symbol of the propagator, see Theorem 2.25.

5. We apply our construction to maximally symmetric spaces of constant curvature in 2D, the standard 2-sphere and the hyperbolic plane, see Section 2.11.

6. Using our complex-valued phase function, we provide a geometric construction which allows us to visualise the analytical circumvention of topological obstructions, see Theorem 2.31.

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 2.3 (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

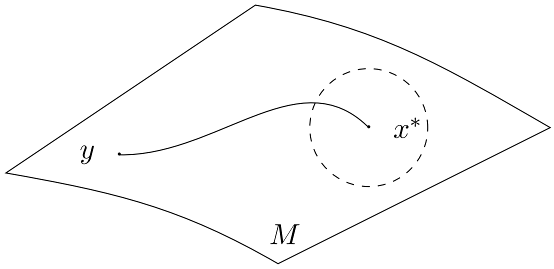
$$\varphi(t,x;y,\eta;\epsilon) := \int_\gamma \zeta \,\mathrm{d}z + \frac{i\,\epsilon}{2}\, h(y,\eta)\, \operatorname{dist}^2(x, x^*(t;y,\eta)) \tag{2.4.1}$$

when x lies in a geodesic neighbourhood[1] of $x^*(t;y,\eta)$ and continued smoothly elsewhere in such a way that $\operatorname{Im}\varphi \ge 0$. 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 $\epsilon = 0$.

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

[1] Here and further on 'geodesic neighbourhood of z' means 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.



reads locally

$$\varphi(t,x;y,\eta;\epsilon) = (x - x^*(t;y,\eta))^\alpha\, \xi^*_\alpha(t;y,\eta) \\ + \frac{i\,\epsilon}{2}\, h(y,\eta)\, \delta_{\mu\nu}\, (x - x^*(t;y,\eta))^\mu (x - x^*(t;y,\eta))^\nu. \quad (2.4.2)$$

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 compatible 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 Theorem 2.18.

Remark 2.4. The real-valued Levi–Civita phase function appears, in various forms, in [77], [104] and [85]. Note, however, that the geometric phase function used in the parametrix construction in [119] and [31] is not the same as (2.4.1) for $\epsilon = 0$: the phase function appearing in [119] and [31] 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 2.5. *We have*

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

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

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

□

In view of Lemma 2.5, we can recast the Levi-Civita phase function (2.4.1) in the more explicit form

$$\varphi(t,x;y,\eta;\epsilon) := -\frac{1}{2}\langle \xi^*, \operatorname{grad}_z[\operatorname{dist}^2(x,z)]\big|_{z=x^*}\rangle + \frac{i\,\epsilon}{2}\,h(y,\eta)\,\operatorname{dist}^2(x^*,x)\,, \tag{2.4.3}$$

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

As briefly discussed in Section 2.2, 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 2.6. *In any coordinate systems x and y, $\varphi_{x^\alpha\eta_\beta}$ along the flow is given by*

$$\varphi_{x^\alpha\eta_\beta}\big|_{x=x^*} = \frac{\partial \xi^*_\alpha}{\partial\eta_\beta} - \Gamma^\mu{}_{\alpha\nu}(x^*)\,\xi^*_\mu\,\frac{\partial x^{*\nu}}{\partial\eta_\beta} - i\,\epsilon\,h(y,\eta)\,g_{\alpha\nu}(x^*)\,\frac{\partial x^{*\nu}}{\partial\eta_\beta}\,, \tag{2.4.4}$$

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

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

Formula (2.4.4) now follows by direct differentiation. □

The explicit formula established in Theorem 2.6 is quite useful. In fact, it offers a direct way of investigating the topology of Λ_h and computing the Maslov index. We will come back to this later on.

2.5 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 (2.3.1) and (2.3.2), let us consider the Lagrangian distribution

$$\mathcal{I}_\varphi(\mathfrak{a}) = \int_{T_y^*M} e^{i\varphi(t,x;y,\eta;\epsilon)}\, \mathfrak{a}(t;y,\eta;\epsilon)\, \chi(t,x;y,\eta)\, w(t,x;y,\eta;\epsilon)\, đ\eta\,, \tag{2.5.1}$$

where the quantities on the RHS are defined as follows.

- φ is the Levi-Civita phase function (2.4.3).
- $\mathfrak{a} \in S^0_{\mathrm{ph}}(\mathbb{R}\times T'M\times\mathbb{R}_+)$ is a polyhomogeneous symbol with asymptotic expansion

$$\mathfrak{a}(t;y,\eta;\epsilon) \sim \sum_{k=0}^{\infty} \mathfrak{a}_{-k}(t;y,\eta;\epsilon), \tag{2.5.2}$$

  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 the geodesic flow and away from the origin $\eta = 0$. 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 (2.5.1) only come from a neighbourhood of the set

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

  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

$$w(t,x;y,\eta;\epsilon) := [\rho(x)]^{-1/2}\,[\rho(y)]^{-1/2}\,\left[\det{}^2\!\left(\varphi_{x^\alpha\eta_\beta}(t,x;y,\eta;\epsilon)\right)\right]^{1/4} \tag{2.5.3}$$

with ρ from (2.1.1). 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 [77, 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 (2.5.1) 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 [104, 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 2.7. The reason we write $\left[\det{}^2\big(\varphi_{x^\alpha\eta_\beta}\big)\right]^{1/4}$ in formula (2.5.3) 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

$$\mathcal{P}:=\partial_t^2-\Delta_x \tag{2.5.4}$$

to (2.5.1). The result is an oscillatory integral

$$\mathcal{I}_\varphi(a)=\mathcal{P}\,\mathcal{I}_\varphi(\mathfrak{a}) \tag{2.5.5}$$

of the same form but with a different amplitude

$$a(t,x;y,\eta;\epsilon)=\frac{e^{-i\varphi(t,x;y,\eta;\epsilon)}}{w(t,x;y,\eta;\epsilon)}\,\mathcal{P}\left(e^{i\varphi(t,x;y,\eta;\epsilon)}\,\mathfrak{a}(t;y,\eta;\epsilon)\,w(t,x;y,\eta;\epsilon)\right).$$

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 $(-i\,\partial_t+\sqrt{-\Delta})$ is justified by [104, 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 (2.5.5) up to an infinitely smooth term:

$$\mathcal{I}_\varphi(\mathfrak{b}) \overset{\mathrm{mod}\ C^\infty}{=} \mathcal{I}_\varphi(a). \tag{2.5.6}$$

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

Put

$$L_\alpha := \left[(\varphi_{x\eta})^{-1}\right]_\alpha{}^\beta \frac{\partial}{\partial x^\beta} \tag{2.5.7}$$

and define

$$\mathfrak{S}_0 := (\,\cdot\,)|_{x=x^*}\ , \tag{2.5.8a}$$

$$\mathfrak{S}_{-k} := \mathfrak{S}_0 \left[i\, w^{-1} \frac{\partial}{\partial \eta_\beta}\, w \left(1 + \sum_{1 \le |\boldsymbol{\alpha}| \le 2k-1} \frac{(-\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!\,(|\boldsymbol{\alpha}|+1)}\, L_{\boldsymbol{\alpha}} \right) L_\beta \right]^k . \tag{2.5.8b}$$

Bold Greek letters in (2.5.8b) denote multi-indices in $\mathbb{N}_0^d$, $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_d)$, $|\boldsymbol{\alpha}| = \sum_{j=1}^d \alpha_j$ and $(-\varphi_\eta)^{\boldsymbol{\alpha}} := (-1)^{|\boldsymbol{\alpha}|} (\varphi_{\eta_1})^{\alpha_1} \ldots (\varphi_{\eta_d})^{\alpha_d}$. All differentiations are applied to the whole expression to the right of them. The operator (2.5.8b) is well defined because the differential operators L_α commute, see Lemma 2.14 in Section 2.6.

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

$$\mathfrak{b}_l := \sum_{2-j-k=l} \mathfrak{S}_{-k}\, a_{2-j}, \qquad l = 2, 1, 0, -1, \ldots. \tag{2.5.9}$$

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 (2.5.6) are postponed to Section 2.6.

Step three. Impose the condition that our oscillatory integral (2.5.1) 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 $\mathfrak{b}$:

$$\mathfrak{b}_l = 0, \qquad l = 2, 1, 0, -1, \dots . \tag{2.5.10}$$

Formula (2.5.10) 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 (2.5.1) is, modulo C^∞, the integral kernel of the identity operator — see Section 2.7 for details.

Remark 2.8. One knows *a priori* that the leading homogeneous term in the expansion (2.5.2) is

$$\mathfrak{a}_0(t; y, \eta; \epsilon) = 1. \tag{2.5.11}$$

This is a consequence of the fact that the subprincipal symbol of the Laplace–Beltrami operator is zero, see [77, Theorem 4.1] or [104, Theorem 3.3.2]. Formula (2.5.11) holds for any choice of phase function due to the way (2.5.1) 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 becomes 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 (2.5.1) 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 x is not in the cut locus or conjugate locus of y. 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 2.9. We define the *symbol of the wave propagator* as the scalar function

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

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 topological obstructions arising from caustics.

In Section 2.8 we will see the algorithm in action and perform a detailed analysis of the subprincipal symbol. In Section 2.11 we will apply our algorithm to two explicit examples.

Remark 2.10. The remainder terms in the asymptotic formulae provided in this Chapter 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 2.11 (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 2.12. By carrying out the integration in η in (2.5.1) for x sufficiently close to y one obtains the well-known Hadamard expansion, see, e.g., [19] and [13, Remark 2.5.5]. Our construction provides an explicit global version of the known local expansion.

2.6 The amplitude-to-symbol operator

In this Section we will provide proofs and rigorous justification to the amplitude reduction algorithm described in Section 2.5, developing ideas outlined in [104].

With the notation established earlier in the thesis, 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

$$\mathcal{I}_\varphi(a) = \int_{T^*_y M} \mathrm{e}^{i\varphi(t,x;y,\eta)}\, a(t,x;y,\eta)\, w(t,x;y,\eta)\, đ\eta\, , \tag{2.6.1}$$

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,

$$\mathcal{I}_\varphi(a) \overset{\mathrm{mod}\, C^\infty}{=} \int_{T^*_y M} e^{i\varphi(t,x;y,\eta)}\, \mathfrak{a}(t;y,\eta)\, w(t,x;y,\eta)\, đ\eta, \tag{2.6.2}$$

for some $\mathfrak{a} = \mathfrak{a}(t; y, \eta)$. We call the a in (2.6.1) *amplitude* and the $\mathfrak{a}$ in (2.6.2) *symbol*.

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

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

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

Theorem 2.13. *The amplitude-to-symbol operator* $\mathfrak{S}$ *reads*

$$\mathfrak{S} \sim \sum_{k=0}^{\infty} \mathfrak{S}_{-k}, \tag{2.6.3}$$

where

$$\mathfrak{S}_0 = (\,\cdot\,)|_{x=x^*}\,, \tag{2.6.4}$$

$$\mathfrak{S}_{-k} = \mathfrak{S}_0 \left[i\, w^{-1} \frac{\partial}{\partial \eta_\beta}\, w \left(1 + \sum_{1 \le |\boldsymbol{\alpha}| \le 2k-1} \frac{(-\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!\,(|\boldsymbol{\alpha}|+1)}\, L_{\boldsymbol{\alpha}} \right) L_\beta \right]^k \tag{2.6.5}$$

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 $\det(\varphi_{x^\alpha \eta_\beta}) \neq 0$ 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

$$a = a^* + (x - x^*)^\alpha\, b_\alpha \tag{2.6.6}$$

for some covector $b = b(t, x; y, \eta)$. Plugging (2.6.6) into (2.6.1), we obtain

$$\begin{aligned} \mathcal{I}_\varphi(a) &= \int_{T'_yM} e^{i\varphi}\, a^*\, w\, đ\eta + \int_{T'_yM} e^{i\varphi}\, (x-x^*)^\alpha\, b_\alpha\, w\, đ\eta \\ &= \int_{T'_yM} e^{i\varphi}\, a^*\, w\, đ\eta + \int_{T'_yM} e^{i\varphi}\, \varphi_{\eta_\alpha}\, \widetilde{b}_\alpha\, w\, đ\eta \\ &= \int_{T'_yM} e^{i\varphi}\, a^*\, w\, đ\eta + \int_{T'_yM} \frac{1}{i}\left(\frac{\partial}{\partial\eta_\alpha} e^{i\varphi}\right) \widetilde{b}_\alpha\, w\, đ\eta \\ &= \int_{T'_yM} e^{i\varphi}\, a^*\, w\, đ\eta + \int_{T'_yM} e^{i\varphi}\, i\, w^{-1}\left(\frac{\partial}{\partial\eta_\alpha}\widetilde{b}_\alpha\, w\right) w\, đ\eta\,, \end{aligned} \tag{2.6.7}$$

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

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

The first integral on the RHS of (2.6.7) 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

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

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

Note that the b and $\widetilde{b}$ 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 $\widetilde{b}_\alpha$ 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 (2.6.6). A crucial point worth stressing is that the whole construction is global and covariant.

Before addressing the proof of Theorem 2.13 we need to state and prove a preparatory lemma.

Lemma 2.14. *The operators*

$$L_\alpha = (\varphi_{x\eta}^{-1})_\alpha{}^\beta \frac{\partial}{\partial x^\beta} \tag{2.6.8}$$

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

$$[L_\alpha, L_\beta] = 0. \tag{2.6.9}$$

Proof. We have

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

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

$$\begin{aligned} (\varphi_{x\eta})_\gamma{}^\alpha\, (\varphi_{x\eta})_\rho{}^\beta\, [L_\alpha, L_\beta] &= \left((\varphi_{x\eta})_\rho{}^\beta [(\varphi_{x\eta}^{-1})_\beta{}^\mu]_{x^\gamma} - (\varphi_{x\eta})_\gamma{}^\alpha\, [(\varphi_{x\eta}^{-1})_\alpha{}^\mu]_{x^\rho}\right) \frac{\partial}{\partial x^\mu} \\ &= \left(-[(\varphi_{x\eta})_\rho{}^\beta]_{x^\gamma} (\varphi_{x\eta}^{-1})_\beta{}^\mu + [(\varphi_{x\eta})_\gamma{}^\alpha]_{x^\rho}\, (\varphi_{x\eta}^{-1})_\alpha{}^\mu\right) \frac{\partial}{\partial x^\mu} \\ &= \left(-\varphi_{x^\rho x^\gamma \eta_\beta}\, (\varphi_{x\eta}^{-1})_\beta{}^\mu + \varphi_{x^\gamma x^\rho \eta_\alpha}\, (\varphi_{x\eta}^{-1})_\alpha{}^\mu\right) \frac{\partial}{\partial x^\mu} \\ &= \left(-\varphi_{x^\rho x^\gamma \eta_\alpha}\, (\varphi_{x\eta}^{-1})_\alpha{}^\mu + \varphi_{x^\gamma x^\rho \eta_\alpha}\, (\varphi_{x\eta}^{-1})_\alpha{}^\mu\right) \frac{\partial}{\partial x^\mu} \\ &= 0. \end{aligned} \tag{2.6.10}$$

Since $\varphi_{x\eta}$ is non-degenerate, (2.6.10) is equivalent to (2.6.9). □

We are now in a position to prove Theorem 2.13.

Proof of Theorem 2.13. The first step is to show that it is possible to write, modulo $O(\|x - x^*\|^\infty)$, the amplitude a as

$$a(t, x; y, \eta) = a(t, x^*(t; y, \eta); y, \eta) + \varphi_{\eta_\alpha}(t, x; y, \eta)\, \widetilde{b}_\alpha(t, x; y, \eta) \tag{2.6.11}$$

for some $\widetilde{b}$.

In order to write down explicitly the $\widetilde{b}$ appearing in formula (2.6.11), let us introduce the operators

$$F_0 := 1, \tag{2.6.12}$$

$$F_k := \sum_{|\boldsymbol{\alpha}|=k} \frac{(\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!} L_{\boldsymbol{\alpha}}\,, \tag{2.6.13}$$

where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \dots, \alpha_d) \in \mathbb{N}_0^d$ is a multi-index, $(\varphi_\eta)^{\boldsymbol{\alpha}} = (\varphi_{\eta_1})^{\alpha_1} (\varphi_{\eta_2})^{\alpha_2} \cdots (\varphi_{\eta_d})^{\alpha_d}$, $\boldsymbol{\alpha}! = \alpha_1!\, \alpha_2! \cdots \alpha_d!\,$, $L_{\boldsymbol{\alpha}} = (L_1)^{\alpha_1} (L_2)^{\alpha_2} \cdots (L_d)^{\alpha_d}$. In view of Lemma 2.14, 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 (2.6.13) are the ones from the algebraic multinomial expansion

$$(z_1+\ldots+z_d)^k = k!\sum_{|\boldsymbol{\alpha}|=k}\frac{1}{\boldsymbol{\alpha}!}\,z^{\boldsymbol{\alpha}}, \tag{2.6.14}$$

a generalisation of the binomial expansion.

Formulae (2.6.13) and (2.6.14) imply

$$(k+1)F_{k+1} = \sum_{\gamma=1}^{d}\varphi_{\eta_\gamma}F_k\,L_\gamma\,. \tag{2.6.15}$$

Furthermore, we have

$$\begin{aligned}
F_1\,F_k - k\,F_k &= \left(\sum_{\gamma=1}^{d}\varphi_{\eta_\gamma}\,L_\gamma\right)F_k - k\,F_k\\
&= \sum_{\gamma,\mu=1}^{d}\varphi_{\eta_\gamma}(\varphi_{x\eta}^{-1})_\gamma{}^\mu\sum_{|\boldsymbol{\alpha}|=k}\frac{[(\varphi_\eta)^{\boldsymbol{\alpha}}]_{x^\mu}}{\boldsymbol{\alpha}!}L_{\boldsymbol{\alpha}}\\
&+\sum_{\gamma=1}^{d}\varphi_{\eta_\gamma}\sum_{|\boldsymbol{\alpha}|=k}\frac{(\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!}L_\gamma L_{\boldsymbol{\alpha}} - k\,F_k\\
&= k\,F_k + \sum_{\gamma=1}^{d}\varphi_{\eta_\gamma}\sum_{|\boldsymbol{\alpha}|=k}\frac{(\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!}L_{\boldsymbol{\alpha}}L_\gamma - k\,F_k\\
&= \sum_{\gamma=1}^{d}\varphi_{\eta_\gamma}F_k\,L_\gamma\,.
\end{aligned} \tag{2.6.16}$$

Combining formulae (2.6.15) and (2.6.16), we arrive at a recurrent formula for our operators F_k :

$$(k+1)F_{k+1} = F_1\,F_k - k\,F_k\,. \tag{2.6.17}$$

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

$$F_k(\varphi_\eta)^{\boldsymbol{\alpha}} = \begin{cases} 0, & |\boldsymbol{\alpha}|<k,\\ \binom{|\boldsymbol{\alpha}|}{k}(\varphi_\eta)^{\boldsymbol{\alpha}}, & |\boldsymbol{\alpha}|\ge k. \end{cases} \tag{2.6.18}$$

Formula (2.6.18) 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 (2.6.17) and the inductive assumption. If

$|\boldsymbol{\alpha}| \geq n$, then formula (2.6.17) and the inductive assumption give us

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

as required.

Formula (2.6.18) 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 (2.6.18) imply

$$(\varphi_\eta)^{\boldsymbol{\alpha}} = -\left(\sum_{k=1}^{|\boldsymbol{\alpha}|}(-1)^k F_k\right)(\varphi_\eta)^{\boldsymbol{\alpha}} = -\left(\sum_{k=1}^{\infty}(-1)^k F_k\right)(\varphi_\eta)^{\boldsymbol{\alpha}}, \qquad \forall \boldsymbol{\alpha} \neq 0. \quad (2.6.19)$$

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

$$a \simeq \sum_{|\boldsymbol{\alpha}| \geq 0} \frac{(\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!}\,[L_{\boldsymbol{\alpha}} a]|_{x=x^*}\,. \qquad (2.6.20)$$

The symbol $\simeq$ in (2.6.20) indicates that we are dealing with an asymptotic expansion. Namely, it means that for any $r \in \mathbb{N}_0$ we have

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

Formula (2.6.19) allows us to rewrite the asymptotic expansion (2.6.20) as

$$a \simeq a|_{x=x^*} - \sum_{k=1}^{\infty} (-1)^k F_k \, a. \tag{2.6.21}$$

The advantage of (2.6.21) over (2.6.20) is that the restriction operator $(\,\cdot\,)|_{x=x^*}$ appears only in one place, in the first term on the RHS of (2.6.21). Formula (2.6.21) is a generalisation of the formula

$$a(x) \simeq a(0) + x a'(x) - \frac{x^2}{2} a''(x) + \frac{x^3}{6} a'''(x) + \ldots \tag{2.6.22}$$

from the analysis of functions of one variable. Namely, formula (2.6.21) turns into (2.6.22) 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 (2.6.8) 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 (2.6.21) also maps scalar functions to scalar functions.

Using formulae (2.6.15) and (2.6.12), (2.6.13), we can rewrite (2.6.21) as

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

where $a^* = a|_{x=x^*}$. Thus, we have represented our amplitude in the form (2.6.11) with

$$\widetilde{b}_\gamma \simeq \sum_{|\boldsymbol{\alpha}|\ge 0} \frac{(-\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}! \, (|\boldsymbol{\alpha}|+1)} L_{\boldsymbol{\alpha}} \, L_\gamma \, a \,. \tag{2.6.23}$$

Combining (2.6.1) with (2.6.11) and (2.6.23) and by using the identity

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

we get, upon integration by parts,

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

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 (2.6.3)–(2.6.5). The cut-off on the possible values of $|\boldsymbol{\alpha}|$ in (2.6.5) follows from incorporating the information that $\varphi_\eta|_{x=x^*} = 0$. □

2.7 Invariant representation of the identity operator

Step three of our algorithm described in Section 2.5 involves initial conditions determined by the symbol of the identity operator, which appears in our construction as a pseudodifferential operator written in the form

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

with the Levi-Civita phase function and some symbol $\mathfrak{s}$, cf. (2.5.1). Recall that χ is a cut-off and w is defined by formula (2.5.3). 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 [85] and [49], 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

$$\mathfrak{s}_0(y,\eta) = 1, \tag{2.7.1}$$

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 2.15. *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

$$(\mathfrak{I}_{\phi,s}\, f)(x) = \int_{T'M} e^{i\,\phi(x;y,\eta)}\, \mathfrak{s}(y,\eta)\, \chi(x;y,\eta)\, v(x;y,\eta)\, f(y)\, \mathrm{d}y\, \text{đ}\eta\,, \tag{2.7.2}$$

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

$$v(x;y,\eta) = \rho(x)^{-1/2}\, \rho(y)^{1/2}\, [\det{}^2 \phi_{x\eta}]^{1/4}\,. \tag{2.7.3}$$

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

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

Remark 2.16. It is easy to see that the quantity defined by formula (2.7.3) 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 2.15. Let us define the dual pseudodifferential operator $\mathfrak{I}'_{\phi,s}$ via the identity

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

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

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

where

$$u(x;y,\eta) = \rho(x)\, \rho(y)^{-1}\, v(x;y,\eta) = \rho(x)^{1/2}\, \rho(y)^{-1/2}\, [\det{}^2 \phi_{x\eta}]^{1/4}\,. \tag{2.7.4}$$

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

$$k \mapsto (\mathfrak{I}'_{\phi,s}\, k)(0). \tag{2.7.5}$$

The map (2.7.5) is a distribution, a continuous linear functional. We want the distribution (2.7.5) to approximate, modulo C^∞, the delta distribution, i.e. we want

$$\int e^{i\,\phi(x;0,\eta)}\,\mathfrak{s}(0,\eta)\,\chi(x;0,\eta)\,u(x;0,\eta)\,k(x)\,\mathrm{d}x\,đ\eta\;=k(0) \tag{2.7.6}$$

modulo a smooth functional. Substituting (2.7.4) into (2.7.6) we rewrite the latter as

$$\int e^{i\,\phi(x;0,\eta)}\,\mathfrak{s}(0,\eta)\,\chi(x;0,\eta)\,\kappa(x)\,\sqrt{\det\phi_{x\eta}}\;\mathrm{d}x\,đ\eta\;=\kappa(0)\,, \tag{2.7.7}$$

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 2.7. Formula (2.7.7) is, in turn, equivalent to

$$\int e^{i\,\phi(x;0,\eta)}\,\mathfrak{s}(0,\eta)\,\chi(x;0,\eta)\,\sqrt{\det\phi_{x\eta}}\;đ\eta\;=\int e^{i\,x^\alpha\eta_\alpha}\,đ\eta\,. \tag{2.7.8}$$

The integrals in (2.7.8) are understood as distributions in the variable x and equality is understood as equality modulo a smooth distribution.

The complex exponential in (2.7.8) admits the expansion

$$e^{i\,\phi(x;0,\eta)}=e^{i\,x^\alpha\eta_\alpha}\left[1+\frac{i}{2}\,\phi_{x^\mu x^\nu}(0;0,\eta)\,x^\mu\,x^\nu+O(\|x\|^3)\right]. \tag{2.7.9}$$

Furthermore,

$$\sqrt{\det\phi_{x\eta}}\,(x;0,\eta)=1+\frac{1}{2}\,\phi_{x^\alpha x^\beta\eta_\alpha}(0;0,\eta)\,x^\beta+O(\|x\|^2). \tag{2.7.10}$$

Substituting (2.7.9) and (2.7.10) into the LHS of (2.7.8) and integrating by parts we get

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

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 $\mathfrak{s}_{-1}(y,\eta)=0$, $\forall(y,\eta)\in T'M$. $\square$

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

Theorem 2.17. *The sub-subleading contribution to the symbol of the identity operator written as a pseudodifferential operator* (2.7.2) *with the Levi-Civita phase function* $\varphi(0, x; y, \eta; \epsilon)$ *is*

$$\mathfrak{s}_{-2}(y, \eta) = \frac{(d-1)\,(d-2)\,\epsilon^2}{8\,g^{\alpha\beta}(y)\,\eta_\alpha\eta_\beta}\,. \tag{2.7.11}$$

Proof. Let us fix a point $P \in M$ and argue as in the proof of Theorem 2.15, arriving at (2.7.8). 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 (2.7.8) 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 (2.4.2).

The complex exponential in (2.7.8) admits the expansion

$$e^{i\,\phi(x;0,\eta)} = e^{i\,x^\alpha\eta_\alpha}\left[1 - \frac{\epsilon}{2}\,\|\eta\|\,\|x\|^2 + \frac{\epsilon^2}{8}\,\|\eta\|^2\,\|x\|^4 + O(\|x\|^6)\right]. \tag{2.7.12}$$

We have

$$(\phi_{x^\alpha\eta_\beta})(x; 0, \eta) = \delta_\alpha{}^\beta + i\,\epsilon\,\delta_{\alpha\mu}\,\delta^{\beta\nu}\,\frac{\eta_\nu}{\|\eta\|}\,x^\mu\,. \tag{2.7.13}$$

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

$$\det(I + A) = 1 + \operatorname{tr} A + \frac{1}{2}\big[(\operatorname{tr} A)^2 - \operatorname{tr}(A^2)\big] + O(\|A\|^3). \tag{2.7.14}$$

Formulae (2.7.13) and (2.7.14) imply

$$\sqrt{\det \phi_{x\eta}}\,(x; 0, \eta) = 1 + \frac{i\epsilon}{2\|\eta\|}\,x^\alpha\eta_\alpha + \frac{\epsilon^2}{8\|\eta\|^2}\,(x^\beta\eta_\beta)^2 + O(\|x\|^3). \tag{2.7.15}$$

Substituting (2.7.12) and (2.7.15) into the LHS of (2.7.8) and integrating by parts we get

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

which gives us (2.7.11). $\square$

The algorithm described in the proof of Theorem 2.17 allows one to calculate explicitly $\mathfrak{s}_{-3}, \mathfrak{s}_{-4}, \ldots$ but the calculations become cumbersome. We list the resulting formulae for the special case $d = 2$:

$$\begin{aligned}
\mathfrak{s}_{-3}(y,\eta) &= \frac{1}{2^3}\,\frac{\epsilon^3}{(g^{\alpha\beta}(y)\,\eta_\alpha\eta_\beta)^{3/2}}\,, & \mathfrak{s}_{-4}(y,\eta) &= 0\,,\\
\mathfrak{s}_{-5}(y,\eta) &= \frac{3^2\times 5}{2^6}\,\frac{\epsilon^5}{(g^{\alpha\beta}(y)\,\eta_\alpha\eta_\beta)^{5/2}}\,, & \mathfrak{s}_{-6}(y,\eta) &= 0\,,\\
\mathfrak{s}_{-7}(y,\eta) &= \frac{3^2\times 5^2\times 13}{2^{10}}\,\frac{\epsilon^7}{(g^{\alpha\beta}(y)\,\eta_\alpha\eta_\beta)^{7/2}}\,, & \mathfrak{s}_{-8}(y,\eta) &= 0\,,\\
\mathfrak{s}_{-9}(y,\eta) &= \frac{3^3\times 5^2\times 7^2\times 47}{2^6}\,\frac{\epsilon^9}{(g^{\alpha\beta}(y)\,\eta_\alpha\eta_\beta)^{9/2}}\,, & \mathfrak{s}_{-10}(y,\eta) &= 0\,.
\end{aligned} \tag{2.7.16}$$

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.

Theorem 2.18. *The full symbol of the identity operator written as a pseudodifferential operator* (2.7.2) *with the real-valued Levi-Civita phase function* $\varphi(0, x; y, \eta; 0)$ *is*

$$\mathfrak{s}(y, \eta) = 1. \tag{2.7.17}$$

Proof. Formula (2.7.17) is established by arguing as in the proof of Theorem 2.17. □

2.8 The 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 2.5 for the special case of the subprincipal symbol.

Definition 2.19. We call the scalar function $\mathfrak{a}_{-1}(t; y, \eta; \epsilon)$ appearing in Definition 2.9 the *subprincipal symbol of the wave propagator.*

Acting with the wave operator (2.5.4) on the oscillatory integral

$$\int e^{i\,\varphi(t,x;y,\eta;\epsilon)}\,(1 + \mathfrak{a}_{-1}(t; y, \eta; \epsilon))\; w(t, x; y, \eta; \epsilon)\, đ\eta, \tag{2.8.1}$$

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

$$a = (1 + \mathfrak{a}_{-1})\, e^{-i\,\varphi} \left[\mathcal{P}\,(e^{i\,\varphi}\, w)\right] w^{-1} + (\mathfrak{a}_{-1})_{tt} + 2\,(\mathfrak{a}_{-1})_t \left(i\,\varphi_t + w_t\, w^{-1}\right) . \tag{2.8.2}$$

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

Lemma 2.20. *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*

$$b_2 = -\,(\varphi_t)^2 + g^{\alpha\beta}(x)\,(\nabla_\alpha\,\varphi)\,(\nabla_\beta\,\varphi)\,, \tag{2.8.3a}$$

$$b_1 = i\left[\varphi_{tt} - g^{\alpha\beta}(x)\,\nabla_\alpha\nabla_\beta\,\varphi + 2\,(\log w)_t\,\varphi_t - 2\,g^{\alpha\beta}(x)\,[\nabla_\alpha(\log w)]\,(\nabla_\beta\,\varphi)\right], \tag{2.8.3b}$$

$$b_0 = w^{-1}\left[w_{tt} - g^{\alpha\beta}(x)\,\nabla_\alpha\nabla_\beta\, w\right], \tag{2.8.3c}$$

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. In view of formula (2.1.2) the contribution to b from the Laplacian reads

$$-\frac{e^{-i\,\varphi}}{w}\,\Delta\left(e^{i\,\varphi}\,w\right) = -i\,g^{\mu\nu}(x)\,\varphi_{x^\mu x^\nu} + g^{\mu\nu}(x)\,\varphi_{x^\mu}\,\varphi_{x^\nu} - g^{\mu\nu}(x)\,w_{x^\mu x^\nu}\,w^{-1}$$
$$-\,2\,i\,g^{\mu\nu}(x)\,\varphi_{x^\mu}\,w_{x^\nu}\,w^{-1} - \rho(x)^{-1}\,[\rho(x)\,g^{\mu\nu}(x)]_{x^\mu}\left(i\,\varphi_{x^\nu} - w_{x^\nu}\,w^{-1}\right) . \tag{2.8.4}$$

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

$$\frac{e^{-i\,\varphi}}{w}\,\frac{\partial^2}{\partial t^2}\left(e^{i\,\varphi}\,w\right) = -\,(\varphi_t)^2 + i\,\varphi_{tt} + 2\,i\,\varphi_t\,w_t\,w^{-1} + w_{tt}\,w^{-1}\,. \tag{2.8.5}$$

Combining (2.8.4) and (2.8.5), singling out terms with the same degree of homogeneity and using the chain of identities

$$\rho(x)^{-1}\,(\rho(x)\,g^{\mu\nu}(x))_{x^\mu} = [g^{\mu\nu}(x)]_{x^\mu} + \frac{1}{2}g^{\mu\nu}(x)\,[\ln(\det g_{\kappa\lambda}(x))]_{x^\mu} = -\Gamma^\nu{}_{\alpha\beta}(x)\,g^{\alpha\beta}(x)$$

we arrive at (2.8.3a)–(2.8.3c). □

In terms of the homogeneous components of b, formula (2.8.2) reads

$$\begin{aligned} a &= b_2 \\ &\quad + b_1 + b_2\,\mathfrak{a}_{-1} \\ &\quad + b_0 + b_1\,\mathfrak{a}_{-1} + 2\,i\,(\mathfrak{a}_{-1})_t\,\varphi_t \\ &\quad + b_0\,\mathfrak{a}_{-1} + (\mathfrak{a}_{-1})_{tt} + 2\,\mathfrak{a}_{-1}\,w_t\,w^{-1}\,, \end{aligned} \tag{2.8.6}$$

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 2.21. *We have*

$$\varphi_t|_{x=x^*} = -h(y,\eta). \tag{2.8.7}$$

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 (2.8.7) now follows from the fact that the Hamiltonian is preserved along the flow. □

Lemma 2.22. *The function b_2 defined by (2.8.3a) 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 2.21 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 2.21. The problem at hand is now down to showing that

$$\left(\varphi_{tx^\mu} + [h(x,\nabla\varphi)]_{x^\mu}\right)\big|_{x=x^*} = 0. \tag{2.8.8}$$

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

$$\varphi = (x - x^*)^\alpha \, \xi^*_\alpha + \frac{1}{2} \, [H_\varphi]_{\mu\nu} \, (x - x^*)^\mu \, (x - x^*)^\nu + O(\|x - x^*\|^3), \qquad (2.8.9)$$

with

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

Combining (2.8.9) with Hamilton's equations, we get

$$\varphi_{tx^\alpha}|_{x-x^*} = \dot{\xi}^*_\alpha - [H_\varphi]_{\alpha\mu} \, \dot{x}^{*\mu} = -h_{x^\alpha}(x^*, \xi^*) - [H_\varphi]_{\alpha\mu} \, h_{\xi_\mu}(x^*, \xi^*). \qquad (2.8.10)$$

Moreover, we have

$$\begin{aligned} [h(x, \nabla\varphi)]_{x^\alpha}|_{x=x^*} =& h_{x^\alpha}(x^*, \xi^*) + h_{\xi_\mu}(x^*, \xi^*) \;\; \varphi_{x^\alpha x^\mu}|_{x=x^*} \\ =& h_{x^\alpha}(x^*, \xi^*) + [H_\varphi]_{\alpha\mu} \, h_{\xi_\mu}(x^*, \xi^*). \end{aligned} \qquad (2.8.11)$$

Substitution of (2.8.10) and (2.8.11) into (2.8.8) concludes the proof. □

Lemmata 2.21 and 2.22 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 2.5, in view of formulae (2.5.9) and (2.8.6) we have

$$\mathfrak{b}_2 = \mathfrak{S}_0 \, b_2 \, , \qquad (2.8.12a)$$

$$\mathfrak{b}_1 = \mathfrak{S}_{-1} \, b_2 + \mathfrak{S}_0 \, b_1 \, , \qquad (2.8.12b)$$

$$\mathfrak{b}_0 = \mathfrak{S}_{-2} \, b_2 + \mathfrak{S}_{-1} \, b_1 + \mathfrak{S}_0 \, b_0 - 2\, i \, h \, (\mathfrak{a}_{-1})_t + \mathfrak{a}_{-1} \, \mathfrak{b}_1 \, . \qquad (2.8.12c)$$

Note that homogeneous components of the symbol $\mathfrak{a}_{-k}$ with degree of homogeneity less than -1, even if taken into account in (2.8.1), would not contribute to (2.8.12a)–(2.8.12c). Note also the appearance of the x-independent term $\mathfrak{a}_{-1} \, \mathfrak{b}_1$ on the RHS of (2.8.12c): it can be traced back to the fact that Lemma 2.22 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 2.22.

Lemma 2.23. *The first transport equation (FTE)* $\mathfrak{b}_1 = 0$ *can be equivalently rewritten as*

$$(\varphi_{tt} - \Delta\varphi)|_{x=x^*} = 2\, h\, \frac{\mathrm{d}(\log\, w^*)}{\mathrm{d}t} + \frac{1}{2}\, (x^*_{\eta_\alpha})^\gamma \left[[(\varphi_{x\eta})^{-1}]_\alpha{}^\beta\, (b_2)_{x^\beta x^\gamma} \right]\Big|_{x=x^*}\,, \qquad (2.8.13)$$

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

Proof. Consider the operator $\mathfrak{S}_{-1}$ defined in (2.5.8b). When acting on a function with a second order zero along the flow, it can be simplified to read

$$\mathfrak{S}_{-1}\, b_2 = i\, \frac{\partial(L_\beta\, b_2)}{\partial\eta_\beta}\Big|_{x=x^*} - \frac{i}{2}\, [\varphi_{\eta_\alpha\eta_\beta}\, L_\alpha L_\beta\, b_2]\,|_{x=x^*}\,. \qquad (2.8.14)$$

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 (2.5.7), we obtain

$$\begin{aligned} -\frac{i}{2}\, [\varphi_{\eta_\alpha\eta_\beta}\, L_\alpha L_\beta\, b_2]\,|_{x=x^*} &= \frac{i}{2} (x^*_{\eta_\alpha})^\gamma\, (\Phi_{x\eta})_\gamma{}^\beta\, (\Phi^{-1}_{x\eta})_\alpha{}^\delta\, (\Phi^{-1}_{x\eta})_\beta{}^\rho\, (H_{b_2})_{\delta\rho} \\ &= \frac{i}{2} (x^*_{\eta_\alpha})^\gamma\, \delta_\gamma{}^\rho\, (\Phi^{-1}_{x\eta})_\alpha{}^\delta\, (H_{b_2})_{\delta\rho} \\ &= \frac{i}{2} (x^*_{\eta_\alpha})^\rho\, (\Phi^{-1}_{x\eta})_\alpha{}^\delta\, (H_{b_2})_{\delta\rho}\,. \end{aligned} \qquad (2.8.15)$$

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 (2.8.14) becomes

$$i\, \frac{\partial(L_\beta\, b_2)}{\partial\eta_\beta}\Big|_{x=x^*} = -i\, (x^*_{\eta_\alpha})^\gamma\, (\Phi^{-1}_{x\eta})_\alpha{}^\mu\, (H_{b_2})_{\mu\gamma}\,. \qquad (2.8.16)$$

By substituting (2.8.15) and (2.8.16) into (2.8.14) we arrive at the last summand on the LHS of (2.8.13). As for the remaining terms, they correspond to $\mathfrak{S}_0\, b_1$ in (2.8.12b) and are obtained by evaluating (2.8.3b) 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 (2.8.13) 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 (2.8.1), the FTE would be an ordinary differential equation allowing for the (unique) determination thereof. Lemma 2.23 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 subprincipal symbol $\mathfrak{a}_{-1}(t; y, \eta; \epsilon)$. To the end of computing the 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 (2.5.8a) and (2.5.8b). Put

$$\mathfrak{B}_{-1} := i\, w^{-1} \frac{\partial}{\partial \eta_\alpha}\, w\, L_\alpha - \frac{i}{2}\, \varphi_{\eta_\alpha \eta_\beta}\, L_\alpha\, L_\beta\, . \tag{2.8.17}$$

Then we have

$$\mathfrak{S}_{-1} = \mathfrak{S}_0\, \mathfrak{B}_{-1}\, , \tag{2.8.18}$$

$$\mathfrak{S}_{-2} = \mathfrak{S}_0\, \mathfrak{B}_{-1} \left[i\, w^{-1} \frac{\partial}{\partial \eta_\beta}\, w \left(1 + \sum_{1 \le |\boldsymbol{\alpha}| \le 3} \frac{(-\varphi_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!(|\boldsymbol{\alpha}|+1)}\, L_{\boldsymbol{\alpha}} \right) L_\beta \right], \tag{2.8.19}$$

and these representations can now be used in formula (2.8.12c).

The last ingredient needed to write down the subprincipal symbol is the initial condition at $t = 0$, extensively discussed in Section 2.7. The Levi-Civita phase function evaluated at $t = 0$, $\varphi(0, x; y, \eta; \epsilon)$, clearly satisfies the assumptions (a) and (b) of Theorem 2.15, hence $\mathfrak{a}_{-1}|_{t=0} = 0$. Integrating in time, we arrive at the following theorem.

Theorem 2.24. *The global invariantly defined subprincipal symbol of the wave propagator is*

$$\mathfrak{a}_{-1}(t; y, \eta; \epsilon) = -\frac{i}{2\, h} \int_0^t \left[\mathfrak{S}_{-2}\, b_2 + \mathfrak{S}_{-1}\, b_1 + \mathfrak{S}_0\, b_0 \right] (\tau; y, \eta; \epsilon)\, \mathrm{d}\tau\, . \tag{2.8.20}$$

The functions b_k, $k = 2, 1, 0$, are defined by (2.8.3a)–(2.8.3c), (2.4.3), (2.5.3), while the operators $\mathfrak{S}_{-2}$, $\mathfrak{S}_{-1}$ and $\mathfrak{S}_0$ are given by (2.8.17)–(2.8.19) and (2.5.7), (2.5.8a).

2.9 Small time expansion for the 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 subprincipal symbol when t tends to zero. In Section 2.10 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 2.25. *The subprincipal symbol of the wave propagator admits the following expansion for small times:*

$$\mathfrak{a}_{-1}(t; y, \eta) = \frac{i}{12\, h(y, \eta)}\, \mathcal{R}(y)\, t + O(t^2)\,, \tag{2.9.1}$$

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

$$\mathfrak{a}_{-1}(t; 0, \eta) = \frac{i}{12\, h(0, \eta)}\, \mathcal{R}(0)\, t + O(t^2) \tag{2.9.2}$$

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.

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

$$x^{*\alpha} = \frac{\eta^\alpha}{h}\, t\,, \tag{2.9.3}$$

where $\eta^\alpha = \delta^{\alpha\beta}\eta_\beta$. Substituting (2.9.3) into the first Hamilton's equation (2.2.1) we get

$$\begin{aligned} \xi^*_\alpha &= g_{\alpha\beta}(x^*)\,\eta^\beta \\ &= \left[g_{\alpha\beta}\left(\frac{\eta}{h}\,t\right)\right]\eta^\beta \\ &= \left(\delta_{\alpha\beta} - \frac{1}{3}\,R_{\alpha\mu\beta\nu}(0)\,\frac{\eta^\mu\eta^\nu}{h^2}\,t^2 + O(t^3)\right)\eta^\beta \\ &= \eta_\alpha + O(t^3). \end{aligned} \tag{2.9.4}$$

The simplifications in the above calculations are due to the properties of normal coordinates and the (anti)symmetries of the Riemann curvature tensor R.

Arguing as in the proof of Theorem 2.6 and using formula (2.9.3), one concludes that the initial velocity of the (unique) geodesic connecting x^* to x is

$$\begin{aligned} \dot\gamma(0)^\alpha &= (x-x^*)^\alpha + \frac{1}{2}\,\Gamma^\alpha{}_{\beta\gamma}(x^*)\,(x-x^*)^\beta\,(x-x^*)^\gamma \\ &+ \frac{1}{2}\,(\partial_{x^\mu}\Gamma^\alpha{}_{\beta\gamma})(x^*)\,(x-x^*)^\mu\,(x-x^*)^\beta\,(x-x^*)^\gamma \\ &+ O(\|x-x^*\|^4) \\ &= x^\alpha - \frac{\eta^\alpha}{h}\,t + \frac{1}{2}(\partial_{x^\mu}\Gamma^\alpha{}_{\beta\gamma})(0)\,\frac{\eta^\mu}{h}\,t\,\left(x-\frac{\eta}{h}\,t\right)^\beta\left(x-\frac{\eta}{h}\,t\right)^\gamma \\ &+ \frac{1}{2}(\partial_{x^\mu}\Gamma^\alpha{}_{\beta\gamma})(0)\left(x-\frac{\eta}{h}\,t\right)^\mu\left(x-\frac{\eta}{h}\,t\right)^\beta\left(x-\frac{\eta}{h}\,t\right)^\gamma + O(\|x\|^4+t^4) \\ &= x^\alpha - \frac{\eta^\alpha}{h}\,t - (\partial_{x^\mu}\Gamma^\alpha{}_{\beta\gamma})(0)\,\frac{\eta^\beta}{h}\,t\,x^\mu\,x^\gamma + \frac{1}{2}(\partial_{x^\mu}\Gamma^\alpha{}_{\beta\gamma})(0)\,\frac{\eta^\beta\,\eta^\gamma}{h^2}\,t^2\,x^\mu \\ &+ \frac{1}{2}(\partial_{x^\mu}\Gamma^\alpha{}_{\beta\gamma})(0)\,x^\mu x^\beta x^\gamma + O(\|x\|^4+t^4) \\ &= x^\alpha - \frac{\eta^\alpha}{h}\,t + \frac{1}{3\,h}\,R^\alpha{}_{\gamma\beta\mu}(0)\,\eta^\beta\,t\,x^\gamma x^\mu - \frac{1}{3}R^\alpha{}_{\beta\gamma\mu}(0)\,\frac{\eta^\beta\,\eta^\gamma}{h^2}\,t^2\,x^\mu \\ &+ O(\|x\|^4+t^4)\,. \end{aligned} \tag{2.9.5}$$

Here at the last step we resorted to the identity

$$(\partial_{x^\mu}\Gamma^\alpha{}_{\beta\gamma})(0) = -\frac{1}{3}\,(R^\alpha{}_{\beta\gamma\mu}(0) + R^\alpha{}_{\gamma\beta\mu}(0)). \tag{2.9.6}$$

Lemma 2.5 and formulae (2.9.4), (2.9.5) imply that our real-valued Levi-Civita phase function admits the following Taylor expansion in powers of x and t:

$$\varphi(t,x;0,\eta) = x^\alpha\,\eta_\alpha - t\,h + \frac{1}{3\,h}\,R^\alpha{}_\mu{}^\beta{}_\nu(0)\,\eta_\alpha\,\eta_\beta\,t\,x^\mu\,x^\nu + O(\|x\|^4+t^4)\,. \tag{2.9.7}$$

The next step is computing the homogeneous functions b_2, b_1 and b_0 defined by (2.8.3a)–(2.8.3c) at $t=0$.

Direct inspection tells us that

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

and

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

Adding up the above two formulae, we get

$$b_2(0,x;0,\eta) = R^\alpha{}_\mu{}^\beta{}_\nu(0)\,\eta_\alpha\,\eta_\beta\,x^\mu\,x^\nu + O(\|x\|^3). \tag{2.9.8}$$

Let us now move on to b_1. Direct differentiation of (2.9.7) reveals that

$$\varphi_{tt}|_{t=0} = O(\|x\|^2), \qquad \varphi_t|_{t=0} = -h + O(\|x\|^2)\,, \qquad \varphi_{xx}|_{t=0} = O(\|x\|^2)\,. \tag{2.9.9}$$

Furthermore, we have

$$\varphi_{x^\rho\eta_\sigma} = \delta_\rho{}^\sigma + t\,\frac{2}{3h}\Big(R^\sigma{}_\rho{}^\beta{}_\nu(0)\,\eta_\beta + R^\alpha{}_\rho{}^\sigma{}_\nu(0)\,\eta_\alpha\Big)\,x^\nu + O(\|x\|^3 + |t|^3) \tag{2.9.10}$$

and, consequently,

$$\det\varphi_{x^\rho\eta_\sigma} = 1 - t\,\frac{2}{3h}\,\mathrm{Ric}^\alpha{}_\nu(0)\,\eta_\alpha\,x^\nu + O(\|x\|^3 + |t|^3). \tag{2.9.11}$$

Plugging (2.9.11) into (2.5.3) and expanding the Riemannian density in normal geodesic coordinates, one eventually obtains

$$w = 1 + \frac{1}{12}\,\mathrm{Ric}_{\mu\nu}(0)\,x^\mu\,x^\nu - \frac{t}{3h}\,\mathrm{Ric}^\alpha{}_\nu(0)\,\eta_\alpha\,x^\nu + O(\|x\|^3 + |t|^3). \tag{2.9.12}$$

Formulae (2.9.6), (2.9.7), (2.9.9) and (2.9.12) give us

$$\begin{aligned} -ig^{\alpha\beta}(x)\,\nabla_\alpha\nabla_\beta\,\varphi\Big|_{t=0} &= -\,ig^{\alpha\beta}(x)\,\big(-\Gamma^\gamma{}_{\alpha\beta}(x)\,\varphi_{x^\gamma}|_{t=0} + O(\|x\|^2)\big)\\ &= -\,\frac{i}{3}\,\delta^{\alpha\beta}\,(R^\gamma{}_{\alpha\beta\mu}(0) + R^\gamma{}_{\beta\alpha\mu}(0))\,x^\mu\,\eta_\gamma + O(\|x\|^2) \\ &= \frac{2\,i}{3}\,\mathrm{Ric}^\gamma{}_\mu(0)\,\eta_\gamma\,x^\mu + O(\|x\|^2), \end{aligned} \tag{2.9.13}$$

$$2\,i(\log w)_t\,\varphi_t|_{t=0} = \frac{2\,i}{3}\,\mathrm{Ric}^\alpha{}_\nu(0)\,\eta_\alpha\,x^\nu + O(\|x\|^2), \tag{2.9.14}$$

$$-2\,i\,g^{\alpha\beta}(x)\,[\nabla_\alpha(\log w)]\,\nabla_\beta\,\varphi\Big|_{t=0} = -\frac{i}{3}\,\mathrm{Ric}^\alpha{}_\nu(0)\,\eta_\alpha\,x^\nu + O(\|x\|^2). \tag{2.9.15}$$

Substitution of (2.9.9) and (2.9.13)–(2.9.15) into (2.8.3b) yields

$$b_1(0,x;0,\eta) = i\ \mathrm{Ric}^{\alpha}{}_{\mu}(0)\,\eta_\alpha\,x^\mu + O(\|x\|^2). \tag{2.9.16}$$

Finally, let us deal with b_0. Formula (2.9.12) 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 (2.8.3c), we get

$$b_0(0,x;0,\eta) = -\frac{1}{6}\,\mathcal{R}(0) + O(\|x\|). \tag{2.9.17}$$

Theorem 2.24 tells us that

$$\mathfrak{a}_{-1}(t;0,\eta) = -\frac{i}{2\,h}\,[\mathfrak{S}_{-2}\,b_2 + \mathfrak{S}_{-1}\,b_1 + \mathfrak{S}_0\,b_0]|_{t=0}\,t + O(t^2)\,. \tag{2.9.18}$$

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 (2.9.18) is easy. Namely, using (2.9.17), we get

$$[\mathfrak{S}_0\,b_0]|_{t=0} = b_0(0,0;0,\eta) = -\frac{1}{6}\,\mathcal{R}(0)\,. \tag{2.9.19}$$

Calculating the first two terms in the square brackets in (2.9.18) 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

$$[\mathfrak{S}_{-1}\,(\,\cdot\,)]|_{t=0} \;=\; \left.\left[i\,\frac{\partial}{\partial\eta_\alpha}\frac{\partial}{\partial x^\alpha}\,(\,\cdot\,)\right]\right|_{t=0,\ x=0}, \tag{2.9.20}$$

$$[\mathfrak{S}_{-2}\,(\,\cdot\,)]|_{t=0} \;=\; \frac{1}{2}\left.\left[\left(i\,\frac{\partial}{\partial\eta_\alpha}\frac{\partial}{\partial x^\alpha}\right)^2(\,\cdot\,)\right]\right|_{t=0,\ x=0}. \tag{2.9.21}$$

Substituting (2.9.8) and (2.9.16) into (2.9.20) and (2.9.21) respectively, we get

$$[\mathfrak{S}_{-2}\,b_2]|_{t=0} = \mathcal{R}(0)\,, \qquad [\mathfrak{S}_{-1}\,b_1]|_{t=0} = -\mathcal{R}(0)\,. \tag{2.9.22}$$

Formulae (2.9.18), (2.9.19) and (2.9.22) imply (2.9.2). □

2.10 Weyl coefficients

The aim of this Section is show that the small time expansion for the subprincipal symbol of the propagator (Theorem 2.25) allows us to recover in a straightforward manner the first three Weyl coefficients and that our result agrees with those obtained by the heat kernel method.

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

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

the one-dimensional Fourier transform and by

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

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 [8, 41, 51, 68, 69, 70, 104] that the function $(N' * \mu)(y, \lambda)$ admits an asymptotic expansion in integer powers of λ:

$$(N' * \mu)(y, \lambda) = c_{d-1}(y)\, \lambda^{d-1} + c_{d-2}(y)\, \lambda^{d-2} + c_{d-3}(y)\, \lambda^{d-3} + \dots \quad \text{as} \quad \lambda \to +\infty. \tag{2.10.1}$$

Definition 2.26. We call the coefficients $c_k(y)$ appearing in formula (2.10.1) *local Weyl coefficients.*

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

Integrating (2.10.1) in λ and using the fact that $(N' * \mu)(y, \lambda)$ decays faster than any power of λ as $\lambda \to -\infty$, we get

$$\begin{aligned}(N * \mu)(y, \lambda) = \frac{c_{d-1}(y)}{d}\, \lambda^{d} + \frac{c_{d-2}(y)}{d-1}\, \lambda^{d-1} + \dots + c_0(y)\, \lambda + c_{-1}(y)\, \ln \lambda + b \\ - c_{-2}(y)\, \lambda^{-1} - \frac{c_{-3}(y)}{2}\, \lambda^{-2} - \dots \quad \text{as} \quad \lambda \to +\infty,\end{aligned} \tag{2.10.2}$$

where b is some constant. Our Definition 2.26 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 (2.10.2) Weyl coefficients rather than those in the asymptotic expansion (2.10.1). However, for the purposes of this thesis we will stick with Definition 2.26.

A separate question is whether one can get rid of the mollifier in (2.10.2). It is known [102, 104] that under appropriate geometric conditions on loops we do indeed have

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

See also Remark 3.6 for a brief discussion regarding the third unmollified term. We shall not discuss unmollified spectral asymptotics in this thesis.

We have

$$(N' * \mu)(y, \lambda) = \mathcal{F}^{-1}\left[\mathcal{F}\left[(N' * \mu)\right]\right](y, \lambda) = \mathcal{F}^{-1}\left[u(t, y, y)\, \hat{\mu}(t)\right], \tag{2.10.3}$$

where u is the Schwartz kernel (2.1.6) of the propagator (2.1.5). At each point of the manifold the quantity $u(t, y, y)$ is a distribution in the variable t — more precisely, an element in $C^\infty(M_x \times M_y; \mathcal{D}'(\mathbb{R}))$ — and the construction presented in previous sections allows us to write down this distribution explicitly, modulo a smooth function. Hence, formula (2.10.3) opens the way to the calculation of Weyl coefficients.

Theorem 2.27. *The first three Weyl coefficients are*

$$c_{d-1}(y) = \frac{S_{d-1}}{(2\pi)^d}\,, \tag{2.10.4}$$

$$c_{d-2}(y) = 0\,, \tag{2.10.5}$$

$$c_{d-3}(y) = \frac{d-2}{12}\,\mathcal{R}(y)\,c_{d-1}(y)\,, \tag{2.10.6}$$

where

$$S_{d-1} = \frac{2\pi^{d/2}}{\Gamma(\frac{d}{2})} \tag{2.10.7}$$

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 (2.3.1), (2.3.2) 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 (2.3.1) 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 2.17, we work in geodesic normal coordinates centred at our chosen point.

