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Semiclassical dynamics of wave equations in curved spacetime

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Oliver Stöckl BSc

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Dr. Marius Adrian Oancea

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Abstrakt

Diese Masterarbeit beschäftigt sich mit der Generalisierung der Werkzeuge zur Untersuchung der Dynamik von Wellengleichungen in gekrümmter Raumzeit. *Watson* [43] wählt dafür eine Schrödinger Gleichung mit periodischem Potential. Wir werden jedoch einen Ansatz nehmen, der für Szenarien in gekrümmter Raumzeit besser entspricht. Wir setzen mit der Klein Gordon Gleichung an und wählen einen Ansatz, der einen Punkt im Raum mit einer Geodäte über die Beschreibung von Synges World functions beschreibt. In der höchsten Ordnung in einer zwei Parameter Expansion finden wir eine Art Schrödinger Gleichung. Aus *Watson* [43] werden wir einen Ansatz adaptieren. Schließlich finden wir ein System aus zwei gekoppelten partiellen Differentialgleichungen für zwei Matrizen. Diese beinhalten auch eine Matrix, in einer Basis, die orthogonal zu der Ausbreitungsrichtung und proportional zur Krümmung des Raumes ist. Wir untersuchen drei unterschiedliche Fälle der Dynamik um besseres Verständnis über das System und die Veränderungen der Amplitude zu bekommen: radial mit konstantem Winkel φ , orbital mit konstantem Radius r und einer allgemeinen Bewegung in radialer Richtung und Bewegung in φ . Nachdem der Ansatz von einem Vektor v im Exponenten abhängig ist, der in der Basis, die orthogonal zur Ausbreitungsrichtung liegt, ausgedrückt ist, wählen wir verschiedenen Punkte entlang der Trajektorie des Teilchens um das schwarze Loch und untersuchen, wie sich die Formen der Niveaumengen für die Komponenten dieses Vektors in der Amplitude des Ansatzes ändern. Wir finden Deformationen von der der sphärischen Niveaumenge am Start, die stärker werden, je näher die Trajektorie am schwarzen Loch vorbei führt und damit je stärker die Gravitationskräfte werden.

Abstract

In this thesis, we aim to generalize the working tools for studying the dynamics of wave equations in curved spacetime. *Watson* [43] does this by a Schrödinger equation with a periodic potential but we take an approach more appropriate for scenarios in curved spacetime. We introduce the Klein Gordon equation and an Ansatz which connects a point in space with a Geodesic by means of Synge's World functions formalism. In the highest order of a two parameter expansion we find the shape of the high-frequency wave packet is described by a Schrödinger-like equation. *Watson* [43] provides an Ansatz for this equation which we adapt. We ultimately find a system of two coupled partial differential equations for two matrices involving a matrix in a basis orthogonal to the direction of propagation proportional to the curvature of the space-time. To get insight in the dynamics of this system and the amplitude of the introduced Ansatz we look at three different cases of motion around a Schwarzschild black hole: radial with constant angle φ , orbital with constant radius r and general motion in both, radial and angular direction. As the Ansatz depends on a vector v in the exponent which is expressed in the basis orthogonal to the direction of propagation, we choose several points along the path of the particle around a Schwarzschild black hole and analyse how the shape of the level sets for this vector in the amplitude of the Ansatz changes. We find that, the nearer the trajectory passes the black hole the stronger the gravitational tidal forces act on the amplitude and we find deformation of an initial spherical level set.

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1. Introduction

The interest in the description and understanding about the dynamics of waves in different media is present since the beginning of science. In fact, one can find the first attempts to describe the processes which lead to human vision between the years 1011 to 1021 [30] [25]. At this time, emission theory was still a valid theory to describe the human vision but the eyes emitting some form of radiation to objects which then perceive their colour and shape. *Ibn al-Haytham* was very sceptical about the consequences of this theory especially as the human eye could be damaged when looking directly into the sun, which led him to the first attempt of describing light as rays coming from infinite source points [26] [36]. The basic principles of later known *Geometrical optics* were born. At least qualitatively, phenomena like reflection, refraction, the casting of shadows and also changes in perspective could be described.

It took several hundred years after *Ibn al-Haytham*, however, to show the empirical strength of the earlier developments and to get to the point, where the qualitative descriptions of *Ibn al-Haytham* could be made mathematically rigorous. *Newton* provided great quantitative confirmation of the light bending at interfaces of different media depending on its properties [24]. Although not publicly available, *Snell* empirically discovered his famous law of refraction in about 600 years later, giving the first mathematical description of light rays bending at interfaces [15]. It did not take long then for *Pierre de Fermat* to introduce his famous principle of least time, which is the very foundation of ray optics. It is this principle, that tells us exactly, that rays are straight and take the shortest path. In media, however, rays will always bend according to changes in media according to the generalized Snell's law within continuous media. Finally, *Descartes* could combine Snell's law and ray diagrams to describe refraction and lenses.

Ray based optics was not the only approach in the 17. century. *Huygens* chose a different approach. In fact, one could almost see this historical difference as a preview on the later particle-wave duality. For Huygens, light was not a particle moving on a straight line, in fact, it should be a wave propagating through some medium [16]. The front is composed of a set of points with equal phase and at each point, a new source of a spherical wave with the new wavefront being then the envelope of the waves generated at each point. Snell's law could then be regained by constructing envelopes at boundaries, thus showing the compatibility of both theories. This idea of wave based propagation was later empirically tested by *Young* in demonstrating interference behaviour [45] and by *Fresnel* who tested superposition properties and wavefront reconstruction [10].

Huygens work was mostly geometrical, though. The key missing parameter is now a mathematical description of a wave. Although *D'Alembert* is considered the first to publish some kind of wave equation introducing the today well known *D'Alembert operator*

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[32] when he described the vibrations of a string, it was until about a hundred years later, when *Maxwell* introduced his famous *Maxwell equations* that we got a general description for electromagnetic waves [23]. We will focus on the simpler case of the *Klein-Gordon* equation in this thesis [17] [12]. For the massless case, this reduces into the D'Alembert equation. In the massive case, we also find a potential term relating the mass to the wave. The Klein-Gordon equation provides a simple relativistic wave equation closely related to the *Schrödinger equation*. The Klein-Gordon equation provided a good setup for quantizations. First quantization of the Klein Gordon equation, however, introduces different problems. First quantization brings also negative energy and probability solutions, thus one has to restrict oneself to positive energy modes, which makes the inner product and position operator dependent of the form of Lorentz Violation [2]. One can relate the first quantization of the Klein-Gordon equation with a relativistic version of the Schrödinger equation, however. In the second quantization though, when one switches to quantum field theory, a lot of problems of the first quantization are avoided [33].

Solving the Klein-Gordon equation can be quite difficult, however, especially in curved spacetime. Instead of looking for an exact solution, we will use an Ansatz, where we find the amplitude to be approximated in half-orders of a parameter ϵ which encodes the relation between the wavelength and the order of magnitude for variations in the medium to find an asymptotic solution. Thus, what is now missing, is a function as an Ansatz we expect to fulfil the wave equation. For this Ansatz we can make the so called *eikonal approximation*. This states, that the wavelength of our wave is small compared to any size of obstacle, the wave could encounter. Assuming light as a straight line, which makes sense when the wavelength goes to 0 compared to any obstacles, the *image* or $\epsilon\kappa\omega\nu$ *eikōn* is formed by a straight line projection of the object [35]. The eikonal approximation is very closely related to the *WKB approximation* in quantum mechanics. [44] [19] [4]. Both approximations reduce the differential wave equations into a differential equation on variable due to the approximation, that the wave is propagating in one line. This special line can be chosen as a special direction. In the WKB approximation, expansion happens in terms of Planck's constant h , it introduces more complexity, than the eikonal approximation, though, in the fact, that the single variable in the differential equation after the approximation denotes the trajectory of the particle, which can get very complicated. The eikonal approximation, however, stays with a classical trajectory as a straight line forming a semi-classical limit.

While helpful in its regime, the eikonal approximation together with its wave equation as the most trivial separation of the slowly varying amplitude and rapidly varying phase, one quickly reaches its border of satisfactory applicability. The image of light or particles moving on straight rays completely skips wave effects like diffraction, beam spreading or interference at caustics [20] [8] [31]. Apart from that, the wave with mentioned Ansatz is defined globally, which is not in accordance with rays converging which would create regions of infinity intensity in the eikonal approximation leading to caustics. There, the phase function is not single valued any more. Apart from that, in the real world we almost never experience strictly monochrome waves; we always find wave packets as multiple overlying waves. This yield effect like beam spreading, divergence or amplitude variations transverse to the direction of propagation. Finally, paths involving media where the refractive index changes rapidly can not be captured by a global defined phase

function.