The construction presented in the above sections 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

$$\mathfrak{a}_0(t,\eta) = 1 \tag{2.10.8}$$

and, by Theorem 2.25,

$$\mathfrak{a}_{-1}(t,\eta) = \frac{i}{12\,\|\eta\|}\,\mathcal{R}\,t + O(t^2)\,. \tag{2.10.9}$$

The lower order terms $\mathfrak{a}_{-2}, \mathfrak{a}_{-3}, \ldots$ in the expansion (2.5.2) do not affect the first three Weyl coefficients and neither does the remainder term in (2.10.9), so further on we assume that the full symbol of the propagator reads

$$\mathfrak{a}(t,\eta) = 1 + \frac{i}{12\,\|\eta\|}\,\mathcal{R}\,t\,. \tag{2.10.10}$$

Using formula (2.9.7) with $x = y$ we get

$$\varphi(t,\eta) = -\|\eta\|\,t + O(t^4)\,. \tag{2.10.11}$$

Replacing $e^{i\,\varphi(t,\eta)}$ by $e^{-i\,\|\eta\|\,t}$ in the oscillatory integral (2.3.2) does not affect the first three Weyl coefficients: this fact is established by using (2.10.11) and expanding $e^{O(t^4)}$ 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 2.15 and 2.17). Hence, further on we assume that

$$e^{i\varphi(t,\eta)} = e^{-i\|\eta\|t}\,. \tag{2.10.12}$$

Using formula (2.9.10) with $x = y$ we get

$$\varphi_{x^\alpha \eta_\beta}(t,\eta) = \delta_\alpha{}^\beta + O(t^3)\,. \tag{2.10.13}$$

Substitution of (2.10.13) into (2.5.3) gives us

$$w(t,\eta) = 1 + O(t^3)\,. \tag{2.10.14}$$

The remainder term in (2.10.14) does not affect the first three Weyl coefficients, so further on we assume that

$$w(t,\eta) = 1\,. \tag{2.10.15}$$

Substituting (2.10.10), (2.10.12) and (2.10.15) into (2.3.2), we conclude that formula (2.10.3) can now be rewritten as

$$(N' * \mu)(y,\lambda) = \frac{1}{2\pi}\int_{\mathbb{R}^{d+1}} \left(1 + \frac{i}{12\,\|\eta\|}\,\mathcal{R}\,t\right) e^{i(\lambda-\|\eta\|)t}\,\hat{\mu}(t)\,\chi(\|\eta\|)\,đ\eta\,\mathrm{d}t \;+\; O(\lambda^{d-4}). \tag{2.10.16}$$

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 (2.10.16) as

$$(N' * \mu)(y,\lambda) = \frac{S_{d-1}}{(2\pi)^{d+1}}\int_{\mathbb{R}^2} \left(r^{d-1} + \frac{i}{12}\,\mathcal{R}\,r^{d-2}\,t\right) e^{i(\lambda-r)t}\,\hat{\mu}(t)\,\chi(r)\,\mathrm{d}r\,\mathrm{d}t + O(\lambda^{d-4}). \tag{2.10.17}$$

Here r is the radial coordinate and the extra factor $(2\pi)^d$ in the denominator came from (2.2.3).

Observe that

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

so integrating by parts in (2.10.17) we simplify this formula to read

$$(N' * \mu)(y,\lambda) = \frac{S_{d-1}}{(2\pi)^{d+1}} \int_{\mathbb{R}^2} r^{d-1}\, e^{i(\lambda-r)t}\, \hat{\mu}(t)\, \chi(r)\, \mathrm{d}r\, \mathrm{d}t \,+\, O(\lambda^{d-4}) \tag{2.10.18}$$

for $d=2$ and

$$(N' * \mu)(y,\lambda) = \frac{S_{d-1}}{(2\pi)^{d+1}} \int_{\mathbb{R}^2} \left(r^{d-1} + \frac{d-2}{12}\,\mathcal{R}\, r^{d-3} \right) e^{i(\lambda-r)t}\, \hat{\mu}(t)\, \chi(r)\, \mathrm{d}r\, \mathrm{d}t + O(\lambda^{d-4}) \tag{2.10.19}$$

for $d \geq 3$.

It remains only to drop the cut-off χ in formulae (2.10.18) and (2.10.19) as this does not affect the asymptotics when $\lambda \to +\infty$ and to make use of the formula

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

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

We see that formulae (2.10.18) and (2.10.19) give us (2.10.4)–(2.10.6). □

As a final step, let us show that Theorem 2.27 agrees with the classical heat kernel expansion. To this end, let us introduce the (local) heat kernel

$$Z(y,t) := \int_{-\infty}^{+\infty} e^{-t\lambda^2}\, N'(y,\lambda)\, \mathrm{d}\lambda \,=\, \int_0^{+\infty} e^{-t\lambda^2}\, N'(y,\lambda)\, \mathrm{d}\lambda + \frac{1}{\mathrm{Vol}(M,g)}\,. \tag{2.10.20}$$

If we now replace $N'(y,\lambda)$ in formula (2.10.20) with its mollified version $(N' * \mu)(y,\lambda)$ this gives an error, but this error can be easily estimated:

$$Z(y,t) = \int_0^{+\infty} e^{-t\lambda^2}\, (N' * \mu)(y,\lambda)\, \mathrm{d}\lambda \,+\, O(1) \quad \text{as} \quad t \to 0^+. \tag{2.10.21}$$

Substituting (2.10.1) and (2.10.4)–(2.10.6) into (2.10.21), we get

$$Z(y,t) = c_{d-1}(y) \int_0^{+\infty} e^{-t\lambda^2}\, \lambda^{d-1}\, \mathrm{d}\lambda \,+\, O(1) \quad \text{as} \quad t \to 0^+ \tag{2.10.22}$$

for $d=2$,

$$Z(y,t) = \int_0^{+\infty} e^{-t\lambda^2} \left(c_{d-1}(y)\, \lambda^{d-1} + c_{d-3}(y)\, \lambda^{d-3} \right) \mathrm{d}\lambda \,+\, O(|\ln t|) \quad \text{as} \quad t \to 0^+ \tag{2.10.23}$$

for $d = 3$, and

$$Z(y,t) = \int_0^{+\infty} e^{-t\lambda^2} \Big(c_{d-1}(y)\,\lambda^{d-1} + c_{d-3}(y)\,\lambda^{d-3}\Big)\,\mathrm{d}\lambda \,+\, O\big(t^{(3-d)/2}\big) \quad \text{as} \quad t \to 0^+ \tag{2.10.24}$$

for $d \geq 4$.

We have

$$\int_0^{+\infty} e^{-z^2}\, z^{d-1}\,\mathrm{d}z \,=\, \frac{\Gamma(\frac{d}{2})}{2}\,. \tag{2.10.25}$$

We also have

$$\int_0^{+\infty} e^{-z^2}\, z^{d-3}\,\mathrm{d}z \,=\, \frac{\Gamma(\frac{d}{2}-1)}{2} \,=\, \frac{\Gamma(\frac{d}{2})}{d-2} \tag{2.10.26}$$

for $d \geq 3$.

Using (2.10.4)–(2.10.7), (2.10.25) and (2.10.26) we can rewrite formulae (2.10.22)–(2.10.24) as a single formula

$$Z(y,t) = \begin{cases} (4\pi t)^{-d/2} + O(1) \quad \text{for} \quad d = 2, \\ (4\pi t)^{-d/2}\,\big(1 + \frac{1}{6}\,\mathcal{R}(y)\,t\big) + O(|\ln t|) \quad \text{for} \quad d = 3, \\ (4\pi t)^{-d/2}\,\big(1 + \frac{1}{6}\,\mathcal{R}(y)\,t\big) + O\big(t^{(3-d)/2}\big) \quad \text{for} \quad d \geq 4 \end{cases} \tag{2.10.27}$$

as $t \to 0^+$.

It is known [91], [21, Ch. III, E.IV.], [101, Section 3.3], that for all $d \geq 2$ the heat kernel admits the expansion

$$Z(y,t) = (4\pi t)^{-d/2} \left(1 + \frac{1}{6}\,\mathcal{R}(y)\,t\right) + O\big(t^{(4-d)/2}\big) \quad \text{as} \quad t \to 0^+. \tag{2.10.28}$$

We see that our result (2.10.27) agrees with the classical formula (2.10.28).

2.11 Explicit examples

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

2.11.1 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 topological obstructions 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 interesting 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,

$$\sigma : \mathbb{R}^2 \to \mathbb{S}^2 \setminus \begin{pmatrix} 0 \\ 0 \\ 2 \end{pmatrix}, \qquad \begin{pmatrix} u \\ v \end{pmatrix} \mapsto \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \frac{1}{1+K^2} \begin{pmatrix} u \\ v \\ 2K^2 \end{pmatrix}, \tag{2.11.1}$$

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

$$g = \frac{1}{(1+K^2)^2} \left[\mathrm{d}u^2 + \mathrm{d}v^2 \right]. \tag{2.11.2}$$

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

$$z^*(t;\eta) = 2 \, \tan(t/2) \, \frac{\eta}{\|\eta\|}, \tag{2.11.3a}$$

$$\xi^*(t;\eta) = \cos^2(t/2) \, \eta, \tag{2.11.3b}$$

provide a solution to the Hamiltonian system (2.2.1) for the Hamiltonian (2.2.5) 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 2.28. *For the 2-sphere we have*

$$\frac{\rho(y)}{\rho(z)} \det \varphi_{z^\alpha \eta_\beta} \Big|_{z=z^*} = \cos(t) - i \, \epsilon \, \sin(t). \tag{2.11.4}$$

Proof. A key ingredient in the computation of (2.11.4) is formula (2.4.4) from Theorem 2.6. As a first step, we need to compute the Christoffel symbols of g along the geodesic flow.

By means of (2.11.2) and (2.11.3), one obtains

$$\Gamma^u{}_{uu}(u^*,v^*) = -\frac{\sin(t)}{2}\frac{\eta_u}{\|\eta\|},\ \Gamma^u{}_{uv}(u^*,v^*) = -\frac{\sin(t)}{2}\frac{\eta_v}{\|\eta\|},\ \Gamma^u{}_{vv}(u^*,v^*) = \frac{\sin(t)}{2}\frac{\eta_u}{\|\eta\|},$$
$$\Gamma^v{}_{vv}(u^*,v^*) = -\frac{\sin(t)}{2}\frac{\eta_v}{\|\eta\|},\ \Gamma^v{}_{vu}(u^*,v^*) = -\frac{\sin(t)}{2}\frac{\eta_u}{\|\eta\|},\ \Gamma^v{}_{uu}(u^*,v^*) = \frac{\sin(t)}{2}\frac{\eta_v}{\|\eta\|}. \tag{2.11.5}$$

Substituting (2.11.2), (2.11.3) and (2.11.5) into (2.4.4), we get

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

from which it ensues that

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

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

Note that (2.11.4) 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 (2.11.4) 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 topological obstruction.

The result of Lemma 2.28 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 (2.2.7), (2.11.4) we get

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

and, in view of (2.2.8), we conclude that

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

Let us now move on to the calculation of the 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

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

which is nothing but the map (2.11.1) shifted by $(0,0,-1)$. Then the geodesic distance between (u,v) and (u',v') is given by

$$\operatorname{dist}((u,v),(u',v')) = \arccos\left[\,\widetilde{\sigma}(u,v)\,\cdot\,\widetilde{\sigma}(u',v')\,\right], \tag{2.11.6}$$

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

Formulae (2.11.6) and (2.2.1) yield an explicit representation for (2.4.3), which can be used to set up the algorithm described in Section 2.8.

For $\epsilon=1$ the functions appearing on the RHS of (2.8.20) read

$$\mathfrak{S}_{-2}\,b_2 = \frac{1}{4}\left(-3+2e^{2\,i\,t}+e^{4\,i\,t}\right), \tag{2.11.7a}$$

$$\mathfrak{S}_{-1}\,b_1 = \frac{1}{6}\left(7-4e^{2\,i\,t}-3e^{4\,i\,t}\right), \tag{2.11.7b}$$

$$\mathfrak{S}_{0}\,b_0 = \frac{1}{12}\left(-8+e^{2\,i\,t}\right). \tag{2.11.7c}$$

Substitution of (2.11.7a)–(2.11.7c) into (2.8.20) yields a formula for the subprincipal symbol:

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

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

$$\mathfrak{a}_{-1}(t;y,\eta;\epsilon) = \frac{i\,t}{8\,\|\eta\|} + \frac{i\sin(2t)-4\epsilon\sin^2(t)+3\,i\,\epsilon^2\sin(2t)+6\epsilon^3\sin^2(t)}{48\,\|\eta\|\,(\cos(t)-i\epsilon\sin(t))^2}\,. \tag{2.11.8}$$

Formulae (2.11.7a)–(2.11.8) have been obtained using the licensed software Mathematica. The Mathematica script is provided in Appendix A.1

Remark 2.29. For $t \neq \pi/2 + \pi k$, $k \in \mathbb{Z}$, the subprincipal symbol admits the following expansion in powers of ϵ:

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

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

$$\mathfrak{a}_{-1}(t;y,\eta;0) = \frac{i}{24\,\|\eta\|}\,(3t + \tan(t))\,, \tag{2.11.9}$$

which is the subprincipal symbol of the propagator for the real-valued Levi-Civita phase function. Of course, formula (2.11.9) 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 (2.11.9) agrees with (2.9.1), with $\mathcal{R}(y) = 2$.

Let us now run a test for our formula (2.11.8). To this end, let us shift the Laplacian by a quarter,

$$-\Delta \mapsto -\Delta + \frac{1}{4}\,. \tag{2.11.10}$$

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

$$\widetilde{U}(t + 2\pi) = -\widetilde{U}(t). \tag{2.11.11}$$

Going back to Lemma 2.20, we see that the shift of the Laplacian (2.11.10) does not affect b_2 and b_1, but shifts b_0 as

$$b_0 \mapsto b_0 + 1/4\,. \tag{2.11.12}$$

Theorem 2.24 and formula (2.11.12) tell us that the subprincipal symbol of the propagator transforms as

$$\mathfrak{a}_{-1}(t;y,\eta;0) \mapsto \mathfrak{a}_{-1}(t;y,\eta;0) - \frac{i\,t}{8\|\eta\|}\,. \tag{2.11.13}$$

Applying the transformation (2.11.13) to formula (2.11.8), we see that the 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 (2.11.11) of the propagator itself. This is to do with the Maslov index: formulae (2.5.3) and (2.11.4) 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 (2.11.10) 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 [30]. See also [40], [107, Section 3].

2.11.2 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 our thesis 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

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

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

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

Unlike the sphere, the hyperbolic plane does not present caustics due to its negative curvature. Hence, there are no topological 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 $\epsilon \geq 0$

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

and

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

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 (2.8.20) yields a formula for the subprincipal symbol:

$$\mathfrak{a}_{-1}(t; y, \eta; 0) = -\frac{i}{24\,\|\eta\|}\,(3t + \tanh(t))\,. \tag{2.11.16}$$

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 [113], see also [120, Sec. 3.7.2]. Formula (2.11.16) is, of course, in agreement with (2.9.1), with $\mathcal{R}(y) = -2$.

Our explicit examples gave us the opportunity to illustrate, once again, the importance of formula (2.4.4): it allows one to extract topological information by means of a simple direct computation.

2.12 Circumventing topological obstructions: geometric picture

As discussed in the previous sections, the weight w defined by formula (2.5.3) is a crucial object in our mathematical construction in that it carries important topological information. 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 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

$$Q^{\mu\nu}(\eta;t,y) := g_{\alpha\beta}(x^*(\eta))\,q^{\alpha\mu}(\eta;t,y)\,q^{\beta\nu}(\eta;t,y)\,, \tag{2.12.1}$$

where

$$q^{\alpha\mu}(\eta;t,y) := [x^*(\eta)]^\alpha_{\eta_\mu}\,. \tag{2.12.2}$$

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

$$\dot{\gamma}^\alpha(s)\, \nabla_\alpha\, \zeta(\gamma(s))_\beta = \dot{\gamma}^\alpha(s)\, [\partial_\alpha \zeta_\beta(\gamma(s)) - \Gamma^\rho{}_{\alpha\beta}(\gamma(s))\, \zeta_\rho(\gamma(s))] = 0\,, \tag{2.12.3}$$

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 (2.12.3) 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

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

Put

$$p^{\alpha\mu}(\eta; t, y) := g^{\alpha\gamma}(x^*(\eta)) \left[(\xi^*_\gamma(\eta))_{\eta_\mu} - \Gamma^\rho{}_{\gamma\beta}(x^*(\eta))\, \xi^*_\rho(\eta)\, (x^*(\eta))^\beta_{\eta_\mu}\right] \tag{2.12.4}$$

and define the bilinear form

$$P^{\mu\nu}(\eta; t, y) := g_{\alpha\beta}(x^*(\eta))\, p^{\alpha\mu}(\eta; t, y)\, p^{\beta\nu}(\eta; t, y)\,. \tag{2.12.5}$$

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

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

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

Theorem 2.30. *Let a and b be positive parameters. Then the linear combination of the position and momentum forms*

$$ah^2 Q + bP \in C^\infty(\mathcal{T}_y(t); \otimes^2_s T^* \mathcal{T}_y(t)) \tag{2.12.6}$$

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 $ah^2Q + bP$ if and only if $v^\flat$ satisfies

$$[x^*(\eta)]^\alpha_{\eta_\mu}\, v_\mu = 0 \qquad \text{and} \qquad [\xi^*_\alpha(\eta)]_{\eta_\mu}\, v_\mu = 0\,. \tag{2.12.7}$$

Since the Hamiltonian flow is non-degenerate, i.e. it preserves the tautological 1-form, the two conditions (2.12.7) cannot be simultaneously fulfilled unless $v = 0$. Therefore, $ah^2Q + bP$ is non-degenerate. □

The metric $ah^2Q + bP$ 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 2.31. *We have*

$$\varphi_{x^\alpha \eta_\mu}\big|_{x=x^*} = g_{\alpha\beta}(x^*)\left[p^{\beta\mu} - i\,\epsilon\, h\, q^{\beta\mu}\right]. \tag{2.12.8}$$

Proof of Theorem 2.31. The identity (2.12.8) is established by comparing (2.4.4) with (2.12.2) and (2.12.4). □

Example 2.32 (Position and momentum forms for $\mathbb{S}^2$)**.** *With the notation of Sec-*

tion 2.11, the quantities q and p defined by formulae (2.12.2) *and* (2.12.4) *read*

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

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

Consequently, the position and momentum forms are given by

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

We have $\det Q = 0$ *and* $\det P = \cos^2(t)$. *This implies that* P*, which is associated with the real part of* (2.4.4) *via* (2.12.8) *and* (2.12.5)*, 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* (2.12.6) *with* $a = b = 1$ *does not depend on* t.

Chapter 3

The massless Dirac propagator

3.1 Statement of the problem

Let (M,g) be a connected oriented closed Riemannian 3-manifold. We denote by ∇ the Levi-Civita connection, by $\Gamma^\alpha{}_{\beta\gamma}$ the Christoffel symbols and by

$$\rho(x) := \sqrt{g_{\alpha\beta}(x)} \tag{3.1.1}$$

the Riemannian density.

Let e_j, $j=1,2,3$, be a positively oriented global framing, i.e. a set of three orthonormal smooth vector fields[1] whose orientation agrees with the orientation of the manifold. In chosen local coordinates x^α, $\alpha=1,2,3$, we will denote by $e_j{}^\alpha$ the α-th component of the j-th vector field. Throughout this Chapter we use Greek letters for holonomic (tensor) indices and Latin for anholonomic (frame) indices. We adopt Einstein's convention of summation over repeated indices.

Let

$$s^1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = s_1\,, \quad s^2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = s_2\,, \quad s^3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = s_3 \tag{3.1.2}$$

be the standard Pauli matrices and let

$$\sigma^\alpha := s^j\, e_j{}^\alpha \tag{3.1.3}$$

be their projection along the framing. The quantity σ^α is a vector-function with values in the space of trace-free Hermitian 2×2 matrices.

[1]Observe that an orientable 3-manifold is automatically parallelisable [74, 110].

Definition 3.1. We call *massless Dirac operator* the operator

$$W := -i\sigma^\alpha \left(\frac{\partial}{\partial x^\alpha} + \frac{1}{4}\sigma_\beta \left(\frac{\partial \sigma^\beta}{\partial x^\alpha} + {\Gamma^\beta}_{\alpha\gamma}\,\sigma^\gamma \right) \right) : H^1(M;\mathbb{C}^2) \to L^2(M;\mathbb{C}^2). \quad (3.1.4)$$

Here H^1 is the usual Sobolev space of functions which are square integrable together with their first partial derivatives.

In theoretical physics the massless Dirac equation is often referred to as the Weyl equation, which explains our notation. Henceforth, we refer to the massless Dirac operator simply as the Dirac operator, which conforms with the terminology adopted in differential geometry.

Remark 3.2. The Dirac operator admits several equivalent definitions. The most common is the geometric definition written in terms spinor bundles. Our analytic Definition 3.1 is equivalent to the standard geometric one, see [54, Appendix B].

Definition 3.1 depends on the choice of framing and this issue requires clarification.

Let

$$G : M \to \mathrm{SU}(2) \quad (3.1.5)$$

be an arbitrary smooth special unitary matrix-function and let $\widetilde{W}$ be the Dirac operator corresponding to a given framing. Consider the transformation

$$\widetilde{W} \mapsto G^*\widetilde{W}G := W, \quad (3.1.6)$$

where the star indicates Hermitian conjugation. It turns out that W is also a Dirac operator, only corresponding to a different framing.

Let us now look at the matter the other way round. Suppose that $\widetilde{W}$ and W are two Dirac operators. Does there exist a smooth matrix-function (3.1.5) such that $W = G^*\widetilde{W}G$? If the operators $\widetilde{W}$ and W are in a certain sense 'close' then the answer is yes, but in general there are topological obstructions and the answer is no. This motivates the introduction of the concept of spin structure, see Chapter 4.

The gauge transformation (3.1.5), (3.1.6) is the manifestation, at operator level, of the freedom of pointwise rotating the framing in a smooth way,

$$\widetilde{e}_j \mapsto {O_j}^k\,\widetilde{e}_k =: e_j, \qquad O \in C^\infty(M;\mathrm{SO}(3)), \quad (3.1.7)$$

via the double cover

$$\mathrm{SU}(2) \overset{2:1}{\to} \mathrm{SO}(3).$$

The Dirac operator (3.1.4) is uniquely determined by the metric and spin structure modulo an SU(2) gauge transformation.

The Dirac operator is symmetric with respect to the L^2 inner product

$$\langle u, v\rangle := \int_M u^* v\, \rho\, \mathrm{d}x\,, \qquad u, v \in L^2(M; \mathbb{C}^2), \tag{3.1.8}$$

where $\mathrm{d}x = \mathrm{d}x^1 \mathrm{d}x^2 \mathrm{d}x^3$. Furthermore, a simple calculation shows that it is elliptic[2].

It is known that the Dirac operator is self-adjoint and its spectrum is discrete, accumulating to $+\infty$ and to $-\infty$. Let λ_k be the eigenvalues of W and v_k the corresponding orthonormal eigenfunctions, $k \in \mathbb{Z}$. The choice of particular enumeration is irrelevant for our purposes, but what is important is that eigenvalues are enumerated with account of their multiplicity. Note that the Dirac operator has the special property that it commutes with the antilinear operator of charge conjugation

$$v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \mapsto \begin{pmatrix} -\overline{v_2} \\ \overline{v_1} \end{pmatrix} =: \mathrm{C}(v),$$

see [42, Appendix A] for details, and this implies that eigenvalues have even multiplicity.

Definition 3.3. We define the *Dirac propagator* as

$$U(t) := e^{-itW}. \tag{3.1.9}$$

The Dirac propagator is the (distributional) solution of the hyperbolic Cauchy problem

$$\left(-i\,\frac{\partial}{\partial t} + W\right) U = 0\,, \tag{3.1.10a}$$

$$U(0) = \mathrm{Id}\ . \tag{3.1.10b}$$

It is a time-dependent unitary operator which can written via functional calculus as

$$U(t) = \sum_{\lambda_k} e^{-it\lambda_k}\, v_k\, \langle v_k\,,\,\cdot\,\rangle. \tag{3.1.11}$$

[2]Ellipticity means that the determinant of the principal symbol does not vanish on $T^*M \setminus \{0\}$.

The Dirac propagator can be written as a sum of three operators

$$U(t) = U^+(t) + U^0 + U^-(t) \tag{3.1.12}$$

defined as

$$U^+(t) := \sum_{\lambda_k>0} e^{-it\lambda_k}\, v_k\, \langle v_k\,,\,\cdot\,\rangle, \tag{3.1.13a}$$

$$U^0 := \sum_{\lambda_k=0} v_k\, \langle v_k\,,\,\cdot\,\rangle, \tag{3.1.13b}$$

$$U^-(t) := \sum_{\lambda_k<0} e^{-it\lambda_k}\, v_k\, \langle v_k\,,\,\cdot\,\rangle. \tag{3.1.13c}$$

We call the operators (3.1.13a), (3.1.13b) and (3.1.13c) *positive*, *zero mode* and *negative* propagators, respectively. These are time-dependent partial isometries. Note that the operator U^0 is nontrivial only if the Dirac operator has zero modes (i.e. if zero is an eigenvalue).

We define the *positive* (+) and *negative* (−) local counting functions as

$$N_\pm(y;\lambda) := \begin{cases} 0 & \text{for } \lambda \le 0, \\ \sum_{0<\pm\lambda_k<\lambda} [v_k(y)]^*\, v_k(y) & \text{for } \lambda > 0. \end{cases} \tag{3.1.14}$$

Of course, integration over M gives

$$N_\pm(\lambda) := \int_M N_\pm(y;\lambda)\,\rho(y)\,\mathrm{d}y = \begin{cases} 0 & \text{for } \lambda \le 0, \\ \sum_{0<\pm\lambda_k<\lambda} 1 & \text{for } \lambda > 0. \end{cases} \tag{3.1.15}$$

The functions (3.1.15) are the 'global' counting functions, the only difference with the usual definition [104] being that we count the positive and negative eigenvalues separately.

Let $\hat\mu : \mathbb{R} \to \mathbb{C}$ be a smooth function such that $\hat\mu = 1$ in some neighbourhood of the origin and $\operatorname{supp}\hat\mu$ is sufficiently small. Here 'sufficiently small' means that $\operatorname{supp}\hat\mu \subset (-T_0, T_0)$, where T_0 is the infimum of lengths of all the geodesic loops originating from all the points of the manifold.

Following the notation set out in Chapter 2, we write the Fourier transform as

$$\mathcal{F}_{\lambda\to t}[f](t) = \hat f(t) = \int_{-\infty}^{+\infty} e^{-it\lambda} f(\lambda)\,\mathrm{d}\lambda \tag{3.1.16}$$

and the inverse Fourier transform as

$$\mathcal{F}^{-1}_{t\to\lambda}[\hat{f}](\lambda) = f(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{it\lambda}\hat{f}(t)\,\mathrm{d}t. \tag{3.1.17}$$

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

It is known [51, 68, 69, 70, 104] that the mollified derivative of the positive (resp. negative) counting function admits a complete asymptotic expansion in integer powers of λ:

$$(N'_\pm * \mu)(y,\lambda) = c_2^\pm(y)\,\lambda^2 + c_1^\pm(y)\,\lambda + c_0^\pm(y) + \dots \quad \text{as} \quad \lambda \to +\infty. \tag{3.1.18}$$

Here $*$ stands for the convolution in the variable λ.

Definition 3.4. We call *local Weyl coefficients* the smooth functions $c_k^\pm(y)$ appearing in the asymptotic expansions (3.1.18).

Remark 3.5. (i) Our definition of Weyl coefficients does not depend on the choice of mollifier μ. If $\widetilde{\mu}$ is another mollifier with the same support properties, then

$$(N'_\pm * \mu)(y,\lambda) - (N'_\pm * \widetilde{\mu})(y,\lambda) = O(\lambda^{-\infty}) \quad \text{as} \quad \lambda \to +\infty.$$

(ii) Our definition of Weyl coefficients is, in a sense, unusual. The standard convention in the literature is to call local Weyl coefficients the functions appearing in the asymptotic expansion of the mollified counting function $N * \mu$, as opposed to its derivative. The two definitions are, effectively, the same up to integrating factors,

$$\begin{aligned}(N_\pm * \mu)(y,\lambda) &= \int_{-\infty}^{\lambda} (N'_\pm * \mu)(y,\kappa)\,\mathrm{d}\kappa \\ &= \frac{1}{3}\,c_2^\pm(y)\,\lambda^3 + \frac{1}{2}\,c_1^\pm(y)\,\lambda^2 + c_0^\pm(y)\,\lambda + \dots \quad \text{as} \quad \lambda \to +\infty, \end{aligned} \tag{3.1.19}$$

compare (3.1.18) with (3.1.19). As a matter of convenience, we will stick with Definition 3.4 throughout this Chapter.

(iii) It was shown in [42] that

$$c_2^\pm(y) = \frac{1}{2\pi^2}\,, \qquad c_1^\pm(y) = 0. \tag{3.1.20}$$

(iv) The unmollified counting functions $N_\pm(y,\lambda)$ also admit asymptotic expansions as $\lambda \to +\infty$, but here the situation is more delicate because these functions are discontinuous and one encounters number-theoretic issues. It is known [41, 42] that

$$N_\pm(y,\lambda) = \frac{1}{6\pi^2}\,\lambda^3 + O(\lambda^2) \quad \text{as} \quad \lambda \to +\infty \tag{3.1.21}$$

uniformly over $y \in M$ and, furthermore, under appropriate assumptions on geodesic loops,

$$N_\pm(y,\lambda) = \frac{1}{6\pi^2}\,\lambda^3 + o(\lambda^2) \quad \text{as} \quad \lambda \to +\infty. \tag{3.1.22}$$

(v) An important topic in the spectral theory of first order elliptic systems is the issue of spectral asymmetry [2, 3, 4, 5]. Let us mention that to observe spectral asymmetry for our Dirac operator one as to go as far as the sixth Weyl coefficients. This follows from the fact that the eta function

$$\eta(s) := \sum_{\lambda_k \neq 0} \frac{\operatorname{sgn}\lambda_k}{|\lambda_k|^s} = \int_0^{+\infty} \lambda^{-s}(N'_+(\lambda) - N'_-(\lambda))\,\mathrm{d}\lambda$$

is holomrphic in the complex half-plane $\operatorname{Re} s > -2$ [22, 60] and has its first pole at $s = -2$. The value of the residue of the eta function at $s = -2$, which was computed explicitly by Branson and Gilkey [27], describes the difference

$$\int_M (c^+_{-3}(y) - c^-_{-3}(y))\,\rho(y)\,\mathrm{d}y$$

between the sixth (global) Weyl coefficients.

This Chapter has two main objectives.

Objective 1 Construct the propagators $U^\pm(t)$ explicitly, modulo integral operators with infinitely smooth kernels, and do so as a single invariantly defined oscillatory integral global in space and in time.

Objective 2 Compute the third Weyl coefficient $c^\pm_0(y)$.

Remark 3.6. One cannot, in general, identify the third Weyl coefficient by looking at the asymptotic behaviour of the unmollified counting function. In order to illustrate this point, let us consider the 3-torus equipped with standard flat metric. Already in this simple case the mathematical statement

$$N_\pm(y,\lambda) = \frac{1}{6\pi^2}\,\lambda^3 + c_0^\pm(y)\,\lambda + o(\lambda) \quad \text{as} \quad \lambda \to +\infty \tag{3.1.23}$$

is *false*. This fact can be established by writing down the eigenvalues explicitly as in [42, Appendix B] and using standard results [65] from analytic number theory.

3.2 Main results

The study of Dirac operators, arguably the most important operators from the point of view of physical applications alongside the Laplacian, has a long and noble history in the mathematical literature. Excellent introductions to the topic can be found in [79] and [58].

Due to its physical significance, a lot of attention has been attracted by the spectrum of Dirac operators on Riemannian manifolds and numerous researchers have contributed to our current understanding of the topic. One can ask, for example, how the eigenvalues behave under perturbations of the metric [25, 54], how the spectrum depends on the spin structure [12], whether zero modes exist [10], *et cetera*.

In the second part of this Chapter, we will be concerned with the study of the asymptotic behaviour of large (in modulus) eigenvalues of the massless Dirac operator on a closed 3-manifold. In the case of scalar elliptic operators, such as for example the Laplace–Beltrami operator, a wide range of classical techniques are available in the literature to compute spectral asymptotics. However, if one is interested in 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, and even resolvent techniques require major modification [9]. This is why for the Dirac operator — and for non-semibounded operators in general — the so-called wave method described in the previous Chapter, which consists in recovering information about the eigenvalue counting function from the small time behaviour of the wave propagator, is even more natural.

Our goal is to construct the positive and negative Dirac propagators explicitly, in a global — i.e., as a single oscillatory integral — and invariant (under change of coordinates and gauge transformations) fashion.

Our work partly builds upon [41] and [42]. In [41], using the wave method, Chervova, Downes and Vassiliev obtained an explicit formula for the second Weyl coefficient of an elliptic self-adjoint first order pseudodifferential matrix operator, fixing thirty years of incorrect or incomplete publications in the subject, see [41, Section 11]. In [42] the same authors applied the results from [41] to the massless Dirac operator. Unlike in this thesis, the approach from [41] is not geometric in nature and complex-valued phase functions do not appear. Note that some results from [42] were improved by Strohmaier and Li in [83], where the authors studied the second term of the mollified spectral counting function of Dirac type operators and characterised the operators in this class with vanishing second Weyl coefficient.

A fully geometric global construction of the (scalar) wave propagator $e^{-it\sqrt{-\Delta}}$ on closed Riemannian manifolds, as a single oscillatory integral with complex-valued phase function, was the subject of Chapter 2, and has recently been extended to the Lorentzian setting by the author and collaborators in [32].

Our main results are as follows.

1. We present a global construction of each of the two propagators, the positive propagator $U^+(t)$ and the negative propagator $U^-(t)$, as a single invariantly defined oscillatory integral, global in space and in time, with distinguished complex-valued phase function (Theorem 3.9). We provide a closed formula for the principal symbols of the propagators (Theorem 3.26) and an algorithm for the calculation of the subprincipal symbols and all asymptotic components of the amplitude of lower degree of homogeneity in momentum (subsection 3.3.3).

2. We give an explicit small time expansion of principal and subprincipal symbols of positive and negative propagators in terms of geometric invariants (Theorem 3.38).

3. We compute the third local Weyl coefficients in the asymptotic expansion of the two eigenvalue counting functions (3.1.14) (Theorem 3.39).

Along the way, we prove a number of results about general first order elliptic systems and invariant representations of pseudodifferential operators on manifolds.

This Chapter is structured as follows.

In Section 3.3 we characterise positive and negative propagators for a general first order elliptic self-adjoint (pseudo)differential matrix operator A in terms of the eigenvalues of A_{prin}. Then, we explain how to construct them explicitly as a finite sum of oscillatory integrals global in space and time.

In Section 3.4 we deal with the delicate issue of invariant descriptions of pseudodifferential operators acting on scalar functions. In particular, we examine the relation between the g-subprincipal symbol and the standard notion of subprincipal symbol for operators acting on half-densities.

In Section 3.5 we apply the results from Section 3.3 to the massless Dirac operator. A formula for the principal symbol of positive and negative Dirac propagators is provided in Section 3.6, whereas small time expansions for principal and subprincipal symbols of positive and negative propagators are obtained in Section 3.7. Our final results are expressed in terms of geometric invariants: the curvature of the Levi-Civita connection associated with the metric g and the torsion of the Weitzenböck connection generated by the framing defining the Dirac operator.

In Section 3.8 we use the results from Section 3.7 to compute the third local Weyl coefficients for the massless Dirac operator.

Finally, in Section 3.9 we apply our techniques to two explicit examples: $M = \mathbb{S}^3$, where formulae are isotropic in momentum, and $M = \mathbb{S}^2 \times \mathbb{S}^1$, where they are not.

3.3 Preliminary results for general first order systems

In this section we will consider a broader class of first order systems and we will prove fairly general results, which will be later applied to the special case of the Dirac operator. In doing so, we will need some of the technology developed in [41]. The setting of our analysis is somewhat different from that in [41], in that our operators are differential, as opposed to pseudodifferential (see also Remark 3.14), and act on scalar functions on a Riemannian manifold, as opposed to half-densities on a manifold with no metric structure. In particular, the change in the domain of the operator raises delicate issues concerning the invariance of the mathematical objects involved. For these reasons we provide here a modified version of some of the results from [41], adapted to our setting.

Throughout this section, M will be a smooth connected closed Riemannian manifold of dimension $d \geq 2$.

Let A be an elliptic symmetric first order $m \times m$ matrix differential operator acting on m-columns of smooth complex-valued scalar functions $v \in C^\infty(M; \mathbb{C}^m)$ and let $A_{\text{prin}} : T'M \to \operatorname{Herm}(m, \mathbb{C})$ be the principal symbol of A, where $T'M := T^*M \setminus \{0\}$ and $\operatorname{Herm}(m, \mathbb{C})$ is the real vector space of $m \times m$ Hermitian matrices.

We denote by $h^{(j)}(x, \xi)$ the eigenvalues of $A_{\text{prin}}(x, \xi)$ enumerated in increasing order, with positive index $j = 1, 2, \dots, m^+$ for positive $h^{(j)}(x, \xi)$ and negative index $j = -1, -2, \dots, -m^-$ for negative $h^{(j)}(x, \xi)$. We assume that the eigenvalues of the principal symbol A_{prin} are simple. Clearly, $m = m^+ + m^-$, because the ellipticity condition $\det A_{\text{prin}}(x, \xi) \neq 0$ ensures that all eigenvalues are nonzero. In fact, as our operator is differential, one can show [56, Remark 2.1] that m can only be even and that we have

$$m^+ = m^- = \frac{m}{2}\,. \tag{3.3.1}$$

Furthermore, the eigenvalues $h^{(j)}$ of the principal symbol and the corresponding normalised eigenvectors $v^{(j)}$ possess the symmetry

$$h^{(-j)}(x, \xi) = -h^{(j)}(x, -\xi), \quad v^{(-j)}(x, \xi) = v^{(j)}(x, -\xi), \qquad j = 1, \dots, \frac{m}{2}\,. \tag{3.3.2}$$

Under the above assumptions the spectrum of A is discrete and accumulates to $+\infty$ and to $-\infty$. We denote eigenvalues and orthonormalised eigenfunctions of A by λ_k and v_k, respectively, enumerated with account of their multiplicity.

By replacing W with A, one can define the 'full' propagator $U_A(t)$ for A via (3.1.11), as well as the positive, zero mode and negative propagators via (3.1.13a)–(3.1.13c), which we denote by $U_A^+(t)$, U_A^0 and $U_A^-(t)$, respectively.

Each eigenvalue $h^{(j)}(x, \xi)$ of the principal symbol can be interpreted as a Hamiltonian on the cotangent bundle. The corresponding Hamiltonian flow

$$(x^{(j)}(t; y, \eta), \xi^{(j)}(t; y, \eta)),$$

i.e. the (global) solution to Hamilton's equations

$$\dot{x}^{(j)} = h^{(j)}_\xi(x^{(j)}, \xi^{(j)}), \qquad \dot{\xi}^{(j)} = -h^{(j)}_x(x^{(j)}, \xi^{(j)})$$

with initial condition $(x^{(j)}(0;y,\eta),\xi^{(j)}(0;y,\eta))=(y,\eta)$, generates a Lagrangian manifold to which one can, in turn, associate a *global* Lagrangian distribution. See Section 2.2 and references therein for details. In particular, the singularities of the solution to the initial value problem

$$(-i\partial_t + A)v = 0, \qquad v|_{t=0} = v_0 \tag{3.3.3}$$

propagate along Hamiltonian trajectories generated by the eigenvalues of A_{prin}.

3.3.1 Positive and negative propagators: an abstract approach

Our aim is to show that $U_A^+(t)$ and $U_A^-(t)$ can be *separately* approximated by a finite sum of global oscillatory integrals. Before doing so, let us state and prove an abstract preparatory theorem.

Notation 3.7. Let

$$v\in C^\infty(\mathbb{R}\times M_x\times M_y), \qquad (\lambda,x,y)\mapsto v(\lambda,x,y).$$

We write

$$v=O(|\lambda|^{-\infty}) \quad \text{as } \lambda\to\pm\infty \tag{3.3.4}$$

if for every $\alpha>0$, every $k\in\mathbb{N}$ and every linear partial differential operator P with infinitely smooth coefficients of order k on $M_x\times M_y$ there exists a positive constant $C_{\alpha,P}$ such that

$$|Pv|\le C_{\alpha,P}\,|\lambda|^{-\alpha} \quad \text{for } \pm\lambda>1\,, \tag{3.3.5}$$

uniformly over $M_x\times M_y$.

Theorem 3.8. *Let $(T_-,T_+)\subseteq\mathbb{R}$ be an open interval (possibly, the whole real line) and let $u^+(t,x,y)$, $u^-(t,x,y)$, $\widetilde{u}^+(t,x,y)$ and $\widetilde{u}^-(t,x,y)$ be elements of $C^\infty(M_x\times M_y;\mathcal{D}'(T_-,T_+))$, satisfying*

(a) $u^+(t,x,y)+u^-(t,x,y)=\widetilde{u}^+(t,x,y)+\widetilde{u}^-(t,x,y) \mod C^\infty((T_-,T_+)\times M_x\times M_y)$.

Furthermore, assume that for every $\zeta\in C_0^\infty(T_-,T_+)$ we have

(b) $\mathcal{F}^{-1}_{t\to\lambda}[\zeta\,u^\pm]=O(|\lambda|^{-\infty})$ *as* $\lambda\to\mp\infty$,

(c) $\mathcal{F}^{-1}_{t\to\lambda}[\zeta\,\widetilde{u}^{\pm}] = O(|\lambda|^{-\infty})$ *as* $\lambda \to \mp\infty$.

Then

$$u^{\pm}(t,x,y) = \widetilde{u}^{\pm}(t,x,y) \mod C^{\infty}((T_-,T_+)\times M_x \times M_y). \tag{3.3.6}$$

Proof. Let $\zeta \in C_0^{\infty}(T_-,T_+)$. Multiplying (a) by $\zeta(t)$ we get

$$\zeta(t)\,u^{+}(t,x,y) + \zeta(t)\,u^{-}(t,x,y) = \zeta(t)\,\widetilde{u}^{+}(t,x,y) + \zeta(t)\,\widetilde{u}^{-}(t,x,y) \mod C_0^{\infty}(\mathbb{R}\times M_x \times M_y). \tag{3.3.7}$$

Applying the inverse Fourier transform $\mathcal{F}^{-1}_{t\to\lambda}$ to (3.3.7), letting $\lambda \to +\infty$ and using assumptions (b) and (c) we obtain

$$\mathcal{F}^{-1}_{t\to\lambda}[\zeta\,u^{+}] = \mathcal{F}^{-1}_{t\to\lambda}[\zeta\,\widetilde{u}^{+}] + O(|\lambda|^{-\infty}) \qquad \text{as } \lambda \to +\infty. \tag{3.3.8}$$

Here, when dealing with the remainder from (3.3.7), we used the fact that the Fourier transform of a compactly supported smooth function is rapidly decreasing. The compactness of M ensures a uniform estimate in the spatial variables.

Furthermore, (b) and (c) immediately imply

$$\mathcal{F}^{-1}_{t\to\lambda}[\zeta\,u^{+}] = \mathcal{F}^{-1}_{t\to\lambda}[\zeta\,\widetilde{u}^{+}] + O(|\lambda|^{-\infty}) \qquad \text{as } \lambda \to -\infty. \tag{3.3.9}$$

Combining (3.3.8) and (3.3.9) we arrive at

$$\mathcal{F}^{-1}_{t\to\lambda}[\zeta\,(u^{+} - \widetilde{u}^{+})] = O(|\lambda|^{-\infty}) \qquad \text{as } |\lambda| \to +\infty, \tag{3.3.10}$$

which implies

$$\zeta\,(u^{+} - \widetilde{u}^{+}) \in C^{\infty}(\mathbb{R}\times M_x \times M_y). \tag{3.3.11}$$

As $\zeta \in C_0^{\infty}(T_-,T_+)$ in the above formula is arbitrary, we conclude that

$$u^{+} - \widetilde{u}^{+} \in C^{\infty}((T_-,T_+)\times M_x \times M_y). \tag{3.3.12}$$

A similar argument gives

$$u^{-} - \widetilde{u}^{-} \in C^{\infty}((T_-,T_+)\times M_x \times M_y). \tag{3.3.13}$$

□

3.3.2 Construction of positive and negative propagators

Theorem 3.9. *The positive and negative propagators can be written, modulo an infinitely smoothing operator, as a finite sum of oscillatory integrals, global in space and in time. More precisely, we have*

$$U_A^+(t) \overset{\operatorname{mod}\Psi^{-\infty}}{=} \sum_{j=1}^{m^+} U_A^{(j)}(t), \tag{3.3.14}$$

$$U_A^-(t) \overset{\operatorname{mod}\Psi^{-\infty}}{=} \sum_{j=1}^{m^-} U_A^{(-j)}(t), \tag{3.3.15}$$

where

$$U_A^{(j)}(t) := \frac{1}{(2\pi)^d} \int_{T'M} e^{i\varphi^{(j)}(t,x;y,\eta)}\, \mathfrak{a}^{(j)}(t;y,\eta)\, \chi^{(j)}(t,x;y,\eta)\, w^{(j)}(t,x;y,\eta)\ (\,\cdot\,)\, \rho(y)\, \mathrm{d}y\, \mathrm{d}\eta \tag{3.3.16}$$

and

- *by* $\overset{\operatorname{mod}\Psi^{-\infty}}{=}$ *we mean that the operator on the LHS is equal to the operator on the RHS up to an integral operator with infinitely smooth integral kernel;*

- *the phase function* $\varphi^{(j)} \in C^\infty(\mathbb{R} \times M \times T'M; \mathbb{C})$ *satisfies*

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

  (ii) $\varphi^{(j)}_{x^\alpha}\Big|_{x=x^{(j)}} = \xi^{(j)}_\alpha$,

  (iii) $\det \varphi^{(j)}_{x^\alpha \eta_\beta}\Big|_{x=x^{(j)}} \neq 0$,

  (iv) $\operatorname{Im} \varphi^{(j)} \geq 0$*;*

- *the symbol* $\mathfrak{a}^{(j)} \in \mathrm{S}^0_{\mathrm{ph}}(\mathbb{R} \times T'M; \operatorname{Mat}(m;\mathbb{C}))$ *is an element in the class of polyhomogeneous symbols of order zero with values in* $m \times m$ *complex matrices, which means that* $\mathfrak{a}^{(j)}$ *admits an asymptotic expansion in components positively homogeneous in momentum,*

$$\mathfrak{a}^{(j)}(t;y,\eta) \sim \sum_{k=0}^{+\infty} \mathfrak{a}^{(j)}_{-k}(t;y,\eta), \qquad \mathfrak{a}^{(j)}_{-k}(t;y,\alpha\,\eta) = \alpha\, \mathfrak{a}^{(j)}_{-k}(t;y,\eta) \quad \forall \alpha > 0; \tag{3.3.17}$$

- *the function* $\chi^{(j)} \in C^\infty(\mathbb{R} \times M \times T'M)$ *is a cut-off satisfying*

  (I) $\chi^{(j)}(t,x;y,\eta) = 0$ *on* $\{(t,x;y,\eta) \,|\, |h^{(j)}(y,\eta)| \leq 1/2\}$,

(II) $\chi^{(j)}(t,x;y,\eta)=1$ *on the intersection of* $\{(t,x;y,\eta)\,|\,|h^{(j)}(y,\eta)|\ge 1\}$ *with some conical neighbourhood of* $\{(t,x^{(j)}(t;y,\eta);y,\eta)\}$,

(III) $\chi^{(j)}(t,x;y,\alpha\,\eta)=\chi^{(j)}(t,x;y,\eta)$ *for* $\alpha\ge 1$ *on* $\{(t,x;y,\eta)\,|\,|h^{(j)}(y,\eta)|\ge 1\}$;

- *the weight* $w^{(j)}$ *is defined by*

$$w^{(j)}(t,x;y,\eta):=[\rho(x)\,\rho(y)]^{-\frac12}\left[\det{}^2(\varphi^{(j)}_{x^\alpha\eta_\beta})\right]^{\frac14}, \tag{3.3.18}$$

where the smooth branch of the complex root is chosen in such a way that $w(0,y;y,\eta)=[\rho(y)]^{-1}$.

Remark 3.10. Note that the weight $w^{(j)}$ is the inverse of a smooth density in the variable y and a smooth scalar function in all other variables. The powers of the Riemannian density ρ in (3.3.18) are chosen in such a way that the symbol $\mathfrak{a}^{(j)}$ and the integral kernel

$$u^{(j)}(t,x,y):=\frac{1}{(2\pi)^d}\int_{T'_yM}e^{i\varphi^{(j)}(t,x;y,\eta)}\,\mathfrak{a}^{(j)}(t;y,\eta)\,\chi^{(j)}(t,x;y,\eta)\,w^{(j)}(t,x;y,\eta)\,\mathrm{d}\eta \tag{3.3.19}$$

of the operator (3.3.16) are scalar functions in all variables. The fact that the symbol is a genuine scalar function on $\mathbb{R}\times T'M$ is a crucial feature of our construction.

Taking the square and then extracting the fourth root in (3.3.18) serves the purpose of making the weight invariant under inversion of a single coordinate x^α or a single coordinate y^α. Note, however, that if one works on an orientable and oriented manifold, then one can simplify (3.3.18) to read

$$w^{(j)}(t,x;y,\eta)=[\rho(x)\,\rho(y)]^{-\frac12}\left[\det\varphi^{(j)}_{x^\alpha\eta_\beta}\right]^{\frac12}. \tag{3.3.20}$$

Remark 3.11. The existence of a phase function satisfying conditions (i)–(iv) is a nontrivial matter. In fact, the space of phase function satisfying these conditions is nonempty and path-connected, see [77, Lemmata 1.4 and 1.7].

Proof of Theorem 3.9. Suppose that we have constructed the symbols $\mathfrak{a}^{(j)}$ appearing in the oscillatory integrals (3.3.16) so that

$$\widetilde{U}_A(t):=\sum_j U_A^{(j)}(t)=\sum_{j=1}^{m^+}U_A^{(j)}(t)+\sum_{j=1}^{m^-}U_A^{(-j)}(t) \tag{3.3.21}$$

satisfies

$$\left(-i\,\frac{\partial}{\partial t}+A\right)\widetilde{U}_A(t)\overset{\mathrm{mod}\ \Psi^{-\infty}}{=}0\,,\tag{3.3.22a}$$

$$\widetilde{U}_A(0)\overset{\mathrm{mod}\ \Psi^{-\infty}}{=}\mathrm{Id}\,.\tag{3.3.22b}$$

How to achieve this will be explained in subsection 3.3.3.

Put

$$\widetilde{u}^+(t,x,y):=\sum_{j=1}^{m^+}u^{(j)}(t,x,y),\tag{3.3.23}$$

$$\widetilde{u}^-(t,x,y):=\sum_{j=1}^{m^-}u^{(-j)}(t,x,y),\tag{3.3.24}$$

so that the Schwartz kernel of the operator $\widetilde{U}_A(t)$ reads

$$\widetilde{u}(t,x,y)=\widetilde{u}^+(t,x,y)+\widetilde{u}^-(t,x,y).\tag{3.3.25}$$

Let $u(t,x,y)$, $u^+(t,x,y)$ and $u^-(t,x,y)$ be the Schwartz kernels of the operators $U_A(t)$, $U_A^+(t)$, and $U_A^-(t)$, respectively.

Formulae (3.3.22a) and (3.3.22b) imply

$$u(t,x,y)=\widetilde{u}(t,x,y)\quad\mathrm{mod}\ C^\infty(\mathbb{R}\times M_x\times M_y;\mathrm{Mat}(m,\mathbb{C})).\tag{3.3.26}$$

This fact can be established as follows.

Let

$$u_\infty(t,x,y):=u(t,x,y)-\widetilde{u}(t,x,y).\tag{3.3.27}$$

From the construction algorithm, we know that

$$\left[\left(-i\,\frac{\partial}{\partial t}+A^{(x)}\right)u_\infty\right](t,x,y)=f(t,x,y),\tag{3.3.28}$$

$$u_\infty(0,x,y)=\zeta(x,y),\tag{3.3.29}$$

where $f\in C^\infty(\mathbb{R}\times M_x\times M_y;\mathrm{Mat}(m,\mathbb{C}))$ and $\zeta\in C^\infty(M_x\times M_y;\mathrm{Mat}(m,\mathbb{C}))$. Here the superscript in $A^{(x)}$ indicates that the differential operator A acts in the variable x. Using functional calculus, we can write the functions u_∞, f and ζ in terms of the eigenfunctions of A as

$$u_\infty(t,x,y)=\sum_{j,k}a_{jk}(t)\,v_j(x)\,[v_k(y)]^*,\tag{3.3.30}$$

$$f(t,x,y)=\sum_{j,k} b_{jk}(t)\,v_j(x)\,[v_k(y)]^*, \tag{3.3.31}$$

$$\zeta(x,y)=\sum_{j,k} c_{jk}\,v_j(x)\,[v_k(y)]^*. \tag{3.3.32}$$

Here the smooth functions b_{jk} and the constants c_{jk} are given, whereas the functions a_{jk} are our unknowns. Substituting (3.3.30)–(3.3.32) into (3.3.28), (3.3.29) we obtain the family of first order ODEs

$$\left[\left(-i\,\frac{\mathrm{d}}{\mathrm{d}t}+\lambda_j\right)a_{jk}\right](t)=b_{jk}(t), \tag{3.3.33}$$

$$a_{jk}(0)=c_{jk}, \tag{3.3.34}$$

whose solutions are

$$a_{jk}(t)=e^{-i\lambda_j t}\left(c_{jk}+i\int_0^t e^{i\lambda_j s}\,b_{jk}(s)\,\mathrm{d}s\right). \tag{3.3.35}$$

Straightforward integration by parts and the fact that $\lambda_k \sim k^{1/d}$ when $k\to\infty$ allow one to conclude that $a_{j,k}$ decay faster than any power of j and k as $j,k\to\infty$. This implies that the series on the RHS of (3.3.30) defines a function u_∞ which is smooth in all variables. So we arrive at (3.3.26), which gives us assumption (a) in Theorem 3.8 with $(T_-,T_+)=\mathbb{R}$.

Resorting to standard stationary phase arguments — see, e.g., [104, Appendix C] – and using the properties (i)–(iv) of our phase functions, it is easy to see that $u^\pm$ and $\widetilde{u}^\pm$ satisfy assumptions (b) and (c) of Theorem 3.8. Hence, Theorem 3.8 gives us (3.3.14) and (3.3.15).

The fact that the construction is global in time is guaranteed by [77, Lemma 1.2].

□

Remark 3.12. If one is prepared to give up globality in time, Theorem 3.9 and the corresponding proof can be adapted in a straightforward manner to the more customary case of real-valued — as opposed to complex-valued — phase functions. This is achieved by prescribing the phase functions to take values in $\mathbb{R}$, dropping condition (iv) and replacing everywhere in the statement and in the proof the time domain $\mathbb{R}$ with the interval (T_-,T_+), where

$$T_+ := \min_j \inf\{t>0 \,|\, \det \varphi^{(j)}_{x^\alpha\eta_\beta}\big|_{x=x^{(j)}}=0,\ (y,\eta)\in T'M\}\,, \tag{3.3.36}$$

$$T_- := \max_j \sup\{t < 0 \,|\, \det \varphi^{(j)}_{x^\alpha \eta_\beta}\big|_{x=x^{(j)}} = 0,\ (y,\eta) \in T'M\}\,. \tag{3.3.37}$$

The values of $T_\pm$ depend on the choice of particular real-valued phase functions, but we always have $T_- < 0 < T_+$. Observe that Theorem 3.8 was formulated in such a way that it covers both the case of real-valued and complex-valued phase functions.

The reader will have noticed that the zero mode propagator U_A^0 does not appear in our construction. This is due to the fact that, clearly,

$$U_A^0 \overset{\text{mod}\,\Psi^{-\infty}}{=} 0.$$

We end this subsection with the observation that, thanks to the presence of the weight $w^{(j)}$ in formula (3.3.16), the scalar matrix-function $\mathfrak{a}_0^{(j)}$ does not depend on the choice of the phase functions $\varphi^{(j)}$. This motivates the following definition.

Definition 3.13. We call $\mathfrak{a}_0^{(j)}$ the *principal symbol* of the Fourier integral operator (3.3.16).

The above definition agrees with the standard definition of principal symbol of a Fourier integral operator expressed as a section of the Keller–Maslov bundle, see [77, subsection 2.4].

3.3.3 The algorithm

The integral kernel (3.3.19) of $U_A^{(j)}(t)$ can be constructed explicitly as follows.

Step 1. Choose a phase function $\varphi^{(j)}$ compatible with Theorem 3.9. We will see later on that for the special case of the Dirac operator we can identify distinguished phase functions, the *Levi-Civita phase functions*. Furthermore, set $\chi^{(j)} \equiv 1$. In fact, the purpose of the cut-off is to localise integration in a neighbourhood of the $h^{(j)}$-flow and away from the zero section: different choices of $\chi^{(j)}$ result in oscillatory integrals differing by an infinitely smooth function.