A step into the direction of a appropriate wave description lies in the *paraxial approximation*. In this approximation, the wave still moves into a chosen axis, we allow variations into transverse directions, however. These variations should be slow compared to the direction of propagation. In fact, we require them to be so slow, that we can omit second derivatives in the direction of propagation. Depending on the spot size compared to the wavelength of the light, one quickly reaches the limit of satisfactory applicability for this approximation as well [1] [42].

Though reaching the point of validity quickly, the paraxial approximation paves the way to a very strong formalism to represent waves, the so-called *Gaussian beams*. For this, one looks at solutions to the paraxial wave equation with spherical symmetry, mostly in cylindrical coordinates. A possible solution to the *Helmholtz equation* in its paraxial form is then given by these *Gaussian beams* [40] [6]. With this result, we have gained a far more appropriate description of a light or particle wave beam, than before. Instead of a point source, we now have a so-called *beam waist*. This is the point, where the beam is mostly confined. The main difference is, that this region is no longer infinitesimally small, it has a finite Gaussian profile. We still have propagation along a preferred axis, as we would expect, but the beam now no longer decays with the inverse of the radius away from this axis. With Gaussian beams, we find exponential decay.

In the construction of such Gaussian beams we also find a nice insight in the difference between those Ansatzes. Both Ansatzes are constituted from a slow varying amplitude function and a rapidly varying phase exponential with a phase function. In the geometric optics approximation, the amplitude can be complex or real, the phase function, however, is strictly real. Using the Ansatz in the wave equation yields the eikonal equation and the transport equation for the amplitude, which are required to hold strictly. This can be understood in Hamiltonian form, where we can use the method of characteristics to solve it. Looking at the region where the wave is different from 0, we find, that this space gets smaller and smaller over time with the characteristic geodesics getting closer and closer. At some point, these characteristics intersect, which makes the wave function to essentially become a straight line and thus going to infinity. It is this point, we call a *caustic* where the wave function explodes.

For a Gaussian beam, the phase function must explicitly be complex such that we can choose the imaginary part in such a way, that we find exponential decay away from the beam. We again find the eikonal equation and a transport equation for the amplitude, this time, however, they are only valid along some geodesic and must only strictly hold until some large order. Typically, for the second derivative for the eikonal equation and just the equation itself for the transport equation. Thus, also the transport equation dissolves into an ordinary differential equation as we are only solving it along one specific characteristic geodesic. Therefore, we no longer have the problem of different geodesics intersecting at some point, as all equations are only evaluated along one specific geodesic. From the derivatives of the eikonal equation, one also finds restrictions on the transverse parts of the wave [34] [29] [28].

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As we have seen, Gaussian beams provide a very nice way to express the behaviour of waves. There are other interesting properties, though, one should consider when talking about Gaussian beams. A very important item for Gaussian beams is the so called *Rayleigh range*. We know, that Gaussian beams diverge exponentially away from the axis thus giving circular envelope of the beam, which we call the *cross section*. The Rayleigh length then gives the distance at which this envelope, the cross section, has doubled in size. This length is dependent on the beam waist and the wavelength of the wave. It is also this length from which the beam radius grows linearly which makes the area expanding quadratically. With quadratical change in area, also the peak intensity drops quadratically with the distance along the axis of propagation.

As the beam is confined to a specific region, the power or energy transported is localized as well. Depending on the radius we look at, we find a different fraction of power of the beam within this radius.

Gaussian beams also provide the feature, that they can represent diffraction. This effect is best seen when looking at the beam size. When we look at the spot size at the beam waist, we find, that the smaller this spot is, the faster the beam diverges. In fact, the angular divergence of the beam is inversely proportional to its waist.

We now have found a very nice Ansatz to use in wave equations. We can put all together and see, how we handle such a Gaussian beam when inserting it as an Ansatz for a Klein-Gordon equation, for example. For this goal, there is one huge problem remaining. Solving differential equations with such rigorous Ansatzes is often impossible or extremely complicated to do analytically. Simple solutions, like plane waves, are again not locally restrained and while some wave-packet solutions can be written as integrals in Fourier space, it is mostly very cumbersome. And in most cases, we do not really need the complete analytical solution at all, we just want to understand the physics we care about. Thus, we look for asymptotic solutions. We try to make expansions in a way, that the solution then remains within a certain limit around the exact solution [21] [5].

With Gaussian beams, we find two parameters we have to keep track of during expansion. We need the order of change of the amplitude in direction of propagation, as well as in transversal direction to be much smaller then the order of a wavelength. We call such an expansion the *two parameter expansions*. As it can get very cumbersome quite quickly to keep track of both parameters separately, we combine them into one parameter and expand the Ansatz in this parameter [41]. When we then insert the Gaussian beam into a wave equation, we can look at each order separately in this parameter, as two terms of different order can never possibly cancel each other out. For each order we then get additional information of our system. In the usual case in flat spacetime we find the eikonal equation in the lowest order, and then transport equations in the next orders [39].

In flat spacetime, at what we have looked so far, take a simple form with the amplitude only depending on a position in space. When we now move to curved spacetime in the regime of General Relativity, we run into problems. We do not have any kind of global Cartesian frame any more at which we can specify any point. Especially the direction of

the transverse region to the direction of propagation of a wave can change all the time due to curvature. We thus need to be more careful to choose a correct Ansatz. Apart from that we need to consider, that the direction of propagation is now also given by a geodesic.

For our calculations, we will therefore look more closely at the Ansatz provided by *Watson* [43] which we will generalize for the regime of general relativity.

A natural way to take care of the non-existing "general" flat coordinate system in curved spacetime is the concept of *Synge's world function* [18]. These are defined as the half squared geodesic distance between two points. By deriving this world function, we then find the tangent vector to the geodesic which connects these two points. With this concept, we can always define a local coordinate system along any geodesic. Taking the geodesic, which displays the direction of propagation of the wave, as the basis, we can construct a local orthonormal frame also called *tetrad* with the 0th basis vector tangent to the geodesic at any point along this geodesic. Such a coordinate system is then called *Fermi Normal coordinates* [22]. We can use these geodesics then as our world lines in the meaning of Synge's world functions to connect the chosen point along the geodesic with any other point. Any such point can be reached by a space like geodesic orthogonal to the propagation geodesic of the wave.

Taking this approach, makes the given Ansatz from *Watson* [43] a bit more complicated and in fact, it depicts a new approach, independent of geometrical optics or Gaussian beams. The only points, where our Ansatz is similar to geometrical optics lies in the fact, that the phase function is real, and as well as with Gaussian beams, we only want the solutions at each order in epsilon to only hold to a specific high order.

The amplitude of our Ansatz is no longer dependent only on some spacetime point, but also on the tangent vector of the geodesic, which connects this spacetime point to the geodesic, that provides the trajectory of the wave. This complication will indeed manifest in the calculation of the derivatives when inserting the new adjusted Ansatz into a wave equation. Apart from that, one has to be careful with the terms at each expansion parameter. It may happen, that some terms do not appear at the appropriate order, where they would belong. Specific properties of Synge's world functions may be needed to bring them to the correct order, as we will see later in the calculations.

Apart from the complications, we also get new insights after insertion of the Ansatz into the wave equation. In the case of curved spacetime, we find the mass condition in the lowest order. The next order then yields a parallel propagation law for the wave vector along the geodesic, which provides the world line for the wave. The biggest difference is happens in the next order. Inserting the Ansatz with the geometrical optics approximation as well as in the Gaussian beam approximation yields a transport law for the amplitude. Our Ansatz, however, provides a generalization of this propagation law in the form of a Schrödinger-like equation. While Gaussian beams are helpful, as this propagation law is formed by an ordinary differential equation as we are only on one geodesic, we again find a partial differential equation, as it was the case in geometrical optics approximation.

These results are not specific to general relativity, however, indeed one gets similar results

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for any kind of inhomogeneous media, as well as inhomogeneous periodic media [43].

The new Schrödinger-like equation needs another Gaussian beam like Ansatz which is retrieved from the literature [43] [14] [13]. As the amplitude is only reaching into the transverse space of propagation, we find an ansatz which incorporates the structure of the space in a matrix which is then contracted with two copies of tangent vector of the geodesics of the Fermi Normal coordinate system. Analytic solution of this, however, is not really possible any more.