Step 2. Act with the operator $-i\partial_t + A^{(x)}$ on the oscillatory integral (3.3.19). This produces a new oscillatory integral

$$\frac{1}{(2\pi)^d} \int_{T'_yM} e^{i\varphi^{(j)}(t,x;y,\eta)}\, a^{(j)}(t,x;y,\eta)\, \chi^{(j)}(t,x;y,\eta)\, w^{(j)}(t,x;y,\eta)\, \mathrm{d}\eta \tag{3.3.38}$$

whose amplitude $a^{(j)} \in C^\infty(\mathbb{R} \times M \times T'M; \mathrm{Mat}(m,\mathbb{C}))$ is given by

$$a^{(j)} := e^{-i\varphi^{(j)}}[w^{(j)}]^{-1}\left(-i\partial_t + A^{(x)}\right)\left(e^{i\varphi^{(j)}}\,\mathfrak{a}^{(j)}\,w^{(j)}\right). \tag{3.3.39}$$

By making use of the fact that $\varphi^{(j)}$ and $w^{(j)}$ are positively homogeneous in momentum η of degree 1 and 0, respectively, one can write down an asymptotic expansion for the amplitude $a^{(j)}$ in components positively homogeneous in momentum:

$$a^{(j)}(t,x;y,\eta) \sim \sum_{k=-1}^{+\infty} a^{(j)}_{-k}(t,x;y,\eta), \quad a^{(j)}_{-k}(t,x;y,\alpha\,\eta) = \alpha^{-k}\,a^{(j)}_{-k}(t,x;y,\eta),\ \forall\alpha>0. \tag{3.3.40}$$

Step 3. As $u^{(j)}(t,x,y)$ is to be the (distributional) solution of the hyperbolic equation

$$(-i\partial_t + A^{(x)})u^{(j)}(t,x,y) \overset{\mathrm{mod}\ C^\infty}{=} 0,$$

one would like to impose the condition $a^{(j)}(t,x,y,\eta)=0$. However, the amplitude $a^{(j)}$, unlike the symbol $\mathfrak{a}^{(j)}$, depends on x, and doing so would result in an unsolvable system of partial differential equations (PDEs). The current step consists in excluding the dependence of $a^{(j)}$ on x by means of a procedure known as *reduction of the amplitude*, to the end of reducing the system of PDEs to a system of ordinary differential equations, instead.

Put

$$L^{(j)}_\alpha := \left[(\varphi^{(j)}_{x\eta})^{-1}\right]_\alpha{}^\beta \frac{\partial}{\partial x^\beta} \tag{3.3.41}$$

and define

$$\mathfrak{S}^{(j)}_0 := (\,\cdot\,)|_{x=x^{(j)}}\,, \tag{3.3.42a}$$

$$\mathfrak{S}^{(j)}_{-k} := \mathfrak{S}^{(j)}_0\left[i\,[w^{(j)}]^{-1}\frac{\partial}{\partial\eta_\beta}\,w^{(j)}\left(1+\sum_{1\le|\boldsymbol{\alpha}|\le 2k-1}\frac{(-\varphi^{(j)}_\eta)^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!\,(|\boldsymbol{\alpha}|+1)}\,L^{(j)}_{\boldsymbol{\alpha}}\right)L^{(j)}_\beta\right]^k, \tag{3.3.42b}$$

where $\boldsymbol{\alpha}\in\mathbb{N}^d$, $|\boldsymbol{\alpha}| = \sum_{j=1}^d \alpha_j$ and $(-\varphi^{(j)}_\eta)^{\boldsymbol{\alpha}} := (-1)^{|\boldsymbol{\alpha}|}\,(\varphi^{(j)}_{\eta_1})^{\alpha_1}\dots(\varphi^{(j)}_{\eta_d})^{\alpha_d}$. The operator (3.3.42b) is well defined, because the differential operators $L^{(j)}_\alpha$ commute. Furthermore, the operators $\mathfrak{S}^{(j)}_{-k}$ are invariant under change of local coordinates x and y.

The *amplitude-to-symbol operator* is defined as

$$\mathfrak{S}^{(j)} : C^\infty(\mathbb{R}\times M\times T'M)\to C^\infty(\mathbb{R}\times T'M)\,,$$
$$\mathfrak{S}^{(j)} := \sum_{j=0}^{\infty}\mathfrak{S}^{(j)}_{-k}\,. \tag{3.3.43}$$

When acting on a function positively homogeneous in momentum, the operator $\mathfrak{S}^{(j)}_{-k}$ excludes the dependence on x and decreases the degree of homogeneity by k.

The reduction of the amplitude is achieved by replacing the amplitude $a^{(j)}$ in (3.3.38) by

$$\mathfrak{S}^{(j)} a^{(j)} =: \mathfrak{b}^{(j)}, \tag{3.3.44}$$

with

$$\mathfrak{b}^{(j)}(t;y,\eta)\sim\sum_{k=-1}^{+\infty}\mathfrak{b}^{(j)}_{-k}(t;y,\eta)\,,\qquad \mathfrak{b}^{(j)}_{-k}=\sum_{l+s=k}\mathfrak{S}^{(j)}_{-l}\,a^{(j)}_{-s}\,.$$

The oscillatory integral

$$\frac{1}{(2\pi)^d}\int_{T'_yM} e^{i\varphi^{(j)}(t,x;y,\eta)}\,\mathfrak{b}^{(j)}(t;y,\eta)\,\chi^{(j)}(t,x;y,\eta)\,w^{(j)}(t,x;y,\eta)\,\mathrm{d}\eta \tag{3.3.45}$$

differs from (3.3.38) only by an infinitely smooth function.

We remind the reader that further particulars and detailed proofs concerning the amplitude-to-symbol operator were provided in Section 2.6.

Step 4. Set

$$\mathfrak{b}^{(j)}_{-k}=0,\qquad k=-1,0,1,\dots. \tag{3.3.46}$$

Equations (3.3.46), combined with the initial conditions stemming from the constraint

$$\sum_j U^{(j)}(0)\overset{\mathrm{mod}\ \Psi^{-\infty}}{=}\mathrm{Id}, \tag{3.3.47}$$

yield a hierarchy of (matrix) transport equations for the homogeneous components $\mathfrak{a}^{(j)}_{-k}$.

Let us make a few remarks warranted by formula (3.3.47).

The m oscillatory integrals appearing on the RHS of (3.3.14) and (3.3.15) are not independent of one another, but they 'mix' at $t=0$ via the initial condition (3.3.47).

Now, satisfying (3.3.47) involves representing the identity operator on $C^\infty(M;\mathbb{C}^m)$ in a somewhat nonstandard fashion, as

$$\mathrm{Id} \overset{\mathrm{mod}\ \Psi^{-\infty}}{=} \sum_j \frac{1}{(2\pi)^d} \int_{T'M} e^{i\varphi^{(j)}(0,x;y,\eta)}\, \mathfrak{s}^{(j)}(y,\eta)\, \chi^{(j)}(0,x;y,\eta)\, w^{(j)}(0,x;y,\eta)\, (\,\cdot\,)\, \rho(y)\, \mathrm{d}y\, \mathrm{d}\eta, \tag{3.3.48}$$

with $\mathfrak{s}^{(j)} \in S^0_{\mathrm{ph}}(T'M;\mathrm{Mat}(m;\mathbb{C}))$.

In terms of the symbols $\mathfrak{a}^{(j)}$, the initial condition (3.3.47) reads

$$\mathfrak{a}^{(j)}(0;y,\eta) = \mathfrak{s}^{(j)}(y,\eta). \tag{3.3.49}$$

From the fact that the principal symbol of the identity operator is the identity matrix it follows that

$$\sum_j \mathfrak{a}^{(j)}_0(0;y,\eta) = \sum_j \mathfrak{s}^{(j)}_0(y,\eta) = \mathbf{1}_{m\times m}. \tag{3.3.50}$$

Furthermore, one can show that

$$\mathfrak{s}^{(j)}_0(y,\eta) = v^{(j)}(y,\eta)\, [v^{(j)}(y,\eta)]^*.$$

However, obtaining formulae for subleading components $\mathfrak{s}^{(j)}_{-1}$ is already a challenging task, see [41, subsection 4.2]. In general, lower order components of $\mathfrak{s}^{(j)}$ depend in a nontrivial manner on the eigenvalues and eigenprojections of the matrix-function $A_{\mathrm{prin}}(x,\xi)$ and on the choice of phase functions $\varphi^{(j)}$.

The invariant representation of the identity operator — and, more generally, of pseudodifferential operators — on manifolds is not a well-studied subject. An initial analysis of the scalar case was carried out in Section 2.7. For the case of massless Dirac a more detailed examination of the operator (3.3.48) will be provided in subsection 3.5.2.

Remark 3.14. All statements and results presented in this section carry over verbatim to the case where A is an elliptic symmetric first order $m\times m$ matrix *pseudodifferential* — as opposed to differential — operator, with the following exceptions:

- formulae (3.3.1) and (3.3.2) have to be dropped as they are no longer true;

- 'Step 2.' in subsection 3.3.3 has to be modified to take into account the action of a pseudodifferential operator on an oscillatory integral in an *invariant* manner, along the lines of [18, Section 4.3].

Remark 3.15. Let us point out that in this section we did not use anywhere the fact that M carries a Riemannian structure. If one replaces the Riemannian density (3.1.1) with an arbitrary positive density, all statements and results stay the same.

3.4 Invariant description of pseudodifferential operators acting on scalar functions

In order to prepare ourselves to address the issue of initial conditions for our transport equations in the case of the massless Dirac operator, we need to discuss first the more general question of invariant representation of a pseudodifferential operator. We devote a separate section to this, as we believe this matter to be of independent interest. Note that we treat the case of a scalar operator merely for the sake of presentational convenience: all the formulae and arguments in this subsection remain unchanged for matrix pseudodifferential operators acting on m-columns of scalar functions.

Definition 3.16. We call *time-independent Levi-Civita phase function* the function $\phi \in C^\infty(M \times T'M; \mathbb{C})$ defined by

$$\phi(x; y, \eta) := \int_\gamma \zeta \,\mathrm{d}z + \frac{i\epsilon}{2} h(y, \eta)\ [\mathrm{dist}(x, y)]^2 \tag{3.4.1}$$

when x lies in a geodesic neighbourhood of y and continued smoothly elsewhere in such a way that $\operatorname{Im}\phi \geq 0$. Here γ is the (unique) shortest geodesic connecting y to x, ζ is the parallel transport of η along γ,

$$h(y, \eta) := \sqrt{g^{\alpha\beta}(y)\, \eta_\alpha \eta_\beta}\,, \tag{3.4.2}$$

dist is the geodesic distance and ϵ is a positive parameter.

Let P be a pseudodifferential operator of order p acting on scalar functions over a Riemannian d-manifold. The operator P can be written, modulo an integral operator with smooth kernel, in the form

$$P = \int_{T'M} e^{i\phi(x;y,\eta)}\, \mathfrak{p}(y,\eta)\, \chi_0(x;y,\eta)\, w_0(x;y,\eta)\, (\,\cdot\,)\, \rho(y)\, \mathrm{d}y\, \mathrm{d}\eta, \tag{3.4.3}$$

where ϕ is the time-independent Levi-Civita phase function, $\mathfrak{p} \in S^m_{\mathrm{ph}}(T'M)$, χ_0 is a cut-off localising the integration in a neighbourhood of the diagonal and away from the zero section (see also (I)–(III) in Theorem 3.8) and

$$w_0(x;y,\eta) := [\rho(x)\,\rho(y)]^{-\frac{1}{2}}\left[\det{}^2\phi_{x^\alpha \eta_\beta}(x;y,\eta)\right]^{\frac{1}{4}}. \tag{3.4.4}$$

Here the smooth branch of the complex root is chosen in such a way that $w_0(y;y,\eta) = [\rho(y)]^{-1}$.

Remark 3.17. Note that (3.4.3) is, effectively, a special case of (3.3.16) with $t = 0$.

Formula (3.4.3) provides an invariant representation of the pseudodifferential operator P.

Definition 3.18. We call *full symbol* of the operator P the scalar function

$$\mathfrak{p}(y,\eta) \sim \sum_{k=-p}^{+\infty} \mathfrak{p}_{-k}(y,\eta).$$

Furthermore, we call the homogeneous functions $\mathfrak{p}_p$ and $\mathfrak{p}_{p-1}$ the *g-principal* and *g-subprincipal* symbol, respectively[3].

The notions of principal and subprincipal symbols of a pseudodifferential operator are nowadays standard concepts in microlocal analysis. The former makes sense for operators acting either on scalar functions or on half-densities, whereas the latter is only defined for operators acting on half-densities. We refer the reader to [67] for further details. Note that the concept of subprincipal symbol was introduced by Duistermaat and Hörmander in [52, Eqn. (5.2.8)].

It is easy to see that the concept of principal symbol P_{prin} and that of g-principal symbol $\mathfrak{p}_p$ coincide. As far as the subprincipal symbol is concerned, the situation is more complicated, in that before drawing a comparison we need to turn our operator into an operator acting on half-densities.

[3] Here 'g' is a reference to the Riemannian metric used in the construction of the phase function ϕ.

Put

$$P_{1/2} := \rho^{1/2} \, P \, \rho^{-1/2} \tag{3.4.5}$$

and let P_{sub} be the subprincipal symbol of the operator (3.4.5) defined in accordance with [52, Eqn. (5.2.8)].

A natural question to ask is: what is the relation between P_{sub} and $\mathfrak{p}_{p-1}$?

Theorem 3.19. *The invariant quantities* P_{sub} *and* $\mathfrak{p}_{p-1}$ *are related as*

$$\mathfrak{p}_{p-1} = P_{\mathrm{sub}} + \frac{i}{2}(P_{\mathrm{prin}})_{y^\alpha \eta_\alpha} + \frac{i}{2}\,\Gamma^\alpha{}_{\beta\gamma}\left[\eta_\alpha (P_{\mathrm{prin}})_{\eta_\beta}\right]_{\eta_\gamma} - \frac{\epsilon}{2}\, g_{\beta\gamma}\left[h\,(P_{\mathrm{prin}})_{\eta_\beta}\right]_{\eta_\gamma}. \tag{3.4.6}$$

Theorem 3.19 implies that, in particular, the two notions of subprincipal symbol coincide when the principal symbol does not depend on η, i.e. when P is a pseudodifferential operator of the type "multiplication by a scalar function plus an operator of order -1". Note that the identity operator, whose invariant representation was investigated in Section 2.7, falls into this class. This is why we did not introduce the terminology "g-subprincipal symbol" in Chapter 2.

A tedious, yet straightforward, calculation shows that the RHS of (3.4.6) is a scalar function on the cotangent bundle. In fact, the second and third summands on the RHS of (3.4.6) admit an invariant representation in terms of the Laplace–Beltrami operator associated with the *neutral metric* n on the cotangent bundle T^*M, which, in local coordinates $(x^1,\dots,x^d,\xi_1,\dots,\xi_d)$, reads

$$n_{jk}(x,\xi) = \begin{pmatrix} -2\,\xi_\gamma\,\Gamma^\gamma{}_{\alpha\beta}(x) & \delta_\alpha{}^\mu \\ \delta^\nu{}_\beta & 0 \end{pmatrix}, \qquad j,k \in \{1,\dots,2d\}.$$

The adjective 'neutral' refers to the fact that the metric n has signature (d,d).

Proof of Theorem 3.19. Consider the pseudodifferential operator P and turn it into an operator on half-densities $P_{1/2}$ via (3.4.5). In what follows we work in an arbitrary coordinate system, the same for x and y.

Dropping the cut-off, the integral kernel of $P_{1/2}$ now reads

$$\frac{1}{(2\pi)^d}\int_{T'_yM} e^{i\phi(x;y,\eta)}\,\mathfrak{p}(y,\eta)\,\sqrt{\det\phi_{x\eta}}\,\mathrm{d}\eta\,. \tag{3.4.7}$$

Our phase function (3.4.1) admits the expansion

$$\phi(x;y,\eta) = (x-y)^\alpha \eta_\alpha + \frac{1}{2}\Gamma^\alpha{}_{\beta\gamma}\,\eta_\alpha (x-y)^\beta (x-y)^\gamma + \frac{i\epsilon h}{2} g_{\alpha\beta}(x-y)^\alpha (x-y)^\beta + O(\|x-y\|^3), \tag{3.4.8}$$

which implies that

$$\sqrt{\det \phi_{x\eta}} = 1 + \frac{1}{2}[\Gamma^\alpha{}_{\alpha\beta} + i\epsilon h^{-1}\eta_\beta](x-y)^\beta + O(\|x-y\|^2). \tag{3.4.9}$$

Substituting (3.4.8) and (3.4.9) into (3.4.7), we get

$$\frac{1}{(2\pi)^d}\int e^{i(x-y)^\alpha \eta_\alpha} \Big\{ \mathfrak{p}_p + \left(\frac{1}{2}\left[i\Gamma^\alpha{}_{\beta\gamma}\,\eta_\alpha - \epsilon h g_{\beta\gamma}\right](x-y)^\beta (x-y)^\gamma + \frac{1}{2}\left[\Gamma^\alpha{}_{\alpha\beta} + i\epsilon h^{-1}\eta_\beta\right](x-y)^\beta \right)\mathfrak{p}_p + \mathfrak{p}_{p-1} + O(\|\eta\|^{p-2}) \Big\}\, d\eta\,. \tag{3.4.10}$$

Excluding the x-dependence from the amplitude in (3.4.10) by acting with the operator

$$\mathcal{S}_{\text{right}}(\,\cdot\,) := \left[\exp\left(i \frac{\partial^2}{\partial x^\mu\, \partial \eta_\mu} \right)(\,\cdot\,) \right]\Big|_{x=y}, \tag{3.4.11}$$

we arrive at

$$\frac{1}{(2\pi)^d}\int e^{i(x-y)^\alpha \eta_\alpha} \Big\{ \mathfrak{p}_p - \frac{i}{2}\left[\eta_\alpha\, \Gamma^\alpha{}_{\beta\gamma}\,(\mathfrak{p}_p)_{\eta_\beta}\right]_{\eta_\gamma} + \frac{\epsilon}{2}\left[h\, g_{\gamma\beta}\,(\mathfrak{p}_p)_{\eta_\beta}\right]_{\eta_\gamma} + \mathfrak{p}_{p-1} + O(\|\eta\|^{p-2}) \Big\}\, d\eta\,. \tag{3.4.12}$$

Computing the subprincipal symbol of (3.4.12) and using the fact that $\mathfrak{p}_p = P_{\text{prin}} = (P_{1/2})_{\text{prin}}$, we obtain (3.4.6). Note that the sign in front of the correction term

$$\frac{i}{2}(P_{\text{prin}})_{y^\alpha \eta_\alpha}$$

is opposite to the usual one, see, for example, (C.1.3). This is due to the fact that we use here the right — as opposed to left — quantisation. □

3.5 Global propagator for the massless Dirac operator

In this section we will start the analysis of the global propagator for the Dirac operator, specialising Theorem 3.9 to the case $A = W$.

We denote by

$$W_{\mathrm{prin}}(y,\eta) := \sigma^\alpha(y)\,\eta_\alpha \qquad (3.5.1)$$

the principal symbol of W and by

$$W_0(x) := -\frac{i}{4}\sigma^\alpha(x)\sigma_\beta(x)\left(\frac{\partial\sigma^\beta}{\partial x^\alpha}(x) + \Gamma^\beta{}_{\alpha\gamma}(x)\,\sigma^\gamma(x)\right) \qquad (3.5.2)$$

its zero order part, see Definition 3.1.

The principal symbol $W_{\mathrm{prin}}(y,\eta)$ has eigenvalues $h^\pm = \pm h$, where h is given by (3.4.2), compare with (3.3.2). This fact, which can be easily established by writing down (3.5.1) in local coordinates, shows that the Dirac operator is indeed elliptic.

It is well-known that the Hamiltonian flow $(x^+(t;y,\eta),\xi^+(t;y,\eta))$ generated by h is (co-)geodesic. The two flows, $(x^+(t;y,\eta),\xi^+(t;y,\eta))$ and $(x^-(t;y,\eta),\xi^-(t;y,\eta))$, are related as

$$(x^-(t;y,\eta),\xi^-(t;y,\eta)) = (x^+(t;y,-\eta),-\xi^+(t;y,-\eta)). \qquad (3.5.3)$$

Our goal is to write down explicitly the positive and negative propagators (3.1.13a) and (3.1.13c) in the form (3.3.16) for a distinguished choice of phase functions.

To this end, we give the following definition (see also Section 2.4).

Definition 3.20. We call *positive* (+), resp. *negative* (−), *Levi-Civita phase function* the infinitely smooth function $\varphi^\pm \in C^\infty(\mathbb{R}\times M\times T'M;\mathbb{C})$ defined by

$$\varphi^\pm(t,x;y,\eta) = \int_{\gamma^\pm} \zeta^\pm\,\mathrm{d}z + \frac{i\,\epsilon}{2}h(y,\eta)\,\mathrm{dist}^2(x,x^\pm(t;y,\eta)) \qquad (3.5.4)$$

for x in a geodesic neighbourhood of $x^\pm(t;y,\eta)$ and continued smoothly elsewhere in such a way that $\mathrm{Im}\,\varphi^\pm \geq 0$. Here dist is the Riemannian geodesic distance, the path of integration $\gamma^\pm$ is the shortest geodesic connecting $x^\pm$ to x, $\zeta^\pm$ is the result of the parallel transport of $\xi^\pm(t;y,\eta)$ along $\gamma^\pm$ and ϵ is a positive parameter.

The positive and negative Levi-Civita phase functions are related as

$$\varphi^-(t,x;y,\eta) = -\overline{\varphi^+(t,x;y,-\eta)}. \qquad (3.5.5)$$

Let us point out that the way one continues $\varphi^\pm$ outside a neighbourhood of the flow does not affect the singular part of the propagators. The choice of a different smooth continuation results in an error $\overset{\mathrm{mod}\,\Psi^{-\infty}}{=} 0$, as one can show by a straightforward (non)stationary phase argument.

Remark 3.21. The time-independent phase function ϕ introduced in the previous section is the restriction to $t = 0$ of the phase functions $\varphi^\pm$,

$$\phi(x; y, \eta) = \varphi^+(0, x; y, \eta) = \varphi^-(0, x; y, \eta). \tag{3.5.6}$$

It is easy to see that the positive and negative Levi-Civita phase functions satisfy conditions (i), (ii) and (iv) from Theorem 3.9. Furthermore, [104, Corollary 2.4.5] implies that condition (iii) is also satisfied. Hence, Theorem 3.9 ensures that the integral kernel of $U^\pm$ can be written as a single oscillatory integral

$$u^\pm(t, x, y) := \frac{1}{(2\pi)^3} \int_{T'_y M} e^{i\varphi^\pm(t,x;y,\eta)}\, \mathfrak{a}^\pm(t; y, \eta)\, \chi^\pm(t, x; y, \eta)\, w^\pm(t, x; y, \eta)\, \mathrm{d}\eta, \tag{3.5.7}$$

where $\varphi^\pm$ is the positive/negative Levi-Civita phase function.

Definition 3.22. We define *the full symbol of the positive* (resp. *negative*) *propagator* to be the scalar matrix-function $\mathfrak{a}^+$ (resp. $\mathfrak{a}^-$), obtained through the algorithm described in Section 3.3.3 with Levi-Civita phase functions.

We define the *subprincipal symbol of the positive* (resp. *negative*) *propagator* to be the scalar matrix-function $\mathfrak{a}^+_{-1}$ (resp. $\mathfrak{a}^-_{-1}$) obtained the same way.

As to the principal symbol, this object was defined earlier, see Definition 3.13.

We stress that the mathematical objects contained in the above definition are uniquely and invariantly defined. They only depend on the phase functions which, in turn, originate from the geometry of M in a coordinate-free covariant manner, cf. Definition 3.5.4.

To the best of our knowledge, there is no accepted definition of full symbol or subprincipal symbol for a Fourier integral operator available in the literature to date. The geometric nature of our construction allows us to provide invariant definitions of full and subprincipal symbol of the Dirac propagator, analyse them, and give explicit formulae. Our work, from this Chapter and the previous one, aims to build towards an invariant theory for pseudodifferential and Fourier integral operators on manifolds.

Before moving on to computing the principal and subprincipal symbols of the positive (resp. negative) Dirac propagator, an important remark is in order. In addition to what was discussed in Section 3.3 for the general case, the construction of the Dirac propagator has to be consistent with the gauge transformation (3.1.5), (3.1.6). In particular, the action of the gauge transformation needs to be carefully accounted for by the construction process.

The transformation (3.1.6) leads to the transformation

$$\mathfrak{a}^{\pm}(t;y,\eta) \mapsto G^{*}(x)\,\mathfrak{a}^{\pm}(t;y,\eta)\,G(y). \tag{3.5.8}$$

in the oscillatory integral (3.5.7). Note that this introduces an x-dependence which has to be handled by means of amplitude-to-symbol reduction (3.3.43).

3.5.1 Transport equations

By acting with the Dirac operator W on (3.5.7) in the variable x and dropping the cut-off, we obtain

$$Wu^{\pm}(t,x,y) = \frac{1}{(2\pi)^3}\int_{T'_yM} e^{i\varphi^{\pm}(t,x;y,\eta)}\,a^{\pm}(t;y,\eta)\,w^{\pm}(t,x;y,\eta)\,\mathrm{d}\eta, \tag{3.5.9}$$

where

$$\begin{aligned} a &= -ie^{-i\varphi^{\pm}}(w^{\pm})^{-1}\partial_t\left(e^{i\varphi^{\pm}}\,\mathfrak{a}^{\pm}\,w^{\pm}\right) + \left[-ie^{-i\varphi^{\pm}}(w^{\pm})^{-1}\sigma^{\alpha}\partial_{x^\alpha}\left(e^{i\varphi^{\pm}}\,w^{\pm}\right) + W_0\right]\mathfrak{a}^{\pm} \\ &= \left(\varphi^{\pm}_t + \sigma^{\alpha}\varphi^{\pm}_{x^\alpha}\right)\mathfrak{a}^{\pm} - i\mathfrak{a}^{\pm}_t + \left[-i(w^{\pm})^{-1}\left(w^{\pm}_t + \sigma^{\alpha}w^{\pm}_{x^\alpha}\right) + W_0\right]\mathfrak{a}^{\pm}. \end{aligned} \tag{3.5.10}$$

Put

$$a \sim \sum_{k=-1}^{+\infty} a_{-k}, \tag{3.5.11}$$

where

$$a^{\pm}_1 := \left(\varphi^{\pm}_t + W_{\mathrm{prin}}(x,\varphi^{\pm}_x)\right)\mathfrak{a}^{\pm}_0 \tag{3.5.12}$$

and

$$a^{\pm}_{-k} := \left(\varphi^{\pm}_t + W_{\mathrm{prin}}(x,\varphi^{\pm}_x)\right)\mathfrak{a}^{\pm}_{-k-1} - i(\mathfrak{a}^{\pm}_{-k})_t + \left[-i(w^{\pm})^{-1}\left(w^{\pm}_t + \sigma^{\alpha}w^{\pm}_{x^\alpha}\right) + W_0\right]\mathfrak{a}^{\pm}_{-k} \tag{3.5.13}$$

for $k \ge 0$. Note that the $a^\pm_{-k}$, $k \ge -1$, are positively homogeneous in momentum of degree $-k$.

Our transport equations read

$$\mathfrak{S}^\pm_0 a^\pm_1 = 0, \tag{3.5.14}$$

$$\mathfrak{S}^\pm_{-1} a^\pm_1 + \mathfrak{S}^\pm_0 a^\pm_0 = 0, \tag{3.5.15}$$

$$\mathfrak{S}^\pm_{-2} a^\pm_1 + \mathfrak{S}^\pm_{-1} a^\pm_0 + \mathfrak{S}^\pm_0 a^\pm_{-1} = 0, \tag{3.5.16}$$

$$\dots$$

Recalling that $v^\pm$ are the normalised eigenvectors of W_{prin} corresponding to the eigenvalues $\pm h$, denote by

$$P^\pm(y,\eta) := v^\pm(y,\eta)\,[v^\pm(y,\eta)]^*. \tag{3.5.17}$$

the spectral projections along the eigenspaces spanned by $v^\pm$. Of course,

$$W_{\mathrm{prin}} = h\,(P^+ - P^-), \tag{3.5.18}$$

$$\mathrm{Id} = P^+ + P^-, \tag{3.5.19}$$

and

$$P^\pm = \frac{1}{2}\left(\mathrm{Id} \pm \frac{W_{\mathrm{prin}}}{h}\right). \tag{3.5.20}$$

Let us label the transport equations with nonnegative integer numbers in increasing order, so that (3.5.14) is the zeroth transport equation, (3.5.15) is the first transport equation and so on. Direct inspection of (3.5.12) and (3.5.13) reveals that

- multiplication of the n-th transport equation by $P^\mp(x^\pm,\xi^\pm)$ on the left allows one to determine
$$P^\mp(x^\pm,\xi^\pm)\mathfrak{a}^\pm_{-n}(t;y,\eta), \qquad n \ge 0, \tag{3.5.21}$$
algebraically;
- multiplication of the $(n+1)$-th transport equation by $P^\pm(x^\pm,\xi^\pm)$ on the left and the use of (3.5.21), allows one to determine
$$P^\pm(x^\pm,\xi^\pm)\mathfrak{a}^\pm_{-n}(t;y,\eta), \qquad n \ge 0, \tag{3.5.22}$$
upon solving a matrix ordinary differential equation in the variable t.

Summing up (3.5.21) and (3.5.22) one obtains $\mathfrak{a}^\pm_{-k}(t;y,\eta)$, in view of (3.5.19).

3.5.2 Pseudodifferential operators $U^\pm(0)$

This subsection is devoted to the examination of operators $U^\pm(0)$. We need to examine these operators because, as explained in subsection 3.3.3, their full symbols determine the initial conditions $\mathfrak{a}^\pm_{-k}(0;y,\eta)$ for our transport equations.

We have

$$U^\pm(0)=\theta(\pm W), \tag{3.5.23}$$

where

$$\theta(\lambda):=\begin{cases}1 & \text{for} \quad \lambda>0,\\ 0 & \text{for} \quad \lambda\le 0.\end{cases} \tag{3.5.24}$$

We see that the operators $U^\pm(0)$ are self-adjoint pseudodifferential operators of order zero, orthogonal projections onto the positive/negative eigenspaces of the operator W. The operator $\mathrm{Id}-U^+(0)-U^-(0)$ is the orthogonal projection onto the nullspace of the operator W, hence

$$U^+(0)+U^-(0) \overset{\mod \Psi^{-\infty}}{=} \mathrm{Id}. \tag{3.5.25}$$

The principal symbols of the operators $U^\pm(0)$ read

$$[U^\pm(0)]_{\mathrm{prin}}=P^\pm(y,\eta), \tag{3.5.26}$$

where $P^\pm$ are the orthogonal projections onto the positive/negative eigenspaces of the principal symbol of the operator W, see (3.5.17).

The analysis of the *full* symbol of $U^\pm(0)$ is a delicate task which was investigated, to a certain extent and in a somewhat different setting, in [41]. In order to develop the ideas from [41] we have to address a number of issues.

- We are now dealing with scalar fields as opposed to half-densities.
- We are now making full use of Riemannian structure.
- We are now working in the special setting of a system of two equations in dimension three with trace-free principal symbol.
- Unlike [41, 42], we are aiming to evaluate the actual matrix-functions $[U^\pm(0)]_{\mathrm{sub}}$ and not only their traces.

In order to calculate the subprincipal symbols of the pseudodifferential operators $U^{\pm}(0)$ we will need the following auxiliary result.

Theorem 3.23. *Fix a point $y \in M$ and let $\{\widetilde{e}\}_{j=1}^{3}$ be a framing on M. Let $G \in C^{\infty}(M; SU(2))$ be a gauge transformation such that $G(y) = \mathrm{Id}$ and let*

$$e_j{}^{\alpha} := \frac{1}{2}\,\mathrm{tr}(s_j\, G^*\, s^k\, G)\, \widetilde{e}_k{}^{\alpha}. \tag{3.5.27}$$

Then

$$\nabla_{\alpha} G(y) = -\frac{i}{2}\left[\overset{*}{K}_{\alpha\beta}(y) - \overset{*}{\widetilde{K}}_{\alpha\beta}(y)\right]\,\sigma^{\beta}(y), \tag{3.5.28}$$

where K (resp. $\widetilde{K}$) is the contorsion tensor of the Weitzenböck connection (see Appendix B.1) associated with the framing $\{e_j\}_{j=1}^{3}$ (resp. $\{\widetilde{e}_j\}_{j=1}^{3}$), the star stands for the Hodge dual applied in the first and third indices, see formula (B.1.7), and $\sigma^{\alpha}(y)$ is defined by (3.1.3).

Proof. The proof is provided in Appendix B.2.1. □

Remark 3.24. Let $\{\widetilde{e}\}_{j=1}^{3}$ and $\{e\}_{j=1}^{3}$ be a pair of framings related in accordance with (3.5.27), and let $\widetilde{W}$ and W be the corresponding massless Dirac operators, see Definition 3.1. Then

$$W = G^* \widetilde{W} G. \tag{3.5.29}$$

The following theorem is the main result of this subsection.

Theorem 3.25. *We have*

$$[U^{\pm}(0)]_{\mathrm{sub}}(y,\eta) = \pm \frac{1}{4(h(y,\eta))^3}\, \overset{*}{T}{}^{\alpha\beta}(y)\, \eta_{\alpha}\eta_{\beta}\, \mathrm{Id}\,, \tag{3.5.30}$$

where T is the torsion tensor of the Weitzenböck connection (see Appendix B.1) associated with the framing $\{e_j\}_{j=1}^{3}$ encoded within the massless Dirac operator W (see Definition 3.1) and the star stands for the Hodge dual applied in the second and third indices, see formula (B.1.6).

Proof. Let us fix a point $y \in M$ and choose normal geodesic coordinates x centred at y such that $e_j{}^{\alpha}(y) = \delta_j{}^{\alpha}$. Consider the (local) operator with constant coefficients

$$\widetilde{W} := -is^{\alpha}\,\frac{\partial}{\partial x^{\alpha}}\,, \tag{3.5.31}$$

where the s^α are the standard Pauli matrices (3.1.2). Let us choose a smooth special unitary 2×2 matrix-function G such that

$$G(0)=\mathrm{Id}, \tag{3.5.32}$$

$$[W]_{\mathrm{prin}}=[G^*\widetilde{W}G]_{\mathrm{prin}}+O(\,\|\eta\|\,\|x\|^2\,)\,, \tag{3.5.33}$$

compare with (3.5.29). It is easy to see that such a matrix-function $G(x)$ exists and is defined uniquely modulo $O(\|x\|^2)$.

Let us now compare the subprincipal symbols of the pseudodifferential operators $\theta(\pm W)$ and $\theta(\pm G^*\widetilde{W}G)$, with $G^*\widetilde{W}G$ understood as an operator acting in Euclidean space (constant metric tensor $g_{\alpha\beta}(x)=\delta_{\alpha\beta}$). It can be shown that at the origin we have

$$[W]_{\mathrm{sub}}(0,\eta)=[G^*\widetilde{W}G]_{\mathrm{sub}}(0,\eta).$$

Thus, the proof of the Theorem 3.25 has been reduced to the case when we are in Euclidean space and the operator W is given by formulae (3.5.29) and (3.5.31).

We have

$$\theta(\pm\widetilde{W})=\frac{1}{(2\pi)^3}\int_{T'\mathbb{R}^3} e^{i(x-z)^\alpha\eta_\alpha}\,P^\pm(\eta)\,(\,\cdot\,)\,\mathrm{d}z\,\mathrm{d}\eta\,, \tag{3.5.34}$$

where

$$P^\pm(\eta)=\frac{1}{2}\left(\mathrm{Id}\pm\frac{1}{\|\eta\|}s^\beta\eta_\beta\right). \tag{3.5.35}$$

Formulae (3.5.34) and (3.5.35) imply that

$$\theta(\pm G^*\widetilde{W}G)=\frac{1}{(2\pi)^3}\int_{T'\mathbb{R}^3} e^{i(x-z)^\alpha\eta_\alpha}\,Q^\pm(x,z,\eta)\,(\,\cdot\,)\,\mathrm{d}z\,\mathrm{d}\eta\,, \tag{3.5.36}$$

where

$$Q^\pm(x,z,\eta)=G^*(x)\,P^\pm(\eta)\,G(z)=\frac{1}{2}\,G^*(x)\left(\mathrm{Id}\pm\frac{1}{\|\eta\|}s^\beta\eta_\beta\right)G(z)\,. \tag{3.5.37}$$

Excluding the z-dependence from the amplitude $Q^\pm$ by acting with the operator

$$\mathcal{S}_{\mathrm{left}}(\,\cdot\,):=\left.\left[\exp\left(-i\frac{\partial^2}{\partial z^\mu\,\partial\eta_\mu}\right)(\,\cdot\,)\right]\right|_{z=x}, \tag{3.5.38}$$

compare with (3.4.11), we arrive at

$$\theta(\pm G^*\widetilde{W}G)=\frac{1}{(2\pi)^3}\int_{T'\mathbb{R}^3} e^{i(x-z)^\alpha\eta_\alpha}\,\mathcal{Q}^\pm(x,\eta)\,(\,\cdot\,)\,\mathrm{d}z\,\mathrm{d}\eta\,, \tag{3.5.39}$$

where

$$\mathcal{Q}^{\pm}(x,\eta) = \mathcal{Q}^{\pm}_0(x,\eta) + \mathcal{Q}^{\pm}_{-1}(x,\eta) + O(\|\eta\|^{-2})\,, \tag{3.5.40}$$

$$\mathcal{Q}^{\pm}_0(x,\eta) = \frac{1}{2}\,G^*(x)\left(\mathrm{Id} \pm \frac{1}{\|\eta\|}s^\beta\eta_\beta\right)G(x)\,, \tag{3.5.41}$$

$$\mathcal{Q}^{\pm}_{-1}(x,\eta) = -\frac{i}{2}\,G^*(x)\left(\mathrm{Id} \pm \frac{1}{\|\eta\|}s^\beta\eta_\beta\right)_{\eta_\mu} G_{x^\mu}(x)\,. \tag{3.5.42}$$

In the Euclidean setting the standard formula [52, Eqn. (5.2.8)] for the subprincipal symbol reads

$$[\theta(\pm G^*\widetilde{W}G)]_{\mathrm{sub}} = \mathcal{Q}^{\pm}_{-1} + \frac{i}{2}(\mathcal{Q}^{\pm}_0)_{x^\mu\eta_\mu}\,. \tag{3.5.43}$$

Substituting (3.5.41) and (3.5.42) into (3.5.43) and setting $x=0$, we get

$$\begin{aligned}[\theta(\pm G^*\widetilde{W}G)]_{\mathrm{sub}} &= \pm\frac{i}{4}\left[G^*_{x^\mu}\left(\frac{1}{\|\eta\|}s^\beta\eta_\beta\right)_{\eta_\mu} - \left(\frac{1}{\|\eta\|}s^\beta\eta_\beta\right)_{\eta_\mu} G_{x^\mu}\right]\\ &= \pm\frac{i(\delta_\beta{}^\mu\|\eta\|^2 - \eta_\beta\,\eta^\mu)}{4\|\eta\|^3}\left[G^*_{x^\mu}s^\beta - s^\beta G_{x^\mu}\right]. \end{aligned} \tag{3.5.44}$$

Theorem 3.23 tells us that $G_{x^\mu} = \frac{i}{2}\overset{*}{K}_{\mu\nu}\,s^\nu$. Substituting this into (3.5.44), and using standard properties of Pauli matrices and (B.1.10), we get

$$\begin{aligned}[\theta(\pm G^*\widetilde{W}G)]_{\mathrm{sub}} &= \pm\frac{\delta_\beta{}^\mu\|\eta\|^2 - \eta_\beta\,\eta^\mu}{8\|\eta\|^3}\left[s^\nu s^\beta + s^\beta s^\nu\right]\overset{*}{K}_{\mu\nu}\\ &= \pm\frac{1}{4\|\eta\|^3}\left(\overset{*}{K}{}^\gamma{}_\gamma\delta_{\mu\nu} - \overset{*}{K}_{\mu\nu}\right)\eta^\mu\eta^\nu\,\mathrm{Id}\\ &= \pm\frac{1}{4\|\eta\|^3}\overset{*}{T}_{\mu\nu}\,\eta^\mu\,\eta^\nu\,\mathrm{Id}\,. \end{aligned} \tag{3.5.45}$$

The above argument combined with (3.5.23) yields (3.5.30). □

Observe that formula (3.5.30) implies

$$\mathrm{tr}\,[U^\pm(0)]_{\mathrm{sub}}(y,\eta) = \pm\frac{1}{2(h(y,\eta))^3}\overset{*}{T}{}^{\alpha\beta}(y)\,\eta_\alpha\eta_\beta\,, \tag{3.5.46}$$

which agrees with [41, formula (1.20)] and [42, formula (4.1) with $\mathbf{c}=+1$].

3.6 Principal symbol of the global Dirac propagator

In this section we provide an explicit geometric characterisation of the principal symbols of the positive and negative Dirac propagators.

Theorem 3.26. *The principal symbols of the positive and negative Dirac propagators are*

$$\mathfrak{a}_0^\pm(t;y,\eta) = \zeta^\pm(t;y,\eta)\,[v^\pm(y,\eta)]^*, \tag{3.6.1}$$

where $\zeta^\pm(t;y,\eta)$ is the parallel transport of $v^\pm(y,\eta)$ along $x^\pm$ with respect to the spin connection, i.e.

$$\left(\frac{\mathrm{d}}{\mathrm{d}t} + [\dot{x}^\pm]^\alpha \, \frac{1}{4}\sigma_\beta \left(\frac{\partial \sigma^\beta}{\partial x^\alpha} + \Gamma^\beta{}_{\alpha\gamma}\sigma^\gamma\right)\right)\zeta^\pm = 0, \qquad \zeta^\pm|_{t=0} = v^\pm. \tag{3.6.2}$$

Proof. It is known [102, 93] that the principal symbols $\mathfrak{a}_0^\pm$ are independent of the choice of the phase function and read

$$\mathfrak{a}_0^\pm(t;y,\eta) = v^\pm(x^\pm,\xi^\pm)\,[v^\pm(y,\eta)]^*\, e^{-i\int_0^t q^\pm(x^\pm(\tau;y,\eta),\xi^\pm(\tau;y,\eta))\,d\tau}, \tag{3.6.3}$$

where

$$q^\pm = [v^\pm]^*\, W_{\mathrm{sub}}\, v^\pm - \frac{i}{2}\{[v^\pm]^*, W_{\mathrm{prin}} - h^\pm, v^\pm\} - i\,[v^\pm]^*\{v^\pm, h^\pm\}\,, \tag{3.6.4}$$

and

$$W_{\mathrm{sub}}(y) := W_0(y) + \frac{i}{2}\sigma^\alpha(y)\,\Gamma^\beta{}_{\alpha\beta}(y) + \frac{i}{2}[W_{\mathrm{prin}}(y,\eta)]_{y^\alpha\eta_\alpha}. \tag{3.6.5}$$

In formula (3.6.4) curly brackets denote the Poisson bracket

$$\{B, C\} := B_{y^\alpha} C_{\eta_\alpha} - B_{\eta_\alpha} C_{y^\alpha} \tag{3.6.6}$$

and the generalised Poisson bracket

$$\{B, C, D\} := B_{y^\alpha} C D_{\eta_\alpha} - B_{\eta_\alpha} C D_{y^\alpha} \tag{3.6.7}$$

on matrix-functions on the cotangent bundle. In formula (3.6.5) the second term on the RHS is the result of switching to half-densities, see (3.4.5).

Introducing the shorthand $q^\pm(t) := q^\pm(x^\pm(t;y,\eta),\xi^\pm(t;y,\eta))$, the task at hand is to show that

$$\zeta^\pm(t;y,\eta) = e^{-i\int_0^t q^\pm(\tau)\,d\tau}\, v^\pm(x^\pm,\xi^\pm).$$

More explicitly, we need to show that

$$e^{i\int_0^t q^\pm(\tau)\,d\tau}\left(\frac{\mathrm{d}}{\mathrm{d}t} + [\dot{x}^\pm]^\alpha \, \frac{1}{4}\sigma_\beta \left(\frac{\partial \sigma^\beta}{\partial x^\alpha} + \Gamma^\beta{}_{\alpha\gamma}\sigma^\gamma\right)\right)\left[e^{-i\int_0^t q^\pm(\tau)\,d\tau}\, v^\pm(x^\pm,\xi^\pm)\right] = 0, \tag{3.6.8}$$

where we premultiplied our expression by $e^{i\int_0^t q^\pm(\tau)\,d\tau}$ for the sake of convenience.

We shall prove (3.6.1) for $\mathfrak{a}_0^+$, which corresponds to the upper choice of signs in (3.6.8). The proof for $\mathfrak{a}_0^-$ is analogous.

Let us begin by computing

$$e^{i\int_0^t q^+(\tau)}\frac{\mathrm{d}}{\mathrm{d}t}\left(e^{-i\int_0^t q^+(\tau)\,d\tau}\,v^+(x^+,\xi^+)\right) = -iq^+(t)\,v^+ + v^+_{x^\alpha}[\dot{x}^+]^\alpha + v^+_{\xi_\alpha}[\dot{\xi}^+]_\alpha$$
$$= -iq^+(t)\,v^+ + \{v^+,h\}. \tag{3.6.9}$$

To this end, let us choose geodesic normal coordinates centred at $x^+(t;y,\eta) = 0$ and such that $[\xi^+(t;y,\eta)]_\alpha = \delta_{3\alpha}$. Furthermore, up to a global rigid rotation of the framing, we can assume that

$$e_j{}^\alpha(0) = \delta_j{}^\alpha. \tag{3.6.10}$$

In our special coordinate system we have

$$v^+(0,\xi^+) = \begin{pmatrix}1\\0\end{pmatrix}, \qquad v^-(0,\xi^+) = \begin{pmatrix}0\\1\end{pmatrix}, \tag{3.6.11}$$

and we can expand our framing about $x^+ = 0$ as

$$\begin{pmatrix} e_1{}^1(x) & e_1{}^2(x) & e_1{}^3(x)\\ e_2{}^1(x) & e_2{}^2(x) & e_2{}^3(x)\\ e_3{}^1(x) & e_3{}^2(x) & e_3{}^3(x)\end{pmatrix} = \begin{pmatrix} 1 & l^3(x) & -l^2(x)\\ -l^3(x) & 1 & l^1(x)\\ l^2(x) & -l^1(x) & 1\end{pmatrix} + O(\|x\|^2) \quad \text{as } x\to 0, \tag{3.6.12}$$

where $l^k(x) = O(\|x\|)$, $k = 1,2,3$.

The fact that $([v^+]^*v^+)(x,\xi) = 1$ implies

$$\{[v^+]^*,P^+,v^+\}(0,\xi^+) = [v^+_{x^\alpha}]^*\,v^+\,[v^+]^*\,v^+_{\xi_\alpha} - [v^+_{\xi_\alpha}]^*\,v^+\,[v^+]^*\,v^+_{x^\alpha} = 0, \tag{3.6.13}$$

which, in turn, yields

$$\{[v^+]^*,W_{\mathrm{prin}},v^+\} = h\,\{[v^+]^*,2P^+-\mathrm{Id},v^+\} = -h\,\{[v^+]^*,v^+\}. \tag{3.6.14}$$

A standard perturbation argument gives us

$$h\,\{[v^+]^*,v^+\}(0,\xi^+) = -\frac{i}{2}\left(\frac{\partial l^1}{\partial x^1}+\frac{\partial l^2}{\partial x^2}\right)\Big|_{x=0} \tag{3.6.15}$$

and

$$\{v^+, h\}(0, \xi^+) = \frac{i}{2} \begin{pmatrix} 0 \\ \dfrac{\partial l^1}{\partial x^3} + i \dfrac{\partial l^2}{\partial x^3} \end{pmatrix} \Bigg|_{x=0} . \tag{3.6.16}$$

Furthermore, combining (3.6.12) with (3.1.3) and (3.6.5), we get

$$W_{\mathrm{sub}}(0) = -\frac{1}{2} \left(\frac{\partial l^1}{\partial x^1} + \frac{\partial l^2}{\partial x^2} + \frac{\partial l^3}{\partial x^3} \right) \Bigg|_{x=0} \mathrm{Id}. \tag{3.6.17}$$

Substituting (3.6.11), (3.6.14) and (3.6.15)–(3.6.17) into (3.6.4), and then (3.6.4) and (3.6.16) into (3.6.9), we conclude that

$$e^{i \int_0^t q^+(\tau)} \frac{\mathrm{d}}{\mathrm{d}t} \left(e^{-i \int_0^t q^+(\tau)\, d\tau}\, v^+(x^+, \xi^+) \right) = \frac{i}{2} \begin{pmatrix} \dfrac{\partial l^3}{\partial x^3} \\ 0 \end{pmatrix} \Bigg|_{x=0} + \frac{i}{2} \begin{pmatrix} 0 \\ \dfrac{\partial l^1}{\partial x^3} + i \dfrac{\partial l^2}{\partial x^3} \end{pmatrix} \Bigg|_{x=0} . \tag{3.6.18}$$

Similarly, in our special coordinate system we have

$$\begin{aligned} [\dot{x}^+]^\alpha \frac{1}{4} \sigma_\beta \left(\frac{\partial \sigma^\beta}{\partial x^\alpha} + \Gamma^\beta{}_{\alpha\gamma} \sigma^\gamma \right) v^+ \Big|_{x=0,\ \xi=\xi^+} &= \frac{1}{4} \sigma_\beta \left(\frac{\partial \sigma^\beta}{\partial x^3} \right) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Bigg|_{x=0} \\ &= -\frac{i}{2} \begin{pmatrix} \dfrac{\partial l^3}{\partial x^3} \\ \dfrac{\partial l^1}{\partial x^3} + i \dfrac{\partial l^2}{\partial x^3} \end{pmatrix} \Bigg|_{x=0} . \end{aligned} \tag{3.6.19}$$

Summing up (3.6.18) and (3.6.19) we arrive at (3.6.8). □

3.7 Explicit small time expansion of the symbol

Even though the presence of gauge degrees of freedom represents an additional challenge in the analysis of the propagator, one can put this freedom to use and exploit it to obtain a small time expansion for the propagator.

Our strategy goes as follows.

1. Compute the principal and subprincipal symbol of the positive (resp. negative) propagator for a conveniently chosen framing;
2. Using the gauge transformation (3.1.7), (3.1.6), switch to an arbitrary framing with the same orientation[4];
3. Express the final result in terms of geometric invariants.

[4]Recall that in this Chapter the orientation is prescribed from the beginning.

3.7.1 Special framing

Let us fix an arbitrary point $y \in M$ and let $V_j \in T_yM$, $j = 1, 2, 3$ be defined by

$$V_j := e_j(y). \tag{3.7.1}$$

Definition 3.27 (Levi-Civita framing)**.** Let $\mathcal{U}$ be a geodesic neighbourhood of y. For $x \in \mathcal{U}$, let $\widetilde{e}_j^{\mathrm{loc}}(x)$, $j = 1, 2, 3$, be the parallel transport of V_j along the shortest geodesic connecting y to x. We define the *Levi-Civita framing generated by* $\{e_j\}_{j=1}^3$ *at* y to be the equivalence class of framings coinciding with $\{\widetilde{e}_j^{\mathrm{loc}}\}_{j=1}^3$ in a neighbourhood of y.

With slight abuse of notation, in the following we will confuse the Levi-Civita framing with one of its representatives, denoted by $\{\widetilde{e}_j\}_{j=1}^3$. The choice of a particular representative does not affect our results.

Using the Levi-Civita framing is especially convenient due to the following property.

Lemma 3.28. *In normal coordinates centred at y, the Levi-Civita framing admits the following expansion:*

$$\widetilde{e}_j{}^{\alpha}(x) = e_j{}^{\alpha}(y) + \frac{1}{6} e_j{}^{\beta}(y)\, R^{\alpha}{}_{\mu\beta\nu}(y)\, x^{\mu} x^{\nu} + O(\|x\|^3), \qquad j = 1, 2, 3, \tag{3.7.2}$$

where R is the Riemann curvature tensor.

Proof. In normal geodesic coordinates centred at y, the unique geodesic connecting y to x can be written as

$$\gamma^{\alpha}(t) = \frac{x^{\alpha}}{\|x\|_E}\, t,$$

where $\|\cdot\|_E$ is the Euclidean norm, so that $\gamma(\|x\|_E) = x$. Assuming t and $\|x\|_E$ to be small and of the same order, let us perform an expansion in powers of t of $\widetilde{e}_j$.

The parallel transport equation defining the framing $\{\widetilde{e}_j\}_{j=1}^3$ reads

$$\dot{\widetilde{e}}_j{}^{\alpha}(\gamma(t)) = -\dot{\gamma}^{\beta}(t)\, \Gamma^{\alpha}{}_{\beta\mu}(\gamma(t))\; \widetilde{e}_j{}^{\mu}(\gamma(t)), \qquad j = 1, 2, 3. \tag{3.7.3}$$

Since $\widetilde{e}_j(0) = V_j$ and $\Gamma(0) = 0$, at linear order in t we have $\dot{\widetilde{e}}_j(\gamma(t)) = 0 + O(t)$, which implies

$$\widetilde{e}_j(\gamma(t)) = V_j + O(t^2). \tag{3.7.4}$$

Substituting (3.7.4) into (3.7.3), we get

$$\dot{\widetilde{e}}_j{}^\alpha(\gamma(t)) = -\frac{x^\beta\, x^\nu}{\|x\|_E^2}\partial_\nu \Gamma^\alpha{}_{\beta\mu}(0)\, V_j{}^\mu\, t + O(t^2), \tag{3.7.5}$$

so that

$$\widetilde{e}_j{}^\alpha(\gamma(t)) = V_j - \frac{1}{2}\frac{x^\beta x^\nu}{\|x\|_E^2}\partial_\nu \Gamma^\alpha{}_{\beta\mu}(0)\, V_j{}^\mu\, t^2 + O(t^3) \tag{3.7.6}$$

and

$$\widetilde{e}_j{}^\alpha(x) = \widetilde{e}_j{}^\alpha(\gamma(\|x\|_E)) = V_j{}^\alpha - \frac{1}{2}\partial_\nu \Gamma^\alpha{}_{\beta\mu}(0)\, V_j{}^\mu\, x^\beta x^\nu + O(\|x\|^3), \qquad j=1,2,3. \tag{3.7.7}$$

Formula (3.7.2) follows at once from (3.7.7) and the elementary identity

$$\partial_\nu \Gamma^\alpha{}_{\beta\mu}(0) = -\frac{1}{3}(R^\alpha{}_{\beta\mu\nu} + R^\alpha{}_{\mu\beta\nu})(0). \tag{3.7.8}$$

□

Corollary 3.29. *In normal coordinates x centred at y, the Pauli matrices $\widetilde{\sigma}^\alpha(x)$ projected along the Levi-Civita framing (see (3.1.3)) satisfy*

$$\widetilde{\sigma}^\alpha(y) = \sigma^\alpha(y), \quad [\widetilde{\sigma}^\alpha]_{x^\beta}(y) = 0, \quad [\widetilde{\sigma}^\alpha]_{x^\mu x^\nu}(y) = \frac{1}{6}\,[R^\alpha{}_{\nu\beta\mu}(y) + R^\alpha{}_{\mu\beta\nu}(y)]\,\sigma^\beta(y). \tag{3.7.9}$$

Proof of Corollary 3.29. Formula (3.7.9) follows immediately from (3.7.2). □

Corollary 3.30. *Let $\widetilde{W}$ be the Dirac operator (3.1.4) corresponding to the choice of the Levi-Civita framing. Then, in normal coordinates centred at y, its zero order part $\widetilde{W}_0$ (see formula (3.5.2)) admits the following expansion:*

$$\widetilde{W}_0(x) = \frac{i}{4}\,\mathrm{Ric}_{\alpha\beta}(y)\,\widetilde{\sigma}^\beta(y)\,x^\alpha + O(\|x\|^2). \tag{3.7.10}$$

3.7.2 Small time expansion of the principal symbols

The first step towards computing small time expansions for principal and subprincipal symbols of W is to obtain an expression for these objects in a neighbourhood of a given point $y \in M$ for the choice of the Levi-Civita framing generated by our framing $\{e_j\}_{j=1}^3$ at y. Observe that, as we are after a small time expansion of the symbols, it is enough to restrict our attention to a small open neighbourhood of y.

In the following, we will denote with a tilde objects associated with the Dirac operator $\widetilde{W}$ corresponding to the choice of the Levi-Civita framing.

Theorem 3.31. *We have*

$$\widetilde{\mathfrak{a}}_0^\pm(t;y,\eta)=\widetilde{P}^\pm(y,\eta)+O(t^3). \tag{3.7.11}$$

Proof. In view of formula (3.6.1), we need to show that

$$\widetilde{\zeta}^\pm(t;y,\eta)=\widetilde{v}^\pm(y,\eta)+O(t^3). \tag{3.7.12}$$

Once this is achieved, (3.7.11) follows from the fact that $\widetilde{W}_{\mathrm{prin}}(y,\eta)=W_{\mathrm{prin}}(y,\eta)$.