From this stage, numerical simulation gives good insight. One finds interesting results, when the wave propagates around some non trivial geometry, like around a black hole. When the world line goes straight into the black hole, the forces of the black hole get stronger and therefore the changes in the medium. This has influence on the shape of the Gaussian beam [3] [37]. For a particle, orbiting at a specified radius around the black hole, this means, that due to the gravitational forces and therefore the shape of the medium, the beam gets focused by spacetime curvature and also distorted as the black hole distorts the transverse modes. If we look at the level sets of the vectors tangent to the geodesics which form the Fermi Normal frame, this means, that from a starting state, where they may all be equally long, they get distorted rapidly until a point, where one may reach a caustic which leads the Gaussian beam approximation to break up. Higher order Gaussian beam modes like *Hermite*- or *Laguerre*- Gaussian beams may provide better behaviour but can still lead to breaking of the approximation near points of strong curvature or caustics.

For world lines of particles moving radially only we find essentially two similar cases. When the particle moves inwards, the level sets of the tangent vectors get distorted more and more until, at some point, the particle reaches the point, at which the stretching and focusing reaches a caustic point and the approximation breaks apart.

A different images is found, when the particle moves outwards. We still find distortion of the level sets, however, at this case, the difference between the distortions of two different points along the trajectory get smaller and smaller with increasing distance from the black hole. This gives very intuitive insight. The tidal forces decrease with $\frac{1}{r^3}$ as they are proportional to the second derivative of the gravitational potential. Thus, after some distance, we can actually approximate the metric, which presented a lot of curvature, with the flat Minkowski metric. As the difference from the flat metric gets smaller and smaller with the distance from the black hole, also the influence of the tidal forces get smaller, thus the difference between two consecutive level shells of the tangent vectors get smaller until at infinite distance, the difference gets 0.

The thesis will take following way to describe aforementioned concepts. We will first take a revising look at the basics and concepts of *Geometrical optics* in 2. This will also include a construction of the beam more specific to the later calculations. In chapter 3, we will revise the basics and concepts of *Gaussian beams* and conclude with a section of a construction for the beam and differential equation more related to later calculations. Section 4 we will finally introduce the Klein-Gordon equation and discuss our specific Ansatz. We will look at the derivatives of the Ansatz in detail and express the con-

sequences of the equation parts for each order in our two parameter expansion. This chapter will end with the definition of the differential equations, the matrices for the Ansatz for the Schrödinger-like equation must satisfy. The next chapter, 5 will discuss how we proceeded with numerical calculation of geodesic equation and the differential equation for these matrices to plot the level sets of the tangent vectors. We will discuss the resulting plots and the reasons for their behaviour in detail. In the end chapter 6 we will then give an outlook of what the next steps would be.

2. Geometric optics

Following the approach by *Thorne* [41] we will introduce the concept of Geometric optics by looking at Waves in homogeneous medium which we will then generalize to the inhomogeneous case. Here, we will find important notions like the eikonal equation. These sections are followed by a discussion of how we can use the geometric optics approximation for general waves and we will see where the approximation breaks. Finally we will take a look at the famous Fermat's principle and polarizations until, in the end, we construct an Ansatz for the proceeding calculations.

2.1. Introduction

With its simplification of light propagating as rays instead of waves, *geometric optics* is the oldest approach to study the dynamics in the field of optics. Although assuming multiple simplifications, it has still its region of validity, namely exactly where the wavelength and the periods of the waves are far smaller than the length- and timescales of changes in the medium in which the wave propagates. Thus, geometric optics provides a very good approximation for scenarios in the region of general relativity. As long, as we stay away from singularities, the frame stays more or less quasi-Cartesian so changes are very small and we get good results when studying the track of light emitted from quasars travelling through spacetime. Lensing effects by galaxies or even scattering at black holes can be described fairly well by the approximations of geometric optics.

Before we start into the topic, however, we will start with a quick review of wave propagation in a homogeneous medium, which will be followed by the derivation of the *propagation equations* of geometric optics and the *eikonal approximation*. Ultimately, we will find a connection to quantum theory, where classical rays can be interpreted as a flux of quanta when we look at *Hamilton Jacobi Theory*. We will conclude this chapter by deducing the propagation law for the polarization vector which will lead us to a classical version of *geometric phases*.

2.2. Waves in homogeneous medium

The most trivial way to get insight into the field of geometric optics is to look at a monochromatic wave, i.e. a wave of only one single wavelength, propagating through a

2. Geometric optics

homogeneous medium. We can describe such a wave by a simple plane wave

$$\psi = Ae^{ik\hat{x}-\omega t} \equiv Ae^{i\varphi} . \quad (2.2.1)$$

For such a plane wave, A describes the *complex Amplitude* and the *phase* is given by $\varphi = k \cdot x - \omega t$. As usual, t and x describe the time and position, respectively. Apart from these, we have ω as the *angular frequency* and the wave vector k . The norm of the wave vector denotes the wave number and the normalized wavevector then gives the direction of propagation $\hat{k} \equiv \frac{k}{|k|}$ which is orthogonal to the planes of constant phase φ . These planes move with the phase velocity

$$v_{ph} \equiv \left. \frac{\partial x}{\partial t} \right|_{\varphi} = \frac{\omega}{|k|} k . \quad (2.2.2)$$

Using the wave number, we can define the *wavelength* as $\lambda = \frac{2\pi}{k}$ and by dividing the wavelength by 2π we find the reduced wavelength $\bar{\lambda} = \frac{\lambda}{2\pi}$.

Another important item for the description of waves is the dispersion relation Ω . Using it, we find the frequency as

$$\omega = \Omega(k) , \quad (2.2.3)$$

The dispersion relation describes the spreading of the wave especially for wave packets constructed by superpositions of plane waves. The most important examples are

- For electromagnetic waves propagating through isotropic dielectric medium with refraction index n :

$$\omega = \Omega(k) = Ck \equiv C|k|$$

where $C = \frac{c}{n}$ is the base speed and c the light speed in vacuum.

- For waves on the surface of a deep body of water, where the depth is much larger than the reduced wavelength $\bar{\lambda}$. Here, ψ could be the height of the water above equilibrium.

$$\omega = \Omega(k) = \sqrt{gk} = \sqrt{g|k|}$$

with g being the acceleration of gravity.

- For gravitational waves ψ can denote a component of the waves' metric perturbation which describes its stretching and squeezing of space. As they propagate non-dispersively at the speed of light, they have the same dispersion relation as standard magnetic waves. but with C being replaced by the vacuum light speed c .

2.2.1. Wave packets

Monochromatic waves provide a very easy way for an introduction into geometric optics. In the real world, however, one requires very expensive high specialized lasers to produces somewhat monochromatic waves. One generally finds superpositions of different plane

waves. We call such superpositions *wave packets* and we describe them as

$$\psi(x, t) = \int A(k) e^{i\alpha(k)} e^{i(k \cdot x - \omega t)} \frac{d^3 k}{(2\pi)^3} . \quad (2.2.4)$$

In this integral, A and α describe the modulus and phase of the complex amplitude. We find multiple waves with different wave vectors k for such a wave packets, however, the contributions for adjacent wave vectors will cancel out except where the phase factor changes only very little with k . This region describes the place, where the wave is localized and where we exactly find $\nabla_k \text{phase factor} = 0$ we have

$$\left(\frac{\partial \alpha}{\partial k_j} + \frac{\partial}{\partial k_j} (k \cdot x - \omega t) \right) \Big|_{k=k_0} = 0 . \quad (2.2.5)$$

This differential equation can be solved with the help of the dispersion relation which gives

$$\begin{aligned} x_j &= \left(\frac{\partial \Omega}{\partial k_j} \right) \Big|_{k=k_0} \\ t &= - \left(\frac{\partial \alpha}{\partial k_j} \right) \Big|_{k=k_0} = \text{const} \end{aligned} \quad (2.2.6)$$

for the centre of the wave packet. We also find the group velocity

$$V_g = \nabla_k \Omega \quad (2.2.7)$$

or equivalently

$$V_{g,j} = \left(\frac{\partial \Omega}{\partial k_j} \right)_{k=k_0} . \quad (2.2.8)$$

In general, the group and phase velocity are not equal. In fact, for movement in anisotropic media like magnetized plasma, the group velocity may even point into a different direction as the phase velocity.