A perturbation argument shows that if $\widetilde{\zeta}^\pm$ solves (3.6.2) with initial condition $\widetilde{\zeta}^\pm(0;y,\eta)=\widetilde{v}^\pm(y,\eta)$, then

$$\begin{aligned}\widetilde{\zeta}^\pm(t;y,\eta)&=\widetilde{v}^\pm(y,\eta)\\ &\quad-\frac{t^2}{2}\left\{\frac{\eta^\alpha\eta^\mu}{[h(y,\eta)]^2}\left[\widetilde{\sigma}_\beta(0)[\widetilde{\sigma}^\beta(0)]_{x^\alpha x^\mu}+\widetilde{\sigma}_\beta(0)\,\frac{\partial {\Gamma^\beta}_{\alpha\gamma}}{\partial x^\mu}(0)\widetilde{\sigma}^\gamma(0)\right]\right\}\widetilde{v}^\pm(y,\eta)\\ &\quad+O(t^3).\end{aligned} \tag{3.7.13}$$

Using Corollary 3.29 and the identity (3.7.8), we obtain

$$\begin{aligned}&\left[\widetilde{\sigma}_\beta(0)[\widetilde{\sigma}^\beta(0)]_{x^\alpha x^\mu}+\widetilde{\sigma}_\beta(0)\,\frac{\partial {\Gamma^\beta}_{\alpha\gamma}}{\partial x^\mu}(0)\widetilde{\sigma}^\gamma(0)\right]\eta^\alpha\eta^\mu\\ &\quad=\left[\frac{1}{6}({R^\beta}_{\alpha\gamma\mu}+{R^\beta}_{\mu\gamma\alpha})(0)-\frac{1}{3}({R^\beta}_{\alpha\gamma\mu}+{R^\beta}_{\gamma\alpha\mu})(0)\right]\widetilde{\sigma}_\beta(0)\widetilde{\sigma}^\gamma(0)\,\eta^\alpha\eta^\mu\\ &\qquad=\left[\frac{1}{6}\,2{R^\beta}_{\alpha\gamma\mu}(0)-\frac{1}{3}\,{R^\beta}_{\alpha\gamma\mu}(0)\right]\widetilde{\sigma}_\beta(0)\widetilde{\sigma}^\gamma(0)\,\eta^\alpha\eta^\mu\\ &\qquad=0.\end{aligned} \tag{3.7.14}$$

Substituting (3.7.14) into (3.7.13) we arrive at (3.7.12). □

3.7.3 Small time expansion of the subprincipal symbols

Let us now turn our attention to the subprincipal symbols $\widetilde{\mathfrak{a}}_{-1}^\pm$.

Unlike the principal symbols, the subprincipal symbol depends on the choice of the phase function. As here we are only interested in small time expansions and the injectivity radius $\operatorname{Inj}(M,g)$ is strictly positive, we can work, without loss of generality, in a neighbourhood of y with no conjugate points to y. The absence of conjugate points allows us to construct positive and negative propagators for small times by means of the algorithm described in subsection 3.3.3 for the choice of *real-valued*

Levi-Civita phase functions

$$\varphi^{\pm}(t,x;y,\eta)=\int_{\gamma^{\pm}}\zeta^{\pm}\,\mathrm{d}z, \tag{3.7.15}$$

cf. Definition 3.20 for $\epsilon=0$.

In the remainder of this subsection we adopt the same coordinates for x and y and we choose normal geodesic coordinates centred at y. We remind the reader that, in such coordinates,

$$[x^{\pm}]^{\alpha}(t;0,\eta)=\pm\frac{\eta^{\alpha}}{h}\,t. \tag{3.7.16}$$

According to (2.9.7) and (2.9.12), we have

$$\varphi^{\pm}(t,x;0,\eta)=x^{\alpha}\eta_{\alpha}\mp h\,t\pm\frac{1}{3h}R^{\alpha}{}_{\mu}{}^{\beta}{}_{\nu}(0)\eta_{\alpha}\eta_{\beta}\,x^{\mu}x^{\nu}+O(\|x\|^{4}+t^{4}) \tag{3.7.17}$$

and

$$w^{\pm}(t,x;0,\eta)=1+\frac{1}{12}\operatorname{Ric}_{\mu\nu}(0)\,x^{\mu}\,x^{\nu}\mp\frac{t}{3h}\operatorname{Ric}^{\mu}{}_{\nu}(0)\,\eta_{\mu}\,x^{\nu}+O(\|x\|^{3}+|t|^{3}). \tag{3.7.18}$$

Recall that the weight w is defined by (3.3.18).

As explained in subsection 3.5.1, the subprincipal symbols are determined by the first and the second transport equations, (3.5.14) and(3.5.15). More precisely, if we are interested in expansions with remainder $O(t^2)$, we need to determine the RHS of (3.5.15) at zero order in t and the RHS of (3.5.14) up to first order in t.

To this end, we begin by observing that formulae (3.7.17) and (3.7.18), see (3.3.42), imply that the differential evaluation operators $\mathfrak{S}^{\pm}_{-2}$ and $\mathfrak{S}^{\pm}_{-1}$ admit the following expansions in normal coordinates centred at y.

Lemma 3.32. *We have*

(a)

$$\mathfrak{S}^{\pm}_{-2}=\frac{1}{2}\left[i\frac{\partial^{2}}{\partial x^{\alpha}\partial\eta_{\alpha}}\right]^{2}(\,\cdot\,)\bigg|_{t=0,\,x=0}+O(t), \tag{3.7.19}$$

(b)

$$\mathfrak{S}^{\pm}_{-1}=i\,\mathfrak{S}^{\pm}_{0}\left(\frac{\partial^{2}}{\partial x^{\alpha}\partial\eta_{\alpha}}\pm\frac{t}{2}\,h_{\eta_{\alpha}\eta_{\beta}}\frac{\partial^{2}}{\partial x^{\alpha}\partial x^{\beta}}\right)+O(t^{2}). \tag{3.7.20}$$

Proof. (a) It is an immediate consequence of (3.7.16), (3.7.18) and

$$L^{\pm}_{\alpha}=\frac{\partial}{\partial x^{\alpha}}+O(\|x\|+|t|). \tag{3.7.21}$$

(b) Substituting (3.7.18) into (3.3.42) with $k=1$ and recalling that $\varphi^\pm_\eta|_{x=x^\pm}=0$, we get

$$\mathfrak{S}^\pm_{-1}=\mathfrak{S}^\pm_0\left[i\frac{\partial^2}{\partial x^\alpha\partial\eta_\alpha}-\frac{i}{2}\varphi^\pm_{\eta_\alpha\eta_\beta}L^\pm_\alpha L^\pm_\beta\right]+O(t^2). \tag{3.7.22}$$

Formula (3.7.21) and the fact that

$$\varphi^\pm_{\eta_\alpha\eta_\beta}\Big|_{x=x^\pm}=\mp t\,h_{\eta_\alpha\eta_\beta}+O(t^3) \tag{3.7.23}$$

yield (3.7.20). □

In order to be able to compute the subprincipal symbols, we need to determine the initial condition $\widetilde{\mathfrak{a}}^\pm_{-1}|_{t=0}$ first.

Lemma 3.33. *For the choice of real-valued Levi-Civita phase functions, the positive and negative subprincipal symbols $\widetilde{\mathfrak{a}}^\pm_{-1}$ vanish at $t=0$:*

$$\widetilde{\mathfrak{a}}^\pm_{-1}(0;y,\eta)=0. \tag{3.7.24}$$

Proof. The subprincipal symbols are scalar functions, so it enough to establish (3.7.24) in one specific coordinate system. Let us choose normal coordinates centred at $y=0$ such that $\widetilde{e}_j{}^\alpha(0)=\delta_j{}^\alpha$. We observe that the torsion of the Weitzenböck connection generated by the Levi-Civita framing at y vanishes at y, as a consequence of the fact that the first derivatives of the framing are zero, cf. (3.7.2) and (B.1.2)-(B.1.3). Therefore, Theorem 3.25 tells us that

$$[U^\pm(0)]_{\mathrm{sub}}(0,\eta)=0. \tag{3.7.25}$$

A straightforward perturbation argument shows that

$$(v^\pm)_{x^\alpha}(0,\eta)=0. \tag{3.7.26}$$

Substituting (3.7.25) and (3.7.26) into (3.4.6) with $P=U^\pm(0)$ and $\epsilon=0$ and using the fact that Christoffel symbols vanish at y, we arrive at (3.7.24). □

We are now in a position to examine the first transport equation.

Lemma 3.34. *The projection onto the negative (resp. positive) eigenspace of $\widetilde{W}_{\mathrm{prim}}$ of the subprincipal symbol of the positive (resp. negative) propagator is given by*

$$\widetilde{P}^\mp(x^\pm,\xi^\pm)\widetilde{\mathfrak{a}}^\pm_{-1}(t;y,\eta)=$$
$$\pm\, it\,\widetilde{P}^\mp(y,\eta)\left[\frac{1}{8h^3}\,\mathrm{Ric}_{\alpha\beta}(y)\,\eta^\alpha\eta^\beta-\frac{1}{4h}\,\mathrm{Ric}_{\alpha\beta}(y)\,\eta^\alpha\widetilde{P}^\pm_{\eta_\beta}(y,\eta)\right]+O(t^2). \tag{3.7.27}$$

Proof. We will establish formula (3.7.27) by expanding the first transport equation (3.5.14) up to first order in t and then acting with $\widetilde{P}^{\mp}$ on the left. Recall that $a_{-k}^{\pm}$ is defined by (3.5.13).

Working in normal coordinates centred at y and using (3.7.17)-(3.7.18), we obtain

$$\begin{aligned}\mathfrak{S}_0^{\pm}\widetilde{a}_0^{\pm}(t;0,\eta) &= \Big\{\Big(\varphi_t^{\pm} + \widetilde{W}_{\mathrm{prin}}(x,\varphi_x^{\pm})\Big)\,\widetilde{\mathfrak{a}}_{-1}^{\pm} - i(\widetilde{\mathfrak{a}}_{-0}^{\pm})_t \\ &\quad + \Big[-i(w^{\pm})^{-1}\left(w_t^{\pm} + \sigma^{\alpha}w_{x^{\alpha}}^{\pm}\right) + \widetilde{W}_0\Big]\,\widetilde{\mathfrak{a}}_{-0}^{\pm}\Big\}\Big|_{x=x^{\pm}} \\ &= (\widetilde{W}_{\mathrm{prin}}(x^{\pm},\xi^{\pm}) \mp h)\,\widetilde{\mathfrak{a}}_{-1}^{\pm}(t;0,\eta) \\ &\quad + \frac{i\,t}{3h^2}\,\mathrm{Ric}_{\alpha\nu}(0)\left(\eta^{\alpha}\eta^{\nu} \pm \frac{1}{2}h\,\eta^{\alpha}\,\widetilde{\sigma}^{\nu}(0)\right)\widetilde{P}^{\pm}(y,\eta) \\ &\quad \pm \frac{t\,\eta^{\alpha}}{h}(\widetilde{W}_0)_{x^{\alpha}}(0)\,\widetilde{P}^{\pm}(y,\eta) + O(t^2).\end{aligned} \tag{3.7.28}$$

Furthermore, in view of Theorem 3.26 and Lemma 3.32(b), we have

$$\begin{aligned}\mathfrak{S}_{-1}^{\pm}\widetilde{a}_1^{\pm}(t;0,\eta) &= \left[\frac{\partial^2}{\partial x^{\alpha}\partial\eta_{\alpha}} \pm \frac{t}{2}\,h_{\eta_{\alpha}\eta_{\beta}}\frac{\partial^2}{\partial x^{\alpha}\partial x^{\beta}}\right]\Big(\varphi_t^{\pm} + \widetilde{W}_{\mathrm{prin}}(x,\varphi_x^{\pm})\Big)\,\widetilde{\mathfrak{a}}_0^{\pm}\Big|_{x=x^*} \\ &\quad + O(t^2) \\ &= -\frac{2it}{3h^2}\,\mathrm{Ric}_{\alpha\nu}(0)\,\eta^{\alpha}\eta^{\nu}\widetilde{P}^{\pm} \pm \mathrm{i}t\left[\frac{2}{3h}R^{\mu}{}_{\alpha}{}^{\nu}{}_{\beta}(0)\,\eta_{\mu}\eta_{\nu}\,\widetilde{\sigma}^{\beta}(0)\widetilde{P}^{\pm}\right]_{\eta_{\alpha}} \\ &\quad \pm it\frac{\eta^{\beta}}{h}\left[(\widetilde{W}_{\mathrm{prin}})_{x^{\alpha}x^{\beta}}(0,\eta)\widetilde{P}^{\pm}\right]_{\eta_{\alpha}} \\ &\quad + \mathrm{i}\,t\left[\frac{h_{\eta_{\alpha}\eta_{\beta}}}{3h}\,R^{\mu}{}_{\alpha}{}^{\nu}{}_{\beta}(0)\,\eta_{\mu}\eta_{\nu} \pm \frac{1}{2}h_{\eta_{\alpha}\eta_{\beta}}(\widetilde{W}_{\mathrm{prin}})_{x^{\alpha}x^{\beta}}(0,\eta)\right]\widetilde{P}^{\pm} + O(t^2).\end{aligned} \tag{3.7.29}$$

Adding up (3.7.28) and (3.7.29) and projecting along $\widetilde{P}^{\mp}$, we arrive at

$$\begin{aligned}\widetilde{P}^{\mp}\widetilde{\mathfrak{a}}_{-1}^{\pm}(t;0,\eta) &= \frac{it}{h}\widetilde{P}^{\mp}\Big\{\frac{1}{12h}\,\mathrm{Ric}_{\alpha\nu}(0)\,\eta^{\alpha}\widetilde{\sigma}^{\nu}(0)\widetilde{P}^{\pm} - \frac{i\eta^{\alpha}}{2h}(\widetilde{W}_0)_{x^{\alpha}}(0)\,\widetilde{P}^{\pm} \\ &\quad + \left[\frac{1}{3h}R^{\mu}{}_{\alpha}{}^{\nu}{}_{\beta}(0)\,\eta_{\mu}\eta_{\nu}\,\widetilde{\sigma}^{\beta}(0)\,\widetilde{P}^{\pm}\right]_{\eta_{\alpha}} + \frac{\eta^{\beta}}{2h}\left[(\widetilde{W}_{\mathrm{prin}})_{x^{\alpha}x^{\beta}}(0,\eta)\widetilde{P}^{\pm}\right]_{\eta_{\alpha}} \\ &\quad + \frac{1}{4}h_{\eta_{\alpha}\eta_{\beta}}\,(\widetilde{W}_{\mathrm{prin}})_{x^{\alpha}x^{\beta}}(0,\eta)\,\widetilde{P}^{\pm}\Big\} + O(t^2).\end{aligned} \tag{3.7.30}$$

Let us compute the summands in (3.7.30) separately. To this end, let us put

$$\begin{aligned} &A_1 := \frac{1}{12h}\,\mathrm{Ric}_{\alpha\nu}(0)\,\eta^{\alpha}\widetilde{\sigma}^{\nu}(0)\widetilde{P}^{\pm}, \qquad A_2 := -\frac{i\eta^{\alpha}}{2h}(\widetilde{W}_0)_{x^{\alpha}}(0)\,\widetilde{P}^{\pm}, \\ &A_3 := \left[\frac{1}{3h}R^{\mu}{}_{\alpha}{}^{\nu}{}_{\beta}(0)\,\eta_{\mu}\eta_{\nu}\,\widetilde{\sigma}^{\beta}(0)\,\widetilde{P}^{\pm}\right]_{\eta_{\alpha}}, \quad A_4 := \frac{\eta^{\beta}}{2h}\left[(\widetilde{W}_{\mathrm{prin}})_{x^{\alpha}x^{\beta}}(0,\eta)\widetilde{P}^{\pm}\right]_{\eta_{\alpha}}, \\ &A_5 := \frac{1}{4}h_{\eta_{\alpha}\eta_{\beta}}\,(\widetilde{W}_{\mathrm{prin}})_{x^{\alpha}x^{\beta}}(0,\eta)\,\widetilde{P}^{\pm}.\end{aligned} \tag{3.7.31}$$

- A_1: It ensues from elementary properties of $\widetilde{P}^{\pm}$ that

$$\widetilde{P}^{\mp}\widetilde{\sigma}^{\alpha}\widetilde{P}^{\pm}=\widetilde{P}^{\mp}[\widetilde{W}_{\mathrm{prin}}\widetilde{P}^{\pm}]_{\eta_\alpha}-\widetilde{P}^{\mp}\widetilde{W}_{\mathrm{prin}}\widetilde{P}^{\pm}_{\eta_\alpha}=\pm 2h\,\widetilde{P}^{\mp}\widetilde{P}^{\pm}_{\eta_\alpha}. \tag{3.7.32}$$

Hence

$$\widetilde{P}^{\mp}A_1=\widetilde{P}^{\mp}\left(\pm\frac{1}{6}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^{\alpha}\widetilde{P}^{\pm}_{\eta_\beta}\right). \tag{3.7.33}$$

- A_2: Combining Lemma 3.30 with the identity

$$h_{\eta_\alpha\eta_\beta}=\frac{h^2\,\delta^{\alpha\beta}-\eta^{\alpha}\eta^{\beta}}{h^3} \tag{3.7.34}$$

and using (3.7.32), we get

$$\widetilde{P}^{\mp}A_2=\widetilde{P}^{\mp}\left(\pm\frac{1}{4}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^{\alpha}\widetilde{P}^{\pm}_{\eta_\beta}\right). \tag{3.7.35}$$

- A_3: We have

$$\begin{aligned}A_3&=\left[\frac{1}{3h}R^{\mu}{}_{\alpha}{}^{\nu}{}_{\beta}(0)\,\eta_\mu\eta_\nu\,\widetilde{\sigma}^{\beta}(0)\,\widetilde{P}^{\pm}\right]_{\eta_\alpha}=\frac{1}{3h}R^{\mu}{}_{\alpha}{}^{\nu}{}_{\beta}(0)\,\widetilde{\sigma}^{\beta}(0)\left[\eta_\mu\eta_\nu\,\widetilde{P}^{\pm}\right]_{\eta_\alpha}\\&=-\frac{1}{3h}\,\mathrm{Ric}_{\mu\nu}(0)\,\eta^{\mu}\,\widetilde{\sigma}^{\nu}(0)\,\widetilde{P}^{\pm}\pm\frac{1}{6\,h^2}\,\mathrm{Ric}_{\mu\beta}(0)\,\eta^{\mu}\eta^{\beta}\,\mathrm{Id},\end{aligned} \tag{3.7.36}$$

so that, by (3.7.32),

$$\widetilde{P}^{\mp}A_3=\widetilde{P}^{\mp}\left(\mp\frac{2}{3}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^{\alpha}\widetilde{P}^{\pm}_{\eta_\beta}\pm\frac{1}{6\,h^2}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^{\alpha}\eta^{\beta}\right). \tag{3.7.37}$$

- A_4: Recalling (3.7.9), we have

$$\begin{aligned}A_4&=\frac{\eta^{\beta}}{2h}(\widetilde{\sigma}^{\mu})_{x^\alpha x^\beta}(0)\left[\eta_\mu\,\widetilde{P}^{\pm}\right]_{\eta_\alpha}\\&=-\frac{1}{12h}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^{\alpha}\widetilde{\sigma}^{\beta}(0)\,\widetilde{P}^{\pm}\mp\frac{1}{24\,h^2}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^{\alpha}\eta^{\beta}\,\mathrm{Id},\end{aligned} \tag{3.7.38}$$

so that, by (3.7.32),

$$\widetilde{P}^{\mp}A_4=\widetilde{P}^{\mp}\left(\mp\frac{1}{6}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^{\alpha}\widetilde{P}^{\pm}_{\eta_\beta}\mp\frac{1}{24\,h^2}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^{\alpha}\eta^{\beta}\right). \tag{3.7.39}$$

- A_5: In view of (3.7.34) and (3.7.9), we have

$$\begin{aligned}A_5&=\frac{1}{4}\left(\frac{\delta^{\alpha\beta}}{h}-\frac{\eta^{\alpha}\eta^{\beta}}{h^3}\right)\frac{1}{6}\left[R^{\mu}{}_{\beta\nu\alpha}+R^{\mu}{}_{\alpha\nu\beta}\right](0)\,\widetilde{\sigma}^{\nu}(0)\,\eta_\mu\,\widetilde{P}^{\pm}\\&=\frac{1}{12\,h}\,\mathrm{Ric}_{\mu\nu}(0)\,\eta^{\mu}\widetilde{\sigma}^{\nu}(0)\,\widetilde{P}^{\pm},\end{aligned} \tag{3.7.40}$$

so that, by (3.7.32),

$$\widetilde{P}^{\mp}A_5=\widetilde{P}^{\mp}\left(\pm\frac{1}{6}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^{\alpha}\widetilde{P}^{\pm}_{\eta_\beta}\right). \tag{3.7.41}$$

Substituting (3.7.33), (3.7.35), (3.7.37), (3.7.39) and (3.7.41) into (3.7.30) we arrive at (3.7.27). □

Let us now move to the second transport equation.

Lemma 3.35. *The projection onto the positive (resp. negative) eigenspace of $\widetilde{W}_{\mathrm{prin}}$ of the subprincipal symbol of the positive (resp. negative) propagator is given by*

$$\widetilde{P}^\pm(x^\pm,\xi^\pm)\widetilde{\mathfrak{a}}^\pm_{-1}(t;y,\eta) =$$
$$\mp it\,\widetilde{P}^\pm\left[\frac{1}{24h}\mathcal{R}(0)+\frac{1}{8h^3}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^\alpha\,\eta^\beta+\frac{1}{4h}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^\alpha\,\widetilde{P}^\pm_{\eta_\beta}\right]+O(t^2). \qquad (3.7.42)$$

Proof. We will establish formula (3.7.42) by computing the second transport equation (3.5.14) at zero order in t and then acting with $\widetilde{P}^\pm$ on the left.

With account of Lemma 3.32, we have

$$\begin{aligned}
\mathfrak{S}^\pm_{-2}\widetilde{a}^\pm_1|_{t=0} &= -\frac{1}{2}\frac{\partial^4}{\partial x^\alpha\partial\eta_\alpha\partial x^\beta\partial\eta_\beta}\left(\varphi^\pm_t+\widetilde{W}_{\mathrm{prin}}(x,\varphi^\pm_x)\right)\mathfrak{a}^\pm_0\Big|_{x=0,t=0}\\
&= -\frac{1}{2}\frac{\partial^4}{\partial x^\alpha\partial\eta_\alpha\partial x^\beta\partial\eta_\beta}\Big(\mp h\pm\frac{1}{3\,h}\,R^\gamma{}_\mu{}^\rho{}_\nu(0)\,\eta_\gamma\,\eta_\rho\,x^\mu\,x^\nu+O(\|x\|^3)\\
&\quad+\widetilde{\sigma}^\alpha(0)(\eta_\alpha+O(\|x\|^3))\widetilde{P}^\pm\Big)\Big|_{x=0,t=0}\\
&= -\frac{\partial^2}{\partial\eta_\alpha\partial\eta_\beta}\left(\pm\frac{1}{3\,h}\,R^\gamma{}_\alpha{}^\rho{}_\beta(0)\,\eta_\gamma\,\eta_\rho+\frac{1}{2}(\widetilde{W}_{\mathrm{prin}})_{x^\alpha x^\beta}(0,\eta)\right)\widetilde{P}^\pm,
\end{aligned} \qquad (3.7.43)$$

$$\begin{aligned}
\mathfrak{S}^\pm_{-1}\widetilde{a}^\pm_0|_{t=0} &= i\,\frac{\partial^2}{\partial x^\alpha\partial\eta_\alpha}\Big[\left(\mp h+\widetilde{W}_{\mathrm{prin}}(x,\eta)\right)\widetilde{\mathfrak{a}}^\pm_{-1}(0;y,\eta)-i(\widetilde{\mathfrak{a}}^\pm_0)_t\\
&\quad+\left(\pm\frac{i\eta_\mu}{3h}\,\mathrm{Ric}^\mu{}_\nu(0)\,x^\nu+-\frac{i}{6}\,\mathrm{Ric}_{\mu\nu}(0)\,\widetilde{\sigma}^\mu(0)\,x^\nu+O(\|x\|^2)\right)\widetilde{P}^\pm\\
&\quad+\widetilde{W}_0(x)\widetilde{P}^\pm\Big]\Big|_{t=0,x=0}\\
&= \mp\frac{\partial}{\partial\eta_\alpha}\left(\frac{\eta_\mu}{3h^{(j)}}\,\mathrm{Ric}^\mu{}_\alpha(0)\widetilde{P}^\pm\right)+\frac{1}{6}\,\mathrm{Ric}_{\alpha\mu}(0)\,\widetilde{\sigma}^\mu(0)\,\widetilde{P}^\pm_{\eta_\alpha}+i\,(\widetilde{W}_0)_{x^\alpha}(0)\widetilde{P}^\pm_{\eta_\alpha}
\end{aligned} \qquad (3.7.44)$$

and

$$\mathfrak{S}^\pm_0\widetilde{a}^\pm_{-1}\big|_{t=0} = (\mp h+\widetilde{W}_{\mathrm{prin}}(0,\eta))\widetilde{\mathfrak{a}}^\pm_{-2}(0)-i\,(\widetilde{\mathfrak{a}}^\pm_{-1})_t|_{t=0}. \qquad (3.7.45)$$

In carrying out the above calculations we used Theorem 3.31 and Lemma 3.33. Note that, when multiplying on the left by $\widetilde{P}^\pm$, the terms containing $\widetilde{\mathfrak{a}}^\pm_{-2}$ disappear.

Summing up (3.7.43), (3.7.44) and (3.7.45), and projecting along $\widetilde{P}^\pm$, we obtain

$$\begin{aligned}(\widetilde{P}^\pm \widetilde{\mathfrak{a}}^\pm_{-1})_t\,(0;y,\eta) =& i\widetilde{P}^\pm \frac{\partial^2}{\partial\eta_\alpha\partial\eta_\beta}\left[\left(\pm\frac{1}{3h}\,R^\gamma{}_\alpha{}^\rho{}_\beta(0)\,\eta_\gamma\,\eta_\rho + \frac{1}{2}(\widetilde{W}_{\mathrm{prin}})_{x^\alpha x^\beta}(0,\eta)\right)\widetilde{P}^\pm\right]\\ &\pm i\widetilde{P}^\pm \frac{\partial}{\partial\eta_\alpha}\left[\frac{\eta_\mu}{3h}\,\mathrm{Ric}^\mu{}_\alpha(0)\widetilde{P}^\pm\right] - \frac{i}{6}\,\mathrm{Ric}_{\alpha\mu}(0)\,\widetilde{\sigma}^\mu(0)\,\widetilde{P}^\pm_{\eta_\alpha}\\ &+\widetilde{P}^\pm(\widetilde{W}_0)_{x^\alpha}(0)\widetilde{P}^\pm_{\eta_\alpha} + O(t).\end{aligned} \tag{3.7.46}$$

Using the identity

$$\pm\frac{\partial}{\partial\eta_\beta}\left[\frac{1}{3h}\,R^\gamma{}_\alpha{}^\rho{}_\beta(0)\,\eta_\gamma\,\eta_\rho\widetilde{P}^\pm\right] = \mp\frac{\eta_\mu}{3h}\,\mathrm{Ric}^\mu{}_\alpha(0)\widetilde{P}^\pm \pm \frac{1}{3h}\,R^\gamma{}_\alpha{}^\rho{}_\beta(0)\,\eta_\gamma\,\eta_\rho\widetilde{P}^\pm_{\eta_\beta},$$

formula (3.7.46) becomes

$$\begin{aligned}(\widetilde{P}^\pm \widetilde{\mathfrak{a}}^\pm_{-1})_t\,(0;y,\eta) =& \frac{i}{2}\widetilde{P}^\pm \frac{\partial^2}{\partial\eta_\alpha\partial\eta_\beta}\left[(\widetilde{W}_{\mathrm{prin}})_{x^\alpha x^\beta}(0,\eta)\widetilde{P}^\pm\right]\\ &\pm i\widetilde{P}^\pm \frac{\partial}{\partial\eta_\alpha}\left[\frac{1}{3h}\,R^\gamma{}_\alpha{}^\rho{}_\beta(0)\,\eta_\gamma\,\eta_\rho\,\widetilde{P}^\pm_{\eta_\beta}\right]\\ &-\frac{i}{6}\,\mathrm{Ric}_{\alpha\mu}(0)\,\widetilde{\sigma}^\mu(0)\,\widetilde{P}^\pm_{\eta_\alpha} + \widetilde{P}^\pm(\widetilde{W}_0)_{x^\alpha}(0)\widetilde{P}^\pm_{\eta_\alpha} + O(t).\end{aligned} \tag{3.7.47}$$

Let us put

$$\begin{aligned}&B_1 := \frac{i}{2}\left[(\widetilde{W}_{\mathrm{prin}})_{x^\alpha x^\beta}(0,\eta)\widetilde{P}^\pm\right]_{\eta_\alpha\eta_\beta}, \qquad B_2 := \frac{i}{3h}\,R^\gamma{}_\alpha{}^\rho{}_\beta(0)\,\eta_\gamma\,\eta_\rho\,\widetilde{P}^\pm_{\eta_\beta},\\ &B_3 := -\frac{i}{6}\,\mathrm{Ric}_{\alpha\mu}(0)\,\widetilde{\sigma}^\mu(0)\,\widetilde{P}^\pm_{\eta_\alpha} + (\widetilde{W}_0)_{x^\alpha}(0)\widetilde{P}^\pm_{\eta_\alpha}.\end{aligned} \tag{3.7.48}$$

- B_1: It follows from (3.5.20), Corollary 3.29 and (3.7.34) that

$$\begin{aligned}\widetilde{P}^\pm\,B_1 &= \frac{i}{6}\widetilde{P}^\pm\left[R^\mu{}_{\beta\nu\alpha}\,\eta_\mu\,\widetilde{\sigma}^\nu\frac{1}{2}\left(\mathrm{Id}\pm\frac{\eta_\rho\,\widetilde{\sigma}^\rho}{h}\right)\right]_{\eta_\alpha\eta_\beta}\\ &= \pm\frac{i}{12}\widetilde{P}^\pm R^\mu{}_{\beta\nu\alpha}\,\widetilde{\sigma}^\nu\,\widetilde{\sigma}^\rho\left(\frac{\eta_\mu\,\eta_\rho}{h}\right)_{\eta_\alpha\eta_\beta}\\ &= \pm\left(-\frac{i}{12h}\mathcal{R}(0) + \frac{i}{12h^3}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^\alpha\eta^\beta\right)\widetilde{P}^\pm.\end{aligned} \tag{3.7.49}$$

- B_2: Differentiating (3.5.20) with respect to η_β yields

$$\begin{aligned}\widetilde{P}^\pm_{\eta_\beta} &= \pm\frac{1}{2h}(\widetilde{W}_{\mathrm{prin}})_{\eta_\beta} \mp \frac{\eta^\beta}{2h^3}\widetilde{W}_{\mathrm{prin}}\\ &= \pm\frac{1}{2}\left(\frac{\widetilde{\sigma}^\beta}{h} - \frac{\eta^\beta\,\eta_\rho\,\widetilde{\sigma}^\rho}{h^3}\right).\end{aligned} \tag{3.7.50}$$

  Substituting (3.7.50) into B_2 in (3.7.48) we obtain

$$\begin{aligned}\pm\widetilde{P}^\pm\,B_2 &= \frac{i}{6}\widetilde{P}^\pm\,R^\mu{}_\alpha{}^\nu{}_\beta\left[\widetilde{\sigma}^\beta\left(\frac{\eta_\mu\eta_\nu}{h^2}\right)_{\eta_\alpha} + \widetilde{\sigma}^\rho\left(\frac{\eta_\mu\eta_\nu\eta^\beta\eta_\rho}{h^4}\right)_{\eta_\alpha}\right]\\ &= -\frac{i}{6\,h^2}\widetilde{P}^\pm\,\mathrm{Ric}^\mu{}_\beta(0)\,\eta_\mu\,\widetilde{\sigma}^\beta(0).\end{aligned} \tag{3.7.51}$$

- B_3: By means of Corollary 3.30 and formula (3.7.50) we get

$$\begin{aligned} B_3 &= \left(\pm\frac{i}{4}\,\mathrm{Ric}_{\alpha\beta}(0)\,\sigma^\alpha \mp \frac{i}{6}\,\mathrm{Ric}_{\alpha\beta}(0)\,\sigma^\alpha\right)\frac{1}{2}\left(\frac{\sigma^\beta}{h} - \frac{\eta^\beta\,\sigma^\rho\eta_\rho}{h^3}\right) \\ &= \pm\frac{i}{24}\,\mathrm{Ric}_{\alpha\beta}(0)\,\sigma^\alpha\left(\frac{\sigma^\beta}{h} - \frac{\eta^\beta\,\sigma^\rho\eta_\rho}{h^3}\right) \\ &= \pm\left(\frac{i}{24h}\mathcal{R}(0)\,\mathrm{Id} - \frac{i}{24h^3}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^\beta\eta_\rho\sigma^\alpha(0)\,\sigma^\rho(0)\right). \end{aligned} \tag{3.7.52}$$

Now, since $\widetilde{P}^\pm\,\widetilde{\sigma}^\rho(0)\eta_\rho = \widetilde{P}^\pm\,\widetilde{W}_{\mathrm{prin}}(0,\eta) = \pm h\,\widetilde{P}^\pm$ and $\widetilde{\sigma}^\alpha\widetilde{\sigma}^\rho = -\widetilde{\sigma}^\rho\widetilde{\sigma}^\alpha + 2\,\delta^{\alpha\rho}\,\mathrm{Id}$, formula (3.7.52) implies

$$\widetilde{P}^\pm B_3 = \widetilde{P}^\pm\left(\pm\frac{i}{24\,h}\mathcal{R}(0) + \frac{i}{24\,h^2}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^\alpha\,\widetilde{\sigma}^\beta \mp \frac{i}{12h^3}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^\alpha\eta^\beta\right). \tag{3.7.53}$$

Summing up (3.7.49), (3.7.51) and (3.7.53) we arrive at

$$(\widetilde{P}^\pm\widetilde{\mathfrak{a}}^\pm_{-1})_t\,(0;y,\eta) = i\widetilde{P}^\pm\left(\mp\frac{1}{24h}\mathcal{R}(0) - \frac{1}{8h^2}\,\mathrm{Ric}_{\alpha\beta}(0)\,\eta^\alpha\,\widetilde{\sigma}^\beta(0)\right) + O(t). \tag{3.7.54}$$

A straightforward calculation shows that

$$\widetilde{P}^\pm\widetilde{\sigma}^\alpha = \pm\widetilde{P}^\pm\left(\frac{\eta^\alpha}{h} + 2h\widetilde{P}^\pm_{\eta_\alpha}\right). \tag{3.7.55}$$

Substituting the above equation into (3.7.54) and integrating in time with initial condition (3.7.24), we obtain (3.7.42).

□

The pieces of information from Lemma 3.34 and Lemma 3.35 can be combined to give the following result.

Theorem 3.36. *For the choice of the Levi-Civita framing, the subprincipal symbols of the positive and negative propagators admit the following small time expansion:*

$$\widetilde{\mathfrak{a}}^\pm_{-1}(t;y,\eta) = \mp it\left(\frac{1}{24\,h}\mathcal{R}(y)\,\widetilde{P}^\pm(y,\eta) - \frac{1}{8h^2}\,\mathrm{Ric}_{\alpha\beta}(y)\,\eta^\alpha\,(\widetilde{W}_{\mathrm{prin}})_{\eta_\beta}(y,\eta)\right) + O(t^2)\,. \tag{3.7.56}$$

Proof. Summing up formulae (3.7.27) and (3.7.42), we obtain

$$\begin{aligned} \widetilde{\mathfrak{a}}^\pm_{-1}(t;y,\eta) = &\mp\frac{it}{24\,h}\mathcal{R}(y)\,\widetilde{P}^\pm(y,\eta) \mp \frac{it}{8h^4}\,\mathrm{Ric}_{\alpha\beta}(y)\,\eta^\alpha\,\eta^\beta\,\widetilde{W}_{\mathrm{prin}}(y,\eta) \\ &- \frac{it}{4h}\,\mathrm{Ric}_{\alpha\beta}(y)\,\eta^\alpha\,\widetilde{P}^\pm_{\eta_\beta}(y,\eta) + O(t^2)\,. \end{aligned} \tag{3.7.57}$$

The substitution of (3.7.50) into the RHS of the above equation gives (3.7.56). □

Note that if the manifold is Ricci-flat then $\widetilde{\mathfrak{a}}^\pm_{-1}(t;y,\eta) = O(t^2)$.

3.7.4 Invariant reformulation

In the previous subsections, we derived the quite elegant and compact formulae (3.7.11) and (3.7.56), which have been obtained under the assumption that the chosen framing is the Levi-Civita framing at y. The task at hand is now to obtain similar formulae for the Dirac operator W corresponding to an arbitrary positively oriented framing $\{e_j\}_{j=1}^3$.

Given a framing $\{e_j\}_{j=1}^3$ and a point $y \in M$, there exits a special unitary matrix-function G, defined in a neighbourhood of y, such that $\{e_j\}_{j=1}^3$ and the Levi-Civita framing $\{\widetilde{e}_j\}_{j=1}^3$ generated by $\{e_j\}_{j=1}^3$ at y are related in accordance with

$$e_j{}^\alpha(x) = \frac{1}{2}\operatorname{tr}(s_j\, G^*(x)\, s^k\, G(x))\, \widetilde{e}_k{}^\alpha(x). \tag{3.7.58}$$

The symbols $\widetilde{\mathfrak{a}}^\pm$ and $\mathfrak{a}^\pm$ are related as

$$\mathfrak{a}^\pm = \mathfrak{S}^\pm[G^*(x)\, \widetilde{\mathfrak{a}}^\pm\, G(y)], \tag{3.7.59}$$

cf. Section 3.5. Note that on the RHS of (3.7.59) the transformed symbol is acted upon by amplitude-to-symbol operators (3.3.43). In fact, the gauge transformation G introduces an x-dependence in the amplitude, which needs to be excluded.

Working in normal coordinates centred at y, formula (3.7.59), combined with (3.7.16) and (3.7.11), implies

$$\begin{aligned}
\mathfrak{a}_0^\pm &= G^*(x^\pm)P^\pm\, G(y) + O(t^3)\\
&= P^\pm \pm \frac{t\,\eta^\alpha}{h} G^*_{x^\alpha}(y)P^\pm + \frac{t^2}{2}\frac{\eta^\alpha\eta^\beta}{h^2} G^*_{x^\alpha x^\beta}(0)P^\pm + O(t^3)\\
&= P^\pm \pm \frac{t\,\eta^\alpha}{h}\, \nabla_\alpha G^*(y)\, P^\pm + \frac{t^2}{2}\frac{\eta^\alpha\eta^\beta}{h^2} \nabla_\alpha\nabla_\beta G^*(0) P^\pm + O(t^3).
\end{aligned} \tag{3.7.60}$$

Similarly, by means of (3.7.16) and Lemma 3.32, from (3.7.59) we get

$$\begin{aligned}
\mathfrak{a}_{-1}^\pm &= \mathfrak{S}_{-1}^\pm[G^*(x)\, \widetilde{\mathfrak{a}}_0^\pm\, G(y)] + \mathfrak{S}_0^\pm[G^*(x)\, \widetilde{\mathfrak{a}}_{-1}^\pm\, G(y)]\\
&= i\, G^*_{x^\alpha}(y)\, P^\pm_{\eta_\alpha} \pm it\, G^*_{x^\alpha x^\beta}(y) \left(h_{\eta_\beta}\, P^\pm_{\eta_\alpha} + \frac{1}{2} h_{\eta_\alpha\eta_\beta}\, P^\pm\right)\\
&\quad + \widetilde{\mathfrak{a}}_{-1}^\pm + O(t^2)\\
&= i\,\nabla_\alpha G^*(y)\, P^\pm_{\eta_\alpha} \pm it\,\nabla_\alpha\nabla_\beta G^*(y) \left(h_{\eta_\beta}\, P^\pm_{\eta_\alpha} + \frac{1}{2} h_{\eta_\alpha\eta_\beta}\, P^\pm\right)\\
&\quad + \widetilde{\mathfrak{a}}_{-1}^\pm + O(t^2).
\end{aligned} \tag{3.7.61}$$

The last step towards expressing (3.7.60) and (3.7.61) invariantly is writing ∇G and $\nabla\nabla G$ in terms of geometric invariants. Theorem 3.23 tells us that

$$\nabla_\alpha G(y) = -\frac{i}{2}\overset{*}{K}_{\alpha\beta}(y)\,(W_\mathrm{prin})_{\eta_\beta}. \tag{3.7.62}$$

The following theorem provides an expression for the second covariant derivatives of the gauge transformation.

Theorem 3.37. *Let us fix a point y and let G be a special unitary matrix-function such that our framing $\{e_j\}_{j=1}^3$ and the Levi-Civita framing $\{\widetilde{e}_j\}_{j=1}^3$ generated by $\{e_j\}_{j=1}^3$ at y are related in accordance with (3.7.58) in a neighbourhood of y. Then we have*

$$\nabla_\alpha\nabla_\beta\, G(y) = -\frac{i}{4}\left(\nabla_\alpha\overset{*}{K}_{\beta\mu}(y) + \nabla_\beta\overset{*}{K}_{\alpha\mu}(y)\right)\sigma^\mu(y) - \frac{1}{4}\overset{*}{K}_{\alpha\mu}(y)\overset{*}{K}_\beta{}^\mu(y)\,\mathrm{Id}, \tag{3.7.63}$$

where K is the contorsion tensor of the Weitzenböck connection (see Appendix B.1) associated with the framing $\{e_j\}_{j=1}^3$ and the star stands for the Hodge dual applied in the first and third indices (see formula (B.1.7)).

Proof. The proof is given in Appendix B.2.2. □

Substituting (3.7.62) and (3.7.63) into (3.7.60) and (3.7.61) we arrive at the following result.

Theorem 3.38. *Let W be the massless Dirac operator (3.1.4). Then the the principal and subprincipal symbols of the positive and negative propagators admit the following small time expansion:*

$$\begin{aligned}\mathfrak{a}_0^\pm &= \left[\mathrm{Id} \pm \frac{it}{2} h_{\eta_\alpha}\,\overset{*}{K}_{\alpha\beta}\,(W_\mathrm{prin})_{\eta_\beta}\right] P^\pm \\ &+ \frac{t^2}{8}\frac{\eta^\alpha\eta^\beta}{h^2}\left[i\big(\nabla_\alpha\overset{*}{K}_{\beta\mu}(y) + \nabla_\beta\overset{*}{K}_{\alpha\mu}(y)\big)(W_\mathrm{prin})_{\eta_\mu} - \overset{*}{K}_{\alpha\mu}(y)\overset{*}{K}_\beta{}^\mu(y)\right] P^\pm + O(t^3),\end{aligned} \tag{3.7.64}$$

$$\begin{aligned}\mathfrak{a}_{-1}^\pm &= -\frac{1}{2}\overset{*}{K}_{\alpha\beta}\,(W_\mathrm{prin})_{\eta_\beta}\,P^\pm_{\eta_\alpha} \\ &\mp it\left(\frac{1}{24\,h}\mathcal{R}\,P^\pm - \frac{1}{8h^2}\,\mathrm{Ric}_{\alpha\beta}\,\eta^\alpha\,(W_\mathrm{prin})_{\eta_\beta}\right) \\ &\mp \frac{t}{4}\left(\nabla_\alpha\overset{*}{K}_{\beta\mu} + \nabla_\beta\overset{*}{K}_{\alpha\mu}\right)(W_\mathrm{prin})_{\eta_\mu}\left(h_{\eta_\beta}\,P^\pm_{\eta_\alpha} + \frac{1}{2}h_{\eta_\alpha\eta_\beta}\,P^\pm\right) \\ &\mp \frac{it}{4}\overset{*}{K}_{\alpha\mu}\overset{*}{K}_\beta{}^\mu\left(h_{\eta_\beta}\,P^\pm_{\eta_\alpha} + \frac{1}{2}h_{\eta_\alpha\eta_\beta}\,P^\pm\right) \\ &+ O(t^2),\end{aligned} \tag{3.7.65}$$

where $\overset{*}{K}$ denotes the Hodge dual in the first and third indices of the contorsion tensor of the Weitzenböck connection associated with the framing $\{e_j\}_{j=1}^3$.

3.8 Spectral asymptotics

In this section, we will compute the third Weyl coefficient for the massless Dirac operator. In doing so we will use the same notation as in Section 3.1 — recall in particular formulae (3.1.18), (3.1.14) and the definition of the function μ.

Theorem 3.39. *The third local Weyl coefficients for the massless Dirac operator are*

$$c_0^\pm(y) = -\frac{1}{48\pi^2}\mathcal{R}(y), \tag{3.8.1}$$

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

Proof. Let us fix a point $y \in M$ and choose normal geodesic coordinates x centred at y. Let us also choose a Levi-Civita framing $\{\widetilde{e}_j\}_{j=1}^3$, see Definition 3.27; here we make use of the fact that Weyl coefficients do not depend on the choice of framing. The same proof, but for a general framing, is given in Appendix B.3.

We have

$$(N'_+ * \mu)(y,\lambda) = \mathcal{F}^{-1}\left[\mathcal{F}\left[(N'_+ * \mu)\right]\right](y,\lambda) = \mathcal{F}^{-1}\left[\operatorname{tr} u_+(t,y,y)\,\hat{\mu}(t)\right], \tag{3.8.2}$$

$$(N'_- * \mu)(y,\lambda) = \mathcal{F}^{-1}\left[\mathcal{F}\left[(N'_- * \mu)\right]\right](y,\lambda) = \mathcal{F}^{-1}\left[\operatorname{tr} \overline{u_-(t,y,y)}\,\hat{\mu}(t)\right], \tag{3.8.3}$$

where $u_\pm$ is the Schwartz kernel of the propagator $U^\pm$ and tr stands for the matrix trace. Note that at each point of the manifold the quantity $\operatorname{tr} u_\pm(t,y,y)$ is a distribution in the variable t and the construction presented in preceding sections allows us to write down this distribution explicitly, modulo a smooth function.

Our task is to substitute (3.5.7) into the right-hand sides of (3.8.2) and (3.8.3) and expand the resulting quantities in powers of λ as $\lambda \to +\infty$. Thus, the problem reduces to the analysis of explicit integrals in four variables, η_1, η_2, η_3 and t, depending on the parameter λ. In what follows we drop the y in our intermediate calculations.

The construction presented in preceding sections tells us that the only singularity of the distribution $\operatorname{tr} u_\pm(t,y,y)\,\hat{\mu}(t)$ 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 functions $\varphi^\pm$.

Theorems 3.31 and 3.36 imply that

$$\operatorname{tr}\widetilde{\mathfrak{a}}_0^\pm(t;\eta) = 1 + O(t^3)\,, \tag{3.8.4}$$

$$\operatorname{tr}\widetilde{\mathfrak{a}}_{-1}^\pm(t;\eta) = \mp\frac{i}{24\,\|\eta\|}\,\mathcal{R}\,t + O(t^2)\,. \tag{3.8.5}$$

Formula (2.10.11) reads $\varphi^+(t,\eta) = -\|\eta\|\,t + O(t^4)$, which, in view of (3.5.5), implies

$$\varphi^\pm(t,\eta) = \mp\|\eta\|\,t + O(t^4)\,. \tag{3.8.6}$$

Using formulae (3.8.2)–(3.8.6) and arguing as in Section 2.10, we conclude that

$$(N'_\pm * \mu)(y,\lambda) = \frac{S_2}{(2\pi)^4}\int_{\mathbb{R}^2}\left(r^2 - \frac{1}{24}\,\mathcal{R}\right)e^{i(\lambda-r)t}\,\hat{\mu}(t)\,\mathrm{d}r\,\mathrm{d}t \\ + O(\lambda^{-1}) \quad \text{as} \quad \lambda\to+\infty, \tag{3.8.7}$$

where $S_2 = 4\pi$ is the surface area of the 2-sphere. But

$$\frac{1}{2\pi}\int_{\mathbb{R}^2} r^m\,e^{i(\lambda-r)t}\,\hat{\mu}(t)\,\mathrm{d}r\,\mathrm{d}t = \lambda^m, \qquad m = 0,1,2,\ldots, \tag{3.8.8}$$

so (3.8.7) can be rewritten as

$$(N'_\pm * \mu)(y,\lambda) = \frac{1}{2\pi^2}\,\lambda^2 - \frac{1}{48\pi^2}\,\mathcal{R}(y) + O(\lambda^{-1}) \quad \text{as} \quad \lambda\to+\infty.$$

□

Remark 3.40. Let us compare the spectrum of the massless Dirac operator with the spectrum of the Laplacian. Working on the same 3-manifold, let Δ be the Laplace–Beltrami operator and let $N(y,\lambda)$ be the local counting function for the operator $\sqrt{-\Delta}$. Then

$$(N' * \mu)(y,\lambda) = c_2(y)\,\lambda^2 + c_1(y)\,\lambda + c_0(y) + \ldots \quad \text{as} \quad \lambda\to+\infty,$$

where the values of the first three Weyl coefficients are provided by Theorem 2.27. Comparing these with (3.1.20) and (3.8.1), we conclude that

$$c_2^\pm(y) = c_2(y)\,, \qquad c_1^\pm(y) = c_1(y) = 0\,, \qquad c_0^\pm(y) = -\frac{1}{2}\,c_0(y)\,.$$

We see that the large (in modulus) eigenvalues of the massless Dirac operator are distributed approximately the same way as the eigenvalues of the operator $\sqrt{-\Delta}$, differing only in the third Weyl coefficient.

3.9 Examples

In this Section we present two explicit examples, which show how our constructions work in practice and which give us an opportunity to double-check our formulae.

The specific choice of examples is motivated by the fact that the first, $M = \mathbb{S}^3$, is isotropic in momentum whereas the second, $M = \mathbb{S}^2 \times \mathbb{S}^1$, is anisotropic in momentum.

3.9.1 The case $M = \mathbb{S}^3$

Let $\mathbb{R}^4$ be Euclidean space equipped with Cartesian coordinates x^α, $\alpha = 1, 2, 3, 4$, and put

$$\widehat{e}_4 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

Consider the 3-sphere[5]

$$\mathbb{S}^3 := \{x + \widehat{e}_4 \in \mathbb{R}^4 \,|\, \|x\| = 1\}$$

equipped with the standard round metric g and with the global framings $\{V_{\pm,k}\}_{k=1}^3$ defined as the restriction to $\mathbb{S}^3$ of the vector fields in $\mathbb{R}^4$

$$\begin{aligned}
\mathbf{V}_{\pm,1} &:= (1 - x^4)\frac{\partial}{\partial x^1} \mp x^3 \frac{\partial}{\partial x^2} \pm x^2 \frac{\partial}{\partial x^3} + x^1 \frac{\partial}{\partial x^4}, \\
\mathbf{V}_{\pm,2} &:= \pm x^3 \frac{\partial}{\partial x^1} + (1 - x^4)\frac{\partial}{\partial x^2} \mp x^1 \frac{\partial}{\partial x^3} + x^2 \frac{\partial}{\partial x^4}, \\
\mathbf{V}_{\pm,3} &:= \mp x^2 \frac{\partial}{\partial x^1} \pm x^1 \frac{\partial}{\partial x^2} + (1 - x^4)\frac{\partial}{\partial x^3} + x^3 \frac{\partial}{\partial x^4}.
\end{aligned} \tag{3.9.1}$$

It is easy to check that the vector fields (3.9.1) are tangent to $\mathbb{S}^3$, so that they restrict to smooth vector fields on the 3-sphere. Note that (3.9.1) is an adaptation of [54, Eqn. (C.1)] to the case at hand.

Let us introduce coordinates on $\mathbb{S}^3$ with the north pole excised by stereographically projecting it onto the tangent hyperplane to the south pole. The stereographic

[5] We shifted the sphere so as to place the south pole at the origin.

map is given by

$$\sigma : \mathbb{R}^3 \to \mathbb{S}^3 \setminus \begin{pmatrix} 0 \\ 0 \\ 0 \\ 2 \end{pmatrix}, \qquad \begin{pmatrix} u \\ v \\ w \end{pmatrix} \mapsto \begin{pmatrix} x^1 \\ x^2 \\ x^3 \\ x^4 \end{pmatrix} = \frac{1}{1+f^2} \begin{pmatrix} u \\ v \\ w \\ 2f^2 \end{pmatrix}, \tag{3.9.2}$$

where

$$f^2 := \frac{1}{4}\,(u^2+v^2+w^2). \tag{3.9.3}$$

In stereographic coordinates, the metric reads

$$g = \frac{1}{(1+f^2)^2}\left[\mathrm{d}u^2 + \mathrm{d}v^2 + \mathrm{d}w^2\right] \tag{3.9.4}$$

and our framings are given by

$$\begin{aligned} 2V_{\pm,1} &= (2-2f^2+u^2)\frac{\partial}{\partial u} + (uv \mp 2w)\frac{\partial}{\partial v} + (uw \pm 2v)\frac{\partial}{\partial w}, \\ 2V_{\pm,2} &= (uv \pm 2w)\frac{\partial}{\partial u} + (2-2f^2+v^2)\frac{\partial}{\partial v} + (vw \mp 2u)\frac{\partial}{\partial w}, \\ 2V_{\pm,3} &= (uw \mp 2v)\frac{\partial}{\partial u} + (vw \pm 2u)\frac{\partial}{\partial v} + (2-2f^2+w^2)\frac{\partial}{\partial w}. \end{aligned} \tag{3.9.5}$$

A straightforward calculation shows that $\{V_{\pm,k}\}_{k=1}^3$ are positively oriented framings formed by (orthonormal) smooth Killing vector fields with respect to the metric g.

The framings $\{V_{\pm,k}\}_{k=1}^3$ define, via (3.1.4), two Dirac operators $W_\pm$ related in accordance with

$$W_- = G^* W_+ G, \tag{3.9.6}$$

where

$$G := \frac{1}{4(1+f^2)} \begin{pmatrix} u^2+v^2+(w-2\mathrm{i})^2 & 4(v-\mathrm{i}u) \\ -4(v+\mathrm{i}u) & u^2+v^2+(w+2\mathrm{i})^2 \end{pmatrix}. \tag{3.9.7}$$

is the $SU(2)$ gauge transformation relating the two framings via (3.7.58) with $\widetilde{e}_k = V_{+,k}$ and $e_k = V_{-,k}$.

For definiteness, let us focus on W_+. On account of the symmetries of the 3-sphere, we will write formulae for principal and subprincipal symbols of the propagator of W_+ at the south pole ($y = (0,0,0)$) for the choice of momentum $\overline{\eta} = (0,0,1)$.

The principal symbol $(W_+)_{\mathrm{prin}}$ has eigenvalues $h^\pm(y,\eta) = \pm\|\eta\|$, whose Hamiltonian flows in stereographic coordinates read

$$z^\pm(t;0,\eta) = \pm 2\tan(t/2)\frac{\eta}{\|\eta\|}, \qquad \xi^\pm(t;0,\eta) = \cos^2(t/2)\,\eta, \tag{3.9.8}$$

see also formula (3.5.3). Direct inspection of the parallel transport equation reveals that the parallel transport of

$$v^+(0,\overline{\eta}) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad v^-(0,\overline{\eta}) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

along z^+ and z^-, respectively, is given by

$$\zeta^+(t;0,\overline{\eta}) = e^{-\frac{it}{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \zeta^-(t;0,\overline{\eta}) = e^{\frac{it}{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{3.9.9}$$

so that Theorem 3.26 gives us

$$\mathfrak{a}_0^+(t;0,\overline{\eta}) = e^{-\frac{it}{2}} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad \mathfrak{a}_0^-(t;0,\overline{\eta}) = e^{\frac{it}{2}} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{3.9.10}$$

The principal symbol of positive and negative propagators of W_- at $(t;0,\overline{\eta})$ can be obtained from (3.9.10) by means of the gauge transformation (3.9.7) evaluated at $z^\pm(t;0,\overline{\eta})$,

$$G|_{(u,v,w)=z^\pm(t;0,\overline{\eta})} = \begin{pmatrix} e^{\mp it} & 0 \\ 0 & e^{\pm it} \end{pmatrix}.$$

Let us now move to the subprincipal symbol. From (3.9.5) we get

$$\overset{*}{K}_{\alpha\beta}(y) = -\delta_{\alpha\beta}, \qquad \nabla_\gamma \overset{*}{K}_{\alpha\beta}(y) = 0, \tag{3.9.11}$$

so that Theorem 3.38 gives us

$$\mathfrak{a}_{-1}^\pm(t;0,\eta) = \pm\frac{1}{4\|\eta\|}\,\mathrm{Id} \mp it \left(\frac{1}{2\,\|\eta\|}\, P^\pm - \frac{1}{4\|\eta\|^2}\,(W_+)_{\mathrm{prin}} \right) + O(t^2), \tag{3.9.12}$$

and, in turn,

$$\mathfrak{a}_{-1}^+(t;0,\overline{\eta}) = \frac{1}{4} \begin{pmatrix} 1-it & 0 \\ 0 & 1-it \end{pmatrix} + O(t^2), \qquad \mathfrak{a}_{-1}^-(t;0,\overline{\eta}) = -\frac{1}{4} \begin{pmatrix} 1+it & 0 \\ 0 & 1-3it \end{pmatrix} + O(t^2). \tag{3.9.13}$$

Let us run a test for Theorem 3.39. It is well known [11, 12, 111, 114] that the eigenvalues of the Dirac operator on the round 3-sphere are

$$\pm\left(k+\frac{1}{2}\right), \qquad k \in \mathbb{N}\setminus\{0\},$$

with multiplicity $k(k+1)$. Therefore, in view of (3.8.2), we have

$$\mathcal{F}_{\lambda\to t}[N'_+ * \mu](y,t) = \frac{1}{2\pi^2} e^{-\frac{it}{2}} \sum_{k=1}^{\infty} k(k+1) e^{-ikt}. \tag{3.9.14}$$

Taking the Fourier transform of the RHS of (3.9.14) we get

$$\begin{aligned}
\mathcal{F}^{-1}_{t\to\lambda}\left[\frac{1}{2\pi^2} e^{-\frac{it}{2}} \sum_{k=1}^{\infty} (k^2+k) e^{-ikt} \hat{\mu}(t)\right] &= \frac{1}{4\pi^3} \sum_{k=1}^{\infty} \int_{-\infty}^{+\infty} e^{it(\lambda-\frac{1}{2}-k)} \, (k^2+k)\, \hat{\mu}(t)\, \mathrm{d}t \\
&= \frac{1}{2\pi^2}\left((\lambda-\frac{1}{2})^2 + (\lambda-\frac{1}{2}) + O(\lambda^{-\infty}) \right) \\
&= \frac{1}{2\pi^2}\left(\lambda^2 - \frac{1}{4} + O(\lambda^{-\infty}) \right).
\end{aligned} \tag{3.9.15}$$

Combining (3.9.15) and (3.9.14) we arrive at

$$[N'_+ * \mu](y,\lambda) = \frac{1}{2\pi^2}\left(\lambda^2 - \frac{1}{4} + O(\lambda^{-\infty}) \right) \qquad \text{as } \lambda \to +\infty. \tag{3.9.16}$$

Formula (3.9.16) is in agreement with (3.8.1) with $\mathcal{R}(y) = 6$.

3.9.2 The case $M = \mathbb{S}^2 \times \mathbb{S}^1$

Let $M = \mathbb{S}^2 \times \mathbb{S}^1$ be endowed with the metric $g = g_{\mathbb{S}^2} + d\varphi^2$, where $g_{\mathbb{S}^2}$ is the round metric on the 2-sphere. Let $y \in M$ be given. In this subsection we shall compute a small time expansion for the subprincipal symbols of the Dirac propagator $\widetilde{W}$ associated with a Levi-Civita framing at y. In this case, the result will not be isotropic in momentum η, because, unlike the previous example, $(\mathbb{S}^2 \times \mathbb{S}^1, g)$ is not an Einstein manifold.

Without loss of generality, we assume that y coincides with the north pole when projected onto $\mathbb{S}^2$. The exponential map $\exp_y : T_yM \to M$ is realised explicitly by

$$(u,v,w) \mapsto (\theta = \sqrt{u^2+v^2}, \phi = \arctan(v/u), \varphi = w). \tag{3.9.17}$$

Formula (3.9.17) defines geodesic normal coordinates in a neighbourhood of y. In such coordinates, the metric g reads

$$g(u,v,z) = \frac{1}{u^2+v^2} \begin{pmatrix} u^2 + \frac{v^2 \sin^2(\sqrt{u^2+v^2})}{u^2+v^2} & uv\left(1 - \frac{\sin^2(\sqrt{u^2+v^2})}{u^2+v^2}\right) & 0 \\ uv\left(1 - \frac{\sin^2(\sqrt{u^2+v^2})}{u^2+v^2}\right) & v^2 + \frac{u^2 \sin^2(\sqrt{u^2+v^2})}{u^2+v^2} & 0 \\ 0 & 0 & u^2+v^2 \end{pmatrix}. \tag{3.9.18}$$

We will assume that normal coordinates are chosen so that the Levi-Civita framing satisfies $\widetilde{e}_j{}^\alpha(y) = \delta_j{}^\alpha$. In this case, the Hamiltonian flows generated by the eigenvalues of $\widetilde{W}_{\mathrm{prin}}$ read, simply,

$$x^\pm(t;0,\eta) = \pm t\frac{\eta}{\|\eta\|}, \qquad \xi^\pm(t;0,\eta) = \eta.$$

The Ricci curvature of g in normal coordinates is given by

$$\mathrm{Ric}(u,v,w) = \frac{1}{45}\begin{pmatrix} v^2\left(2u^2+2v^2-15\right)+45 & uv\left(15-2\left(u^2+v^2\right)\right) & 0 \\ uv\left(15-2\left(u^2+v^2\right)\right) & u^2\left(2u^2+2v^2-15\right)+45 & 0 \\ 0 & 0 & 0 \end{pmatrix} + O(\|(u,v,w)\|^5). \quad (3.9.19)$$

Hence, Theorem 3.36 tells us that

$$\widetilde{\mathfrak{a}}^\pm_{-1}(t;0,\eta) = \mp it\left(\frac{1}{12\|\eta\|}\,\widetilde{P}^\pm - \frac{1}{8\|\eta\|^2}(\eta_1\,s^1+\eta_2\,s^2)\right) + O(t^2)\,. \qquad (3.9.20)$$

Let us stress once again that, even though the intermediate steps depend on the choice of coordinates, the final result (3.9.20) is a scalar matrix-function, thus independent of the choice of coordinates.

Chapter 4

Classification of first order sesquilinar forms

4.1 Introduction

A natural way to obtain a system of partial differential equations on a manifold is to vary a suitably defined sesquilinear form. If one is only interested in first order systems, say, of the type described in Chapter 3, then one can concentrate on a subclass of Hermitian forms acting on smooth m-columns over a smooth d-dimensional manifold without boundary. A natural question is: can one classify such forms up to (local) $GL(m,\mathbb{C})$ gauge equivalence? In this Chapter we study sesquilinear forms that generate first order systems of partial differential equations on manifolds, with a particular focus on the this question.

In order to provide motivation for our analysis, let us first recall some basic facts from linear algebra in finite dimension.

Working in a finite dimensional complex vector space V, consider an Hermitian form

$$S : V \times V \to \mathbb{C}, \quad (u,v) \mapsto S(u,v).$$

Here S is assumed to be antilinear in the first argument and linear in the second. Variation of the real-valued action $S(v,v)$ produces the following linear field equation for v:

$$S(u,v) = 0, \qquad \forall u \in V. \tag{4.1.1}$$

Suppose now that our vector space V is equipped with an additional structure, an inner product $\langle \cdot\,,\,\cdot \rangle$. Then the sesquilinear form S and inner product $\langle \cdot\,,\,\cdot \rangle$ uniquely define a self-adjoint linear operator $L : V \to V$ via the formula

$$S(u, v) = \langle u, Lv \rangle, \qquad \forall u, v \in V. \tag{4.1.2}$$

The argument also works the other way round: a self-adjoint linear operator uniquely defines an Hermitian sesquilinear form via formula (4.1.2). Thus, in an inner product space the concepts of Hermitian sesquilinear form and self-adjoint linear operator are equivalent.

Given a linear operator L, we can consider the linear equation

$$Lv = 0. \tag{4.1.3}$$

If S and L are related as in (4.1.2), then equations (4.1.1) and (4.1.3) are equivalent.

It may seem that there is no point in working with Hermitian sesquilinear forms and that one can work with self-adjoint linear operators instead, which would be easier for practical purposes. However, the more abstract take is justified by the fact that the statement regarding the equivalence of linear equations (4.1.1) and (4.1.3) is based on the use of an inner product. The concept of an Hermitian sesquilinear form is more fundamental than the concept of a self-adjoint linear operator in that it does not require an inner product for its definition. One can formulate and study the linear equation (4.1.1) without introducing an inner product.

In the class of problems we are interested in, the above toy model translates into the study of partial differential equations on manifolds in a setting when there is no natural definition of an inner product invariant under relevant gauge transformations. Such a situation arises, for instance, when dealing with physically meaningful problems in 4-dimensional Lorentzian spacetime, see Sections 4.9 and 4.10. Fully relativistic equations of mathematical physics are not always associated with a natural inner product, not even an indefinite non-degenerate one.

In more precise terms, our goal is to study and classify sesquilinear forms acting on compactly supported smooth sections of the trivial $\mathbb{C}^m$-bundle over a smooth manifold M, whose coordinate representation involves the sections themselves and their first derivatives but no products of first derivatives. Adopting a non-canonical approach, we ask the question: when do two sesquilinear forms written in their coordinate representation correspond to the same abstract sesquilinear form? In other words, we are interested in establishing when two sesquilinear forms can be obtained one from the other by a pointwise change of basis in the fibre depending smoothly on the base point. As it turns out, this problem can be solved thanks to the interplay of techniques from algebraic topology, geometry and analysis of partial differential equations.

Our work builds upon results from [7], where the authors provide an analytic definition of spin structure in the more restrictive operator setting.

This Chapter is structured as follows.

In Section 4.2 we provide a precise definition of the class of sesquilinear forms we work with using the language of analysis of partial differential equations.

In Section 4.3 we formulate the mathematical problem we want to address, namely, the classification of first order sesquilinear forms, distinguishing the two different types of classification we will be looking at.

Section 4.4 contains a brief description of the main result of the Chapter: our classification theorems in dimension four.

Sections 4.5 and 4.6 comprise preparatory work towards the proof of the main theorems. In Section 4.5 we analyse properties of sesquilinear forms, identifying geometric and topological objects naturally encoded in their analytic definition. In Section 4.6 we recast our analytic definition of equivalence of sesquilinear forms in a purely algebraic topological fashion, proving the equivalence of the two formulations.

Our main theorems are proved in Section 4.7.

Section 4.8 is concerned with a similar analysis in dimension three, under suitable additional conditions. We also examine two explicit examples.

In Section 4.9 we revisit the sesquilinear forms vs linear operators issue in the context of our main results.

In conclusion, in Section 4.10 we briefly mention some physically meaningful applications of our results.

The main text of the Chapter is complemented by Appendix C.1 where we explain the relation between the traditional definitions of symbols of (pseudo)differential operators and our definitions for sesquilinear forms.

4.2 First order sesquilinear forms

Let M be a real connected smooth d-manifold without boundary, not necessarily compact. Local coordinates on M will be denoted by x^α, $\alpha = 1, \dots, d$.

We will be working with compactly supported smooth functions $u : M \to \mathbb{C}^m$. Such functions can be thought of as sections of the trivial $\mathbb{C}^m$-bundle over M or as m-columns of smooth complex-valued scalar fields. They form an (infinite-dimensional) vector space $C_0^\infty(M;\mathbb{C}^m)$.

Definition 4.1. A first order sesquilinear form is a functional

$$S(u,v) := \int_M [u^*\,\mathbf{A}^\alpha\,v_{x^\alpha} + u^*_{x^\alpha}\,\mathbf{B}^\alpha\,v + u^*\,\mathbf{C}\,v]\,\mathrm{d}x\,, \qquad u,v \in C_0^\infty(M;\mathbb{C}^m), \tag{4.2.1}$$

where $\mathbf{A}^\alpha(x)$, $\mathbf{B}^\alpha(x)$ and $\mathbf{C}(x)$ are some prescribed smooth complex $n \times n$ matrix-functions, the subscript x^α indicates partial differentiation, the star stands for Hermitian conjugation and $\mathrm{d}x = \mathrm{d}x^1 \dots \mathrm{d}x^d$. As in previous chapters, we adopt the summation convention over repeated indices.

In formula (4.2.1) the elements of the matrix-function $\mathbf{C}$ are densities, whereas the elements of the matrix-functions $\mathbf{A}$ are $\mathbf{B}$ are vector densities. Here and further on we use bold script for density-valued quantities.

Performing integration by parts, one can rewrite the sesquilinear form (4.2.1) in many different ways. We define the canonical representation of a first order sesquilinear form to be

$$S(u,v) = \int_M \left[-\frac{i}{2}\,u^*\,\mathbf{E}^\alpha\,v_{x^\alpha} + \frac{i}{2}u^*_{x^\alpha}\,\mathbf{E}^\alpha\,v + u^*\,\mathbf{F}\,v\right]\mathrm{d}x\,. \tag{4.2.2}$$

The matrix-functions in (4.2.1) and (4.2.2) are related by formulae

$$\mathbf{E}^\alpha = i(\mathbf{A}^\alpha - \mathbf{B}^\alpha), \qquad \mathbf{F} = \mathbf{C} - \frac{1}{2}\frac{\partial(\mathbf{A}^\alpha + \mathbf{B}^\alpha)}{\partial x^\alpha}\,.$$

Recall the well-known fact that if $\mathbf{w}^\alpha$ is a vector density then $\partial\mathbf{w}^\alpha/\partial x^\alpha$ is a density, so elements of the matrix-function $\mathbf{F}(x)$ are densities.

We define the principal, subprincipal and full symbols of the sesquilinear form (4.2.2) as

$$\mathbf{S}_{\mathrm{prin}}(x,p) := \mathbf{E}^\alpha(x)\,p_\alpha\,, \tag{4.2.3}$$

$$\mathbf{S}_{\text{sub}}(x) := \mathbf{F}(x), \tag{4.2.4}$$

$$\mathbf{S}_{\text{full}}(x,p) := \mathbf{S}_{\text{prin}}(x,p) + \mathbf{S}_{\text{sub}}(x), \tag{4.2.5}$$

respectively. Here p_α, $\alpha = 1, \ldots, m$, is the dual variable (momentum) and all the above symbols are well defined on the cotangent bundle T^*M. It is easy to see that the full symbol uniquely determines our first order sesquilinear form and that our sesquilinear form is Hermitian (that is, $S(u,v) = \overline{S(v,u)}$) if and only if its full symbol is Hermitian.

Establishing a correspondence between a sesquilinear form or a (pseudo)differential operator on the one hand and a (full) symbol on the other hand is often referred to as *quantisation*. The argument in the above paragraph shows that first order sesquilinear forms admit a particularly convenient and natural quantisation.

Further on we work with Hermitian first order sesquilinear forms.

An Hermitian first order sesquilinear form $S(u,v)$ defines a real-valued action $S(v,v)$. Variation of this action produces field equations for v. This is a system of m linear scalar first order partial differential equations for m unknown complex-valued scalar fields.

Remark 4.2. Note that, according to Definition 4.1, a first order sesquilinear form does not contain the term $u^*_{x^\alpha}\,\mathbf{D}^{\alpha\beta}\,v_{x^\beta}$. The presence of such a term would fundamentally change the corresponding field equations, making them second order.

Definition 4.3. We say that the sesquilinear form S is *non-degenerate* if

$$\mathbf{S}_{\text{prin}}(x,p) \neq 0, \qquad \forall (x,p) \in T^*M \setminus \{0\}. \tag{4.2.6}$$

Condition (4.2.6) means that $\mathbf{S}_{\text{prin}}$ does not vanish as a matrix, i.e. for any $(x,p) \in T^*M \setminus \{0\}$ the matrix $\mathbf{S}_{\text{prin}}(x,p)$ has at least one nonzero element. This is the weakest possible non-degeneracy condition.

Further on we work with non-degenerate Hermitian first order sesquilinear forms.

4.3 Statement of the problem

4.3.1 General linear classification

Consider a smooth matrix-function

$$G : M \to GL(m, \mathbb{C}). \tag{4.3.1}$$

Given a sesquilinear form (4.2.2) we can now define another sesquilinear form

$$\widetilde{S}(u, v) := S(Gu, Gv). \tag{4.3.2}$$

We interpret this new sesquilinear form as a different representation of our original sesquilinear form. What we did is we changed, fibrewise, the basis in our $\mathbb{C}^m$-bundle over M using the gauge transformation G.

The explicit formula for $\widetilde{S}(u, v)$ reads

$$\widetilde{S}(u, v) = \int_M \left[-\frac{i}{2}\, u^* \,\widetilde{\mathbf{E}}^\alpha\, v_{x^\alpha} + \frac{i}{2} u^*_{x^\alpha}\, \widetilde{\mathbf{E}}^\alpha\, v + u^*\, \widetilde{\mathbf{F}}\, v \right] \mathrm{d}x\,,$$

where

$$\widetilde{\mathbf{E}}^\alpha = G^*\, \mathbf{E}^\alpha G, \qquad \widetilde{\mathbf{F}} = G^*\, \mathbf{F} G + \frac{i}{2} \left[G^*_{x^\alpha}\, \mathbf{E}^\alpha G - G^*\, \mathbf{E}^\alpha G_{x^\alpha} \right].$$

The corresponding full symbol is

$$\widetilde{\mathbf{S}}_{\mathrm{full}} = G^*\, \mathbf{S}_{\mathrm{full}}\, G + \frac{i}{2} \left[G^*_{x^\alpha} (\mathbf{S}_{\mathrm{full}})_{p_\alpha} G - G^* (\mathbf{S}_{\mathrm{full}})_{p_\alpha} G_{x^\alpha} \right]. \tag{4.3.3}$$

Our goal is to perform the above argument the other way round, solving, effectively, an 'inverse problem'. Namely, suppose we are given two full symbols, $\mathbf{S}_{\mathrm{full}}(x, p)$ and $\widetilde{\mathbf{S}}_{\mathrm{full}}(x, p)$. Do they describe the same sesquilinear form? In order to deal with this question rigorously we introduce the following definition.

Definition 4.4. We say that two full symbols $\mathbf{S}_{\mathrm{full}}(x, p)$ and $\widetilde{\mathbf{S}}_{\mathrm{full}}(x, p)$ are GL-*equivalent* if there exists a smooth matrix-function (4.3.1) such that (4.3.3) is satisfied.

4.3.2 Special linear classification

We will also deal with the problem of equivalence of symbols in a more restrictive, special linear setting.

Definition 4.5. We say that two full symbols $\mathbf{S}_{\mathrm{full}}(x,p)$ and $\widetilde{\mathbf{S}}_{\mathrm{full}}(x,p)$ are *SL-equivalent* if there exists a smooth matrix-function

$$G : M \to SL(m,\mathbb{C}) \tag{4.3.4}$$

such that (4.3.3) is satisfied.

Let elaborate a bit on the motivation for Definition 4.5.

Suppose that we have an additional structure in our mathematical model, a complex-valued volume form, namely, a non-vanishing map

$$\mathrm{vol} : M \to \bigwedge^{n,0}(\mathbb{C}^m), \qquad \mathrm{vol}(x) = c(x)\,\mathrm{d}z^1 \wedge \ldots \wedge \mathrm{d}z^n,$$

where $c(x)$ is some prescribed smooth non-vanishing complex scalar field.

The transformation $u \to Gu$, where G is a matrix-function (4.3.1), turns vol into the complex-valued volume form $\widetilde{\mathrm{vol}}(x) = \widetilde{c}(x)\,\mathrm{d}z^1 \wedge \ldots \wedge \mathrm{d}z^n$ with $\widetilde{c}(x) = c(x)\,\det G(x)$.

As in the previous Subsection, we consider the 'inverse' problem which now involves both the sesquilinear form and the complex-valued volume form. Namely, consider two symbols $\mathbf{S}_{\mathrm{full}}(x,p)$ and $\widetilde{\mathbf{S}}_{\mathrm{full}}(x,p)$ and two non-vanishing scalar fields $c(x)$ and $\widetilde{c}(x)$. Does there exist a smooth matrix-function (4.3.1) which turns $(\mathbf{S}_{\mathrm{full}}, c)$ into $(\widetilde{\mathbf{S}}_{\mathrm{full}}, \widetilde{c})$?

One way of addressing the above question is as follows. Choose an arbitrary smooth matrix-function $Q : M \to GL(m,\mathbb{C})$ such that $\det Q(x) = c(x)/\widetilde{c}(x)$ (for example, one can take $Q(x) = \mathrm{diag}\,(c(x)/\widetilde{c}(x), 1, \ldots, 1)\,)$ and view the sesquilinear form $\widetilde{\mathbf{S}}(Qu, Qv)$ as the 'new' sesquilinear form $\widetilde{\mathbf{S}}$. The two complex-valued volume forms now have the same representation. After this we can only apply $SL(m,\mathbb{C})$-transformations (4.3.4) to establish whether the two sesquilinear forms $\mathbf{S}_{\mathrm{full}}(x,p)$ and $\widetilde{\mathbf{S}}_{\mathrm{full}}(x,p)$ are equivalent, because we do not want to change the complex-valued volume form. This reduces the problem to checking whether the symbols are SL-equivalent in the sense of Definition 4.5.

Alternatively, we can do the argument the other way round. Take an arbitrary smooth matrix-function $Q : M \to GL(m,\mathbb{C})$ such that $\det Q(x) = \widetilde{c}(x)/c(x)$ and view the sesquilinear form $\mathbf{S}(Qu, Qv)$ as the 'new' sesquilinear form $\mathbf{S}$ etc.

It is easy to see that the outcome of this exercise does not depend on which way we proceed or which Q we choose. In group-theoretic language, this corresponds to the fact that the group of matrix-functions (4.3.4) is a normal subgroup of the group of matrix-functions (4.3.1). The matrix-function Q picks a particular element in each of the left cosets (or, equivalently, right cosets) of $C^\infty(M, GL(m,\mathbb{C}))/C^\infty(M, SL(m,\mathbb{C}))$.

4.4 Main results

The main problem addressed in the current Chapter is to give necessary and sufficient conditions for a pair of full symbols to be GL-equivalent or SL-equivalent. Our explicit non-canonical approach will eventually produce a full classification of equivalence classes of sesquilinear forms for the special case

$$d = 4, \qquad m = 2, \tag{4.4.1}$$

i.e. the case when we are dealing with a pair of complex-valued scalar fields over a 4-manifold.

Under the assumption (4.4.1) we have the following two theorems, which represent the main result of this Chapter.

Theorem 4.6. *Two full symbols* $\mathbf{S}_{\mathrm{full}}(x,p)$ *and* $\widetilde{\mathbf{S}}_{\mathrm{full}}(x,p)$ *are* GL-equivalent *if and only if*

(i) the metrics encoded within these symbols belong to the same conformal class,

(ii) the electromagnetic covector potentials encoded within these symbols belong to the same cohomology class in $H^1_{\mathrm{dR}}(M)$*,*

(iii) their topological charges are the same,

(iv) their temporal charges are the same and

(v) they have the same 2-torsion spin^c *structure.*

Theorem 4.7. *Two full symbols* $\mathbf{S}_{\mathrm{full}}(x,p)$ *and* $\widetilde{\mathbf{S}}_{\mathrm{full}}(x,p)$ *are* SL-equivalent *if and only if*

(i) the metrics encoded within these symbols are the same,

(ii) the electromagnetic covector potentials encoded within these symbols are the same,

(iii) their topological charges are the same,

(iv) their temporal charges are the same and

(v) they have the same spin structure.

The geometric and topological objects appearing in (i)–(v) in Theorems 4.6 and 4.7 will be introduced in Section 4.5 and examined further in Section 4.6. The proof of the above theorems will be given in Section 4.7.

The construction presented in Sections 4.5–4.7 is not straightforward and comes in several steps which combine techniques from differential geometry, algebraic topology and analysis of partial differential equations.

4.5 Invariant objects encoded within sesquilinear forms

4.5.1 Geometric objects

Let us first explain what makes the case (4.4.1) special.

We start by observing that having the weaker constraint

$$d = m^2 \tag{4.5.1}$$

already brings about important geometric consequences. Namely, under the condition (4.5.1) a manifold M admits a non-degenerate Hermitian first order sesquilinear form if and only if it is parallelisable. The proof of this statement retraces that of [7, Lemma 1.2].

Hence, without loss of generality, further on we assume that our manifold M is parallelisable. Without this assumption we would not have any non-degenerate Hermitian first order sesquilinear forms to work with.

Setting $m = 2$ and $d = 4$ has even more profound geometric consequences. Namely, observe that the determinant of the principal symbol is a quadratic form in momentum p:

$$\det \mathbf{S}_{\mathrm{prin}}(x,p) = -\mathbf{g}^{\alpha\beta}(x)\, p_\alpha p_\beta\,, \tag{4.5.2}$$

where $\mathbf{g}^{\alpha\beta}(x)$ is a real symmetric 4×4 matrix-function with values in 2-densities. More precisely, $\mathbf{g}$ is a rank two symmetric tensor density of weight two.

The quadratic form $\mathbf{g}^{\alpha\beta}$ has Lorentzian signature $(+,+,+,-)$ [55, Lemma 2.1]. This implies, in particular, that

$$\det \mathbf{g}^{\alpha\beta}(x) < 0, \qquad \forall x \in M.$$

Put

$$\rho(x) := (-\det \mathbf{g}^{\mu\nu}(x))^{1/6}. \tag{4.5.3}$$

The quantity (4.5.3) is a density. This observation allows us to define the Lorentzian metric

$$g^{\alpha\beta}(x) := (\rho(x))^{-2}\ \mathbf{g}^{\alpha\beta}(x). \tag{4.5.4}$$

Of course, formula (4.5.3) can now be rewritten in more familiar form as

$$\rho(x) = (-\det g_{\mu\nu}(x))^{1/2}.$$

We see that the case (4.4.1) is special in that there is a Lorentzian metric encoded within our sesquilinear form. This Lorentzian metric g is defined by the explicit formulae (4.5.4), (4.5.3), (4.5.2).

Let $g^{\alpha\beta}$ be the contravariant metric tensor encoded within the sesquilinear for S. Then the contravariant metric tensor $\widetilde{g}^{\alpha\beta}$ encoded within the sesquilinear form $\widetilde{S}$ defined by (4.3.2) is

$$\widetilde{g}^{\alpha\beta} = |\det G|^{-2/3}\, g^{\alpha\beta}. \tag{4.5.5}$$

We see that the metric transforms conformally under the action of G as in (4.3.1). In particular, it is invariant under (4.3.4).

The second geometric object encoded within our sesquilinear form is the electromagnetic covector potential. In order to single it out we first introduce the concept of covariant subprincipal symbol

$$\mathbf{S}_{\mathrm{csub}} := \mathbf{S}_{\mathrm{sub}} + \frac{i}{16}\,\mathbf{g}_{\alpha\beta}\{\mathbf{S}_{\mathrm{prin}}, \operatorname{adj}\mathbf{S}_{\mathrm{prin}}, \mathbf{S}_{\mathrm{prin}}\}_{p_\alpha p_\beta}, \tag{4.5.6}$$

where $\mathbf{g}_{\alpha\beta}$ is the inverse of $\mathbf{g}^{\alpha\beta}$,

$$\{F, G, H\} := F_{x^\alpha} G H_{p_\alpha} - F_{p_\alpha} G H_{x^\alpha}$$

is the generalised Poisson bracket on matrix-functions and adj is the operator of matrix adjugation

$$F = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \mapsto \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} =: \operatorname{adj} F.$$

We define the electromagnetic covector potential A as the — unique, due to (4.2.6) — real-valued solution of

$$\mathbf{S}_{\mathrm{csub}}(x) = \mathbf{S}_{\mathrm{prin}}(x, A(x)). \tag{4.5.7}$$

Note that (4.5.7) is a system of four linear algebraic equations for the four components of A.

Lemma 4.8. *The electromagnetic covector potential is given explicitly by the following formula*

$$A_\alpha = -\frac{1}{2}\, \mathbf{g}_{\alpha\beta} \operatorname{tr}\left([\mathbf{S}_{\mathrm{csub}}]\, [\operatorname{adj}(\mathbf{S}_{\mathrm{prin}})_{p_\beta}] \right). \tag{4.5.8}$$

Proof. In view of (4.5.2), multiplication of both sides of (4.5.7) by $\operatorname{adj}(\mathbf{S}_{\mathrm{prin}}(x,p))$ gives

$$\begin{aligned} [\mathbf{S}_{\mathrm{csub}}(x)]\, [\operatorname{adj}(\mathbf{S}_{\mathrm{prin}}(x,p))] &= [\mathbf{S}_{\mathrm{prin}}(x, A(x))]\, [\operatorname{adj}(\mathbf{S}_{\mathrm{prin}}(x,p)] \\ &= (-\mathbf{g}^{\mu\nu}(x)\, A_\mu(x)\, p_\nu)\, \mathrm{Id}. \end{aligned} \tag{4.5.9}$$

Differentiating both sides of (4.5.9) with respect to p_β, taking the matrix trace and lowering the index with the ((-2)-density valued) metric yields (4.5.8). □

Formulae (4.5.2), (4.5.6) and (4.5.7) tell us that the full symbol is completely determined by principal symbol and electromagnetic covector potential.

Lemma 4.9. *Let A be the electromagnetic covector potential encoded within the sesquilinear form S. Then the electromagnetic covector potential $\widetilde{A}$ encoded within the sesquilinear form $\widetilde{S}$ defined by* (4.3.2) *is*

$$\widetilde{A} = A + \frac{1}{2} \operatorname{grad}(\arg \det G). \tag{4.5.10}$$

Proof. From [55, formulae (5.1), (5.2), (D.4)–(D.6)] it follows that

$$\widetilde{\mathbf{S}}_{\mathrm{csub}} = G^* \mathbf{S}_{\mathrm{csub}} G - \mathbf{Q} - \mathbf{Q}^*, \tag{4.5.11}$$

with

$$\mathbf{Q} = -\frac{i}{8}\,\mathbf{g}_{\alpha\beta}\,G^*\,(\mathbf{S}_{\mathrm{prin}})_{p_\alpha}\,G_{x^\gamma}\,G^{-1}\,(\operatorname{adj}\mathbf{S}_{\mathrm{prin}})_{p_\beta}\,(\mathbf{S}_{\mathrm{prin}})_{p^\gamma}\,G. \tag{4.5.12}$$

The matrix-function G can be written locally as

$$G(x) = r(x)\,e^{i\varphi(x)}\,G_1(x), \tag{4.5.13}$$

where $r, \varphi : M \to \mathbb{R}$ and $G_1 : M \to SL(2,\mathbb{C})$ are smooth real and matrix-valued functions respectively. In particular, $\varphi(x) = \frac{1}{2}\arg\det G(x)$. From (4.5.13) we obtain

$$G_{x^\gamma}\,G^{-1} = (G_1)_{x^\gamma}\,G_1^{-1} + \frac{r_{x^\gamma}}{r}\,\mathrm{Id} + i\,\varphi_{x^\gamma}\,\mathrm{Id}\,. \tag{4.5.14}$$

The first term on the RHS of (4.5.14) is trace-free and hence, by [55, formula (C.1)], it does not contribute to (4.5.12). The second term is real, and, when multiplied by i, it does not contribute to $\mathbf{Q}+\mathbf{Q}^*$. Therefore, by substituting (4.5.14) into (4.5.12) and, in turn, (4.5.12) into (4.5.11), we obtain

$$\widetilde{\mathbf{S}}_{\mathrm{csub}} = G^*\mathbf{S}_{\mathrm{csub}}G + G^*(\mathbf{S}_{\mathrm{prin}})_{p^\gamma}\,\varphi_{x^\gamma}G, \tag{4.5.15}$$

from which (4.5.10) ensues. □

Remark 4.10. The use of the term 'electromagnetic covector potential' for the covector field A is motivated by the fact that this A is, in our context, a counterpart of what in gauge theory is a $U(1)$-connection, see formula (4.5.10).

4.5.2 Topological objects

As explained in the beginning of the previous subsection, our manifold M is *a priori* parallelisable, hence orientable. We specify an orientation on our manifold and define the topological charge of our sesquilinear form as

$$c_{\mathrm{top}} := -\frac{i}{2}\sqrt{-\det\mathbf{g}_{\alpha\beta}}\;\operatorname{tr}\big((\mathbf{S}_{\mathrm{prin}})_{p_1}(\mathbf{S}_{\mathrm{prin}})_{p_2}(\mathbf{S}_{\mathrm{prin}})_{p_3}(\mathbf{S}_{\mathrm{prin}})_{p_4}\big), \tag{4.5.16}$$

where tr stands for the matrix trace. Straightforward calculations show that the number c_{top} can take only two values, $+1$ or -1. It describes the orientation of the principal symbol relative to our chosen orientation of local coordinates $x = (x^1, x^2, x^3, x^4)$.

Our Lorentzian 4-manifold (M, g) does, in fact, possess an additional property: it is automatically time-orientable, i.e. it admits a timelike (co)vector field. Indeed, consider the quantity

$$f_x(p) := \frac{1}{\rho(x)} \operatorname{tr} \mathbf{S}_{\mathrm{prin}}(x, p).$$

We are looking at a linear map

$$f_x : T_x^* M \to \mathbb{R}, \qquad p \mapsto f_x(p),$$

depending smoothly on $x \in M$. Non-degeneracy of our principal symbol implies that

$$\operatorname{range} f_x \neq \{0\}, \qquad \forall x \in M.$$

By duality the linear map f_x can be represented in terms of a nonvanishing vector field t,

$$f_x(p) = t(p) = t^\alpha(x)\, p_\alpha\,,$$

which can be shown to be timelike.

Let us specify a time orientation by choosing a reference timelike covector field q. We define the temporal charge of our sesquilinear form as

$$c_{\mathrm{tem}} := \operatorname{sgn} t(q). \tag{4.5.17}$$

It describes the orientation of the principal symbol relative to our chosen time orientation.

Definition 4.11. Consider symbols corresponding to metrics from a given conformal class and with the same topological and temporal charges. We define *2-torsion* spin^c *structure* to be the equivalence class of symbols

$$[\mathbf{S}] = \{\widetilde{\mathbf{S}} \mid \widetilde{\mathbf{S}}_{\mathrm{prin}} = G^* \mathbf{S}_{\mathrm{prin}} G,\ G \in C^\infty(M, GL(m, \mathbb{C}))\}\,. \tag{4.5.18}$$

Definition 4.12. Consider symbols corresponding to a given metric and with the same topological and temporal charges. We define *spin structure* to be the equivalence class of symbols

$$[\mathbf{S}] = \{\widetilde{\mathbf{S}} \mid \widetilde{\mathbf{S}}_{\mathrm{prin}} = G^* \mathbf{S}_{\mathrm{prin}} G,\ G \in C^\infty(M, SL(m, \mathbb{C}))\}\,. \tag{4.5.19}$$

In the above definitions we use topological terminology, even though the definitions themselves are stated in a purely analytic fashion. A rigorous justification for this is provided in the next Section.

4.6 Transition from analysis to topology

The aim of this section is to perform an analysis of Definitions 4.11 and 4.12, so as to show that these analytic definitions are equivalent to standard topological ones. We will establish this equivalence by rewriting the principal symbol of a sesquilinear form in a way that is better suited for revealing topological content, see formula (4.6.1) below.

4.6.1 Framings and their equivalence

Let M be an oriented time-oriented Lorentzian 4-manifold. By a *frame* at a point $x \in M$ we mean a positively oriented and positively time-oriented orthonormal, in the Lorentzian sense, frame e_j, $j = 1, 2, 3, 4$, in the tangent space T_xM:

$$\det {e_j}^\alpha > 0, \qquad q(e^4) > 0,$$

$$g_{\alpha\beta}\,{e_j}^\alpha {e_k}^\beta = \begin{cases} 0 & \text{if} \quad j \neq k, \\ +1 & \text{if} \quad j = k \neq 4, \\ -1 & \text{if} \quad j = k = 4. \end{cases}$$

Here each vector e_j has coordinate components ${e_j}^\alpha$, $\alpha = 1, 2, 3, 4$. By a *framing* of M we mean a choice of frame at every point $x \in M$ depending smoothly on the point. Of course, the contravariant metric tensor is expressed via the framing as

$$g^{\alpha\beta} = {e_1}^\alpha {e_1}^\beta + {e_2}^\alpha {e_2}^\beta + {e_3}^\alpha {e_3}^\beta - {e_4}^\alpha {e_4}^\beta$$

and the Lorentzian density is expressed via the framing as $\rho = (\det {e_j}^\alpha)^{-1}$.

Let

$$s^1 = s_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad s^2 = s_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

$$s^3 = s_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad s^4 = -s_4 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

be the standard basis in the real vector space of 2×2 Hermitian matrices. Then the principal symbols of sesquilinear forms with $c_{\text{top}} = c_{\text{temp}} = +1$ are in one-to-one correspondence with framings. This correspondence is realised explicitly by the formula

$$\mathbf{S}_{\mathrm{prin}}(x,p) = \rho(x)\, s^j\, e_j{}^\alpha(x)\, p_\alpha\,. \tag{4.6.1}$$

The nondegeneracy condition (4.2.6) implies that the vector fields e_j, $j = 1,2,3,4$, are linearly independent. Moreover, they are automatically Lorentz-orthogonal with respect to the metric encoded within $\mathbf{S}_{\mathrm{prin}}$, see [7, Sections 1 and 2]. Thus, the e_j, $j = 1,2,3,4$, provide a framing. Observe that one can also argue the other way around: in view of (4.6.1) a framing completely determines the principal symbol.

The point of the above argument is that instead of working with an analytic object, a principal symbol, we can work with an equivalent geometric object, a framing.

In what follows $SO^+(3,1)$ denotes the identity component of the Lorentz group and $CSO^+(3,1)$ denotes its conformal extension. Here 'conformal extension' refers to multiplication of matrices from $SO^+(3,1)$ by arbitrary positive factors. The Lie group $SO^+(3,1)$ is 6-dimensional, so $CSO^+(3,1)$ is 7-dimensional. The conformal extension of the Lorentz group is needed because gauge transformations (4.3.2), (4.3.1) result in the scaling of the Lorentzian metric encoded within the principal symbol, see formula (4.5.5).

Let us now fix a conformal class of Lorentzian metrics and within this class choose a pair of principal symbols $\mathbf{S}_{\mathrm{prin}}$ and $\widetilde{\mathbf{S}}_{\mathrm{prin}}$. Let e_j and $\widetilde{e}_j$ be the corresponding framings. Then

$$\widetilde{e}_j = O_j{}^k\, e_k \tag{4.6.2}$$

for some uniquely defined smooth matrix-function $O : M \to CSO^+(3,1)$.

Suppose now that there exists a matrix-function $G : M \to GL(2,\mathbb{C})$ such that $\widetilde{\mathbf{S}}_{\mathrm{prin}} = G^*\, \mathbf{S}_{\mathrm{prin}} G$. A straightforward calculation shows that the matrix-function O appearing in (4.6.2) is expressed via G as

$$O_j{}^k = \frac{1}{2} |\det G|^{-4/3}\, \mathrm{tr}(s_j G^* s^k G). \tag{4.6.3}$$

It is convenient to define

$$\mathcal{G} := |\det G|^{2/3}\, G. \tag{4.6.4}$$

Of course, the above formula can be inverted:

$$G = |\det \mathcal{G}|^{-2/7}\, \mathcal{G}. \tag{4.6.5}$$

The advantage of working with the matrix-function

$$\mathcal{G} : M \to GL(2, \mathbb{C})$$

rather than the original matrix-function (4.3.1) is that formula (4.6.3) simplifies and reads now

$$O_j{}^k = \frac{1}{2}\,\mathrm{tr}(s_j \mathcal{G}^* s^k \mathcal{G}). \tag{4.6.6}$$

The switch from G to $\mathcal{G}$ does not affect the topological issues we are addressing, it just makes formulae simpler.

Observe that when $\mathcal{G} \in SL(2,\mathbb{C})$, (4.6.6) is the standard spin homomorphism formula which provides a map

$$\Pi : SL(2,\mathbb{C}) \longrightarrow SO^+(3,1), \quad \Pi(\mathcal{G}) = O. \tag{4.6.7}$$

When we allow $\mathcal{G}$ to take values in $GL(2,\mathbb{C})$, formula (4.6.6) gives us a map

$$\Pi : GL(2,\mathbb{C}) \longrightarrow CSO^+(3,1), \quad \Pi(\mathcal{G}) = O. \tag{4.6.8}$$

We are now in a position to rephrase Definitions 4.11 and 4.12 as follows.

Consider symbols corresponding to metrics from a given conformal class and with the same topological and temporal charges. We define *2-torsion* spin^c *structure* to be the equivalence class of symbols, where two symbols are called equivalent if the matrix-function O relating them, see (4.6.2), can be written in the form (4.6.6) for some $\mathcal{G} : M \to GL(2,\mathbb{C})$. In other words, the matrix-function $O : M \longrightarrow CSO^+(3,1)$ admits a factorisation

$$O : M \xrightarrow{\mathcal{G}} GL(2,\mathbb{C}) \xrightarrow{\Pi} CSO^+(3,1). \tag{4.6.9}$$

If the metric is the same, we define *spin structure* to be the equivalence class of symbols, where two symbols are called equivalent if the matrix-function O relating them can be written in the form (4.6.6) for some $\mathcal{G} : M \to SL(2,\mathbb{C})$.

Remark 4.13. It is easy to see that in the GL case the matrix-function $\mathcal{G}$, if it exists, is defined uniquely modulo multiplication by $e^{i\varphi}$, where φ is an arbitrary smooth real-valued scalar function. In the SL case the matrix-function $\mathcal{G}$, if it exists, is defined uniquely modulo multiplication by ± 1.

It follows from [7] that our definition of spin structure agrees with the accepted topological one[1]. In the remainder of this section we establish a similar result for 2-torsion spin^c structure.

Let us remind the reader that it follows from our assumptions (4.2.6) and (4.4.1) that M is a Lorentzian manifold which is parallelisable and time-orientable. In particular, it is spin. A choice of reference framing on M provides a trivialisation of the tangent bundle TM so that any other framing is related to this reference framing by a smooth function $O : M \to CSO^+(3,1)$. Two framings corresponding to functions O_1 and O_2 are equivalent in the above sense if and only if there exists a smooth function $\mathcal{G} : M \to GL(2,\mathbb{C})$ such that $O_2 \cdot (\Pi \circ \mathcal{G}) = O_1$ as functions $M \to CSO^+(3,1)$.

4.6.2 Topological characterisation

In this Section, we will characterise the equivalence relation we used to define the 2-torsion spin^c structures in purely topological terms. We begin by recalling that the compact subgroups $U(2) \subset GL(2,\mathbb{C})$ and $SO(3) \subset CSO^+(3,1)$ are deformation retracts of the respective non-compact Lie groups compatible with the map (4.6.8) in the sense that the following diagram commutes

$$\begin{array}{ccc} U(2) & \longrightarrow & GL(2,\mathbb{C}) \\ \Big\downarrow \mathrm{Ad} & & \Big\downarrow \Pi \\ SO(3) & \longrightarrow & CSO^+(3,1) \end{array} \tag{4.6.10}$$

Here we used the fact that the restriction of the map (4.6.8) to the subgroup $U(2)$ coincides with the adjoint map $\mathrm{Ad} : U(2) \longrightarrow SO(3)$. The two vertical arrows in this diagram are principal $U(1)$–bundles, the action being multiplication by a diagonal matrix; see Remark 4.13.

Lemma 4.14. *The principal $U(1)$–bundles*

$$U(2) \to SO(3) \quad \textit{and} \quad GL(2,\mathbb{C}) \to CSO^+(3,1)$$

[1] The map called $\mathrm{Ad} : SL(2,\mathbb{C}) \to SO^+(3,1)$ in [7] should in fact be understood as the spin homomorphism Π.

are non-trivial.

Proof. A principal bundle is known to be trivial if and only if it admits a section. Assuming that the bundle $U(2) \to SO(3)$ admits a section $s : SO(3) \to U(2)$, we immediately obtain a contradiction because the composition

$$H^2(SO(3);\mathbb{Z}) \xrightarrow{\mathrm{Ad}^*} H^2(U(2);\mathbb{Z}) \xrightarrow{s^*} H^2(SO(3);\mathbb{Z})$$

must be identity while $H^2(U(2);\mathbb{Z}) = \mathbb{Z}$ and $H^2(SO(3);\mathbb{Z}) = \mathbb{Z}/2$. The argument for the other bundle is similar. □

We will be mostly interested in the bundle $GL(2,\mathbb{C}) \to CSO^+(3,1)$. Given a map $f : M \to CSO^+(3,1)$, associate with it the cohomology class $\mathcal{O}(f) = f^*(1) \in H^2(M;\mathbb{Z})$, where $1 \in H^2(CSO^+(3,1);\mathbb{Z}) = \mathbb{Z}/2$ is the generator. Note that $\mathcal{O}(f)$ is an element of order at most two in $H^2(M;\mathbb{Z})$; in particular, it automatically vanishes whenever the group $H^2(M;\mathbb{Z})$ has no 2-torsion.

Proposition 4.15. *A map $f : M \to CSO^+(3,1)$ admits a factorisation (4.6.9) if and only if $\mathcal{O}(f) = 0$.*

Proof. We begin by constructing, for a given map $f : M \to CSO^+(3,1)$, the pull back principal bundle

$$\begin{array}{ccc} E(f) & \longrightarrow & GL(2,\mathbb{C}) \\ \downarrow \pi & & \downarrow \Pi \\ M & \xrightarrow{f} & CSO^+(3,1) \end{array}$$

where $E(f) = \{\,(x,p) \,|\, f(x) = \Pi(p)\,\} \subset M \times GL(2,\mathbb{C})$ and the maps $\pi : E(f) \to M$ and $E(f) \to GL(2,\mathbb{C})$ are projections onto the respective factors. It is well known (and can be checked by comparing the definitions) that $f : M \to CSO^+(3,1)$ admits a factorisation (4.6.9) if and only if the bundle $\pi : E(f) \to M$ admits a section. Since $\pi : E(f) \to M$ is a principal bundle it admits a section if and only if it is trivial. The latter happens if and only if the first Chern class $c_1(E(f)) \in H^2(M;\mathbb{Z})$ vanishes. Since c_1 is natural with respect to pull backs, $c_1(E(f))$ is the pul back via $f^* : H^2(CSO^+(3,1);\mathbb{Z}) \to H^2(M;\mathbb{Z})$ of the first Chern class of the bundle $GL(2,\mathbb{C}) \to CSO^+(3,1)$. According to Lemma 4.14, the latter bundle is non-trivial, hence its first Chern class must be the generator $1 \in H^2(CSO^+(3,1);\mathbb{Z}) = \mathbb{Z}/2$ and $c_1(E(f)) = f^*(1) = \mathcal{O}(f)$. □

Proposition 4.16. *Every element of $H^2(M;\mathbb{Z})$ of order two can be realised as $\mathcal{O}(f)$ for some map $f : M \to CSO^+(3,1)$.*

Proof. Let us consider the short exact sequence $0 \longrightarrow \mathbb{Z} \xrightarrow{\cdot 2} \mathbb{Z} \longrightarrow \mathbb{Z}/2 \longrightarrow 0$. The associated long exact sequence

$$\ldots \longrightarrow H^1(M;\mathbb{Z}/2) \xrightarrow{\partial} H^2(M;\mathbb{Z}) \xrightarrow{\cdot 2} H^2(M;\mathbb{Z}) \longrightarrow H^2(M;\mathbb{Z}/2) \longrightarrow \ldots$$

implies that every element $b \in H^2(M;\mathbb{Z})$ of order two belongs to the image of the Bockstein homomorphism $\partial : H^1(M;\mathbb{Z}/2) \longrightarrow H^2(M;\mathbb{Z})$. We will show that every cohomology class $a \in H^1(M;\mathbb{Z}/2)$ is of the form $a = f^*(1)$ for some $f : M \to SO^+(3,1)$ and $1 \in H^1(SO^+(3,1);\mathbb{Z}/2) = \mathbb{Z}/2$. The result will then follow from the commutative diagram

$$\begin{array}{ccc} H^1(SO^+(3,1);\mathbb{Z}/2) & \xrightarrow{\partial} & H^2(SO^+(3,1);\mathbb{Z}) \\ \downarrow f^* & & \downarrow f^* \\ H^1(M;\mathbb{Z}/2) & \xrightarrow{\partial} & H^2(M;\mathbb{Z}) \end{array} \tag{4.6.11}$$

whose upper row is an isomorphism, and the fact that $SO^+(3,1) \subset CSO^+(3,1)$ is a deformation retract.

Let us consider the double covering $SL(2,\mathbb{C}) \to SO^+(3,1)$ given by the spin homomorphism (4.6.7) and its associated fibration sequence (see, for instance, [47, Lemma 8.23])

$$\mathbb{Z}/2 \longrightarrow SL(2,\mathbb{C}) \longrightarrow SO^+(3,1) \longrightarrow K(\mathbb{Z}/2,1) \longrightarrow BSL(2,\mathbb{C}),$$

where $K(\mathbb{Z}/2,1)$ is the Eilenberg–MacLane space and $BSL(2,\mathbb{C})$ the classifying space of the Lie group $SL(2,\mathbb{C})$. It gives rise to the exact sequence of homotopy sets (see [47, Theorem 6.29])

$$[M, SO^+(3,1)] \longrightarrow H^1(M;\mathbb{Z}/2) \longrightarrow [M, BSL(2,\mathbb{C})]$$

using the fact that $H^1(M;\mathbb{Z}/2) = [M, K(\mathbb{Z}/2,1)]$. We wish to show that the first map in this sequence is surjective or, equivalently, that the second map is zero. Write $H^1(M;\mathbb{Z}/2) = [M,\mathbb{R}\mathrm{P}^\infty]$ using the homotopy equivalence between $K(\mathbb{Z}/2,1)$ and the real projective space $\mathbb{R}\mathrm{P}^\infty$. Also observe that, up to homotopy equivalence, $BSL(2,\mathbb{C}) = BSU(2) = \mathbb{H}\mathrm{P}^\infty$, the quaternionic projective space. Then the question becomes whether, for any continuous map $M \to \mathbb{R}\mathrm{P}^\infty$, the composition $M \to \mathbb{R}\mathrm{P}^\infty \to \mathbb{H}\mathrm{P}^\infty$ with the natural inclusion $\mathbb{R}\mathrm{P}^\infty \to \mathbb{H}\mathrm{P}^\infty$ is homotopic to zero. Since $\dim M = 4$ and the 5–skeleton of the CW–complex $\mathbb{H}\mathrm{P}^\infty$ is $\mathbb{H}\mathrm{P}^1 = S^4$, the cellular approximation theorem reduces this question to an identical question about the composition $M \to \mathbb{R}\mathrm{P}^4 \to S^4$. By the Hopf theorem, a map $M \to S^4$ is homotopic to zero if and only if the induced map $H^4(S^4;\mathbb{Z}) \to H^4(M;\mathbb{Z})$ is zero. In our case, this last map splits as the composition

$$H^4(S^4;\mathbb{Z}) \longrightarrow H^4(\mathbb{R}\mathrm{P}^4;\mathbb{Z}) \longrightarrow H^4(M;\mathbb{Z}),$$

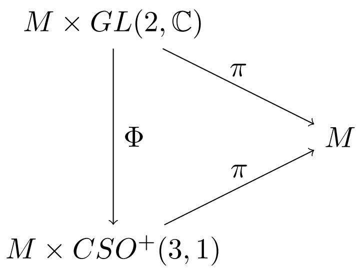
with $H^4(\mathbb{R}\mathrm{P}^4;\mathbb{Z}) = \mathbb{Z}/2$. Since M is orientable, $H^4(M;\mathbb{Z})$ is a free abelian group, hence the second map in this composition must vanish.

It is worth mentioning that the orientability of M in this argument is essential: in general, realisability of cohomology classes in $H^2(M;\mathbb{Z})$ can be obstructed by the non-trivial quadruple cup-product on $H^1(M;\mathbb{Z}/2)$. $\square$

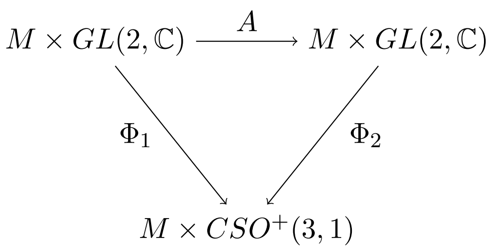
Corollary 4.17. *The set of 2-torsion* spin^c *structures on M is in a bijective correspondence with the 2-torsion subgroup of $H^2(M;\mathbb{Z})$.*

4.6.3 Differential geometric characterisation

Our goal in this Subsection is to identify the equivalence classes of framings with the 2-torsion spin^c structures on M, whose definition is modelled after that in Riemannian geometry [79]; see Remark 4.19 below. In the special case at hand, when the tangent bundle TM is trivialised via the reference frame, it reads as follows. A 2-torsion spin^c structure on M is an equivalence class of commutative diagrams



where π stands for the projection onto the first factor, and the map Φ is equivariant in that $\Phi(x,g) = \Phi(x,1) \cdot \Pi(g)$ for all $x \in M$ and $g \in GL(2,\mathbb{C})$. Two diagrams as above with the vertical maps Φ_1 and Φ_2 are called equivalent if there is a commutative diagram



such that $\pi \circ A = \pi$ and the map A is equivariant in that $A(x,g) = A(x,1) \cdot g$ for all $x \in M$ and $g \in GL(2,\mathbb{C})$.

Theorem 4.18. *For parallelisable time-orientable Lorentzian 4-manifolds, the equivalence classes of framings as above are in bijective correspondence with the 2-torsion* spin^c *structures.*

Proof. Using the commutativity of the first diagram, write $\Phi(x,g) = (x, \phi(x,g))$ for some function $\phi : M \times GL(2,\mathbb{C}) \to CSO^+(3,1)$ and observe that the equivariance condition on Φ translates into the equation $\phi(x,g) = \phi(x,1) \cdot \Pi(g)$. Therefore, the map Φ is uniquely determined by the map $\psi : M \to CSO^+(3,1)$ given by $\psi(x) = \phi(x,1)$.

Similarly, write $A(x,g) = (x, \alpha(x,g))$ and observe that the equivariance condition on A translates into the equation $\alpha(x,g) = \alpha(x,1) \cdot g$. Therefore, the map A is uniquely determined by the map $\beta : M \to GL(2,\mathbb{C})$ given by $\beta(x) = \alpha(x,1)$. One can easily check that the second commutative diagram then simply means that $\psi_2 \cdot \Pi(\beta) = \psi_1$ as functions $M \to CSO^+(3,1)$. □

Theorem 4.18 rigorously shows, in view of (4.6.1), the equivalence of two definitions of 2-torsion spin^c structure, the standard topological one and Definition 4.11. Note that the equivalence we established is not canonical in that it depends on the choice of reference frame.

Remark 4.19. It may be worth explaining the origin of the term '2-torsion spin^c structure'. Following the analogy with Riemannian geometry, one can define a spin^c structure on M as the equivalence class of lifts of the principal frame bundle of M to a $GL(2,\mathbb{C})$ bundle; even though the frame bundle of M is trivial, it may lift to a non-trivial $GL(2,\mathbb{C})$ bundle. Among these lifts is the lift to an $SL(2,\mathbb{C})$ bundle P associated with the spin structure on M. The bundle P must be trivial for topological reasons: it is classified by its second Chern class $c_2(P)$, and we know that $4c_2(P) = -p_1(TM) = 0 \in H^4(M;\mathbb{Z})$. As in the Riemannian case, one can use P to establish a bijective correspondence between spin^c structures on M and the group $H^2(M;\mathbb{Z})$. Under this correspondence, the spin^c structure corresponding to a cohomology class $a \in H^2(M;\mathbb{Z})$ lives in a Hermitian rank-two bundle with the first Chern class $c_1(P) + 2a = 2a \in H^2(M;\mathbb{Z})$. Since we restrict ourselves to trivial bundles, the class $2a$ must vanish. This means that $a \in H^2(M;\mathbb{Z})$ is a 2-torsion, hence the name of the corresponding spin^c structure.

4.7 Proofs of main theorems

4.7.1 Proof of Theorem 4.6

Necessity

Let us first show that conditions (i)–(v) of Theorem 4.6 are necessary.

(i) Formula (4.5.5) tells us that the conformal class of metrics is preserved under GL transformations, so condition (i) is necessary.

(ii) Lemma 4.9 tells us that condition (ii) is necessary.

(iii)-(iv) In order to deal with conditions (iii) and (iv) we observe that the two charges, topological (4.5.16) and temporal (4.5.17), can be expressed via the framing as

$$c_{\text{top}} = \operatorname{sgn} \det e_j{}^{\alpha}, \qquad c_{\text{tem}} = \operatorname{sgn} q(e^4).$$

We showed in Section 4.6 that under GL transformations the framing stays within the original connected component of the conformally extended Lorentz group, hence conditions (iii) and (iv) are necessary.

(v) As to the necessity of condition (v), it follows immediately from Definition 4.11.

Sufficiency

Let us now show that conditions (i)–(v) of Theorem 4.6 are sufficient.

We need to find a GL transformation which turns one full symbol into the other. As explained in Subsection 4.5.1, a full symbol is completely determined by principal symbol and electromagnetic covector potential. Thus, we need to find a GL transformation which turns one principal symbol into the other and one electromagnetic covector potential into the other.

Conditions (i) and (iii)–(v) ensure that we can find a matrix-function (4.3.1) which turns one principal symbol into the other, see formula (4.5.18). Remark 4.13 and formulae (4.6.4), (4.6.5) tell us that this matrix-function (4.3.1) is defined uniquely modulo multiplication by $e^{i\varphi}$, where φ is an arbitrary smooth real-valued scalar function. In view of condition (ii) this function φ can be chosen so as to turn one electromagnetic covector potential into the other.

All in all, we obtain a matrix-function G defined uniquely modulo multiplication by a constant $c \in \mathbb{C}$, $|c| = 1$. □

4.7.2 Proof of Theorem 4.7

The proof of Theorem 4.7 is similar to that of Theorem 4.6, with only two modifications.

- SL transformations preserve the metric, so the requirement is that the two metrics are the same as opposed to the two metrics being in the same conformal class.

- SL transformations preserve the electromagnetic covector potential, so the requirement is that the two electromagnetic covector potentials are the same as opposed to the two electromagnetic covector potentials being in the same cohomology class in $H^1_{\mathrm{dR}}(M)$.

  All in all, we obtain a matrix-function G defined uniquely modulo multiplication by ± 1. □

4.8 The 3-dimensional Riemannian case

Let us consider first order sesquilinear forms satisfying the additional assumption

$$\operatorname{tr} \mathbf{S}_{\mathrm{prin}}(x,p) = 0, \qquad \forall (x,p) \in T^*M. \tag{4.8.1}$$

In this setting it is natural to look at transformations of symbols generated by matrix-functions

$$G : M \to U(m) \tag{4.8.2}$$

or

$$G : M \to SU(m). \tag{4.8.3}$$

Of course, $U(m) \subset GL(m,\mathbb{C})$ and $SU(m) \subset SL(m,\mathbb{C})$, so (4.8.2) and (4.8.3) are special cases of (4.3.1) and (4.3.4) respectively. We are now more restrictive in our choice of matrix-functions G because we want to preserve condition (4.8.1).

It turns out that for sesquilinear forms with trace-free principal symbol one can perform a classification similar to that described in previous Sections. We list the main results below, skipping detailed proofs as these are modifications of arguments presented earlier in the Chapter.

Condition (4.5.1) is now replaced by

$$d = m^2 - 1. \tag{4.8.4}$$

Under the condition (4.8.4) a manifold M admits a non-degenerate Hermitian first order sesquilinear form with trace-free principal symbol if and only if it is parallelisable. So, as in the four dimensional case, without loss of generality we assume that our manifold is parallelisable.

In this Section we deal with the special case

$$d = 3, \qquad m = 2, \tag{4.8.5}$$

compare with (4.4.1). It is known [110, 74] that a 3-manifold is parallelisable if and only if it is orientable. Therefore, orientability is our only topological restriction on M.

Under the assumption (4.8.1) the non-degeneracy condition (4.2.6) is equivalent to the condition

$$\det \mathbf{S}_{\mathrm{prin}}(x,p) \neq 0, \qquad \forall (x,p) \in T^*M \setminus \{0\}. \tag{4.8.6}$$

But (4.8.6) is the standard ellipticity condition. Thus, we are led to consider formally self-adjoint elliptic first order sesquilinear forms S with trace-free principal symbols which act on sections of the trivial $\mathbb{C}^2$-bundle over a connected smooth oriented 3-manifold M without boundary.

We define $\mathbf{g}^{\alpha\beta}(x)$ via (4.5.2). The quadratic form $\mathbf{g}^{\alpha\beta}$ is positive definite, a fact which implies, in particular, that

$$\det \mathbf{g}^{\alpha\beta}(x) > 0, \qquad \forall x \in M.$$

Put

$$\rho(x) := (\det \mathbf{g}^{\mu\nu}(x))^{1/4}. \tag{4.8.7}$$

The quantity (4.8.7) is a density. This observation allows us to define the Riemannian metric

$$g^{\alpha\beta}(x) := (\rho(x))^{-2}\, \mathbf{g}^{\alpha\beta}(x).$$

Of course, formula (4.8.7) can now be rewritten in more familiar form as $\rho(x) = (\det g_{\mu\nu}(x))^{1/2}$. And it is easy to see that our metric tensor is invariant under transformations (4.3.2), (4.8.2).

We define the covariant subprincipal symbol in accordance with formula (4.5.6). The magnetic covector potential $A = (A_1, A_2, A_3)$ and electric potential A_4 are defined as the solution of

$$\mathbf{S}_{\mathrm{csub}}(x) = \mathbf{S}_{\mathrm{prin}}(x, A(x)) + A_4\, \mathrm{Id}\,,$$

compare with (4.5.7). For the magnetic potential we still have the explicit formula (4.5.8) and for the electric potential we have

$$A_4 = \frac{1}{2}\,\operatorname{tr}\mathbf{S}_{\mathrm{csub}}\,.$$

The full symbol is completely determined by principal symbol, magnetic covector potential and electric potential. The electric potential is invariant under transformations (4.3.2), (4.8.2), whereas the magnetic covector potential transforms in accordance with formula (4.5.10).

We specify an orientation on our manifold and define the topological charge of our sesquilinear form as

$$c_{\mathrm{top}} := -\frac{i}{2}\sqrt{\det \mathbf{g}_{\alpha\beta}}\,\operatorname{tr}\big((\mathbf{S}_{\mathrm{prin}})_{p_1}(\mathbf{S}_{\mathrm{prin}})_{p_2}(\mathbf{S}_{\mathrm{prin}})_{p_3}\big) = \operatorname{sgn}\det {e_j}^{\alpha}, \tag{4.8.8}$$

compare with (4.5.16).

Definition 4.20. Consider symbols corresponding to a given metric and with the same topological charge. We define *2-torsion* spin^c *structure* to be the equivalence class of symbols

$$[\mathbf{S}] = \{\widetilde{\mathbf{S}} \mid \widetilde{\mathbf{S}}_{\mathrm{prin}} = G^*\mathbf{S}_{\mathrm{prin}}G,\ G \in C^\infty(M, U(2))\}\,. \tag{4.8.9}$$

Definition 4.21. Consider symbols corresponding to a given metric and with the same topological charge. We define *spin structure* to be the equivalence class of symbols

$$[\mathbf{S}] = \{\widetilde{\mathbf{S}} \mid \widetilde{\mathbf{S}}_{\mathrm{prin}} = G^*\mathbf{S}_{\mathrm{prin}}G,\ G \in C^\infty(M, SU(2))\}\,. \tag{4.8.10}$$

Our analytic definition of 2-torsion spin^c structure in dimension three, Definition 4.20, is equivalent to the standard topological one. This follows by the argument of Section 4.6.2 and Section 4.6.3 once the map $GL(2,\mathbb{C}) \to CSO^+(3,1)$ is replaced by the map $U(2) \to SO(3)$. Our analytic definition of spin structure in dimension three, Definition 4.21, is also equivalent to the standard topological one, which follows from [7] with the help of Diagram 4.6.10.

We define U-equivalence and SU-equivalence of symbols as in Definition 4.4, replacing (4.3.1) by (4.8.2) and (4.8.3) respectively.

We have the following analogues of Theorems 4.6 and 4.7.

Theorem 4.22. *Two full symbols* $\mathbf{S}_{\mathrm{full}}(x,p)$ *and* $\widetilde{\mathbf{S}}_{\mathrm{full}}(x,p)$ *are* U-equivalent *if and only if*

(i) the metrics encoded within these symbols are the same,

(ii) the electric potentials encoded within these symbols are the same,

(iii) the magnetic covector potentials encoded within these symbols belong to the same cohomology class in $H^1_{\mathrm{dR}}(M)$,

(iv) their topological charges are the same and

(v) they have the same 2-torsion spin^c *structure.*

Theorem 4.23. *Two full symbols* $\mathbf{S}_{\mathrm{full}}(x,p)$ *and* $\widetilde{\mathbf{S}}_{\mathrm{full}}(x,p)$ *are* SU-equivalent *if and only if*

(i) the metrics encoded within these symbols are the same,

(ii) the electric potentials encoded within these symbols are the same,

(iii) the magnetic covector potentials encoded within these symbols are the same,

(iv) their topological charges are the same and

(v) they have the same spin structure.

4.8.1 Explicit examples

To conclude this Section, let us examine two explicit examples. The first one illustrates how topological obstructions may arise when classifying symbols in accordance with (4.8.9), the second demonstrates the difference between spin and spin^c.

The Lie group $SO(3)$

Let $M = SO(3)$. We claim that $SO(3)$ has more than one 2-torsion spin^c structure. This follows from Corollary 4.17 and the non-vanishing of the group $H^2(SO(3);\mathbb{Z})$ but can also be seen directly as follows. With reference to Section 4.6.2, consider the identity map

$$\mathrm{Id} : M \to SO(3).$$

The map Id does not lift to a map $SO(3) \to U(2)$, namely, there does not exist a map $s : SO(3) \to U(2)$ such that the diagram

$$\begin{array}{ccc} & & U(2) \\ & \overset{s}{\nearrow} & \downarrow \pi \\ SO(3) & \xrightarrow{\text{Id}} & SO(3) \end{array}$$

commutes. A cohomological argument can be found in the proof of Lemma 4.14. Another way to see this is as follows. Let us restrict ourselves to $SU(2)$ matrices with zero trace. These matrices form a sphere $S^2 \subset SU(2)$, which can also be viewed as the conjugacy class of $\text{diag}(i, -i) \in SU(2)$. Explicitly, the matrices in S^2 are of the form

$$A = \begin{pmatrix} ia & b + ic \\ -b + ic & -ia \end{pmatrix},$$

where a, b, and c are real numbers such that $a^2 + b^2 + c^2 = 1$. The adjoint representation sends matrices A and $-A \in S^2$ to the same matrix, giving rise to the double covering $S^2 \to \mathbb{R}\mathrm{P}^2$ of the real projective plane. We shall show that the bundle $U(2) \to SO(3)$ does not admit a section even over the subset $\mathbb{R}\mathrm{P}^2 \subset \mathrm{SO}(3)$. The issue one encounters with finding such a section is adjusting for the signs of $SU(2)$ matrices in S^2 mapping to the same matrix in $\mathbb{R}\mathrm{P}^2$. To make this adjustment, we need to find a continuous function $h : S^2 \to U(1)$ such that $h(-x) = -h(x)$, where $-x$ stands for the antipodal map on the sphere. If such a function h existed, its composition with the standard inclusion $U(1) \to \mathbb{R}^2$ would give rise to a function $f : S^2 \to \mathbb{R}^2$ with the property that $f(-x) = -f(x)$. However, such a function does not exist by the Borsuk–Ulam theorem [64, Theorem 1.10]: the Borsuk–Ulam theorem states that, for any continuous function $f : S^2 \to \mathbb{R}^2$, there exists $x \in S^2$ such that $f(-x) = f(x)$. Combined with $f(-x) = -f(x)$, this means that $f(x) = 0$ for some x, which contradicts the fact that the image of f belongs to the unit circle.

In fact, one can show that $SO(3)$ has precisely two distinct 2-torsion spin^c structures and precisely two distinct spin structures because $H^2(SO(3); \mathbb{Z}) = \mathbb{Z}/2$ and $H^1(SO(3); \mathbb{Z}/2) = \mathbb{Z}/2$. In this particular case, spin^c and spin structures are matched via the Bockstein isomorphism $H^1(SO(3);\mathbb{Z}/2) \to H^2(SO(3);\mathbb{Z})$, cf. Diagram (4.6.11).

The 3-torus

Let $M = \mathbb{T}^3$ be the 3-dimensional torus parameterised by $\bmod 2\pi$ coordinates x^α, $\alpha = 1, 2, 3$. Put

$$\mathbf{S}(x,p) = \mathbf{S}_{\text{prin}}(x,p) := \begin{pmatrix} p_3 & p_1 - ip_2 \\ p_1 + ip_2 & -p_3 \end{pmatrix},$$

$$\widetilde{\mathbf{S}}(x,p) = \widetilde{\mathbf{S}}_{\text{prin}}(x,p) := \begin{pmatrix} p_3 & e^{ix^3}(p_1 - ip_2) \\ e^{-ix^3}(p_1 + ip_2) & -p_3 \end{pmatrix}.$$

We have

$$\det \mathbf{S}_{\text{prin}}(x,p) = \det \widetilde{\mathbf{S}}_{\text{prin}}(x,p) = -\left(p_1^2 + p_2^2 + p_3^2\right),$$

which means that the metric encoded within the symbols $\mathbf{S}$ and $\widetilde{\mathbf{S}}$ is the same, namely, the Euclidean metric. Furthermore, the topological charge (4.8.8) encoded within the symbols $\mathbf{S}$ and $\widetilde{\mathbf{S}}$ is the same, $+1$. Do these symbols have the same spin^c structure? The answer is yes, because if we take

$$G(x) = \begin{pmatrix} e^{-ix^3} & 0 \\ 0 & 1 \end{pmatrix} \in C^\infty(M, U(2))$$

we get

$$\widetilde{\mathbf{S}}_{\text{prin}} = G^* \mathbf{S}_{\text{prin}} G. \tag{4.8.11}$$

However, it is easy to see that there does not exist an $G \in C^\infty(M, SU(2))$ which would give (4.8.11), so our two symbols, $\mathbf{S}$ and $\widetilde{\mathbf{S}}$, have different spin structure.

In fact, it follows from Corollary 4.17 that the 3-torus has a unique 2-torsion spin^c structure because the cohomology group $H^2(\mathbb{T}^3;\mathbb{Z}) = \mathbb{Z}^3$ has no 2-torsion, but it has eight distinct spin structures because the cohomology group $H^1(\mathbb{T}^3;\mathbb{Z}/2) = (\mathbb{Z}/2)^3$ has eight elements.

4.9 Sesquilinear forms vs linear operators

Having developed our theory, we are now in a position to connect the motivational ideas outlined in the Section 4.1 with the theory of partial differential equations.

Consider an Hermitian first order sequilinear form of the type (4.2.2) on the infinite-dimensional vector space $C_0^\infty(M;\mathbb{C}^2)$.

4.9.1 Four-dimensional case

In dimension $d=4$, introduce an inner product

$$\langle u,v\rangle := \int_M u^* B v \,\rho\,\mathrm{d}x\,, \tag{4.9.1}$$

where B is some positive definite Hermitian 2×2 matrix-function and ρ is the Lorentzian density defined as in Subsection 4.5.1. Our first order Hermitian sesquilinear form S and inner product (4.9.1) define a formally self-adjoint first order linear differential operator L. The problem here is that it is impossible to choose B so as to have

$$G^*BG=B, \qquad \forall G\in GL(2,\mathbb{C})$$

or even

$$G^*BG=B, \qquad \forall G\in SL(2,\mathbb{C}),$$

i.e. one cannot introduce an inner product compatible with our gauge transformations. Hence, in the 4-dimensional case the construction presented above defines a linear field equation but not a linear operator.

4.9.2 Three-dimensional case

Working in dimension $d=3$ and within the framework of Section 4.8 (see, in particular, formulae (4.8.1)–(4.8.3)), introduce the inner product

$$\langle u,v\rangle := \int_M u^* v \,\rho\,\mathrm{d}x\,, \tag{4.9.2}$$

where ρ is the Riemannian density encoded within our sesquilinear form in accordance with formulae (4.5.2) and (4.8.7). Now (4.9.2) is compatible with our gauge transformations. Hence, in the 3-dimensional case our construction defines a formally self-adjoint elliptic first order linear differential operator.

4.10 Applications

In dimension $d = 4$ a distinguished physically meaningful sesquilinear form is the *Weyl form*. It is defined by the condition that the electromagnetic covector potential is zero. The gauge group is $SL(2,\mathbb{C})$. One cannot use here the gauge group $GL(2,\mathbb{C})$ because the electromagnetic covector potential is not invariant under the action of this group, see Lemma 4.9. The corresponding linear field equation is called *Weyl's equation*, the accepted mathematical model for the massless neutrino in curved spacetime. The condition $A = 0$ translates, in physical terms, into the neutrino having no electric charge and, therefore, not interacting with the electromagnetic field.

In dimension $d = 3$ and under the assumption (4.8.1) a distinguished physically meaningful sesquilinear form is the *massless Dirac form*. It is defined by the condition that the electric potential and magnetic covector potential are both zero. By analogy with the previous paragraph, the gauge group here is $SU(2)$ and one cannot use $U(2)$ because the magnetic covector potential is not invariant under the action of the latter. The corresponding linear differential operator is the massless Dirac operator, studied in Chapter 3.

Chapter 5

Lorentzian elasticity

5.1 Introduction

The aim of this Chapter is to propose a new mathematical model for a class of field theories in the Lorentzian setting. Inspired by the classical theory of elasticity (see, e.g., [43, 44]), we construct a Lagrangian out of a pair of metrics related by a spacetime diffeomorphism, which, in turn, represents the unknown of our model. The variation of our Lagrangian under the volume preservation condition produces a system of nonlinear partial differential equations, the field equations, whose analysis constitutes the main subject of the Chapter.

Our work possesses several elements of novelty. Firstly, in spite of relying on ideas from Riemannian elasticity, our theory is fully Lorentzian in that it deals with diffeomorphisms of the whole spacetime into itself, giving detailed account of the issues arising due to the indefinite signature. Secondly, our model incorporates a volume preservation condition into a theory of elasticity, leading to interesting mathematical consequences. Thirdly, we suggest new techniques for solving nonlinear PDEs, ones of possibly broader relevance. Lastly, our construction gives rise to solutions that appear to be physically meaningful, with potential applications in the realm of theoretical and particle physics.

For the case of Minkowski spacetime, we provide two classes of explicit solutions, massless and massive, which, at least at a formal level, offer a natural physical interpretation in terms of elementary particles, namely, neutrino/antineutrino and electron/positron. Our massive solution contains two free parameters. Even though these parameters can be interpreted as quantum mechanical mass and electric charge, our model does not allow for their values to be determined. We attribute this to the large number of symmetries implicitly present in our theory. One would hope that appropriate symmetry breaking could overcome this shortcoming of our mathematical model.

Our model is, effectively, a nonlinear version of Maxwell's theory. The only dimensional parameter is the speed of light: it is encoded in the Minkowski metric when we consider the case of flat spacetime. All other parameters are dimensionless and are contained in our Largrangian.

We develop our theory in dimension $d = 4$ and for pseudo-Riemannian manifolds of Lorentzian signature. In principle, neither assumption is necessary for its formulation. However, the physical conclusions we derive are specific to dimension $3 + 1$. In particular, dimension $3 + 1$ appears to be the lowest in which one observes propagating massless solutions.

This Chapter is structured as follows. In Section 5.2 we present the mathematical formulation of our model. In Section 5.3 we derive the corresponding nonlinear field equations, accounting for the volume preservation condition. Section 5.4 is devoted to discussing the role of displacements and rotations; in particular, we perform a detailed analysis of the deformation gradient in terms of its Lorentzian polar decomposition. Section 5.5 contains our first main result: the linearised field equations and their connection with Maxwell's equations. For Ricci-flat Lorentzian manifolds our model gives, in the linear approximation, Maxwell's equations in the Lorenz gauge with exact current. In Sections 5.6 and 5.7 we introduce the concept of homogeneous diffeomorphism and special subgroups of the Poincaré group respectively. These represent the group-theoretic tools which lie at the foundation of our construction of solutions to nonlinear PDEs. Explicit solutions for Minkowski spacetime are presented in Sections 5.8 and 5.9. Massless solutions described in Section 5.8 come into two types: right-handed and left-handed. Massive solutions described in Section 5.9 contain two free parameters: a positive parameter which has the geometric meaning of quantum mechanical mass and a real parameter which may be interpreted as electric charge. Finally, in Section 5.10 and Section 5.11 we present a formal argument, showing that our massless and massive solutions can be associated with spinors satisfying the massless and massive Dirac equations respectively. This constitutes the first step towards possible future applications of our model in theoretical and particle physics. In order to make the presentation smoother, we have moved notation and auxiliary technical results into Appendices D.1–D.4.

5.2 Mathematical model

Let M be a connected 4-manifold. Local coordinates on M will be denoted by $x = (x^1, x^2, x^3, x^4)$ or $y = (y^1, y^2, y^3, y^4)$.

We assume that our manifold M is equipped with Lorentzian metric g with signature $+++-$. Throughout this Chapter the metric g is assumed to be prescribed.

The unknown quantity in our mathematical model is a diffeomorphism $\phi : M \to M$. We will denote the group of diffeomorphisms by $\mathrm{Diff}(M)$.

Let us introduce a new (perturbed) Lorentzian metric h defined as the pullback of g via ϕ, $h := \phi^* g$. In local coordinates this new metric is written as follows. Take an arbitrary point $P \in M$ and choose local coordinates x and y in the neighbourhoods of P and $\phi(P)$ respectively. Our diffeomorphism ϕ can then be written locally as

$$y = \phi(x). \tag{5.2.1}$$

The new metric tensor reads

$$h_{\alpha\beta}(x) := g_{\mu\nu}(\phi(x)) \frac{\partial \phi^\mu}{\partial x^\alpha} \frac{\partial \phi^\nu}{\partial x^\beta} \,. \tag{5.2.2}$$

The $g_{\mu\nu}$ in the RHS of (5.2.2) is the representation of the metric tensor g in local coordinates y. The metric h describes the interval between points of the deformed continuum.

Having at our disposal two Lorentzian metrics, g and h, we can now write down an action. To this end, let us first introduce some definitions.

Definition 5.1. The tensor

$$S^\alpha{}_\beta(x) := [g^{\alpha\gamma}(x)]\,[h_{\gamma\beta}(x)] - \delta^\alpha{}_\beta \tag{5.2.3}$$

is called *strain*.

The concept of strain tensor originates from the papers of Cauchy [38, 39]. The strain tensor describes, pointwise, a linear map in the fibres of the tangent bundle,

$$v^\alpha \mapsto S^\alpha{}_\beta\, v^\beta. \tag{5.2.4}$$

The linear algebraic motivation for the introduction of the map (5.2.4) is given in Appendix D.2.1.

Let us now construct scalars out of a strain tensor. This can be done in many different ways but only four, at most, will be independent. An arbitrary scalar can be expressed, possibly in a nonlinear fashion, via the four chosen independent scalars. The obvious way of choosing four independent scalars is $\operatorname{tr}(S^k)$, $k = 1, 2, 3, 4$, but such a choice is inconvenient as it would make subsequent calculations cumbersome. The most convenient choice of four scalar invariants is

$$e_1(\phi) := \operatorname{tr} S, \tag{5.2.5a}$$

$$e_2(\phi) := \frac{1}{2}\left[(\operatorname{tr} S)^2 - \operatorname{tr}(S^2)\right], \tag{5.2.5b}$$

$$e_3(\phi) := \operatorname{tr}\operatorname{adj} S, \tag{5.2.5c}$$

$$e_4(\phi) := \det S. \tag{5.2.5d}$$

Here tr is the matrix trace and adj is the operator of matrix adjugation from linear algebra.

The reasoning behind the particular choice (5.2.5a)–(5.2.5d) becomes clear if we rewrite these invariants in terms of the eigenvalues of strain. The strain tensor (5.2.3), viewed as a linear operator (5.2.4) acting in $\mathbb{C}^4$ has eigenvalues λ_k, $k = 1, 2, 3, 4$, enumerated with account of their algebraic multiplicity. Note that some eigenvalues may be complex, in which case they come in complex conjugate pairs. It is easy to see that formulae (5.2.5a)–(5.2.5d) can be rewritten as

$$e_1(\phi) = \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4\,, \tag{5.2.6a}$$

$$e_2(\phi) = \lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_1\lambda_4 + \lambda_2\lambda_3 + \lambda_2\lambda_4 + \lambda_3\lambda_4\,, \tag{5.2.6b}$$

$$e_3(\phi) = \lambda_1\lambda_2\lambda_3 + \lambda_1\lambda_2\lambda_4 + \lambda_1\lambda_3\lambda_4 + \lambda_2\lambda_3\lambda_4\,, \tag{5.2.6c}$$

$$e_4(\phi) = \lambda_1\lambda_2\lambda_3\lambda_4\,. \tag{5.2.6d}$$

The advantage of choosing scalar invariants in this particular way is that the polynomials appearing in the right-hand sides of formulae (5.2.6a)–(5.2.6d) are elementary symmetric polynomials.

Note that our scalars e_k are spectral invariants: we are looking at quantities that are determined by the spectrum of the linear map (5.2.4). Our definition of scalar invariants is similar to that in [108, (3.56)], the only difference being that we have four scalar invariants instead of three — a consequence of us adopting a 4-dimensional relativistic approach.

Our action then is

$$\mathcal{J}(\phi) := \int_M \mathcal{L}\big(e_1(\phi), e_2(\phi), e_3(\phi), e_4(\phi)\big) \sqrt{-\det g_{\mu\nu}(x)}\, \mathrm{d}x\,, \tag{5.2.7}$$

where $\mathcal{L}$ is some prescribed smooth real-valued function of four real variables such that $\mathcal{L}(0,0,0,0) = 0$ and $\mathrm{d}x := \mathrm{d}x^1\mathrm{d}x^2\mathrm{d}x^3\mathrm{d}x^4$. Variation of (5.2.7) with respect to the unknown diffeormorphism $\phi \in \mathrm{Diff}(M)$ generates field equations which can be thought of as a Lorentzian version of nonlinear elasticity.

The physical assumptions underlying our choice of action (5.2.7) are isotropy and homogeneity of our 4-dimensional continuum. Isotropy is expressed mathematically in that the integrand $\mathcal{L}$ in (5.2.7) is a symmetric function of the eigenvalues of the map (5.2.4). Homogeneity is expressed mathematically in that the integrand $\mathcal{L}$ in (5.2.7) does not depend explicitly on x.

Two important examples of Lagrangians are given below.

Example 5.2 (Linear Lagrangian)**.** *The unique, up to rescaling, Lagrangian linear in strain is*

$$\mathcal{L}(e_1, e_2, e_3, e_4) = e_1. \tag{5.2.8}$$

This is the action of a harmonic map, see [53, 14], the only difference being that here the metric has Lorentzian signature.

Example 5.3 (Quadratic Lagrangian)**.** *The general form of a Lagrangian quadratic (homogeneous of degree two) in strain is*

$$\mathcal{L}(e_1, e_2, e_3, e_4) = \alpha(e_1)^2 + \beta\, e_2\,, \tag{5.2.9}$$

where $\alpha, \beta \in \mathbb{R}$ are parameters. In the 3-dimensional Riemannian setting the above Lagrangian is used in the theory of elasticity: it describes a static isotropic homogeneous elastic continuum that is physically linear but geometrically nonlinear. The *standard assumption in elasticity theory is*

$$\beta \neq 0. \tag{5.2.10}$$

Under the assumption (5.2.10) *the Lagrangian* (5.2.9) *contains, up to rescaling, only one dimensionless parameter,* α/β*. In elasticity theory the parameters* $\lambda = 2\alpha + \beta$ *and* $\mu = -\beta/2$ *are called* Lamé parameters *and the parameter* $\nu = \frac{2\alpha+\beta}{4\alpha+\beta}$ *is called* Poisson's ratio.

Remark 5.4. Our mathematical model does not involve the concepts of connection and curvature. Moreover, it is easy to see that if the unperturbed metric g is flat then the perturbed metric h is flat as well. Our model is quite different from those commonly used in theories of bimetric gravity [100, 48, 63, 105], even though the mathematical formalism is somewhat similar.

Field equations for the action (5.2.7) are not the equations that we will be studying. We choose to impose, in addition, the volume preservation constraint

$$\det g_{\alpha\beta}(x) = \det h_{\mu\nu}(x). \tag{5.2.11}$$

In other words, we choose to restrict our analysis to the subgroup of volume-preserving diffeomorphisms $\mathrm{Diff}_\rho(M) \subset \mathrm{Diff}(M)$. Here

$$\rho(x) := \sqrt{-\det g_{\alpha\beta}(x)} \tag{5.2.12}$$

is the Lorentzian density of the unperturbed metric.

The condition for a diffeomorphism to be volume preserving reads, locally,

$$\rho(x) = \rho(\phi(x)) \left| \det \left(\frac{\partial \phi^\alpha}{\partial x^\beta} \right) \right| . \tag{5.2.13}$$

The ρ in the LHS of (5.2.13) is the representation of the density ρ in local coordinates x, whereas the ρ in the RHS of (5.2.13) is the representation of the density ρ in local coordinates y.

The idea of imposing the volume preservation condition (5.2.11) is not new. For instance, it appears in unimodular theories of gravity, see [57, 29].

In spectral-theoretic fashion, the volume preservation constraint (5.2.11) can be equivalently rewritten as

$$e_1(\phi) + e_2(\phi) + e_3(\phi) + e_4(\phi) = 0\,. \tag{5.2.14}$$

Formula (5.2.14) allows us to express one of the four scalar invariants via the other three. It is convenient to express e_1 via e_2, e_3 and e_4. Then our action (5.2.7) takes the form

$$J(\phi) = \int_M L\big(e_2(\phi), e_3(\phi), e_4(\phi)\big)\, \rho(x)\, \mathrm{d}x\,, \tag{5.2.15}$$

where

$$L(e_2, e_3, e_4) = \mathcal{L}(-e_2 - e_3 - e_4, e_2, e_3, e_4). \tag{5.2.16}$$

Our mathematical model is formulated as follows: vary the action (5.2.15) over volume preserving diffeomorphisms $\mathrm{Diff}_\rho(M)$ and seek critical points. The L appearing in formula (5.2.15) is some prescribed smooth real-valued function of three real variables which characterises the physical properties of our 4-dimensional isotropic homogeneous continuum.

We shall now impose two conditions on the choice of the Lagrangian L.

Condition 1 We assume that

$$\left.\frac{\partial L}{\partial e_2}\right|_{e_2=e_3=e_4=0} \ne 0, \tag{5.2.17a}$$

which is the minimal non-degeneracy condition. This will be required in Section 5.5 where we will show that in a Ricci-flat spacetime our linearised field equations reduce to Maxwell's equations. Without loss of generality we assume further on that

$$\left.\frac{\partial L}{\partial e_2}\right|_{e_2=e_3=e_4=0} = -1, \tag{5.2.17b}$$

which can always be achieved by rescaling.

Condition 2 We assume that the function of one variable $L(e_2, 0, 0)$ has a critical point on the positive real axis:

$$\left.\frac{\partial L}{\partial e_2}\right|_{e_2=c,\ e_3=e_4=0} = 0 \quad \text{for some} \quad c > 0. \tag{5.2.18}$$

This will be required in Section 5.9 where we will construct explicit massive solutions of our nonlinear field equations in Minkowski spacetime.

Example 5.5 (Examples 5.2 and 5.3 continued)**.** *For the Lagrangian* (5.2.16)*,* (5.2.8) *we get precisely* (5.2.17b)*, whereas for the Lagrangian* (5.2.16)*,* (5.2.9) *we get*

$$\left.\frac{\partial L}{\partial e_2}\right|_{e_2=e_3=e_4=0} = \beta,$$

so condition (5.2.17a) is satisfied when we have (5.2.10).

As to condition (5.2.18), it is not satisfied for the Lagrangian (5.2.16), (5.2.8), whereas for the Lagrangian (5.2.16), (5.2.9) it is satisfied if and only if $\alpha\beta < 0$.

5.3 Nonlinear field equations

Recall that the action in our mathematical model is defined by formula (5.2.15). Our field equations are obtained by varying this action with respect to the unknown diffeomorphism ϕ subject to the volume preservation constraint (5.2.11).

In order to write down the field equations let us initially disregard the constraint (5.2.11) and argue along the lines of [73, Chapter 8]. In local coordinates our action (5.2.15) can be written as

$$J(\phi) = \int f\left(x^\alpha, \phi^\beta, \frac{\partial \phi^\gamma}{\partial x^\kappa}\right) \rho(x)\,\mathrm{d}x\,, \tag{5.3.1}$$

where ϕ^β is the local representation (5.2.1) of our diffeomorphism and f is some function of x, $\phi(x)$ and the first partial derivatives of $\phi(x)$. We vary $\phi(x)$ as

$$\phi^\beta(x) \mapsto \phi^\beta(x) + \Delta\phi^\beta(x), \tag{5.3.2}$$

where $\Delta\phi^\beta(x)$ is a small smooth perturbation with small compact support. Standard variational arguments involving integration by parts give us the variation of (5.3.1) in the form

$$\Delta J(\phi) = \int E_\lambda\left(x^\alpha, \phi^\beta, \frac{\partial \phi^\gamma}{\partial x^\kappa}, \frac{\partial^2 \phi^\sigma}{\partial x^\mu \partial x^\nu}\right) \Delta\phi^\lambda\,\rho(x)\,\mathrm{d}x\,. \tag{5.3.3}$$

The quantity E_λ appearing in the RHS of (5.3.3) is a two-point tensor: it behaves as a scalar under changes of local coordinates x and as a covector under changes of local coordinates y. Hence,

$$\phi \mapsto E_\lambda\left(x^\alpha, \phi^\beta, \frac{\partial \phi^\gamma}{\partial x^\kappa}, \frac{\partial^2 \phi^\sigma}{\partial x^\mu \partial x^\nu}\right) \tag{5.3.4}$$

is an invariantly defined map from diffeomorphisms to covector fields.

We write the RHS of (5.3.4) in concise form as $E(\phi)$. Thus, the field equations for the unconstrained action (5.2.15) read

$$E(\phi) = 0. \tag{5.3.5}$$

This is a system of four nonlinear second order partial differential equations for four unknowns, the functions $\phi^\alpha(x)$, $\alpha = 1, 2, 3, 4$, appearing in the local representation (5.2.1) of our diffeomorphism ϕ.

An algorithm for the construction of the nonlinear differential operator E is provided in Appendix D.4. However, we do not need the explicit form of E for our purposes. Even when we will be writing particular solutions of our nonlinear field equations — see Sections 5.8 and 5.9 — we will do this without using the explicit form of the operator E.

Remark 5.6. A straightforward analysis shows that the identity map is a solution of (5.3.5). Furthermore, any isometry from (M, g) to itself is a solution.

Let us now incorporate the volume preservation constraint (5.2.11) by adding to our original action (5.2.15) the term

$$K(\phi, p) := \int \big[p(\phi(x))\big] \big[\rho_\phi(x) - \rho(x)\big] \,\mathrm{d}x\,, \tag{5.3.6}$$

where $\rho_\phi(x) := \sqrt{-\det h_{\alpha\beta}(x)}$ and $p : M \to \mathbb{R}$ is an additional unknown scalar function playing the role of a Lagrange multiplier. The function p can be interpreted as pressure, cf. [94].

We will now vary our diffeomorphism as in (5.3.2).

Lemma 5.7. *The formula for the variation of the functional* (5.3.6) *reads*

$$\Delta K(\phi, p) = -\int \left[\frac{\partial p}{\partial y^\alpha}(\phi(x))\right] \big[\Delta\phi^\alpha(x)\big] \big[\rho(x)\big] \,\mathrm{d}x\,. \tag{5.3.7}$$

Proof. Observe that the diffeomorphism ϕ appears in formula (5.3.6) twice, so

$$\Delta K(\phi, p) = \Delta K_1(\phi, p) + \Delta K_2(\phi, p), \tag{5.3.8}$$

where

$$K_1(\phi, p) := \int \big[p(\phi(x))\big] \big[\rho_{\boldsymbol{\phi}}(x) - \rho(x)\big] \,\mathrm{d}x\,, \tag{5.3.9}$$

$$K_2(\phi, p) := \int \big[p(\boldsymbol{\phi}(x))\big] \big[\rho_\phi(x)\big] \,\mathrm{d}x\,, \tag{5.3.10}$$

the bold script indicating that this particular occurrence of ϕ is not subject to variation (5.3.2).

Variation of (5.3.9) gives us

$$\Delta K_1(\phi,p)=\int\left[\frac{\partial p}{\partial y^\alpha}(\boldsymbol{\phi}(x))\right]\left[\Delta\phi^\alpha(x)\right]\left[\rho_{\boldsymbol{\phi}}(x)-\rho(x)\right]\mathrm{d}x\,. \tag{5.3.11}$$

In order to calculate the variation of (5.3.10) we switch from local coordinates x to local coordinates y in accordance with $y=\boldsymbol{\phi}(x)$. Formula (5.3.10) now reads

$$K_2(\phi,p)=\int\left[p(y)\right]\left[\mu_\phi(y)\right]dy^1dy^2dy^3dy^4, \tag{5.3.12}$$

where μ_ϕ is the representation of the density ρ_ϕ in local coordinates y. An elementary calculation, see also (5.4.9f) and (5.4.11), shows that

$$\Delta\mu_\phi(y)=\frac{\partial\big(\left[\mu_{\boldsymbol{\phi}}(y)\right]\left[\Delta\phi^\alpha(\boldsymbol{\phi}^{-1}(y))\right]\big)}{\partial y^\alpha}\,. \tag{5.3.13}$$

Substituting (5.3.13) into (5.3.12) and integrating by parts, we get

$$\Delta K_2(\phi,p)=-\int\left[\frac{\partial p}{\partial y^\alpha}(y)\right]\left[\Delta\phi^\alpha(\boldsymbol{\phi}^{-1}(y))\right]\left[\mu_{\boldsymbol{\phi}}(y)\right]dy^1dy^2dy^3dy^4. \tag{5.3.14}$$

It remains only to switch back from local coordinates y to local coordinates x. Formula (5.3.14) becomes

$$\Delta K_2(\phi,p)=-\int\left[\frac{\partial p}{\partial y^\alpha}(\boldsymbol{\phi}(x))\right]\left[\Delta\phi^\alpha(x)\right]\left[\rho_{\boldsymbol{\phi}}(x)\right]\mathrm{d}x\,. \tag{5.3.15}$$

Substituting (5.3.11) and (5.3.15) into (5.3.8) we arrive at (5.3.7). □

Lemma 5.7 tells us that the field equations for the constrained action (5.2.15) read

$$E(\phi)-\mathrm{d}p=0, \tag{5.3.16}$$

where $\mathrm{d}p$ is the gradient of pressure p. Equations (5.3.16) have to be supplemented by the volume preservation condition (5.2.11).

The term $\mathrm{d}p$ appearing in formula (5.3.16) can be written in local coordinates as

$$(\mathrm{d}p)_\alpha(x)=\psi_\alpha{}^\beta(x)\,\frac{\partial(p\circ\phi)}{\partial x^\beta}(x)\,, \tag{5.3.17}$$

where the two-point tensor $\psi_\alpha{}^\beta$ is defined by the identity

$$\psi_\alpha{}^\beta(x)\,\frac{\partial\phi^\alpha}{\partial x^\gamma}(x)=\delta^\beta{}_\gamma\,.$$

Formulae (5.3.16) and (5.2.11) give us a system of five partial differential equations for five unknowns, the functions $\phi^\alpha(x)$, $\alpha=1,2,3,4$, appearing in the local representation (5.2.1) of our diffeomorphism ϕ and the scalar field $(p\circ\phi)(x)$.

5.4 Displacements and rotations

Suppose that our diffeomorphism $\phi : M \to M$ is sufficiently close to the identity map. Then it can be described by a vector field of displacements A. This vector field can be equivalently defined in two different ways.

Take an arbitrary point $P \in M$ and let $\Omega \subset M$ be a normal, with respect to g, neighbourhood of P. As ϕ is close to the identity map we can assume, without loss of generality, that $\phi(P) \in \Omega$. Let $\gamma : [0,1] \to \Omega$ be the geodesic, with respect to g, connecting P and $\phi(P)$, so that $\gamma(0) = P$ and $\gamma(1) = \phi(P)$. Furthermore, let us parameterize our geodesic in such a way that $\gamma(\tau)$ is a solution of the equation

$$\ddot{\gamma}^\lambda + \left\{ \begin{matrix} \lambda \\ \mu\nu \end{matrix} \right\} \dot{\gamma}^\mu \dot{\gamma}^\nu = 0,$$

where the dot stands for differentiation in τ. Then

$$A(P) := \dot{\gamma}(0). \tag{5.4.1}$$

Alternatively, let $W(P,Q)$ be the Ruse–Synge world function [112, Chapter II, §1] with respect to g. Here $P, Q \in M$ are assumed to be sufficiently close. Let $W'(P,Q) := \operatorname{grad}_x W(x,Q)|_{x=P}$ be the gradient of the world function with respect to the first variable. Then

$$A^\flat(P) := -W'(P, \phi(P)). \tag{5.4.2}$$

In formula (5.4.1) A is a vector, whereas in formula (5.4.2) $A^\flat$ is a covector. Raising and lowering tensor indices via the metric g turns one into the other, see Appendix D.1.1 for notation.

Working with a vector field of displacements A rather than an abstract diffeomorphism ϕ makes the physical interpretation clearer.

The field of displacements generates rotations. Describing these rotations mathematically is the subject of finite strain theory in continuum mechanics [116, Section 23]. In what follows we present this construction in a version adapted to Lorentzian signature and curved spacetime.

Consider the quantity

$$\frac{\partial \phi^\nu}{\partial x^\beta}(x)\,. \tag{5.4.3}$$

The quantity (5.4.3) is a two-point tensor: it transforms as a covector under changes of local coordinates x and as a vector under changes of local coordinates y. The two-point tensor (5.4.3) describes a linear map from T_PM to $T_{\phi(P)}M$,

$$v^\alpha \mapsto \frac{\partial\phi^\nu}{\partial x^\beta}\,v^\beta.$$

Let us now parallel transport (5.4.3), in the upper tensor index and with respect to the Levi-Civita connection associated with g, along the geodesic from $\phi(P)$ to P. This gives us a (one-point) (1,1)-tensor $D^\nu{}_\beta(x)$ known in continuum mechanics as the *deformation gradient*. The deformation gradient describes, pointwise, a non-degenerate linear map in the fibres of the tangent bundle,

$$v^\alpha \mapsto D^\nu{}_\beta\, v^\beta. \tag{5.4.4}$$

Moreover, formula (5.2.2) can now be rewritten as

$$h_{\alpha\beta}(x) = [D^\mu{}_\alpha(x)]\,[g_{\mu\nu}(x)]\,[D^\nu{}_\beta(x)]\,. \tag{5.4.5}$$

Further on we assume that the linear map (5.4.4) is sufficiently close to the identity. The issue at hand is to decompose (5.4.4) into a composition of a stretching map and a rotation map. This is achieved by means of the polar decomposition. The concept of polar decomposition is standard in linear algebra, only now it has to be adapted to Lorentzian signature. Some work in this direction was done in [23, 88].

Definition 5.8. We call a linear map $v^\alpha \mapsto B^\alpha{}_\beta\, v^\beta$ *Lorentz–symmetric* if $g_{\alpha\gamma}B^\gamma{}_\beta = g_{\beta\gamma}B^\gamma{}_\alpha$, *Lorentz–antisymmetric* if $g_{\alpha\gamma}B^\gamma{}_\beta = -g_{\beta\gamma}B^\gamma{}_\alpha$ and *Lorentz–orthogonal* if $B^\mu{}_\alpha\, g_{\mu\nu}\, B^\nu{}_\beta = g_{\alpha\beta}$.

Any linear map (5.4.4) sufficiently close to the identity can be uniquely decomposed as

$$D^\alpha{}_\beta = U^\alpha{}_\gamma\, V^\gamma{}_\beta\,, \tag{5.4.6}$$

where U is Lorentz–orthogonal and V is Lorentz–symmetric and close to the identity. The existence of polar decomposition (5.4.6) can be established, for example, by using the power series expansion for the function $\sqrt{1+z}$ with $z = g^{\alpha\gamma}\, D^\mu{}_\gamma\, g_{\mu\nu}\, D^\nu{}_\beta - \delta^\alpha{}_\beta$.

In the setting of classical elasticity theory (Riemannian signature) the tensor V appearing in formula (5.4.6) is called the *right stretch tensor*, see [116, p. 53].

Formula (5.4.6) and the fact that D and V are close to the identity imply that U is close to the identity as well. Therefore, U can be uniquely represented as

$$U = e^F, \tag{5.4.7}$$

where F is Lorentz–antisymmetric and small. The tensor F can be recovered from the tensor U by using the power series expansion for the function $\ln(1+z)$ with $z = U^\alpha{}_\beta - \delta^\alpha{}_\beta$.

Applying the above procedure to the deformation gradient we arrive at a Lorentz–antisymmetric (1,1)-tensor $F^\alpha{}_\beta(x)$. Lowering the first tensor index via g, we get a covariant antisymmetric tensor $F_{\alpha\beta}(x)$ which can be viewed as a 2-form. We call it the *rotation 2-form*.

Substituting (5.4.6) into (5.4.5) we get

$$h_{\alpha\beta}(x) = [V^\mu{}_\alpha(x)]\,[g_{\mu\nu}(x)]\,[V^\nu{}_\beta(x)]\,. \tag{5.4.8}$$

Remark 5.9. The order of indices in our polar decomposition (5.4.6) is important. Had we done the polar decomposition the other way round, i.e. as $D^\alpha{}_\beta = V^\alpha{}_\gamma\,U^\gamma{}_\beta\,,$ we wouldn't have gotten (5.4.8).

Formula (5.4.8) tells us that rotations do not appear explicitly in our mathematical model. In other words, the physics described by our action (5.2.15) does not feel rotations. However, we will still have to consider rotations later on in the Chapter because they do not have a life of their own: rotations are generated by displacements, cf. Sections 5.10 and 5.11.

The following lemma provides a list of formulae obtained by linearising in A. Some of them will be used in Section 5.5.

Lemma 5.10. *We have*

$$D_{\alpha\beta} = g_{\alpha\beta} + \nabla_\beta A_\alpha + O(|A|^2), \tag{5.4.9a}$$

$$U_{\alpha\beta} = g_{\alpha\beta} - \frac{1}{2}(\nabla_\alpha A_\beta - \nabla_\beta A_\alpha) + O(|A|^2), \tag{5.4.9b}$$

$$F_{\alpha\beta} = -\frac{1}{2}(\nabla_\alpha A_\beta - \nabla_\beta A_\alpha) + O(|A|^2), \tag{5.4.9c}$$

$$V_{\alpha\beta} = g_{\alpha\beta} + \frac{1}{2}(\nabla_\alpha A_\beta + \nabla_\beta A_\alpha) + O(|A|^2), \tag{5.4.9d}$$

$$S_{\alpha\beta} = \nabla_\alpha A_\beta + \nabla_\beta A_\alpha + O(|A|^2), \tag{5.4.9e}$$

$$\frac{\det h_{\kappa\lambda}}{\det g_{\mu\nu}} = 1 + 2\,\nabla_\alpha A^\alpha + O(|A|^2). \tag{5.4.9f}$$

In the above lemma and further on ∇ is the Levi-Civita connection associated with g and tensor indices are raised and lowered using the metric g. In particular, the tensor in the LHS of formula (5.4.9e) is our original strain tensor (5.2.3) but with the first tensor index lowered. Of course, we have $S_{\alpha\beta} = h_{\alpha\beta} - g_{\alpha\beta}$.

Note that formulae (5.4.9c) and (5.4.9f) can be equivalently rewritten without covariant derivatives using the identities

$$\nabla_\alpha A_\beta - \nabla_\beta A_\alpha = \partial_\alpha A_\beta - \partial_\beta A_\alpha = (\mathrm{d}A^\flat)_{\alpha\beta}\,, \tag{5.4.10}$$

$$\nabla_\alpha A^\alpha = \rho^{-1}\partial_\alpha(\rho A^\alpha) = -\delta A^\flat, \tag{5.4.11}$$

where ρ is our Lorentzian density (5.2.12). See Appendix D.1.1 for exterior calculus notation.

Remark 5.11. There is an alternative way of describing a diffeomorphism in terms of a vector field. This alternative approach is in the spirit of fluid mechanics and is based on Lie-algebraic considerations. Namely, consider a smooth vector field $u^\alpha(x)$, a field of 'velocities', and the autonomous system of ordinary differential equations

$$\begin{cases} \dot{y} = u(y), \\ y|_{\tau=0} = x, \end{cases} \tag{5.4.12}$$

that it generates. Here $\tau \in [0,1]$ is a parameter and the dot stands for differentiation in τ. We denote the solution of (5.4.12) by $y(\tau; x)$. For u small enough the map $x \mapsto y(1;x)$ realises a diffeomorphism close to the identity. At a formal level one would hope to generate an arbitrary diffeomorphism close to the identity by a suitable choice of vector field u. Furthermore, if we choose a divergence-free vector field, i.e. a vector field satisfying $\rho^{-1}\partial_\alpha(\rho u^\alpha) = 0$ (compare with (5.4.9f) and (5.4.11)), then for u small enough the map $x \mapsto y(1;x)$ realises a volume-preserving diffeomorphism close to the identity. Unfortunately, this approach doesn't work: it is known [86, p. 163] that there does not exist a neighbourhood of the identity where the exponential map $\exp : \mathrm{Vect}(M) \to \mathrm{Diff}(M)$, from vector fields u to diffeomorphisms, is surjective. There are simple explicit examples of diffeomorphisms of $\mathbb{S}^1$ arbitrarily close to the identity that cannot be represented in terms of the above flow, see, for example, [90, p. 1017], [16, p. 8–9], [75, p. 456–457]. The description of a diffeomorphism in terms of a vector field of displacements A (see beginning of this section) does not suffer from the deficiencies of the fluid mechanics description (5.4.12). The fundamental difference between the two approaches is that the concept of displacement relies on the use of the metric structure.

5.5 Linearised field equations

Carrying on from Section 5.4, we assume that our diffeomorphism $\phi : M \to M$ is sufficiently close to the identity map, so that it can be described by a vector field of displacements $A(x)$. Furthermore, we can choose the local coordinates y to be the same as x. Our aim in the current Section is to linearise the field equations (5.3.16), (5.2.11) in $A(x)$ and $p(x)$.

Formulae (5.4.9f) and (5.4.11) give us the linearisation of the volume preservation condition (5.2.11):

$$\delta A^\flat = 0. \tag{5.5.1}$$

Formula (5.3.17) now reads

$$(\mathrm{d}p)_\alpha(x) = \frac{\partial p}{\partial x^\alpha}(\phi(x))\,,$$

and its linearisation is the usual gradient

$$\frac{\partial p}{\partial x^\alpha}(x)\,.$$

The issue at hand is the linearisation of $E(\phi)$.

Inspection of formulae (5.2.5b)–(5.2.5d), (5.2.17b) and (5.4.9e) shows that the expansion of our Lagrangian $L\big(e_2(A), e_3(A), e_4(A)\big)$ in terms homogeneous in A starts with the quadratic expression

$$L^{(2)}(A) = -2\,(\nabla_\alpha A^\alpha)^2 + \frac{1}{2}\,(\nabla_\alpha A_\beta + \nabla_\beta A_\alpha)(\nabla^\alpha A^\beta + \nabla^\beta A^\alpha)\,, \tag{5.5.2}$$

so that $L\big(e_2(A), e_3(A), e_4(A)\big) = L^{(2)}(A) + O(|A|^3)$. Variation of the quadratic action

$$J^{(2)}(A) = \int_M L^{(2)}(A)\,\rho(x)\,\mathrm{d}x$$

generates the linearisation $E^{(1)}(A)$ of $E(\phi)$:

$$\Delta J^{(2)}(A) = \int E^{(1)}_\lambda(A)\ \Delta A^\lambda\ \rho(x)\ \mathrm{d}x\,.$$

However, prior to variation it is useful to rewrite (5.5.2) as in the following lemma, whose proof is a straightforward computation.

Lemma 5.12. *The Lagrangian* (5.5.2) *can be equivalently rewritten as*

$$L^{(2)}(A) = \frac{1}{2}\,(\nabla_\alpha A_\beta - \nabla_\beta A_\alpha)(\nabla^\alpha A^\beta - \nabla^\beta A^\alpha) - 2\,\mathrm{Ric}_{\mu\nu}\,A^\mu A^\nu + \nabla_\kappa B^\kappa\,, \tag{5.5.3}$$

where Ric *is the Ricci tensor associated with g and*

$$B^\kappa = -2\,[A^\kappa(\nabla_\gamma A^\gamma) - A^\gamma(\nabla_\gamma A^\kappa)]\,.$$

The divergence term $\nabla_\kappa B^\kappa$ in formula (5.5.3) does not contribute to the field equations, so we can replace our Lagrangian (5.5.2) with

$$\widetilde{L}^{(2)}(A) = \|\mathrm{d}A^\flat\|^2_g - 2\,\mathrm{Ric}(A,A), \tag{5.5.4}$$

see Appendix D.1.1 for exterior calculus notation. The advantage of writing our quadratic Lagrangian in the form (5.5.4) is that this representation does not involve covariant derivatives.

Formula (5.5.4) implies that the linearised operator generated by our action (5.2.15) reads

$$E^{(1)} = 2\delta\mathrm{d} - 4\,\mathrm{Ric}. \tag{5.5.5}$$

In formulae (5.5.4) and (5.5.5) we abuse notation by using the symbol Ric for two different objects, the quadratic form on vectors $\mathrm{Ric}(u,u) := \mathrm{Ric}_{\alpha\beta}u^\alpha u^\beta$ and the linear map on covectors $\mathrm{Ric} : v_\alpha \mapsto \mathrm{Ric}_{\alpha\beta}v^\beta$.

Hence, our linearised field equations (5.3.16), (5.2.11) read

$$\begin{pmatrix} \delta \mathrm{d} - 2\,\mathrm{Ric} & -\frac{1}{2}\mathrm{d} \\ \delta & 0 \end{pmatrix} \begin{pmatrix} A^\flat \\ p \end{pmatrix} = 0.$$

If we introduce a new scalar field

$$\widetilde{p} := -\frac{1}{2}p \tag{5.5.6}$$

the above system takes the form

$$\begin{pmatrix} \delta \mathrm{d} - 2\,\mathrm{Ric} & \mathrm{d} \\ \delta & 0 \end{pmatrix} \begin{pmatrix} A^\flat \\ \widetilde{p} \end{pmatrix} = 0. \tag{5.5.7}$$

Let us now briefly discuss the analytic properties of the 5×5 matrix linear partial differential operator

$$\mathrm{Lin} : \Omega^1(M) \oplus \Omega^0(M) \to \Omega^1(M) \oplus \Omega^0(M), \qquad \begin{pmatrix} v \\ f \end{pmatrix} \mapsto \begin{pmatrix} \delta \mathrm{d} - 2\,\mathrm{Ric} & \mathrm{d} \\ \delta & 0 \end{pmatrix} \begin{pmatrix} v \\ f \end{pmatrix}. \tag{5.5.8}$$

We start with the observation that the operator Lin is formally self-adjoint (symmetric) with respect to the L^2 inner product defined as in Appendix D.1.1.

The more specific properties of a linear differential operator are determined by its principal symbol. In local coordinates, the principal symbol is obtained by leaving only the leading (higher order) derivatives and replacing each partial differentiation $\partial/\partial x^\alpha$ by $i\xi_\alpha$, where ξ is the dual variable (momentum), see [104, subsection 1.1.3]. This gives a (matrix-)function on the cotangent bundle the properties of which determine the basic features of the differential operator such as ellipticity or hyperbolicity. However, for our operator Lin matters are slightly more complicated because it has a block structure

$$\begin{pmatrix} 2^{\text{nd}} \text{ order operator} & 1^{\text{st}} \text{ order operator} \\ 1^{\text{st}} \text{ order operator} & 0 \text{ order operator} \end{pmatrix}$$

with operators of different order in different blocks. Matrix operators with this particular structure are called Agmon-Douglis-Nirenberg type operators [1]. Application of the Agmon–Douglis–Nirenberg construction gives the principal symbol of Lin as the linear map

$$\begin{pmatrix} v \\ f \end{pmatrix} \mapsto \begin{pmatrix} \|\xi\|_g^2\, v - \langle \xi, v\rangle_g\, \xi + i f \xi \\ -i\,\langle \xi, v\rangle_g \end{pmatrix}. \tag{5.5.9}$$

The determinant of the linear map (5.5.9) is

$$-\|\xi\|_g^8 . \tag{5.5.10}$$

Now, if our metric g were Riemannian then the quantity (5.5.10) would not vanish on $T^*M\setminus\{0\}$ and, hence, our operator Lin would be elliptic in the Agmon–Douglis–Nirenberg sense. However, for Lorentzian metric g the quantity (5.5.10) vanishes on light cones, which suggests that our operator Lin is hyperbolic. There is extensive literature dealing with Agmon–Douglis–Nirenberg type operators in the elliptic setting but we are unaware of similar results for the hyperbolic case. A rigorous investigation of well-posedness issues for the operator Lin, though, would require substantial work and possibly constitute a research project of its own. Hence, we will not pursue the matter further in this thesis. For a review of different notions of hyperbolicity in a setting similar to ours see [117, Section 4].

Note that if we replace the 5×5 matrix operator (5.5.8) with the 4×4 matrix operator $\delta\mathrm{d}$, then the principal symbol will be a degenerate matrix whose determinant is identically zero.

Let us now assume that our spacetime (M,g) is Ricci-flat,

$$\mathrm{Ric}=0. \tag{5.5.11}$$

Note that condition (5.5.11) is the definition of vacuum in General Relativity. Moreover, it is easy to see that if (M,g) is Ricci-flat, then so is (M,h).

Under condition (5.5.11) equation (5.5.7) implies

$$\delta\mathrm{d}\widetilde{p}=\square_g\,\widetilde{p}=0.$$

We see that we have a separate equation for the scalar field $\widetilde{p}$, the wave equation. This observation allows us to collect solutions of our system (5.5.7) into equivalence classes corresponding to particular choices of $\widetilde{p}$: we say that two solutions, $\begin{pmatrix}A^\flat\\ \widetilde{p}\end{pmatrix}$ and $\begin{pmatrix}A^{\flat\prime}\\ \widetilde{p}'\end{pmatrix}$, are equivalent if $\widetilde{p}=\widetilde{p}'$.

Let us now fix a particular solution $\widetilde{p}$ of the wave equation and work within the corresponding equivalence class. Then the first four equations from our system

(5.5.7) can be rewritten as

$$\delta \mathrm{d} A^{\flat} = J,$$

where $J := -\mathrm{d}\widetilde{p}$. We have arrived at Maxwell's equations in the Lorenz gauge (5.5.1) and with exact current $J \in \mathrm{d}\Omega^0(M)$. Recovering Maxwell's equations in the Lorenz gauge is not a factitious artefact of our theory, but, in a sense, a natural thing to have: this is what one obtains when looking at irreducible representations of the Poincaré group in the spirit of Wigner's classification, cf. [17, Chapter 21].

5.6 Homogeneous diffeomorphisms

In the remainder of this Chapter we will construct explicit solutions of the nonlinear field equations (5.3.16). Namely, we will write down explicitly volume preserving diffeomorphisms ϕ satisfying (5.3.16) with $p = 0$. In other words, we will present volume preserving solutions of the unconstrained nonlinear field equations (5.3.5).

Seeking such solutions constitutes an overdetermined problem: we are looking at a system of five nonlinear partial differential equations (5.3.5), (5.2.11) for four unknowns, the functions $\phi^\alpha(x)$, $\alpha = 1, 2, 3, 4$, appearing in the local representation (5.2.1) of our diffeomorphism ϕ. We will base our construction on group-theoretic ideas, the essence of which is explained below.

Further on $\mathrm{Isom}(M, g)$ denotes the finite-dimensional subgroup of $\mathrm{Diff}(M)$ comprising diffeomorphisms that are isometries.

Definition 5.13. Let $\phi \in \mathrm{Diff}(M)$. We say that ϕ is *homogeneous* if there exists a subgroup $H \subset \mathrm{Isom}(M, g)$ acting transitively on M and satisfying

$$H \circ \phi = \phi \circ H. \tag{5.6.1}$$

If we have the stronger property

$$\xi \circ \phi = \phi \circ \xi, \qquad \forall \xi \in H, \tag{5.6.2}$$

we say that ϕ is *equivariant*.

In other words, condition (5.6.1) can be rewritten as follows: for any $\xi \in H$ there exists a $\eta \in H$ such that the diagram

$$\begin{array}{ccc} M & \xrightarrow{\ \xi\ } & M \\ {\scriptstyle\phi}\big\downarrow & & \big\downarrow{\scriptstyle\phi} \\ M & \xrightarrow[\ \eta\ ]{} & M \end{array}$$

is commutative.

Theorem 5.14. *Let ϕ be a homogeneous diffeomorphism. Then the scalar invariants* (5.2.5) *are constant. Furthermore, if the covector field $E(\phi)$ defined in accordance with formula* (5.3.4) *vanishes at a point then it vanishes identically.*

Proof. Let us prove the second statement first. Let ϕ be a homogeneous diffeomorphism and $x, y \in M$ two arbitrary points. We will assume that $E(\phi)|_x = 0$ and we will show that $E(\phi)|_y = 0$. In view of Definition 5.13, there exist isometries ξ and η such that

$$y = \xi(x), \qquad \phi(y) = \eta(\phi(x)), \tag{5.6.3}$$

and

$$\eta \circ \phi = \phi \circ \xi. \tag{5.6.4}$$

Note that in writing (5.6.3) we only used the transitivity of the action of H on M, whereas (5.6.4) required the use of the additional condition (5.6.1).

It is possible to choose coordinates in some neighbourhoods $\mathcal{U}(x)$ and $\mathcal{U}(\phi(x))$ of x and $\phi(x)$ respectively in such a way that ϕ is locally the identity map:

$$\phi|_{\mathcal{U}(x)} \simeq \mathrm{Id} : \mathcal{U}(x) \to \mathcal{U}(\phi(x)).$$

We can then prescribe coordinates in some neighbourhood $\mathcal{U}(y)$ of y (resp. $\mathcal{U}(\phi(y))$ of $\phi(y)$) via the isometry ξ (resp. η). This has two consequences. Firstly, the map

$$\phi|_{\mathcal{U}(y)} : \mathcal{U}(y) \to \mathcal{U}(\phi(y))$$

is the identity in our local coordinates. Secondly, in this coordinate representation the components of the metric tensor are the same near x and y and near $\phi(x)$ and $\phi(y)$. This can be easily seen by explicitly imposing the isometry conditions $\xi^* g = g$ and $\eta^* g = g$ locally, after observing that $\xi|_{\mathcal{U}(x)} \simeq \mathrm{Id}$ and $\eta|_{\mathcal{U}(\phi(x))} \simeq \mathrm{Id}$ for our choice of coordinates. In particular, the Jacobian of the change of coordinates from coordinates centred at x (resp. $\phi(x)$) to coordinates centred at y (resp. $\phi(y)$) is 1. The local expression (5.3.4) of $E(\phi)$ depends only on the (local representation of the) metric, ϕ and its derivatives. Since such local representations are the same in neighbourhoods of x and y, $E(\phi)|_x = 0$ implies $E(\phi)|_y = 0$.

Finally, let us prove that the scalar invariants are constant. If we compute the scalar invariants in local coordinates, we realise that they only depend on the local representation of the metric, of ϕ and of its first derivatives, see (5.2.3) and (5.2.5). Since such representations can be made the same in the neighbourhood of any pair of points x and y, as described above, it ensues that the scalar invariants take the same value everywhere, namely, they are constant. □

Theorem 5.14 tells us that if we seek a solution of nonlinear field equations (5.3.5) in the form of a homogeneous diffeomorphism then it is sufficient to satisfy these field equations at a single point.

Remark 5.15. Note that our mathematical model is invariant under the action of the group of isometries in the following sense. Let $\varphi \in \mathrm{Diff}_\rho(M)$ and $p : M \to \mathbb{R}$ be a solution of our field equations (5.3.16), and let $\xi \in \mathrm{Isom}(M, g)$ be an arbitrary isometry. Then $\xi \circ \varphi$ and $p \circ \xi^{-1}$ is also a solution.

5.7 Special subgroups of the Poincaré group

In the remainder of the Chapter we work in Minkowski space $\mathbb{M}$ where the metric is $g_{\alpha\beta} = \mathrm{diag}(1, 1, 1, -1)$. Further on $\mathrm{Poinc}(\mathbb{M}) := \mathrm{Isom}(\mathbb{R}^4, g)$ denotes the 10-dimensional group of isometries of $\mathbb{M}$, commonly known as the Poincaré group. Clearly, $\mathrm{Poinc}(\mathbb{M}) = \mathbb{R}^4 \rtimes \mathrm{O}(3, 1)$.

In fact, we will be working with the identity component of the Poincaré group, $\mathrm{ISO}^+(3, 1)$. This is known to be the fundamental symmetry group of physics, in that it turns inertial frames into one another.

The Poincaré group can be realised as a subgroup of the matrix group $\mathrm{SL}(5, \mathbb{R})$ as follows:

$$\mathbb{R}^4 \rtimes \mathrm{O}(3, 1) \ni (v, \Lambda) \mapsto \begin{pmatrix} & \Lambda & & & v \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \in \mathrm{SL}(5, \mathbb{R}).$$

Here the 5×5 matrix acts on $x \in \mathbb{M}$ by matrix vector multiplication after complementing it with 1,

$$\begin{pmatrix} x \\ 1 \end{pmatrix} \mapsto \begin{pmatrix} & \Lambda & & & v \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ 1 \end{pmatrix}.$$

We now introduce special subgroups of the restricted Poincaré group $\mathrm{ISO}^+(3,1)$ which will be used later in Sections 5.8 and 5.9.

Definition 5.16. The *right-handed massless screw group* SG_0^+ and *left-handed massless screw group* SG_0^- are the subgroups of $\mathrm{ISO}^+(3,1)$ realised in matrix representation by

$$\mathrm{SG}_0^{\pm} := \left\{ \begin{pmatrix} \cos(q^3+q^4) & \mp\sin(q^3+q^4) & 0 & 0 & q^1 \\ \pm\sin(q^3+q^4) & \cos(q^3+q^4) & 0 & 0 & q^2 \\ 0 & 0 & 1 & 0 & q^3 \\ 0 & 0 & 0 & 1 & q^4 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \;\middle|\; q \in \mathbb{R}^4 \right\}. \tag{5.7.1}$$

Definition 5.17. Let m be a positive real number. The *massive screw group* SG_m is the subgroup of $\mathrm{ISO}^+(3,1)$ realised in matrix representation by

$$\mathrm{SG}_m := \left\{ \begin{pmatrix} \cos(2mq^4) & -\sin(2mq^4) & 0 & 0 & q^1 \\ \sin(2mq^4) & \cos(2mq^4) & 0 & 0 & q^2 \\ 0 & 0 & 1 & 0 & q^3 \\ 0 & 0 & 0 & 1 & q^4 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \;\middle|\; q \in \mathbb{R}^4 \right\}. \tag{5.7.2}$$

It is easy to see that SG_0^+, SG_0^- and SG_m are indeed subgroups of $\mathrm{ISO}^+(3,1)$ and act transitively on $\mathbb{M}$. Each of these groups is isomorphic to the direct product of $\mathbb{R}$ with a 3-dimensional group of Bianchi type $\mathrm{Bi(VII_0)}$.

Let $\xi \in \mathrm{ISO}^+(3,1)$. Then $\xi^{-1}\,\mathrm{SG}_0^+\,\xi$, $\xi^{-1}\,\mathrm{SG}_0^-\,\xi$ and $\xi^{-1}\,\mathrm{SG}_m\,\xi$ are also subgroups of $\mathrm{ISO}^+(3,1)$. The question we want to address is what happens under conjugation.

Lemma 5.18. *There does not exist a* $\xi \in \mathrm{ISO}^+(3,1)$ *such that* $\xi^{-1}\,\mathrm{SG}_0^+\,\xi = \mathrm{SG}_0^-$.

Proof. The result follows from Lemma D.6: the Hodge dual of axial torsion associated with the two groups lies on opposite sides of the light cone and conjugation by an element of $\mathrm{ISO}^+(3,1)$ cannot change this. □

Lemma 5.18 tells us that the groups SG_0^+ and SG_0^- are genuinely different, in that one cannot be turned into the other by conjugation.

Let us now examine what happens when we conjugate the massive screw group. It turns out that the situation here is completely different. Namely, choose $\xi = \mathrm{diag}(-1,-1,-1,-1,1)$ to be the PT transformation. Then

$$\xi^{-1}\,\mathrm{SG}_m\,\xi = \left\{ \begin{pmatrix} \cos(2mq^4) & -\sin(2mq^4) & 0 & 0 & -q^1 \\ \sin(2mq^4) & \cos(2mq^4) & 0 & 0 & -q^2 \\ 0 & 0 & 1 & 0 & -q^3 \\ 0 & 0 & 0 & 1 & -q^4 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \;\middle|\; q \in \mathbb{R}^4 \right\}$$

$$= \left\{ \begin{pmatrix} \cos(2mq^4) & \sin(2mq^4) & 0 & 0 & q^1 \\ -\sin(2mq^4) & \cos(2mq^4) & 0 & 0 & q^2 \\ 0 & 0 & 1 & 0 & q^3 \\ 0 & 0 & 0 & 1 & q^4 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \;\middle|\; q \in \mathbb{R}^4 \right\}.$$

This means that a different choice of signs in (5.7.2) does not yield a different family of subgroups. The argument presented in this paragraph is in agreement with Lemma D.6: the Hodge dual of axial torsion associated with the massive group is spacelike and conjugation moves this covector without encountering obstructions.

5.8 Explicit massless solutions of nonlinear field equations

Working in Minkowski space $\mathbb{M}$, we will describe our diffeomorphism ϕ by a vector field of displacements

$$\phi : x^\alpha \mapsto x^\alpha + A^\alpha(x). \tag{5.8.1}$$

The concept of a vector field of displacements was introduced in Section 5.4. The special feature of Minkowski space is that we do not need to assume that our diffeomorphism is sufficiently close to the identity map. The only restriction on the choice of vector field A is

$$\det(D^\alpha{}_\beta) \neq 0, \tag{5.8.2}$$

where

$$D^\alpha{}_\beta = \delta^\alpha{}_\beta + \partial A^\alpha / \partial x^\beta \tag{5.8.3}$$

is the deformation gradient, see formula (5.4.4) and associated discussion. Condition (5.8.2) ensures that we do indeed have a diffeomorphism, a smooth invertible map.

We seek volume preserving solutions. Examination of formula (5.4.5) shows that in Minkowski space the volume preservation condition (5.2.11) reduces to

$$|\det(D^\alpha{}_\beta)| = 1,$$

which means that we either have

$$\det(D^\alpha{}_\beta) = +1 \tag{5.8.4a}$$

or

$$\det(D^\alpha{}_\beta) = -1. \tag{5.8.4b}$$

Solutions presented in this section and the next one will possess the property (5.8.4a).

We say that a real lightlike covector $p = (p_1, p_2, p_3, p_4)$ lies on the forward light cone if $p_4 > 0$. We say that a complex vector $u = (u^1, u^2, u^3, u^4)$ is isotropic if $u_\alpha \bar{u}^\alpha > 0$ and $u_\alpha u^\alpha = 0$.

The use of the term 'isotropic' is motivated by Cartan who used it in the 3-dimensional Euclidean setting. If we choose a coordinate system such that $u^4 = 0$ our definition is equivalent to that in [37, Chapter III, Section I].

Theorem 5.19. *Let p be a real lightlike covector on the forward light cone, let u be a complex isotropic vector orthogonal to p and let*

$$\mathbb{A}^\alpha(x) = u^\alpha \, e^{ip_\beta x^\beta}. \tag{5.8.5}$$

Then the diffeomorphism (5.8.1) with

$$A(x) = \mathrm{Re}\,[\mathbb{A}(x)] \tag{5.8.6}$$

is volume preserving and satisfies the nonlinear field equations (5.3.5).

Proof. We can perform a (unique) proper orthochronous Lorentz transformation of coordinates so that formula (5.8.5) reads

$$\mathbb{A}^\alpha(x) = a \begin{pmatrix} 1 \\ \mp i \\ 0 \\ 0 \end{pmatrix} e^{i(x^3+x^4)}, \tag{5.8.7}$$

where $a = \sqrt{u_\alpha \bar{u}^\alpha/2}$. Then (5.8.6) becomes

$$A^\alpha(x) = a \begin{pmatrix} \cos(x^3+x^4) \\ \pm\sin(x^3+x^4) \\ 0 \\ 0 \end{pmatrix}. \tag{5.8.8}$$

Substituting (5.8.8) into (5.8.3) we get the following explicit formula for the deformation gradient:

$$D^\alpha{}_\beta = \begin{pmatrix} 1 & 0 & -a\sin(x^3+x^4) & -a\sin(x^3+x^4) \\ 0 & 1 & \pm a\cos(x^3+x^4) & \pm a\cos(x^3+x^4) \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{5.8.9}$$

where the first tensor index, α, enumerates the rows and the second, β, the columns. It is immediately clear that (5.8.4a) is satisfied. Substituting now (5.8.9) into (5.4.5) and (5.2.3) we get the following explicit formula for the strain tensor:

$$S^\alpha{}_\beta = \begin{pmatrix} 0 & 0 & -a\sin(x^3+x^4) & -a\sin(x^3+x^4) \\ 0 & 0 & \pm a\cos(x^3+x^4) & \pm a\cos(x^3+x^4) \\ -a\sin(x^3+x^4) & \pm a\cos(x^3+x^4) & a^2 & a^2 \\ a\sin(x^3+x^4) & \mp a\cos(x^3+x^4) & -a^2 & -a^2 \end{pmatrix}. \tag{5.8.10}$$

It is easy to check that the matrix (5.8.10) is nilpotent, so all our scalar invariants (5.2.5) vanish identically. Note that the nilpotency index of (5.8.10) is three, which, according to Lemma D.3, is the maximal possible.

We vary the vector field of displacements $A(x)$ as

$$A^\alpha(x) \mapsto A^\alpha(x) + \Delta A^\alpha(x).$$

This generates an increment of our scalar invariants Δe_j and an increment of our Lagrangian

$$\sum_{j=2}^{4} \frac{\partial L}{\partial e_j}\bigg|_{e_2=e_3=e_4=0} \Delta e_j\,.$$

In order to prove that our diffeomorphism satisfies the nonlinear field equations (5.3.5) it is sufficient to prove that

$$\int_{\mathbb{R}^4} \Delta e_j \,\mathrm{d}x \,=0\,, \qquad j=2,3,4. \tag{5.8.11}$$

Straightforward calculations give

$$\Delta e_1 = 2\left(\delta^\beta{}_\alpha + \frac{\partial A_\alpha}{\partial x_\beta}\right)\frac{\partial \Delta A^\alpha}{\partial x^\beta}\,, \tag{5.8.12a}$$

$$\Delta e_2 = -2\left(a^2\,p^\beta\,p_\alpha + \frac{\partial A^\beta}{\partial x^\alpha} + \frac{\partial A_\alpha}{\partial x_\beta}\right)\left(\frac{\partial \Delta A^\alpha}{\partial x^\beta} + \frac{\partial A_\gamma}{\partial x_\alpha}\,\frac{\partial \Delta A^\gamma}{\partial x^\beta}\right), \tag{5.8.12b}$$

$$\Delta e_3 = 2\,a^2\,p^\beta\,p_\alpha\left(\frac{\partial \Delta A^\alpha}{\partial x^\beta} + \frac{\partial A_\gamma}{\partial x_\alpha}\,\frac{\partial \Delta A^\gamma}{\partial x^\beta}\right) = 2\,a^2\,p^\beta\,p_\alpha\frac{\partial \Delta A^\alpha}{\partial x^\beta}\,, \tag{5.8.12c}$$

$$\Delta e_4 = 0\,, \tag{5.8.12d}$$

where $p_\kappa = (0,0,1,1)$. Integrating (5.8.12b)–(5.8.12d) by parts and using the identities

$$\Box A = 0, \qquad \frac{\partial A^\alpha}{\partial x^\alpha} = 0, \qquad \left(p^\alpha\frac{\partial}{\partial x^\alpha}\right)A = 0,$$

we arrive at (5.8.11). □

The crucial element of the above proof is the observation that the scalar invariants (5.2.5) generated by the diffeomorphism (5.8.1), (5.8.8) are constant. We established this fact by means of explicit analytic calculations. However, at a group-theoretic level this follows from Theorem 5.14. Indeed, take an arbitrary $\xi \in \mathrm{SG}_0^\pm$, see formula (5.7.1). This isometry acts as

$$\xi:\begin{pmatrix}x^1\\x^2\\x^3\\x^4\end{pmatrix}\mapsto\begin{pmatrix}x^1\cos(q^3+q^4)\mp x^2\sin(q^3+q^4)\\ \pm x^1\sin(q^3+q^4)+x^2\cos(q^3+q^4)\\ x^3\\ x^4\end{pmatrix}+\begin{pmatrix}q^1\\q^2\\q^3\\q^4\end{pmatrix}.$$

Our diffeomorphism (5.8.1), (5.8.8) acts as

$$\phi_\pm : \begin{pmatrix} x^1 \\ x^2 \\ x^3 \\ x^4 \end{pmatrix} \mapsto \begin{pmatrix} x^1 \\ x^2 \\ x^3 \\ x^4 \end{pmatrix} + a \begin{pmatrix} \cos(x^3 + x^4) \\ \pm\sin(x^3 + x^4) \\ 0 \\ 0 \end{pmatrix}$$

and its inverse acts as

$$\phi_\pm^{-1} : \begin{pmatrix} x^1 \\ x^2 \\ x^3 \\ x^4 \end{pmatrix} \mapsto \begin{pmatrix} x^1 \\ x^2 \\ x^3 \\ x^4 \end{pmatrix} - a \begin{pmatrix} \cos(x^3 + x^4) \\ \pm\sin(x^3 + x^4) \\ 0 \\ 0 \end{pmatrix}.$$

Composing ξ with $\phi_\pm$ we get

$$\xi \circ \phi_\pm : \begin{pmatrix} x^1 \\ x^2 \\ x^3 \\ x^4 \end{pmatrix} \mapsto \begin{pmatrix} x^1\cos(q^3+q^4) \mp x^2\sin(q^3+q^4) \\ \pm x^1\sin(q^3+q^4) + x^2\cos(q^3+q^4) \\ x^3 \\ x^4 \end{pmatrix} + \begin{pmatrix} q^1 \\ q^2 \\ q^3 \\ q^4 \end{pmatrix}$$
$$+ a \begin{pmatrix} \cos(x^3+q^3+x^4+q^4) \\ \pm\sin(x^3+q^3+x^4+q^4) \\ 0 \\ 0 \end{pmatrix}.$$

Finally, a composition with $\phi_\pm^{-1}$ gives us

$$\phi_\pm^{-1} \circ \xi \circ \phi_\pm : \begin{pmatrix} x^1 \\ x^2 \\ x^3 \\ x^4 \end{pmatrix} \mapsto \begin{pmatrix} x^1\cos(q^3+q^4) \mp x^2\sin(q^3+q^4) \\ \pm x^1\sin(q^3+q^4) + x^2\cos(q^3+q^4) \\ x^3 \\ x^4 \end{pmatrix} + \begin{pmatrix} q^1 \\ q^2 \\ q^3 \\ q^4 \end{pmatrix}$$
$$+ a \begin{pmatrix} \cos(x^3+q^3+x^4+q^4) \\ \pm\sin(x^3+q^3+x^4+q^4) \\ 0 \\ 0 \end{pmatrix} - a \begin{pmatrix} \cos(x^3+q^3+x^4+q^4) \\ \pm\sin(x^3+q^3+x^4+q^4) \\ 0 \\ 0 \end{pmatrix},$$

which means that $\phi_\pm^{-1} \circ \xi \circ \phi_\pm = \xi$. Thus, our diffeomorphism $\phi_\pm$ is equivariant as per Definition 5.13 with $H = \mathrm{SG}_0^\pm$.

Observe now that the complex 2-form $p \wedge u^\flat$ is an eigenvector of the Hodge star. This motivates the following definition.

Definition 5.20. We say that a solution from Theorem 5.19 is *right-handed* if $*(p \wedge u^\flat) = i\,(p \wedge u^\flat)$ and *left-handed* if $*(p \wedge u^\flat) = -i\,(p \wedge u^\flat)\,.$

It is easy to see that the upper sign in formula (5.8.8) corresponds to a right-handed solution and the lower sign corresponds to a left-handed one. Note that we defined right/left-handedness for groups (Definition 5.16) and massless solutions (Definition 5.20) in such a way that they agree.

5.9 Explicit massive solutions of nonlinear field equations

Theorem 5.21. *Let m be a positive real number and let p be a real timelike covector with $p_\beta p^\beta = -4m^2$ and $p_4 > 0$. Let u be a complex isotropic vector orthogonal to p, and let v be a real vector orthogonal to p and u. Suppose that*

$$4m^2\left(\frac{1}{2}u_\alpha \bar{u}^\alpha + v_\beta v^\beta\right) = c\,, \tag{5.9.1}$$

where c is a critical point from (5.2.18), and put

$$\mathbb{A}^\alpha(x) = u^\alpha\, e^{ip_\beta x^\beta}. \tag{5.9.2}$$

Then the diffeomorphism (5.8.1) with

$$A(x) = \operatorname{Re}\left[\mathbb{A}(x)\right] + (p_\gamma x^\gamma)\, v \tag{5.9.3}$$

is volume preserving and satisfies the nonlinear field equations (5.3.5).

Remark 5.22. It is easy to see that under the assumptions of Theorem 5.21 the scalar $\|\mathrm{d}A^\flat\|^2_g$ is constant,

$$\|\mathrm{d}A^\flat\|^2_g = -4m^2\left(\frac{1}{2}u_\alpha \bar{u}^\alpha + v_\beta v^\beta\right).$$

Hence, formula (5.9.1) can be equivalently rewritten as

$$\|\mathrm{d}A^\flat\|^2_g = -c\,, \tag{5.9.4}$$

which is a condition on the strength of the field $\mathrm{d}A^\flat$. We see a certain similarity with the Born–Infeld model [24], [72, Section 2.1] which sets constraints on admissible values of $\|\mathrm{d}A^\flat\|^2_g$.

Proof of Theorem 5.21. Arguing as in the proof of Theorem 5.19, we can perform a (unique) proper orthochronous Lorentz transformation of coordinates so that formula (5.9.2) reads

$$\mathbb{A}^\alpha(x) = a \begin{pmatrix} 1 \\ -i \\ 0 \\ 0 \end{pmatrix} e^{2imx^4} \tag{5.9.5}$$

and (5.9.3) becomes

$$A^\alpha(x) = \begin{pmatrix} a\cos(2mx^4) \\ a\sin(2mx^4) \\ 2mbx^4 \\ 0 \end{pmatrix}. \tag{5.9.6}$$

Here

$$a = \sqrt{\frac{u_\alpha \bar{u}^\alpha}{2}}\,, \tag{5.9.7a}$$

$$b = -\frac{i}{4ma^2} *(p \wedge u^\flat \wedge \bar{u}^\flat \wedge v^\flat). \tag{5.9.7b}$$

Note that $|b| = \sqrt{v_\alpha v^\alpha}$. However, in defining the scalar invariant b we used the seemingly more complicated formula (5.9.7b) in order to capture information on the relative orientation of the four covectors p, $\operatorname{Re} u^\flat$, $\operatorname{Im} u^\flat$ and $v^\flat$. With this notation formula (5.9.1) can be rewritten as

$$4m^2(a^2 + b^2) = c\,. \tag{5.9.7c}$$

The corresponding deformation gradient reads

$$D^\alpha{}_\beta = \begin{pmatrix} 1 & 0 & 0 & -2ma\sin(2mx^4) \\ 0 & 1 & 0 & 2ma\cos(2mx^4) \\ 0 & 0 & 1 & 2mb \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{5.9.8}$$

for which (5.8.4a) is satisfied. The resulting strain tensor is

$$S^\alpha{}_\beta = \begin{pmatrix} 0 & 0 & 0 & -2ma\sin(2mx^4) \\ 0 & 0 & 0 & 2ma\cos(2mx^4) \\ 0 & 0 & 0 & 2mb \\ 2ma\sin(2mx^4) & -2ma\cos(2mx^4) & -2mb & -c \end{pmatrix}. \tag{5.9.9}$$

Unlike (5.8.10), the matrix (5.9.9) is not nilpotent: its eigenvalues are zero (algebraic and geometric multiplicity two) and

$$-\frac{c}{2}\pm\frac{\sqrt{c(c-4)}}{2}\,.$$

The matrix is diagonalisable if and only if $c\neq 4$.

The fact that the eigenvalues of the strain tensor (5.9.9) are constant implies that all our scalar invariants (5.2.5) are constant:

$$e_1=-c,\qquad e_2=c,\qquad e_3=e_4=0.$$

Arguing as in the proof of Theorem 5.19, we see that in order to prove that our diffeomorphism satisfies the nonlinear field equations (5.3.5) it is sufficient to show, in view of (5.2.18), that

$$\int_{\mathbb{R}^4}\Delta e_j\,\mathrm{d}x\,=0\,,\qquad j=3,4.$$

It is easy to see that $\Delta e_4=0$, which, in essence, is to do with the fact that zero is a double eigenvalue of (5.9.9).

The formula for Δe_3 reads

$$\Delta e_3=B^\beta{}_\alpha\,\frac{\partial\Delta A^\alpha}{\partial x^\beta}\,,$$

where the $B^\beta{}_\alpha$ is some tensor. The explicit formulae for the components of this tensor are complicated, however for our purposes it suffices to observe that $B^4{}_\alpha=0$ and that the remaining components depend only on the coordinate x^4. Hence, integration by parts yields

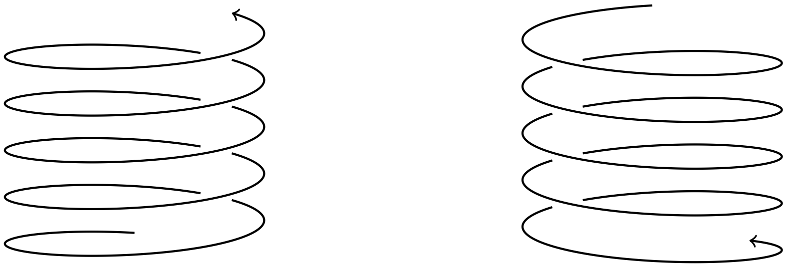
$$\int_{\mathbb{R}^4}\Delta e_3\,\mathrm{d}x\,=-\int_{\mathbb{R}^4}\left(\frac{\partial B^\beta{}_\alpha}{\partial x^\beta}\right)\Delta A^\alpha\,\mathrm{d}x\,=-\int_{\mathbb{R}^4}\left(\frac{\partial B^4{}_\alpha}{\partial x^4}\right)\Delta A^\alpha\,\mathrm{d}x\,=0\,.$$

□

Group-theoretic arguments apply to the massive case as well. Taking an arbitrary $\xi\in\mathrm{SG}_m$, see formula (5.7.2), we get $\phi^{-1}\circ\xi\circ\phi=\eta$, where

$$\mathrm{SG}_m\ni\eta:\begin{pmatrix}x^1\\x^2\\x^3\\x^4\end{pmatrix}\mapsto\begin{pmatrix}x^1\cos(2mq^4)-x^2\sin(2mq^4))\\x^1\sin(2mq^4)+x^2\cos(2mq^4)\\x^3\\x^4\end{pmatrix}+\begin{pmatrix}q^1\\q^2\\q^3-2mbq^4\\q^4\end{pmatrix}.$$

This means that our diffeomorphism ϕ is homogeneous as per Definition 5.13 with $H=\mathrm{SG}_m$. It is equivariant if and only if $b=0$.



(i) $b > 0$ (ii) $b < 0$

Figure 1: Massive solution

Let us discuss the continuum mechanics interpretation of formula (5.9.6). We are looking at a translation (rigid motion without rotation) of 3-dimensional Euclidean space which is a function of the time coordinate x^4. Every point of 3-dimensional Euclidean space moves along a helix, see Figure 1(i) for $b > 0$ and Figure 1(ii) for $b < 0$.

The parameter b could be interpreted as electric charge. Note that for given values of positive parameters m and a the parameter b can take only two values,

$$b = \pm\sqrt{\frac{c}{4m^2} - a^2}\,.$$

5.10 Massless Dirac equation

Let the diffeomorphisms ϕ_+ and ϕ_- be right-handed and left-handed massless solutions as per Definition 5.20. In this section we will calculate the corresponding rotation 2-forms, see Section 5.4, and show that they are equivalent to spinor fields which satisfy massless Dirac equations.

The deformation gradient reads

$$D^\alpha{}_\beta = \delta^\alpha{}_\beta + \operatorname{Re}\left[iu^\alpha p_\beta\, e^{ip_\gamma x^\gamma}\right]. \qquad (5.10.1)$$

In a particular coordinate system the above formula turns to (5.8.9). Performing a polar decomposition (5.4.6), we get

$$U^\alpha{}_\beta = \delta^\alpha{}_\beta - \frac{1}{2}\operatorname{Re}\left[i\,(p^\alpha u_\beta - u^\alpha p_\beta)\,e^{ip_\gamma x^\gamma}\right] - \frac{u_\gamma \bar{u}^\gamma}{16}p^\alpha p_\beta\,, \tag{5.10.2}$$

$$V^\alpha{}_\beta = \delta^\alpha{}_\beta + \frac{1}{2}\operatorname{Re}\left[i\,(p^\alpha u_\beta + u^\alpha p_\beta)\,e^{ip_\gamma x^\gamma}\right] + \frac{3u_\gamma \bar{u}^\gamma}{16}p^\alpha p_\beta\,.$$

On account of formula (5.4.7) one can compute the logarithm of (5.10.2), lower the first index and obtain the following explicit formula for the rotation 2-form:

$$F = -\frac{1}{2}\operatorname{Re}\left[i(p\wedge u^\flat)e^{ip_\gamma x^\gamma}\right] = -\frac{1}{2}\mathrm{d}A^\flat. \tag{5.10.3}$$

We see that the formula for our rotation 2-form is remarkably simple. Recall that for a general diffeomorphism we have $F = -\frac{1}{2}\mathrm{d}A^\flat + O(\|A\|^2)$, see formulae (5.4.9c) and (5.4.10). However the deformation gradient generated by our massless solutions is very special and turns out to be linear in displacements, without any second (or higher) order terms and without any assumptions on the amplitude. The underlying reason for such simplicity is that at any given point of $\mathbb{M}$ one can identify a 2-dimensional invariant subspace of the tangent fibre in which the deformation gradient (5.10.1) differs from the identity map. Furthermore, the restriction of the Minkowski metric to this subspace is degenerate.

Put

$$\mathbb{F} := -\frac{1}{2}\mathrm{d}\mathbb{A}^\flat = -\frac{i}{2}(p\wedge u^\flat)\,e^{ip_\gamma x^\gamma}, \tag{5.10.4}$$

so that $F = \operatorname{Re}\mathbb{F}$. In the remainder of this section we examine the structure of the complex-valued 2-form $\mathbb{F}$.

The 2-form $\mathbb{F}$ is polarised

$$*\,\mathbb{F} = \pm i\,\mathbb{F} \tag{5.10.5}$$

(cf. Definition 5.20) and degenerate

$$\det\mathbb{F} = 0.$$

It is known, see Appendix D.1.3, that such a 2-form is equivalent, modulo sign, to a spinor field which is, effectively, the square root of $\mathbb{F}$. This spinor field is undotted, $\xi = \xi^a$, in the left-handed case (lower sign in (5.10.5)) and dotted, $\eta = \eta_{\dot a}$, in the right-handed case (upper sign in (5.10.5)).

Theorem 5.23. *The spinor field ξ associated with a left-handed massless solution satisfies the massless Dirac equation*

$$\sigma^{\alpha}{}_{\dot{a}b}\,\partial_{x^\alpha}\xi^b = 0. \tag{5.10.6}$$

The spinor field η associated with a right-handed massless solution satisfies the massless Dirac equation

$$\sigma^{\alpha\dot{b}a}\,\partial_{x^\alpha}\eta_{\dot{b}} = 0. \tag{5.10.7}$$

Proof. It is sufficient to establish the identities (5.10.6) and (5.10.7) in one coordinate system, so let us work in the coordinate system in which we have (5.8.7). Plugging (5.8.7) into (5.10.4) we get

$$\mathbb{F}_{\alpha\beta} = -\frac{ia}{2}\begin{pmatrix} 0 & 0 & -1 & -1 \\ 0 & 0 & \pm i & \pm i \\ 1 & \mp i & 0 & 0 \\ 1 & \mp i & 0 & 0 \end{pmatrix} e^{i(x^3+x^4)},$$

where the upper/lower sign corresponds to right-/left-handedness respectively. Using formulae from Appendix D.1.3 we conclude that

$$\xi^a = \pm\sqrt{\frac{a}{2}}\begin{pmatrix} 0 \\ i \end{pmatrix} e^{i(x^3+x^4)/2}, \tag{5.10.8}$$

$$\eta_{\dot{a}} = \pm\sqrt{\frac{a}{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{i(x^3+x^4)/2}. \tag{5.10.9}$$

It remains only to substitute (D.1.1) and (5.10.8) into (5.10.6), and (D.1.2) and (5.10.9) into (5.10.7). □

5.11 Massive Dirac equation

Let the diffeomorphism ϕ be a massive solution as per Theorem 5.21. The corresponding deformation gradient reads

$$D^{\alpha}{}_{\beta} = \delta^{\alpha}{}_{\beta} + \operatorname{Re}\left[iu^{\alpha}p_{\beta}\,e^{ip_\gamma x^\gamma}\right] + v^{\alpha}p_{\beta}. \tag{5.11.1}$$

In a particular coordinate system the above formula turns to (5.9.8). Explicit calculations show that (5.10.1) admits a polar decomposition if and only if $c < 4$. Assuming that $c<4$ and arguing as in Section 5.10 we arrive at the following explicit formula for the rotation 2-form:

$$F = -\frac{1}{\sqrt{c}}\,\operatorname{arctanh}\left(\frac{\sqrt{c}}{2}\right)\left(\operatorname{Re}\left[i(p\wedge u^\flat)e^{ip_\gamma x^\gamma}\right] + (p\wedge v^\flat)\right)$$
$$= -\frac{1}{\sqrt{c}}\,\operatorname{arctanh}\left(\frac{\sqrt{c}}{2}\right)\mathrm{d}A^\flat. \qquad (5.11.2)$$

Observe that unlike the massless case (5.10.3) the prefactor in the RHS of (5.11.2) brings about, effectively, contributions nonlinear in A, see (5.9.4). But apart from the prefactor formula (5.11.2) is quite simple. Here the underlying reason is the same as in the massless case: at any given point of $\mathbb{M}$ one can identify a 2-dimensional invariant subspace of the tangent fibre in which the deformation gradient (5.11.1) differs from the identity map.

Put

$$\mathbb{F} := -\frac{1}{\sqrt{c}}\,\operatorname{arctanh}\left(\frac{\sqrt{c}}{2}\right)\mathrm{d}\mathbb{A}^\flat = -\frac{i}{\sqrt{c}}\,\operatorname{arctanh}\left(\frac{\sqrt{c}}{2}\right)(p\wedge u^\flat)\,e^{ip_\gamma x^\gamma},$$

which captures information about the oscillating part of F. As in the previous section, we will now examine the geometric content of $\mathbb{F}$.

Unlike the massless case, $\mathbb{F}$ is not polarised. However, it can be decomposed into a sum of polarised pieces

$$\mathbb{F} = \mathbb{F}_+ + \mathbb{F}_-\,,$$
$$\mathbb{F}_+ = \frac{\mathbb{F} - i*\mathbb{F}}{2}\,, \qquad \mathbb{F}_- = \frac{\mathbb{F} + i*\mathbb{F}}{2}\,,$$
$$*\,\mathbb{F}_\pm = \pm i\mathbb{F}_\pm\,. \qquad (5.11.3)$$

In our case the two polarised pieces are degenerate, i.e.

$$\det\mathbb{F}_\pm = 0. \qquad (5.11.4)$$

The latter follows easily from the observation that the pair of identities (5.11.4) is equivalent to

$$\det\mathbb{F} = 0, \qquad \mathbb{F}_{\alpha\beta}\,\mathbb{F}^{\alpha\beta} = 0.$$

The 2-form $\mathbb{F}_-$ is equivalent, modulo sign, to an undotted spinor field $\xi=\xi^a$ and the 2-form $\mathbb{F}_+$ is equivalent, modulo sign, to a dotted spinor field $\eta=\eta_{\dot a}$. Since in our case the scalar $\xi^a\bar\eta_a$ is real and nonzero, one can choose the relative sign of ξ and

η so that $\xi^a \bar{\eta}_a > 0$. Thus, our complex-valued 2-form $\mathbb{F}$ is equivalent to a bispinor field (ξ, η). This bispinor field is defined uniquely up to sign and is, effectively, the square root of $\mathbb{F}$.

Theorem 5.24. *The bispinor field (ξ, η) associated with a massive solution satisfies the massive Dirac equation*

$$-\,i\sigma^\alpha{}_{\dot{a}b}\,\partial_{x^\alpha}\xi^b = m\,\eta_{\dot{a}}\,, \qquad -i\sigma^{\alpha\dot{b}a}\,\partial_{x^\alpha}\eta_{\dot{b}} = m\,\xi^a\,. \tag{5.11.5}$$

Proof. Arguing along the same lines as that of Theorem 5.23, in the special coordinate system in which we have (5.9.5) we get

$$\xi^a = \eta_{\dot{a}} = \pm\sqrt{\frac{ma}{\sqrt{c}}\,\operatorname{arctanh}\left(\frac{\sqrt{c}}{2}\right)}\begin{pmatrix}0\\ i\end{pmatrix}e^{imx^4}.$$

The above bispinor field clearly satisfies (5.11.5). □

Remark 5.25. In writing the massive Dirac equation (5.11.5) we adopted the spinor representation, cf. [20, formula (20.2)], as opposed to the standard representation, cf. [20, formulae (21.19), (21.17)].

Appendix A

The wave propagator: complementary material

A.1 The subprincipal symbol for the 2-sphere: Mathematica script

This Appendix contains the Mathematica code implemented to compute the subprincipal symbol of the wave propagator for the 2-sphere, see Section 2.11.1. In the script we adopt the notation $\tau = t/2$.

```
(* Propagator for the 2-sphere: complete scrpit *)
(* (c) Matteo Capoferri -  18 September 2017  *)

SetDirectory[NotebookDirectory[]];

(* Definition of the phase function *)

(* Unit vector in R^3 corresponding to the point (u,v) *)
w[{u_, v_}] := {4 u/(4 + u^2 + v^2), 4 v/(4 + u^2 + v^2), (u^2 + v^2 - 4)(4+ u^2 + v
    ^2)};

(* Towards the taylor expansion for the geodesic distance*)
\[CapitalPsi][{u_, v_}, {x_,y_}] :=
        (Cross[w[{u, v}], w[{x, y}]][[1]])^2 +(Cross[w[{u, v}], w[{x, y}]][[2]])^2
                + (Cross[w[{u, v}], w[{x, y}]][[3]])^2;
```

```
\[Chi][x_] := Normal[Series[ArcSin[Sqrt[x]]/Sqrt[x], {x, 0, 5}]];

(* Distance squared *)
distsq[{u_, v_}, {x_,y_}] := \[CapitalPsi][{u, v}, {x,y}]  \[Chi][\[CapitalPsi][{u, v
    }, {x, y}]]^2;

(* Derivative of the distance squared *)
Ddistsq[\[Tau]_, {u_,v_}, {\[Eta]1_, \[Eta]2_}] :=
        {D[distsq[{u, v}, {x, y}], x], D[distsq[{u, v}, {x, y}], y]}
                /. {x -> 2 Tan[\[Tau]] \[Eta]1/Sqrt[\[Eta]1^2 + \[Eta]2^2],
                        y -> 2 Tan[\[Tau]] \[Eta]2/Sqrt[\[Eta]1^2 + \[Eta]2^2]};

(* Phase function: real part  *)
Re\[CapitalPhi][\[Tau]_, {u_, v_}, {\[Eta]1_, \[Eta]2_}] :=
        -1/2 Cos[\[Tau]]^(-2) {\[Eta]1, \[Eta]2}.Ddistsq[\[Tau], {u, v}, {\[Eta]1, \[
            Eta]2}];

(* Phase function: imaginary part *)
Im\[CapitalPhi][\[Epsilon]_, \[Tau]_, {u_,v_}, {\[Eta]1_, \[Eta]2_}] :=
        1/2 \[Epsilon] Sqrt[\[Eta]1^2 + \[Eta]2^2] distsq[{u, v}, {x,y}]
                /. {x ->2 Tan[\[Tau]] \[Eta]1/Sqrt[\[Eta]1^2 + \[Eta]2^2],
                        y -> 2 Tan[\[Tau]] \[Eta]2/Sqrt[\[Eta]1^2 + \[Eta]2^2]};

(* Phase function: rea partl + imaginary part *)
\[CapitalPhi][\[Epsilon]_, \[Tau]_, {u_, v_}, {\[Eta]1_, \[Eta]2_}] :=
        Re\[CapitalPhi][\[Tau], {u, v}, {\[Eta]1, \[Eta]2}] + I Im\[CapitalPhi][\[
            Epsilon], \[Tau], {u,v}, {\[Eta]1, \[Eta]2}];

(* Taylor expansion of the phase function  *)
Phi0 = Normal[Series[\[CapitalPhi][\[Epsilon],\[Tau],{2 Tan[\[Tau]]+s Z1,s Z2},{1,
    0}],{s,0,7}]]
         /. {s -> 1} // Simplify;

Phi1 = Phi0 /. {Z1 ->z1 Cos[\[Theta]] + z2 Sin[\[Theta]] + (Cos[\[Theta]] \[Minus] 1)
    r,
        Z2 -> \[Minus]z1 Sin[\[Theta]] + z2 Cos[\[Theta]] \[Minus] Sin[\[Theta]] r} //
             Simplify;
```

```
rho = Normal[Series[Sqrt[(1 + s \[Zeta]1)^2 + s^2 \[Zeta]2^2] - 1, {s, 0, 6}]] /. {s
    -> 1};

theta = Normal[Series[ArcTan[s \[Zeta]2 /(1 + s \[Zeta]1)], {s, 0, 6}]] /. {s -> 1};

Zstar = 2 Tan[\[Tau]]
        Normal[Series[{(1 + s \[Zeta]1)/Sqrt[(1 + s \[Zeta]1)^2 + s^2 \[Zeta]2^2],
                s \[Zeta]2/Sqrt[(1 + s \[Zeta]1)^2 + s^2 \[Zeta]2^2]}, {s, 0, 6}]]
                        /. {s -> 1};

Phi2 = Phi1
        /. {Sin[\[Theta]] -> Normal[Sin[\[Theta]] + O[\[Theta]]^7],
                Cos[\[Theta]] -> Normal[ Cos[\[Theta]] + O[\[Theta]]^7]} // Simplify;

Phi3 = (1 + \[Rho]) Normal[Phi2];

Phi4 = Phi3 /. {r -> 2 Tan[\[Tau]], \[Theta] -> theta, \[Rho] -> rho};

Phi5 = Normal[Series[
        Phi4 /. {z1 -> s z1, z2 -> s z2, \[Zeta]1 -> s \[Zeta]1, \[Zeta]2 -> s \[Zeta
            ]2},
                {s, 0, 6}]] /. {s -> 1} // Simplify;

Phi5 >> "PF.m"

(* Taylor expansion of the first time derivative of the phase function \varphi_\tau
    *)
Phi\[Tau]0 = Phi0 /. {Z1 -> x1 - 2 Tan[\[Tau]]};

Phi\[Tau]1 = D[Phi\[Tau]0, \[Tau]];

Phi\[Tau]2 = Phi\[Tau]1 /. {x1 -> Z1 + 2 Tan[\[Tau]]};

Phi\[Tau]3 = Phi\[Tau]2
        /. {Z1 -> z1 Cos[\[Theta]] + z2 Sin[\[Theta]] + (Cos[\[Theta]] \[Minus] 1) r,
                Z2 -> \[Minus]z1 Sin[\[Theta]] + z2 Cos[\[Theta]] \[Minus] Sin[\[Theta
                    ]] r};

Phi\[Tau]4 = Phi\[Tau]3
```

```
        /. {Sin[\[Theta]] -> Normal[Sin[\[Theta]] + O[\[Theta]]^7],
                Cos[\[Theta]] -> Normal[ Cos[\[Theta]] + O[\[Theta]]^7]};

Phi\[Tau]5 = (1 + \[Rho]) Phi\[Tau]4;

Phi\[Tau]6 = Phi\[Tau]5 /. {r -> 2 Tan[\[Tau]], \[Theta] -> theta, \[Rho] -> rho};

Phi\[Tau]7 =  Normal[Series[
        Phi\[Tau]6 /. {z1 -> s z1, z2 -> s z2, \[Zeta]1 -> s \[Zeta]1,
                \[Zeta]2 -> s \[Zeta]2}, {s, 0, 6}]] /. {s -> 1} // Simplify;

Phi\[Tau]7 >> "PFt.m"

(* Taylor expansion of the second time derivative of the phase function \varphi_{\tau\
    tau} *)
Phi\[Tau]\[Tau]1 = D[Phi\[Tau]0, \[Tau], \[Tau]];

Phi\[Tau]\[Tau]2 = Phi\[Tau]\[Tau]1 /. {x1 -> Z1 + 2 Tan[\[Tau]]};

Phi\[Tau]\[Tau]3 =
  Phi\[Tau]\[Tau]2
         /. {Z1 -> z1 Cos[\[Theta]] +  z2 Sin[\[Theta]] + (Cos[\[Theta]] \[Minus] 1) r
              ,
                Z2 -> \[Minus]z1 Sin[\[Theta]] + z2 Cos[\[Theta]] \[Minus] Sin[\[Theta
                    ]] r};

Phi\[Tau]\[Tau]4 = Phi\[Tau]\[Tau]3
        /. {Sin[\[Theta]] -> Normal[Sin[\[Theta]] + O[\[Theta]]^7],
                Cos[\[Theta]] ->   Normal[ Cos[\[Theta]] + O[\[Theta]]^7]};

Phi\[Tau]\[Tau]5 = (1 + \[Rho]) \Phi\[Tau]\[Tau]4;

Phi\[Tau]\[Tau]6 = Phi\[Tau]\[Tau]5 /. {r -> 2 Tan[\[Tau]], \[Theta] -> theta, \[Rho]
    -> rho};

Phi\[Tau]\[Tau]7 = Normal[Series[Phi\[Tau]\[Tau]6
        /. {z1 -> s z1, z2 -> s z2, \[Zeta]1 -> s \[Zeta]1, \[Zeta]2 -> s \[Zeta]2}, {
            s, 0, 6}]]
                /. {s -> 1} // Simplify;
```

```
Phi\[Tau]\[Tau]7 >> "PFtt.m"

(* Taylor expansion of \varphi_{z\eta}^{-1}, \det(\varphi_{z\eta}), \det(\varphi_{z\
    eta}^{-1}) *)
PhaseFunction = << "PF.m";

PhiZzeta = {{D[PhaseFunction, z1, \[Zeta]1], D[PhaseFunction, z1, \[Zeta]2]},{D[
    PhaseFunction, z2, \[Zeta]1],
        D[PhaseFunction, z2, \[Zeta]2]}};

DetPhiZzeta = Det[PhiZzeta];

DetPhiZzeta1 = Normal[Series[
        DetPhiZzeta /. {z1 -> s z1, z2 -> s z2 , \[Zeta]1 -> s \[Zeta]1,
                \[Zeta]2 -> s \[Zeta]2}, {s, 0, 4}]]
                        /. {s -> 1} // Simplify;

X = DetPhiZzeta1 - Cos[\[Tau]]^4 (Cos[2 \[Tau]] - I \[Epsilon] Sin[2 \[Tau]]) //
    Simplify;

Y = X/(Cos[\[Tau]]^4 (Cos[2 \[Tau]] - I \[Epsilon] Sin[2 \[Tau]]));

DetPhiZzetaInv = 1/(Cos[\[Tau]]^4 (Cos[2 \[Tau]] - I \[Epsilon] Sin[2 \[Tau]]))
        (1 - Y + Y^2 - Y^3 + Y^4 - Y^5 + Y^6);

DetPhiZzetaInv1 = Normal[Series[DetPhiZzetaInv
        /. {z1 -> s z1, z2 -> s z2, \[Zeta]1 -> s \[Zeta]1, \[Zeta]2 -> s \[Zeta]2}, {
            s, 0, 4}]]
                /. {s -> 1};

DetPhiZzetaInv2 = DetPhiZzetaInv1 // Simplify;

PhiZzetaInv = DetPhiZzetaInv2
        {{PhiZzeta[[2, 2]], -PhiZzeta[[1, 2]]}, {-PhiZzeta[[2, 1]], PhiZzeta[[1,
            1]]}};

PhiZzetaInv1 = Normal[Series[PhiZzetaInv
```

```
        /. {z1 -> s z1, z2 -> s z2, \[Zeta]1 -> s \[Zeta]1, \[Zeta]2 -> s \[Zeta]2}, {
            s, 0, 4}]]
                /. {s -> 1} // Simplify;

PhiZzetaInv1 >> "PFzZetaInv.m"
DetPhiZzetaInv2 >> "DetPFzZetaInv.m"
DetPhiZzeta1 >> "DetPhizZeta.m"

(* Amplitude-to-symbol operator *)

(* Preliminary definitions  *)
PF = << "PF.m";
PhiZzetaInv = << "PFzZetaInv.m";
DetPhiZzetaInv = << "DetPFzZetaInv.m" ;
DetPhiZzeta = << "DetPhizZeta.m";
PFt = << "PFt.m";
PFtt = << "PFtt.m";

InvMetricComponent = (1 + 1/4 u^2 + 1/4 v^2)^2 /. {u -> z1 + 2 Tan[\[Tau]],
    v -> z2} (* REMARK: we only need this for all practical purposes, as the metric is
         diagonal and a multiple of the identity *);

detg = 1/(1 + 1/4 u^2 + 1/4 v^2)^4 /. {u -> z1 + 2 Tan[\[Tau]], v -> z2};

(* Useful derivatives of the phase function and of the weight *)
PF\[Zeta] = {D[PF, \[Zeta]1], D[PF, \[Zeta]2]};

PF\[Zeta]\[Zeta] = {{D[PF, \[Zeta]1, \[Zeta]1], D[PF, \[Zeta]1, \[Zeta]2]},
        {D[PF, \[Zeta]2, \[Zeta]1], D[PF, \[Zeta]2, \[Zeta]2]}};

DetPFz\[Zeta]\[Tau] = D[PFt, z1, \[Zeta]1] D[PF, z2, \[Zeta]2]
        + D[PF, z1, \[Zeta]1] D[PFt, z2, \[Zeta]2] -  D[PFt, z1, \[Zeta]2] D[PF, z2,
            \[Zeta]1]
                -  D[PF, z1, \[Zeta]2] D[PFt, z2, \[Zeta]1];

DetPFz\[Zeta]\[Tau]\[Tau] = D[PFtt, z1, \[Zeta]1] D[PF, z2, \[Zeta]2]
        + 2 D[PFt, z1, \[Zeta]1] D[PFt, z2, \[Zeta]2] + D[PF, z1, \[Zeta]1] D[PFtt, z2
            , \[Zeta]2]
                - D[PFtt, z1, \[Zeta]2] D[PF, z2, \[Zeta]1]
```

```
                        -  2 D[PFt, z1, \[Zeta]2] D[PFt, z2, \[Zeta]1]
                                - D[PF, z1, \[Zeta]2] D[PFtt, z2, \[Zeta]1];

(* The subscript 0 following the name denotes evaluation at z=z^* *)
PhiZzetaInv0 = {{Sec[\[Tau]]^2,0},{0,Sec[\[Tau]]^2/(Cos[2 \[Tau]] -I \[Epsilon] Sin[2
    \[Tau]])}};

DetPhiZzetaInv0 = Sec[\[Tau]]^4/( Cos[2 \[Tau]] - I \[Epsilon] Sin[2 \[Tau]]);

DetPhiZzeta0 = Cos[\[Tau]]^4 (Cos[2 \[Tau]] - I \[Epsilon] Sin[2 \[Tau]]);

InvMetricComponent0 = Sec[\[Tau]]^4;
DzetaDetPhiZzeta0 = {0, 0};
Phizetazeta0 = {{0,0}, {0,-2 Cos[\[Tau]] Sin[\[Tau]](Cos[2 \[Tau]] -I \[Epsilon] Sin[2
     \[Tau]])}};

(* Differential operators L *)
L[y_] := {PhiZzetaInv[[1, 1]] D[y, z1] + PhiZzetaInv[[1, 2]] D[y, z2],
        PhiZzetaInv[[2, 1]] D[y, z1] + PhiZzetaInv[[2, 2]] D[y, z2]};

L0[y_] := {PhiZzetaInv0[[1, 1]] D[y, z1] + PhiZzetaInv0[[1, 2]] D[y, z2],
        PhiZzetaInv0[[2, 1]] D[y, z1] + PhiZzetaInv0[[2, 2]] D[y, z2]};

(* Differential-evaluation operators \mathfrak{S} *)
S1[y_] := -1/2 Sum[PF\[Zeta][[k]] L[y][[k]], {k, 1, 2}];

S2[y_] := 1/6 Sum[ PF\[Zeta][[k]] PF\[Zeta][[j]] L[L[y][[j]]][[k]], {k, 1, 2}, {j, 1,
    2}];

S3[y_] := -1/24 Sum[PF\[Zeta][[k]] PF\[Zeta][[j]] PF\[Zeta][[i]]
        L[L[L[y][[i]]][[j]]][[k]], {k, 1, 2}, {j, 1, 2}, {i, 1, 2}];

S[y_] := S1[y] + S2[y] + S3[y];

(* NOTATION: here B stands for a facilitated version of \mathfrak{S}, to reduce
    computational effort *)
B1[y_] := I/2 DetPhiZzetaInv
        (D[DetPhiZzeta, \[Zeta]1] (L[y][[1]] + S1[L[y][[1]]])
                + D[DetPhiZzeta, \[Zeta]2] (L[y][[2]] + S1[L[y][[2]]]))
```

```
                        + I (D[L[y][[1]] + S1[L[y][[1]]], \[Zeta]1]
                                + D[L[y][[2]] + S1[L[y][[2]]], \[Zeta]2]);

B2[y_] :=  I/2 DetPhiZzetaInv ( D[DetPhiZzeta, \[Zeta]1] (L[y][[1]] + S[L[y][[1]]])
        + D[DetPhiZzeta, \[Zeta]2] (L[y][[2]] + S[L[y][[2]]])) +  I (D[L[y][[1]]
                + S[L[y][[1]]], \[Zeta]1] + D[L[y][[2]] + S[L[y][[2]]], \[Zeta]2]);

B1b2[y_] := I (L[D[y, \[Zeta]1]][[1]] + L[D[y, \[Zeta]2]][[2]]
        - 1/2 (-2 Cos[\[Tau]] Sin[\[Tau]] (Cos[2 \[Tau]]
                - I \[Epsilon] Sin[2 \[Tau]]) L0[L[y][[2]]][[2]]))
                        (* SPECIAL CASE: B1 when acting on function with a second
                            order zero *);

B1b1[y_] := I (D[L[y][[1]], \[Zeta]1] + D[L[y][[2]], \[Zeta]2]
        - 1/2 (-2 Cos[\[Tau]] Sin[\[Tau]] (Cos[2 \[Tau]]
                - I \[Epsilon] Sin[2 \[Tau]]) L0[L[y][[2]]][[2]]))
                        (* SPECIAL CASE: B1 when acting on b_1 *);

B2self[y_] := I (D[L[y][[1]], \[Zeta]1] + D[L[y][[2]], \[Zeta]2]
        + Cos[\[Tau]] Sin[\[Tau]] (Cos[2 \[Tau]] -  I \[Epsilon] Sin[2 \[Tau]]) L0[L[y
            ][[2]]][[2]])
                (* SPECIAL CASE: B2 when acting on B2b2 *);

(* Homogeneous components of the amplitude b_2, b_1 and b_0  *)
b2 = -1/4 (PFt)^2 + InvMetricComponent ((D[PF, z1])^2 + (D[PF, z2])^2) ;

b1 = I 1/4 PFtt
        -  I InvMetricComponent (D[PF, z1, z1] + D[PF, z2, z2])
                +  I 1/4 DetPhiZzetaInv DetPFz\[Zeta]\[Tau] PFt
                        -  I InvMetricComponent DetPhiZzetaInv (D[DetPhiZzeta, z1] D[
                            PF, z1]
                                + D[DetPhiZzeta, z2] D[PF, z2])
                                        - I (D[InvMetricComponent, z1] D[PF, z1]
                                                + D[InvMetricComponent, z2] D[PF, z2])
                                                    ;

b0 = -1/16 (DetPhiZzetaInv0)^2 ((DetPFz\[Zeta]\[Tau])^2
        - 2 DetPhiZzeta0 DetPFz\[Zeta]\[Tau]\[Tau])
```

```
                + 1/4 (DetPhiZzetaInv0)^2 (1 + Tan[\[Tau]]^2)^2 ((D[DetPhiZzeta, z1])
                    ^2
                        + (D[DetPhiZzeta, z2])^2 - 2 DetPhiZzeta0 (D[DetPhiZzeta, z1,
                            z1]
                                + D[DetPhiZzeta, z2, z2]))
                                        - 1/2 DetPhiZzetaInv0 (D[InvMetricComponent,
                                            z1] D[DetPhiZzeta, z1]
                                                + D[InvMetricComponent, z2] D[
                                                    DetPhiZzeta, z2])
                                                        - (1 + Tan[\[Tau]]^2);

(* Transport equations *)
(* First Transport Equation *)
FTE = B1b2[b2] + b1 /. {z1 -> 0, z2 -> 0, \[Zeta]1 -> 0, \[Zeta]2 -> 0} // Simplify

(* Second Transport Equation *)

(* (B2)^2 [b2] *)
(* It needs to be dealt with differently and separately, because still computationally
     quite expensive *)
b2tay = Normal[Series[b2
        /. {z1 -> s z1, z2 -> s z2, \[Zeta]1 -> s \[Zeta]1, \[Zeta]2 -> s \[Zeta]2}, {
            s, 0, 4}]]
                /. {s -> 1} // Simplify;

Lb2tay = Normal[Series[L[b2]
        /. {z1 -> s z1, z2 -> s z2, \[Zeta]1 -> s \[Zeta]1, \[Zeta]2 -> s \[Zeta]2}, {
            s, 0, 3}]]
                /. {s -> 1};

SLb2tay = Normal[Series[S[Lb2tay]
        /. {z1 -> s z1, z2 -> s z2, \[Zeta]1 -> s \[Zeta]1, \[Zeta]2 -> s \[Zeta]2}, {
            s, 0, 3}]]
                /. {s -> 1};

B2b2 = I/2 DetPhiZzetaInv (D[DetPhiZzeta, \[Zeta]1] (La2tay[[1]]
        + SLb2tay[[1]]) + D[DetPhiZzeta, \[Zeta]2] (Lb2tay[[2]] + SLb2tay[[2]]))
                + I (D[Lb2tay[[1]] + SLb2tay[[1]], \[Zeta]1] + D[Lb2tay[[2]]
                        + SLb2tay[[2]], \[Zeta]2]);
```

```
fraksn1b2 = B2self[B2b2];

B2sqb2 = fraksn1b2 /. {z1 -> 0, z2 -> 0, \[Zeta]1 -> 0, \[Zeta]2 -> 0} // Simplify;

(* Reduced amplitude *)

RA1 = ((8 - 5 \[Epsilon]^2 + (4 - 7 \[Epsilon]^2) Cos[4 \[Tau]] + 3 I (\[Epsilon] + \[
    Epsilon]^3)
        Sin[4 \[Tau]])/(6 (Cos[2 \[Tau]] - I \[Epsilon] Sin[2 \[Tau]])^2))
                (* B2sqb2 evaluated at z=z^* *);

RA2 = B1b1[b1] /. {z1 -> 0, z2 -> 0, \[Zeta]1 -> 0, \[Zeta]2 -> 0} // Simplify;

RA3 = b0 /. {z1 -> 0, z2 -> 0, \[Zeta]1 -> 0, \[Zeta]2 -> 0} // Simplify;

RA = RA1 + RA2 + RA3;

(* ODE for the subprincipal symbol *)
STE = RA - I D[f[\[Tau]], \[Tau]];

DSolve[{STE == 0, f[0] == 0}, f[\[Tau]], \[Tau]] // Simplify
```

Appendix B

The Dirac propagator: complementary material

B.1 The Weitzenböck connection

In this Appendix we recall the main properties of the Weitzenböck connection and fix our signs conventions, which are chosen in agreement with [92].

Let M be an oriented Riemannian 3-manifold and let $\{e_j\}_{j=1}^3$ be a global orthonormal framing.

Definition B.1. The *Weitzenböck connection* is the affine connection ∇^W on M defined by the condition

$$\nabla^W_v(f^i\, e_i) = v(f^i)\, e_i\,, \tag{B.1.1}$$

for every vector field v and $f^i \in C^\infty(M;\mathbb{R})$, $i = 1, 2, 3$.

The Weitzenböck connection is a curvature-free metric-compatible connection. Formula (B.1.1) implies

$$0 = \nabla^W_{e_k} {e_j}^\alpha = {e_k}^\beta \frac{\partial {e_j}^\alpha}{\partial x^\beta} + {e_k}^\beta\, \Upsilon^\alpha{}_{\beta\gamma}\, {e_j}^\gamma,$$

which, in turn, yields a formula for the Weitzenböck connection coefficients $\Upsilon^\alpha{}_{\beta\gamma}$ in terms of the framing:

$$\Upsilon^\alpha{}_{\beta\gamma} = -\, e^j{}_\gamma \frac{\partial {e_j}^\alpha}{\partial x^\beta} = {e_j}^\alpha \frac{\partial e^j{}_\gamma}{\partial x^\beta}\,. \tag{B.1.2}$$

Here $e^j{}_\alpha := \delta^{jk}\, g_{\alpha\beta}\, e_k{}^\beta$. The torsion tensor associated with ∇^W is

$$T^\alpha{}_{\beta\gamma} = \Upsilon^\alpha{}_{\beta\gamma} - \Upsilon^\alpha{}_{\gamma\beta} \tag{B.1.3}$$

and the curvature tensor vanishes identically. The Weitzenböck connection coefficients and the Christoffel symbols are related via the identity

$$\Upsilon^\alpha{}_{\beta\gamma} = \Gamma^\alpha{}_{\beta\gamma} + \frac{1}{2}\,(T^\alpha{}_{\beta\gamma} + T_\beta{}^\alpha{}_\gamma + T_\gamma{}^\alpha{}_\beta)\,, \tag{B.1.4}$$

see [92, Eqn. (7.34)]. The second summand on the RHS of (B.1.4)

$$K^\alpha{}_{\beta\gamma} := \frac{1}{2}\,(T^\alpha{}_{\beta\gamma} + T_\beta{}^\alpha{}_\gamma + T_\gamma{}^\alpha{}_\beta) \tag{B.1.5}$$

is called *contorsion* of ∇^W. Note that the torsion tensor is antisymmetric in the second and third indices, $T^\alpha{}_{\beta\gamma} = -T^\alpha{}_{\gamma\beta}$, whereas the contorsion tensor is antisymmetric in the first and third ones, $K_{\alpha\beta\gamma} = -K_{\gamma\beta\alpha}$. Torsion and contorsion can be expressed one in terms of the other and capture the geometric information encoded within the framing.

In dimension three antisymmetric tensors of order two are equivalent to vectors. Therefore, we define

$$\overset{*}{T}_{\alpha\beta} := \frac{1}{2} T_\alpha{}^{\mu\nu}\, E_{\mu\nu\beta} \tag{B.1.6}$$

and

$$\overset{*}{K}_{\alpha\beta} := \frac{1}{2} K^\mu{}_\alpha{}^\nu\, E_{\mu\nu\beta}\,, \tag{B.1.7}$$

where

$$E_{\alpha\beta\gamma}(x) := \rho(x)\,\varepsilon_{\alpha\beta\gamma}\,, \tag{B.1.8}$$

ρ is the Riemannian density and ε is the totally antisymmetric symbol, $\varepsilon_{123} := +1$. It is often convenient to use (B.1.6) and (B.1.7) instead of T and K because the former have lower order – two instead of three.

As a final remark, we observe that formulae (B.1.6), (B.1.7) and (B.1.5) imply

$$\overset{*}{K}_{\alpha\beta} = \overset{*}{T}_{\alpha\beta} - \frac{1}{2}\overset{*}{T}{}^\gamma{}_\gamma\, g_{\alpha\beta}\,, \tag{B.1.9}$$

$$\overset{*}{T}_{\alpha\beta} = \overset{*}{K}_{\alpha\beta} - \overset{*}{K}{}^\gamma{}_\gamma\, g_{\alpha\beta}\,. \tag{B.1.10}$$

B.2 Some techincal proofs

B.2.1 Proof of Theorem 3.23

In the following, we work in normal coordinates centred at $y=0$ such that

$$e_j{}^\alpha(0)=\widetilde{e}_j{}^\alpha(0)=\delta_j{}^\alpha.$$

Since $G\in C^\infty(M;SU(2))$ and $G(0)=\mathrm{Id}$, there exist smooth real-valued functions A_k, $k=1,2,3$, such that $A_k(0)=0$ and

$$G(x)=e^{is^k A_k(x)} \tag{B.2.1}$$

in a neighbourhood of $y=0$. Differentiating (B.2.1) with respect to x and evaluating the result at 0, we obtain

$$G_{x^\alpha}(0)=is^k F_{k\alpha}, \tag{B.2.2}$$

where $F_{k\alpha}:=[A_k]_{x^\alpha}(0)$.

Now, differentiating (3.5.27) with respect to x and evaluating the result at 0, we obtain

$$\begin{aligned}\frac{\partial e_j{}^\alpha}{\partial x^\beta}(0)&=\frac{1}{2}\operatorname{tr}\left[s_j\,G^*_{x^\beta}(0)\,s^k+s_j\,s^k\,G_{x^\beta}(0)\right]\widetilde{e}_k{}^\alpha(0)+\frac{\partial\widetilde{e}_k{}^\alpha}{\partial x^\beta}(0)\\&=\frac{1}{2}\operatorname{tr}\left[[s_j\,s^k\,G_{x^\beta}(0)]^*+s_j\,s^k\,G_{x^\beta}(0\right]\widetilde{e}_k{}^\alpha(0)+\frac{\partial\widetilde{e}_k{}^\alpha}{\partial x^\beta}(0)\\&=\operatorname{Re}\,\operatorname{tr}\left[s_j\,s^k\,G_{x^\beta}(0)\right]\widetilde{e}_k{}^\alpha(0)+\frac{\partial\widetilde{e}_k{}^\alpha}{\partial x^\beta}(0).\end{aligned} \tag{B.2.3}$$

Contracting (B.2.3) with $e^j{}_\gamma(0)=\widetilde{e}^j{}_\gamma(0)=\delta^j{}_\gamma$, using (B.1.2) and rearranging, we obtain

$$\begin{aligned}\widetilde{\Upsilon}^\alpha{}_{\beta\gamma}(0)-\Upsilon^\alpha{}_{\beta\gamma}(0)&=\operatorname{Re}\operatorname{tr}\left[i\,s_js^ks^l\right]\,F_{l\beta}\,\delta^j{}_\gamma\,\delta_k{}^\alpha\\&=-2\,\varepsilon_\gamma{}^{\alpha l}\,F_{l\beta}.\end{aligned} \tag{B.2.4}$$

In view of (B.1.3), formula (B.2.4) implies

$$T^\alpha{}_{\beta\gamma}(0)-\widetilde{T}^\alpha{}_{\beta\gamma}(0)=2\,\varepsilon_\gamma{}^{\alpha l}\,F_{l\beta}-2\,\varepsilon_\beta{}^{\alpha l}\,F_{l\gamma}. \tag{B.2.5}$$

Contracting (B.2.5) with $\frac{1}{2}E_\sigma{}^{\beta\gamma}(y)=\frac{1}{2}\varepsilon_\sigma{}^{\beta\gamma}$, cf. (B.1.8), we get

$$\begin{aligned}\overset{*}{T}{}^\alpha{}_\sigma(0)-\overset{*}{\widetilde{T}}{}^\alpha{}_\sigma(0)&=2\varepsilon_\sigma{}^{\beta\gamma}\,\varepsilon_\gamma{}^{\alpha l}F_{l\beta}\\&=2\delta^{\beta l}\,F_{l\beta}\,\delta_\sigma{}^\alpha-2\delta_\sigma{}^l\,F_{l\alpha}.\end{aligned} \tag{B.2.6}$$

Inverting (B.2.6) so as to express F in terms of $[\overset{*}{T}-\overset{*}{\widetilde{T}}](0)$, we arrive at

$$\begin{aligned} -2F_{k\beta} &= \delta_k{}^\alpha\,[\overset{*}{T}-\overset{*}{\widetilde{T}}]_{\alpha\beta}(y) - \frac{1}{2}\,\delta_{k\beta}\,[\overset{*}{T}-\overset{*}{\widetilde{T}}]^\gamma{}_\gamma(0) \\ &= \delta_k{}^\alpha\big[\overset{*}{K}-\overset{*}{\widetilde{K}}\big]_{\alpha\beta}(0). \end{aligned} \tag{B.2.7}$$

Substitution of (B.2.7) into (B.2.2) gives (3.5.28).

B.2.2 Proof of Theorem 3.37

By definition of Levi-Civita framing, formula (3.7.58) implies $G(y)=\mathrm{Id}$. In the following, we work in a sufficiently small neighbourhood $\mathcal{U}$ of y and we choose normal coordinates centred at $y=0$ such that $\widetilde{e}_j{}^\alpha(0)=e_j{}^\alpha(0)=\delta_j{}^\alpha$.

Since $G\in C^\infty(M;SU(2))$ and $G(0)=\mathrm{Id}$, there exist smooth real-valued functions A_k, $k=1,2,3$, such that $v_k(0)=0$ and

$$G(x)=e^{is^k\,A_k(x)} \tag{B.2.8}$$

in a neighbourhood of $y=0$. Differentiating (B.2.8) twice with respect to x and evaluating the result at zero we obtain

$$\begin{aligned} G_{x^\alpha x^\beta}(0) &= is^k\,[A_k]_{x^\alpha x^\beta}(0) - \frac{1}{2}s^k\,s^j\,(F_{k\alpha}F_{j\beta}+F_{j\alpha}F_{k\beta}) \\ &= is^k\,H_{k\alpha\beta} - \delta^{jk}\,\mathrm{Id}\,F_{j\alpha}F_{k\beta}. \end{aligned} \tag{B.2.9}$$

Here $H_{k\alpha\beta}:=[A_k]_{x^\alpha x^\beta}(0)$ and $F_{k\alpha}:=[A_k]_{x^\alpha}(0)$. The task at hand is to express H in terms of the contorsion tensor K and its derivatives.

Differentiating the identity

$$\Upsilon^\alpha{}_{\beta\gamma}(x)=e_k{}^\alpha(x)\frac{\partial e^k{}_\gamma}{\partial x^\beta}(x) \tag{B.2.10}$$

with respect to x^μ, evaluating the outcome at $y=0$ and resorting to Lemma 3.7.2, we obtain

$$\begin{aligned} [\Upsilon^\alpha{}_{\beta\gamma}]_{x^\mu}(0) &= \frac{\partial e_k{}^\alpha}{\partial x^\mu}(0)\frac{\partial e^k{}_\gamma}{\partial x^\beta}(0) + e_k{}^\alpha(0)\frac{\partial^2 e^k{}_\gamma}{\partial x^\beta \partial x^\mu}(0) \\ &= -\Upsilon^\alpha{}_{\mu\rho}(0)\,\Upsilon^\rho{}_{\beta\gamma}(0) \\ &+ \delta_k{}^\alpha\,\mathrm{Re}\,\mathrm{tr}[s^k\,G^*_{x^\beta x^\mu}(0)\,s_l + s^k\,G^*_{x^\beta}(0)\,s_l\,G_{x^\mu}(0)]\,\delta^l{}_\gamma \\ &+ \delta_k{}^\alpha\,[\widetilde{e}^k{}_\gamma]_{x^\beta x^\mu}(0) \\ &= -\Upsilon^\alpha{}_{\mu\rho}(0)\,\Upsilon^\rho{}_{\beta\gamma}(0) + \delta_k{}^\alpha\delta^l{}_\gamma\,\mathrm{Re}\,\mathrm{tr}[s_l\,s^k\,G^*_{x^\beta x^\mu}(0)] \\ &+ \delta_k{}^\alpha\delta^l{}_\gamma\,\mathrm{Re}\,\mathrm{tr}[s^k\,G^*_{x^\beta}(0)\,s_l\,G_{x^\mu}(0)] + \delta_k{}^\alpha\,[\widetilde{e}^k{}_\gamma]_{x^\beta x^\mu}(0). \end{aligned} \tag{B.2.11}$$

Straightforward calculations show that

$$\begin{aligned} -\Upsilon^{\alpha}{}_{\mu\rho}(0)\,\Upsilon^{\rho}{}_{\beta\gamma}(0) &= -\operatorname{Re}\,\operatorname{tr}\,[s^{\alpha}\,G^{*}_{x^{\mu}}(0)s_{\rho}]\operatorname{Re}\,\operatorname{tr}\left[s^{\rho}\,G^{*}_{x^{\beta}}(0)s_{\gamma}\right] \\ &= 4\delta^{\alpha}{}_{\gamma}F^{r}{}_{\beta}F_{r\mu} - 4\delta^{\alpha j}\,\delta_{\gamma}{}^{k}\,F_{j\beta}F_{k\mu}, \end{aligned} \tag{B.2.12}$$

$$\delta_{k}{}^{\alpha}\delta^{l}{}_{\gamma}\operatorname{Re}\operatorname{tr}[s_{l}\,s^{k}\,G^{*}_{x^{\beta}x^{\mu}}(0)] = -2\varepsilon^{\alpha}{}_{\gamma}{}^{r}\,H_{r\beta\mu} - 2\delta^{\alpha}{}_{\gamma}\,F^{r}{}_{\beta}\,F_{r\mu} \tag{B.2.13}$$

and

$$\delta_{k}{}^{\alpha}\delta^{l}{}_{\gamma}\operatorname{Re}\operatorname{tr}[s_{l}\,G^{*}_{x^{\beta}}(0)\,s^{k}\,G_{x^{\mu}}(0)] = 2(\delta^{\alpha k}\delta^{j}{}_{\gamma} + \delta^{\alpha j}\delta^{k}{}_{\gamma})\,F_{j\mu}F_{k\beta} - 2\delta^{\alpha}{}_{\gamma}\,F^{r}{}_{\beta}\,F_{r\mu}. \tag{B.2.14}$$

Substituting (B.2.12)–(B.2.14) into (B.2.11) we obtain

$$[\Upsilon^{\alpha}{}_{\beta\gamma}]_{x^{\mu}}\,(0) = -2\varepsilon^{\alpha}{}_{\gamma}{}^{r}\,H_{r\beta\mu} + 2(\delta^{\alpha j}\delta^{k}{}_{\gamma} - \delta^{\alpha k}\delta^{j}{}_{\gamma})\,F_{j\mu}F_{k\beta} + \delta_{k}{}^{\alpha}\,[\widetilde{e}^{k}{}_{\gamma}]_{x^{\beta}x^{\mu}}(0). \tag{B.2.15}$$

Summing up (B.2.15) and (B.2.15) with indices β and μ swapped, we arrive at

$$[\Upsilon^{\alpha}{}_{\beta\gamma}]_{x^{\mu}}\,(0) + [\Upsilon^{\alpha}{}_{\mu\gamma}]_{x^{\beta}}\,(0) = -4\varepsilon^{\alpha}{}_{\gamma}{}^{r}\,H_{r\beta\mu} + 2\delta_{k}{}^{\alpha}\,[\widetilde{e}^{k}{}_{\gamma}]_{x^{\beta}x^{\mu}}(0). \tag{B.2.16}$$

Now, formula (B.1.4) and the fact that the Christoffel symbols vanish at $y=0$ imply

$$\varepsilon_{\alpha}{}^{\gamma}{}_{\rho}\,\Upsilon^{\alpha}{}_{\mu\gamma}(0) = \varepsilon_{\alpha}{}^{\gamma}{}_{\rho}\,K^{\alpha}{}_{\mu\gamma}(0) = 2\overset{*}{K}_{\mu\rho}(0). \tag{B.2.17}$$

Hence, by contracting (B.2.16) with $\varepsilon_{\alpha}{}^{\gamma}{}_{\rho}$, substituting (B.2.17) in, and resorting to the identity

$$\varepsilon_{\alpha}{}^{\gamma}{}_{\rho}\,\varepsilon^{\alpha}{}_{\gamma}{}^{r} = 2\delta_{\rho}{}^{r},$$

we obtain

$$[\overset{*}{K}_{\beta\rho}]_{x^{\mu}}(0) + [\overset{*}{K}_{\mu\rho}]_{x^{\beta}}(0) = -4\,\delta_{\rho}{}^{r}\,H_{r\beta\mu} + \varepsilon_{\alpha}{}^{\gamma}{}_{\rho}\,\delta_{k}{}^{\alpha}\,[\widetilde{e}^{k}{}_{\gamma}]_{x^{\beta}x^{\mu}}(0). \tag{B.2.18}$$

We claim that

$$\varepsilon_{\alpha}{}^{\gamma}{}_{\rho}\,\delta_{k}{}^{\alpha}\,[\widetilde{e}^{k}{}_{\gamma}]_{x^{\beta}x^{\mu}}(0) = 0. \tag{B.2.19}$$

To see this, let us observe that formula (3.7.2) implies

$$\widetilde{e}^{k}{}_{\gamma}(x) = e^{k}{}_{\gamma}(0) - \frac{1}{6}e^{k}{}_{\rho}(0)\,R_{\gamma\tau}{}^{\rho}{}_{\nu}(0)\,x^{\tau}x^{\nu} + O(\|x\|^{3}), \qquad j = 1,2,3,$$

so that

$$\delta_{k}{}^{\alpha}\,[\widetilde{e}^{k}{}_{\gamma}]_{x^{\beta}x^{\mu}}(0) = -\frac{1}{6}\,(R_{\gamma\beta}{}^{\alpha}{}_{\mu} + R_{\gamma\mu}{}^{\alpha}{}_{\beta})\,(0). \tag{B.2.20}$$

The RHS of (B.2.20) is symmetric in α and γ, whereas $\varepsilon_\alpha{}^\gamma{}_\rho$ is antisymmetric in the same indices, so (B.2.19) follows.

All in all, (B.2.9), (B.2.18) and (B.2.19) give us

$$\nabla_\alpha \nabla_\beta\, G(0) = -\frac{i}{4}[\nabla_\alpha \overset{*}{K}_{\beta\rho}(0) + \nabla_\beta \overset{*}{K}_{\alpha\rho}(0)]\sigma^\rho(0) - \delta^{jk}\,\mathrm{Id}\,F_{j\alpha}F_{k\beta}. \tag{B.2.21}$$

Finally, the substitution of (B.2.7) with $\widetilde{K}=0$ (which is the case for the Levi-Civita framing) into (B.2.21) yields (3.7.63).

B.3 Third Weyl coefficient: an alternative derivation

In this Appendix we shall provide an alternative proof for Theorem 3.39 starting from formulae (3.7.64) and (3.7.65), as opposed to formulae (3.7.11) and (3.7.56). This will also serve as a test for formulae (3.7.64) and (3.7.65).

Theorem 3.38 gives us

$$\begin{aligned}\operatorname{tr}\mathfrak{a}_0^\pm =& 1 + \frac{it}{2}\frac{\eta^\alpha\eta^\beta}{h^2}\overset{*}{K}_{\alpha\beta} \pm \frac{it^2}{8}\frac{\eta^\alpha\eta^\beta\eta^\mu}{h^3}\left(\nabla_\alpha \overset{*}{K}_{\beta\mu} + \nabla_\beta \overset{*}{K}_{\alpha\mu}\right)\\ &- \frac{t^2}{8}\frac{\eta^\alpha\eta^\beta}{h^2}\overset{*}{K}_{\alpha\mu}\overset{*}{K}_\beta{}^\mu + O(t^3),\end{aligned} \tag{B.3.1}$$

and

$$\begin{aligned}\operatorname{tr}\mathfrak{a}_{-1}^\pm =& \mp\frac{1}{2}\,h_{\eta_\alpha\eta_\beta}\,\overset{*}{K}_{\alpha\beta} \mp \frac{it}{24\,h}\mathcal{R}\\ &- \frac{t}{4}\left(\nabla_\alpha \overset{*}{K}_{\beta\mu} + \nabla_\beta \overset{*}{K}_{\alpha\mu}\right)\left(h_{\eta_\beta}\,h_{\eta_\alpha\eta_\beta} + \frac{1}{2}h_{\eta_\alpha\eta_\beta}\,h_{\eta_\mu}\right)\\ &\mp \frac{it}{8}\overset{*}{K}_{\alpha\mu}\overset{*}{K}_\beta{}^\mu\,h_{\eta_\alpha\eta_\beta}\\ &+ O(t^2),\end{aligned} \tag{B.3.2}$$

where we used the identities

$$\operatorname{tr}(\sigma^\beta P^\pm) = \pm\frac{\eta^\beta}{h}, \qquad \operatorname{tr}(\sigma^\beta P^\pm_{\eta_\alpha}) = \pm h_{\eta_\alpha\eta_\beta}. \tag{B.3.3}$$

We observe that (B.3.1) and (B.3.2) differ from (3.8.4) and (3.8.5) only in the terms containing contorsion. The task at hand is, therefore, to show that contributions to $N'_\pm * \mu$ coming from terms containing contorsion cancel out.

It is easy to see that there is no term containing contorsion contributing to the first Weyl coefficients, i.e. to order $O(\lambda^2)$.

Arguing as in Section 3.8, we find that the contribution of order $O(\lambda)$ to $N'_\pm * \mu$ is given by

$$\begin{aligned}
&\frac{1}{(2\pi)^4}\int_{\mathbb{R}}\int_{T_y^*M} e^{i(\lambda\mp\|\eta\|)t}\left(\frac{it}{2}\frac{\eta^\alpha\eta^\beta}{h^2}\overset{*}{K}_{\alpha\beta}\mp\frac{1}{2}\,h_{\eta_\alpha\eta_\beta}\overset{*}{K}_{\alpha\beta}\right)\widehat{\mu}(t)\chi(\|\eta\|)\,\mathrm{d}\eta\,\mathrm{d}t\\
&=\frac{1}{(2\pi)^4}\int_{\mathbb{R}}\int_{T_y^*M} e^{i(\lambda-\|\eta\|)t}\left(\pm\frac{it}{2}\frac{\eta^\alpha\eta^\beta}{h^2}\overset{*}{K}_{\alpha\beta}\mp\frac{1}{2}\,h_{\eta_\alpha\eta_\beta}\overset{*}{K}_{\alpha\beta}\right)\widehat{\mu}(\pm t)\,\chi(\|\eta\|)\,\mathrm{d}\eta\,\mathrm{d}t.
\end{aligned} \tag{B.3.4}$$

Switching to polar coordinates $\eta\mapsto(r:=\|\eta\|,\omega:=\eta/\|\eta\|)\in\mathbb{R}\times\mathbb{S}^2$ and dropping the cut-off, (B.3.4) turns into

$$\begin{aligned}
&\frac{1}{(2\pi)^4}\int_{\mathbb{R}}\int_{\mathbb{R}}\int_{\mathbb{S}^2} e^{i(\lambda-r)t}\left(\pm\frac{it}{2}\omega^\alpha\omega^\beta\overset{*}{K}_{\alpha\beta}\mp\frac{1}{2r}\left(\delta^{\alpha\beta}-\omega^\alpha\omega^\beta\right)\overset{*}{K}_{\alpha\beta}\right)\widehat{\mu}(\pm t)\,r^2\,\mathrm{d}\omega\,\mathrm{d}r\,\mathrm{d}t\\
&=\pm\frac{1}{(2\pi)^4}\int_{\mathbb{R}}\int_{\mathbb{R}}\int_{\mathbb{S}^2} e^{i(\lambda-r)t}r\left(\omega^\alpha\omega^\beta\overset{*}{K}_{\alpha\beta}-\frac{1}{2}\left(\delta^{\alpha\beta}-\omega^\alpha\omega^\beta\right)\overset{*}{K}_{\alpha\beta}\right)\widehat{\mu}(\pm t)\,\mathrm{d}\omega\,\mathrm{d}r\,\mathrm{d}t\\
&=\pm\frac{\lambda}{(2\pi)^3}\int_{\mathbb{S}^2}\left(\frac{3}{2}\omega^\alpha\omega^\beta\overset{*}{K}_{\alpha\beta}-\frac{1}{2}\overset{*}{K}{}^\alpha{}_\alpha\right)\mathrm{d}\omega\\
&=\pm\frac{\lambda}{(2\pi)^3}\left(2\pi\overset{*}{K}{}^\alpha{}_\alpha-2\pi\overset{*}{K}{}^\alpha{}_\alpha\right)\\
&=0,
\end{aligned} \tag{B.3.5}$$

which tells us that the second Weyl coefficients vanish. In (B.3.5) we used (3.8.8) and the identity

$$\int_{\mathbb{S}^2}\omega^\alpha\omega^\beta\mathrm{d}\omega=\frac{4\pi}{3}\delta^{\alpha\beta}. \tag{B.3.6}$$

Let us now consider contributions of order $O(1)$, i.e. contribution to the third Weyl coefficients. We observe that the term

$$\pm\frac{it^2}{8}\frac{\eta^\alpha\eta^\beta}{h^2}\left(\nabla_\alpha\overset{*}{K}_{\beta\mu}+\nabla_\beta\overset{*}{K}_{\alpha\mu}\right)\frac{\eta^\mu}{h}$$

from (B.3.1) and the term

$$-\frac{t}{4}\left(\nabla_\alpha\overset{*}{K}_{\beta\mu}+\nabla_\beta\overset{*}{K}_{\alpha\mu}\right)\left(h_{\eta_\beta}\,h_{\eta_\alpha\eta_\beta}+\frac{1}{2}h_{\eta_\alpha\eta_\beta}\,h_{\eta_\mu}\right)$$

from (B.3.2) vanish upon integration because they are odd in momentum.

Hence, we are only left to deal with the last summand before the remainder in (B.3.1) and (B.3.2), respectively. The contribution of the former to $N'_\pm * \mu$ is

$$-\frac{1}{8(2\pi)^4}\int_{\mathbb{R}}\int_{T_y^*M} e^{i(\lambda-\|\eta\|)t}\left(t^2\frac{\eta^\alpha\eta^\beta}{h^2}\overset{*}{K}_{\alpha\mu}\overset{*}{K}_\beta{}^\mu\right)\widehat{\mu}(\pm t)\chi(\|\eta\|)\,\mathrm{d}\eta\,\mathrm{d}t. \tag{B.3.7}$$

Switching to polar coordinates and dropping the cut-off, we get

$$\begin{aligned}
-\frac{\overset{*}{K}_{\alpha\mu}\overset{*}{K}_{\beta}{}^{\mu}}{8(2\pi)^4}\int_{\mathbb{R}}\int_{\mathbb{R}}\int_{\mathbb{S}^2} e^{i(\lambda-r)t}\left(t^2\omega^\alpha\omega^\beta\right)\widehat{\mu}(\pm t)r^2\,\mathrm{d}r\,\mathrm{d}t\,\mathrm{d}\omega \\
&= \frac{\overset{*}{K}_{\alpha\mu}\overset{*}{K}_{\beta}{}^{\mu}}{8(2\pi)^4}\int_{\mathbb{R}}\int_{\mathbb{R}}\int_{\mathbb{S}^2} e^{i(\lambda-r)t}\left(2\omega^\alpha\omega^\beta\right)\widehat{\mu}(\pm t)\,\mathrm{d}r\,\mathrm{d}t\,\mathrm{d}\omega \\
&= \frac{\overset{*}{K}_{\alpha\mu}\overset{*}{K}_{\beta}{}^{\mu}}{4(2\pi)^3}\int_{\mathbb{S}^2}\omega^\alpha\omega^\beta\,\mathrm{d}\omega \\
&= \frac{\overset{*}{K}_{\alpha\mu}\overset{*}{K}_{\beta}{}^{\mu}}{4(2\pi)^3}\frac{4\pi}{3}\delta^{\alpha\beta} \\
&= \frac{\overset{*}{K}_{\alpha\mu}\overset{*}{K}^{\alpha\mu}}{6(2\pi)^2}.
\end{aligned} \tag{B.3.8}$$

The contribution of the last summand on the RHS of (B.3.2) to $N'_\pm * \mu$ is

$$\frac{1}{(2\pi)^4}\int_{\mathbb{R}}\int_{T_y^*M} e^{i(\lambda-\|\eta\|)t}\left(-\frac{it}{8}\overset{*}{K}_{\alpha\mu}\overset{*}{K}_{\beta}{}^{\mu}\,h_{\eta_\alpha\eta_\beta}\right)\widehat{\mu}(\pm t)\chi(\|\eta\|)\,\mathrm{d}\eta\,\mathrm{d}t. \tag{B.3.9}$$

Switching to polar coordinates and dropping the cut-off, we get

$$\begin{aligned}
-\frac{\overset{*}{K}_{\alpha\mu}\overset{*}{K}_{\beta}{}^{\mu}}{8(2\pi)^4}\int_{\mathbb{R}}\int_{\mathbb{R}}\int_{\mathbb{S}^2} e^{i(\lambda-r)t}\,it\left(\frac{\delta^{\alpha\beta}}{r}-\frac{\omega^\alpha\omega^\beta}{r}\right)\widehat{\mu}(\pm t)\,r^2\,\mathrm{d}\omega\,\mathrm{d}r\,\mathrm{d}t \\
&= -\frac{\overset{*}{K}_{\alpha\mu}\overset{*}{K}_{\beta}{}^{\mu}}{8(2\pi)^3}\int_{\mathbb{S}^2}\left(\delta^{\alpha\beta}-\omega^\alpha\omega^\beta\right)\mathrm{d}\omega \\
&= -\frac{\overset{*}{K}_{\alpha\mu}\overset{*}{K}_{\beta}{}^{\mu}}{8(2\pi)^3}\left(4\pi\delta^{\alpha\beta}-\frac{4\pi}{3}\delta^{\alpha\beta}\right) \\
&= -\frac{\overset{*}{K}_{\alpha\mu}\overset{*}{K}^{\alpha\mu}}{6(2\pi)^2}.
\end{aligned} \tag{B.3.10}$$

We see that (B.3.8) and (B.3.10) cancel out. Therefore, third Weyl coefficients computed from (B.3.1) and (B.3.2) are in agreement with Theorem 3.39.

Appendix C

Classification of sesquilinear forms: complementary material

C.1 The concepts of principal and subprincipal symbol

The concepts of principal and subprincipal symbol are widely used in modern analysis, however they are traditionally employed for the description of (pseudo)differential *operators*, see Chapters 2 and 3. In the main text of Chapter 4 we used these concepts for the description of *sesquilinear forms*. We explain below the relation between the two seemingly different versions of, essentially, the same objects.

Let $L^{(1/2)}$ be a first order linear differential operator acting on m-columns of half-densities, i.e. spatially varying complex-valued quantities on M which under changes of local coordinates transform as the square root of a density. In local coordinates this operator reads

$$L^{(1/2)} = -iE^\alpha(x)\frac{\partial}{\partial x^\alpha} + F(x), \tag{C.1.1}$$

where $E^\alpha(x)$ and $F(x)$ are some $m \times m$ matrix-functions, compare with (4.2.2). Here the superscript (1/2) indicates that we are dealing with an operator acting on half-densities.

We define the principal, subprincipal and full symbols of the operator (C.1.1) as

$$L^{(1/2)}_{\mathrm{prin}}(x,p) := E^\alpha(x)\,p_\alpha\,, \tag{C.1.2}$$

$$L^{(1/2)}_{\mathrm{sub}}(x) := F(x) + \frac{i}{2}\big(L^{(1/2)}_{\mathrm{prin}}\big)_{x^\alpha p_\alpha}(x) = F(x) + \frac{i}{2}(E^\alpha)_{x^\alpha}(x)\,, \tag{C.1.3}$$

$$L^{(1/2)}_{\mathrm{full}}(x,p) := L^{(1/2)}_{\mathrm{prin}}(x,p) + L^{(1/2)}_{\mathrm{sub}}(x) \tag{C.1.4}$$

respectively. It is easy to see that the full symbol $L^{(1/2)}_{\mathrm{full}}$ uniquely determines our first order linear differential operator $L^{(1/2)}$.

The definition of the subprincipal symbol (C.1.3) originates from the classical paper [52] of J.J. Duistermaat and L. Hörmander: see formula (5.2.8) in that paper. Unlike [52], we work with matrix-valued symbols, but this does not affect the formal definition of the subprincipal symbol. The correction term $\frac{i}{2}\big(L^{(1/2)}_{\mathrm{prin}}\big)_{x^\alpha p_\alpha}$ plays a crucial role in formula (C.1.3): its presence ensures that the subprincipal symbol is invariant under changes of local coordinates.

Our formulae (4.2.3)–(4.2.5) are analogues of the standard formulae (C.1.2)–(C.1.4). The bold script in the former indicates that we are dealing with density-valued quantities.

In order to establish the relation between symbols of sesquilinear forms and symbols of operators, let us fix a particular positive density μ and introduce the inner product

$$\langle u, v\rangle := \int_M u^* v\, \mu \, \mathrm{d}x \tag{C.1.5}$$

on m-columns of scalar fields. Formulae (4.1.2), (4.2.2) and (C.1.5) define a linear operator L.

The main result of this appendix is the following lemma.

Lemma C.1. *Conditions*

$$L = \mu^{-1/2} L^{(1/2)} \mu^{1/2} \tag{C.1.6}$$

and

$$\mathbf{S}_{\mathrm{full}} = \mu L^{(1/2)}_{\mathrm{full}} \tag{C.1.7}$$

are equivalent.

Proof. Formula (C.1.1) implies

$$\mu^{-1/2} L^{(1/2)} \mu^{1/2} = -iE^\alpha \frac{\partial}{\partial x^\alpha} + F - \frac{i}{2} E^\alpha \,(\ln \mu)_{x^\alpha}\,. \tag{C.1.8}$$

Performing integration by parts, we rewrite formula (4.2.2) as

$$S(u,v) = \int_M u^* \left[\frac{1}{\mu}\left(-i\mathbf{E}^\alpha \frac{\partial}{\partial x^\alpha} + \mathbf{F} - \frac{i}{2}(\mathbf{E}^\alpha)_{x^\alpha}\right) v\right] \mu \, \mathrm{d}x\,,$$

which gives us the following explicit local representation of the operator L:

$$L = \frac{1}{\mu}\left(-i\mathbf{E}^\alpha \frac{\partial}{\partial x^\alpha} + \mathbf{F} - \frac{i}{2}(\mathbf{E}^\alpha)_{x^\alpha}\right). \tag{C.1.9}$$

Substituting (C.1.9) and (C.1.8) into (C.1.6), we see that the latter reduces to the pair of equations

$$\mathbf{E}^\alpha = \mu E^\alpha, \tag{C.1.10}$$

$$\mathbf{F} - \frac{i}{2}(\mathbf{E}^\alpha)_{x^\alpha} = \mu\left(F - \frac{i}{2}\,E^\alpha\,(\ln\mu)_{x^\alpha}\right). \tag{C.1.11}$$

Substituting (C.1.10) into (C.1.11) we rewrite the latter in equivalent form

$$\mathbf{F} = \mu\left(F + \frac{i}{2}(E^\alpha)_{x^\alpha}\right). \tag{C.1.12}$$

In view of (4.2.3)–(4.2.5) and (C.1.2)–(C.1.4) conditions (C.1.10) and (C.1.12) are equivalent to (C.1.7). □

As already pointed out in Section 4.9, in the most general setting of arbitrary d (dimension of the manifold), arbitrary m (number of scalar fields) and arbitrary sesquilinear form the introduction of an inner product of the form (C.1.5) does not make much sense because this inner product is incompatible with general linear and special linear gauge transformations. However, it makes sense in the special case (4.8.5), (4.8.1) because the inner product (C.1.5) is compatible with unitary and special unitary gauge transformations. And in this special case it is natural to take $\mu = \rho$, where ρ is the Riemannian density encoded within our sesquilinear form in accordance with formulae (4.5.2) and (4.8.7).

Appendix D

Lorentzian elasticity: notation and complementary material

D.1 Notation and conventions

D.1.1 Exterior calculus

In this appendix M is a 4-manifold equipped with Lorentzian metric g and Levi-Civita connection ∇.

It is well known that the metric g induces a canonical isomorphism between the tangent bundle TM and the contangent bundle T^*M, the so-called *musical isomorphism*. We denote it by $\flat : TM \to T^*M$ and its inverse by $\sharp : T^*M \to TM$.

Given a scalar field $f \in C^\infty(M)$, its exterior derivative $\mathrm{d}f$ is defined as the gradient. Given a 1-form $A \in \Omega^1(M)$, its exterior derivative $\mathrm{d}A \in \Omega^2(M)$ is defined, componentwise, as

$$(\mathrm{d}A)_{\alpha\beta} = \partial_{x^\alpha} A_\beta - \partial_{x^\beta} A_\alpha \,.$$

Given a pair of rank k covariant antisymmetric tensors Q and T we define their pointwise inner product as

$$\langle Q, T\rangle_g := \frac{1}{k!}\,\overline{Q}_{\alpha_1\ldots\alpha_k}\,T_{\beta_1\ldots\beta_k}\,g^{\alpha_1\beta_1}\cdots g^{\alpha_k\beta_k}\,,$$

and, accordingly,

$$\|Q\|_g^2 := \langle Q, Q\rangle_g\,.$$

We define the L^2 inner product

$$(Q,T)_{L^2} := \int \langle Q,T\rangle_g \sqrt{-\det g_{\mu\nu}}\, \mathrm{d}x\,.$$

Given $U \in \Omega^k(M)$ and $V \in \Omega^{k-1}(M)$ we define the action of the codifferential $\delta : \Omega^k(M) \to \Omega^{k-1}(M)$ in accordance with

$$\langle U, \mathrm{d}V\rangle = \langle \delta U, V\rangle.$$

In particular, when $A \in \Omega^1(M)$ and $F \in \Omega^2(M)$, we get in local coordinates

$$\delta A = -\nabla^\alpha A_\alpha,$$

$$(\delta F)_\alpha = \nabla^\beta F_{\alpha\beta}.$$

For the sake of clarity, let us mention that the wedge product of 1-forms reads

$$(A \wedge B)_{\alpha\beta} = A_\alpha B_\beta - A_\beta B_\alpha\,.$$

We define the action of the Hodge star on a rank k antisymmetric tensor as

$$(*Q)_{\mu_{k+1}\dots\mu_4} := \frac{1}{k!}\sqrt{-\det g_{\alpha\beta}}\; Q^{\mu_1\dots\mu_k}\,\varepsilon_{\mu_1\dots\mu_4}\,,$$

where ε is the totally antisymmetric symbol, $\varepsilon_{1234} := +1$.

D.1.2 Spinors

In this Appendix as well as in Appendix D.1.3 we restrict ourselves to the special case of Minkowski space $\mathbb{M}$. We work with 2-component Weyl spinors as opposed to 4-component Dirac spinors. We recall below the basic ideas and conventions, referring the reader to [20, Section 18] and [28, Section 1.2] for further details.

In line with [20, 28] we treat spinors as holonomic objects. This approach simplifies analysis in the case of flat space and is traditionally used in particle physics.

We adopt the following conventions.

- 'Metric' spinor:

$$\epsilon_{ab} = \epsilon_{\dot a\dot b} = \epsilon^{ab} = \epsilon^{\dot a\dot b} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

- 'Covariant', with respect to spinor indices, Pauli matrices:

$$\sigma^1{}_{\dot a b} := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2{}_{\dot a b} := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3{}_{\dot a b} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma^4{}_{\dot a b} := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{D.1.1}$$

- 'Contravariant', with respect to spinor indices, Pauli matrices:

$$\sigma^{1\dot a b} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \quad \sigma^{2\dot a b} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^{3\dot a b} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma^{4\dot a b} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{D.1.2}$$

Here $\sigma^{\alpha\dot a b} = \epsilon^{\dot a\dot c}\epsilon^{bd}\sigma^\alpha{}_{\dot c d}$.

Pauli matrices satisfy the identities

$$\sigma^{\alpha\dot b a}\,\sigma^\beta{}_{\dot b c} + \sigma^{\beta\dot b a}\,\sigma^\alpha{}_{\dot b c} = -2g^{\alpha\beta}\delta^a{}_c\,, \tag{D.1.3a}$$

$$\sigma^\alpha{}_{\dot a b}\,\sigma^{\beta\dot c b} + \sigma^\beta{}_{\dot a b}\,\sigma^{\alpha\dot c b} = -2g^{\alpha\beta}\delta_{\dot a}{}^{\dot c}\,. \tag{D.1.3b}$$

D.1.3 Spinor representation of 2-forms

Let $\mathbb{F}_-$ and $\mathbb{F}_+$ be polarised complex 2-forms, see (5.11.3). Then $\mathbb{F}_-$ is equivalent to a trace-free undotted rank two spinor $\zeta^b{}_c$,

$$(\mathbb{F}_-)^{\alpha\beta} = -i\sigma^\alpha{}_{\dot a b}\,\zeta^b{}_c\,\sigma^{\beta\dot a c}\,, \tag{D.1.4a}$$

and $\mathbb{F}_+$ is equivalent to a trace-free dotted rank two spinor $\theta_{\dot b}{}^{\dot c}$,

$$(\mathbb{F}_+)^{\alpha\beta} = i\sigma^{\alpha\dot b a}\,\theta_{\dot b}{}^{\dot c}\,\sigma^\beta{}_{\dot c a}\,. \tag{D.1.4b}$$

The identities (D.1.3a) and (D.1.3b) ensure that that the right-hand sides of (D.1.4a) and (D.1.4b), respectively, are antisymmetric in α, β.

Fact D.1. *The following are equivalent.*

(i) $\det \mathbb{F}_- = 0\,.$

(ii) $\det \zeta = 0\,.$

(iii) There exists a rank one spinor ξ^a such that $\zeta^b{}_c = \xi^b\,\xi^d\,\epsilon_{dc}\,.$

Fact D.2. *The following are equivalent.*

(i) $\det \mathbb{F}_+ = 0\,.$

(ii) $\det \theta = 0\,.$

(iii) There exists a rank one spinor $\eta_{\dot a}$ *such that* $\theta_{\dot b}{}^{\dot c} = \eta_{\dot b}\,\eta_{\dot d}\,\epsilon^{\dot d\dot c}\,.$

Facts D.1 and D.2 imply that a degenerate polarised 2-form is equivalent to the square of a rank 1 spinor. The latter is defined uniquely up to sign.

The equivalence between (i) and (ii) in the above statements is a straightforward consequence of (D.1.4a) and (D.1.4b), whereas (iii) is not so obvious. The relevant arguments are presented in Appendix D.2.2.

D.2 Some results in linear algebra

D.2.1 Linear algebra involving a pair of quadratic forms

Working in an n-dimensional real vector space V, consider a pair of non-degenerate symmetric bilinear forms, $g : V \times V \to \mathbb{R}$ and $h : V \times V \to \mathbb{R}$. These uniquely define an invertible linear operator $L : V \to V$ via the formula

$$h(u, v) = g(Lu, v), \qquad \forall u, v \in V.$$

The eigenvalue problem for the operator L

$$Lu = \lambda u$$

can be equivalently reformulated in terms of bilinear forms

$$h(u, v) = \lambda g(u, v), \qquad \forall v \in V.$$

The expression $h - \lambda g$ is called a *linear pencil* of symmetric bilinear forms.

It is well known [59, Section X.6] that if at least one of the forms is sign definite, then L has real eigenvalues and is diagonalisable. In this case the associated pencil is called *regular*.

If neither g nor h is sign definite, then the operator L may have complex eigenvalues and may not be diagonalisable. In particular, the *strain* operator

$$S := L - \mathrm{Id}$$

may be nilpotent. This is a fundamental difference with the regular (sign definite) case where the strain operator cannot be nilpotent.

We now address the question what is the maximal nilpotency index of S.

Lemma D.3. *Suppose that $n \geq 4$ and that both g and h have Lorentzian signature*

$$\underbrace{+\cdots+}_{n-1}-\,.$$

Then the nilpotency index of S is less than or equal to three.

Proof. Observe first that it is sufficient to prove the lemma in the complex setting, where we can use [61, Theorem 8.4.1]. Examination of the latter shows that nilpotency index strictly greater than four is not possible, whereas nilpotency index equal to four is possible only if we have an invariant subspace in which our operator has the structure [61, formula (8.4.19)]. But the matrix N from [61, formula (8.4.19)] with $\lambda = 0$ has nilpotency index at most three. □

Remark D.4. Closer examination shows that in our setting the structure [61, formula (8.4.19)] cannot be realised because the latter describes an operator which is Lorentz–normal but not Lorentz–symmetric. The only way the strain operator can get nilpotency index three is when it has a Jordan block of the type [61, formula (8.4.18)] with $\lambda = r = 0$. As a final observation, let us point out that in dimensions $n = 2$ and $n = 3$ the maximal nilpotency indices two and three can actually be attained.

D.2.2 Nilpotent operators in a 2D symplectic space

Lemma D.5. *Let V be a 2-dimensional complex vector space equipped with a symplectic form ω and let $L : V \to V$ be a linear operator. Then L is nilpotent if and only if there exists a $u \in V$ such that*

$$Lv = u\,\omega(u,v), \qquad \forall v \in V. \tag{D.2.1}$$

Proof. An operator of the form (D.2.1) is clearly nilpotent. So we only need to prove the converse statement.

Let L be nilpotent. Choose a basis in V so that the symplectic form reads

$$\omega(v,w) = \varepsilon_{rs}\, v^r w^s, \tag{D.2.2}$$

where ε is the totally antisymmetric symbol, $\varepsilon_{12} = +1$. The linear operator L is represented in this basis by the matrix

$$L^r{}_s = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{D.2.3}$$

The nilpotency condition is equivalent to the trace and the determinant of L both being zero. Hence, (D.2.3) can be rewritten as

$$L^r{}_s = \begin{pmatrix} \sqrt{-bc} & b \\ c & -\sqrt{-bc} \end{pmatrix} \tag{D.2.4}$$

with appropriate choice of complex square root. The matrix (D.2.4) can be factorised as

$$L^r{}_s = \begin{pmatrix} \sqrt{b} \\ -\sqrt{-c} \end{pmatrix} \begin{pmatrix} \sqrt{b} & -\sqrt{-c} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{D.2.5}$$

where the square roots are chosen in such a way that $\sqrt{b}\,\sqrt{-c} = \sqrt{-bc}$. Formulae (D.2.5) and (D.2.2) give us (D.2.1) with

$$u = \begin{pmatrix} \sqrt{b} \\ -\sqrt{-c} \end{pmatrix}.$$

□

D.3 Differential geometric characterisation of screw groups

Let SG be one of the screw groups SG_0^+, SG_0^- or SG_m defined in Section 5.7. In what follows, the (global) isomorphism $T\mathbb{M} \simeq \mathbb{M} \times \mathbb{M}$ will be tacitly understood. In particular, we will not distinguish between points of M and vectors in the tangent fibres.

Direct inspection shows that for any $P, Q \in \mathbb{M}$ there exists a unique $\xi \in \mathrm{SG}$ such that $\xi(P) = Q$. This allows us to define a map

$$\begin{aligned} \Upsilon : T_P\mathbb{M} &\to T_Q\mathbb{M}\,, \\ V &\mapsto \xi(P+V) - Q, \end{aligned}$$

depending only on P and Q, which, in turn, determine ξ. The map Υ is linear and defines a metric compatible affine connection with vanishing curvature and nonvanishing torsion. Such connections are known as Weitzenböck connections. Weitzenböck connections on orientable Riemannian 3-manifolds were discussed in Appendix B.1.

We define the covariant derivative of a vector field as

$$\frac{\partial v^\alpha}{\partial x^\beta} + \Upsilon^\alpha{}_{\beta\gamma} v^\gamma$$

and torsion in accordance with (B.1.3). It is known [92, formula (7.34)] that a metric compatible affine connection is determined by metric and torsion, so torsion provides a convenient tensorial description of a connection on the Minkowsi space.

Torsion has three irreducible pieces [87, formulae (4.1)–(4.4)]

$$T = T^{\mathrm{ax}} + T^{\mathrm{vec}} + T^{\mathrm{ten}},$$

$$T^{\mathrm{ax}}_{\alpha\beta\gamma} = \frac{1}{3}(T_{\alpha\beta\gamma} + T_{\beta\gamma\alpha} + T_{\gamma\alpha\beta}), \tag{D.3.1}$$

$$T^{\mathrm{vec}}_{\alpha\beta\gamma} = \frac{1}{3}(g_{\alpha\beta} T^\mu{}_{\mu\gamma} - g_{\alpha\gamma} T^\mu{}_{\mu\beta}), \tag{D.3.2}$$

labelled by the adjectives *axial*, *vector* and *tensor* respectively. We remind the reader that we raise and lower tensor indices using the metric g.

Lemma D.6. *For all three groups* SG_0^+, SG_0^- *and* SG_m *torsion is constant and vector torsion is zero. The corresponding formulae for axial torsion read*

$$(*T^{\mathrm{ax}}_\pm)_\alpha = \mp \frac{2}{3}\,(\,0\,,\,0\,,\,1\,,\,1\,)\,,$$

$$(*T^{\mathrm{ax}}_m)_\alpha = -\,\frac{4}{3}\,(\,0\,,\,0\,,\,m\,,0\,)\,.$$

Proof. Straightforward calculations give the following expressions for the nonzero connection coefficients.

- For $\mathrm{SG}_0^\pm$

$$\Gamma^1{}_{32} = \pm 1, \qquad \Gamma^2{}_{31} = \mp 1,$$

$$\Gamma^1{}_{42} = \pm 1, \qquad \Gamma^2{}_{41} = \mp 1.$$

- For SG_m

$$\Gamma^1{}_{42} = 2m, \qquad \Gamma^2{}_{41} = -2m.$$

It remains only to substitute the above expressions into formulae (B.1.3), (D.3.1) and(D.3.2). □

D.4 Explicit formulae for our field equations

In this Appendix we sketch out an algorithm for the derivation of the explicit form of the differential operator $E(\phi)$ introduced in Section 5.3. We will do this for the special case of a Lagrangian of the form (5.2.9) from Example 5.3 and in Minkowski space. Throughout this appendix we shall use the notation $\partial_\alpha = \partial/\partial x^\alpha$.

Substituting (5.2.9) into (5.2.16) we get

$$L(e_2, e_3, e_4) = \alpha(e_2 + e_3 + e_4)^2 + \beta\, e_2\,. \tag{D.4.1}$$

To begin with, let us rewrite the scalars e_3 and e_4 in terms of $\operatorname{tr}(S^k)$, $k = 1, 2, 3, 4$:

$$e_3 = \frac{1}{6}\left[(\operatorname{tr} S)^3 - 3(\operatorname{tr} S)\operatorname{tr}(S^2) + 2\operatorname{tr}(S^3)\right], \tag{D.4.2a}$$

$$e_4 = \frac{1}{24}\left[(\operatorname{tr} S)^4 - 6(\operatorname{tr} S)^2\operatorname{tr}(S^2) + 3(\operatorname{tr}(S^2))^2 + 8(\operatorname{tr} S)\operatorname{tr}(S^3) - 6\operatorname{tr}(S^4)\right]. \tag{D.4.2b}$$

Substituting (5.2.5b), (D.4.2a) and (D.4.2b) into (D.4.1) we get a representation of our Lagrangian L as a linear combination of terms

$$\prod_{j=1}^{k} S^{\alpha_j}{}_{\beta_j}, \tag{D.4.3}$$

where $\{\beta_1, \ldots, \beta_k\}$ is some permutation of $\{\alpha_1, \ldots, \alpha_k\}$. The number k takes values from two to eight. In what follows we write down the contribution to $E(\phi)$ coming from a single term (D.4.3).

The explicit formula for the strain tensor reads

$$S^\alpha{}_\beta = \partial_\beta A^\alpha + \partial^\alpha A_\beta + (\partial^\alpha A_\gamma)(\partial_\beta A^\gamma).$$

Variation $A^\alpha(x) \mapsto A^\alpha(x) + \Delta A^\alpha(x)$ gives us

$$\begin{aligned}\Delta S^\alpha{}_\beta &= \partial_\beta(\Delta A^\alpha) + \partial^\alpha(\Delta A_\beta) + (\partial^\alpha(\Delta A_\gamma))(\partial_\beta A^\gamma) + (\partial^\alpha A_\gamma)(\partial_\beta(\Delta A^\gamma)) \\ &= \delta^\alpha{}_\gamma\, \partial_\beta(\Delta A^\gamma) + g_{\beta\gamma}\, \partial^\alpha(\Delta A^\gamma) + (\partial^\alpha(\Delta A^\gamma))(\partial_\beta A_\gamma) + (\partial^\alpha A_\gamma)(\partial_\beta(\Delta A^\gamma)).\end{aligned}$$

We define the linear differential operator

$$D^\alpha{}_{\beta\gamma} := [g_{\beta\gamma} + (\partial_\beta A_\gamma)]\,\partial^\alpha + [\delta^\alpha{}_\gamma + (\partial^\alpha A_\gamma)]\,\partial_\beta + 2(\partial^\alpha\partial_\beta A_\gamma).$$

The contribution to $E(\phi)$ coming from (D.4.3) reads

$$-\sum_{l=1}^{k} D^{\alpha_l}{}_{\beta_l \gamma} \prod_{\substack{j=1 \\ j\neq l}}^{k} S^{\alpha_j}{}_{\beta_j}.$$

The above algorithm can be easily generalised to spacetimes with x-dependent metric and to Lagrangians of general form.

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