Remark. For simple dispersion relations like the one for electromagnetic waves, the group velocity and phase velocity coincide

$$V_g = V_{ph} = C \hat{k} . \quad (2.2.9)$$

The energy of a wave must always be contained within the wave packet as there cannot be transported any energy where the amplitude vanishes. Thus, the energy must also propagate with the group velocity. Speaking from the quantum mechanical point of view, this is equivalent to the quanta moving with the group velocity. If we denote the wave vector where all wave vectors are concentrated around as k_0 we find the standard quantum mechanical relations

$$\begin{aligned} \epsilon &= \hbar \Omega(k_0) \\ p &= \hbar k_0 . \end{aligned} \quad (2.2.10)$$

2.3. Waves in inhomogeneous, time varying medium, eikonal approximation and geometric optics

We have now looked at waves in homogeneous media, however, this is a very restrictive assumption considering the universe. Our real universe is better described as spatially inhomogeneous with variations in time. To efficiently describe wave propagation in such a regime, we look at the case where the length scale $\mathcal{L}$ and the time scale $\mathcal{T}$ for variations in the medium are very long compared to the reduced wavelength and the period

$$\begin{aligned}\mathcal{L} &\gg \bar{\lambda} = \frac{1}{k} \\ \mathcal{T} &\gg \frac{1}{\omega}.\end{aligned}\tag{2.3.1}$$

As long as this assumption holds, we can treat the waves as planar and monochromatic, at least locally. Even though the medium may introduce variations in the wave vector and frequency, these are not substantial as long as the scales stay beyond $\mathcal{L}$ and $\mathcal{T}$.

We can show this by using the *two length scale expansion* which will also be used in our calculations later. As the name suggests, we expand the wave equation in powers of two parameters

$$\begin{aligned}\frac{\bar{\lambda}}{\mathcal{L}} &= \frac{1}{k\mathcal{L}} \\ \frac{1}{\omega\mathcal{T}} &.\end{aligned}\tag{2.3.2}$$

This is called the *geometrical optics approximation* or *eikonal approximation* which comes from the Greek word for *image*. Apart from that, one also find *WKB approximation* frequently in the literature coming from Gregor Wentzel, Hendrik Anthony Kramers and Léon Brillouin.

This approximation comes handy, as it describes the amplitude as being transported along the trajectories, i.e. the rays. From the view of quantum mechanics these rays describe the world lines of the quanta and indeed, this forms a conservation law. We will now continue to derive the laws of propagation for geometrical optics starting from the wave equation

$$\frac{\partial}{\partial t} \left(W \frac{\partial \psi}{\partial t} \right) - \nabla \cdot (WC^2 \nabla \psi) = 0.\tag{2.3.3}$$

As in the previous chapters, $\psi(x, t)$ describes the oscillating wave. $C(x, t)$ describes the propagation speed which may vary slowly and $W(x, t)$ is a function which sets a weight also slowly varying with the medium.

Remark. While W does not have influence on the dispersion relation, it still influences the transportation law of the amplitude.

Remark. Our chosen equation (2.3.3) describes sound waves which propagate through a static, isentropic, inhomogeneous fluid. Thus, if we think carefully, what such a sound

2.3. Waves in inhomogeneous, time varying medium, eikonal approximation and geometric optics

wave actually is, ψ describes the pressure perturbation. $C(x) = \sqrt{(\frac{\partial P}{\partial \rho})_s}$ then denotes the adiabatic speed of sound and using the fluid's unperturbed density ρ we find $W(x) = \frac{1}{\rho C^2}$.

For time independent W and C , the energy density $U(x, t)$ and the energy flux $F(x, t)$ fulfil the conservation law

$$\frac{\partial U}{\partial t} + \nabla \cdot F = 0 \quad (2.3.4)$$

but if we allow variations in time, we find, that the energy density and flux are given by

$$U = W \left[\frac{1}{2} \left(\frac{\partial \psi}{\partial t} \right)^2 + \frac{1}{2} C^2 (\nabla \psi)^2 \right] \quad (2.3.5)$$

$$F = -WC^2 \frac{\partial \psi}{\partial t} \nabla \psi. \quad (2.3.6)$$

We will now start to weaken our conditions a bit. The fluid may be weakly inhomogeneous and we also allow variations with time. The wave should be planar. For the wave equation (2.3.3) we use a plane wave Ansatz again but we express the wave in the before mentioned eikonal approximation. The Amplitude may vary slowly with the length and timescale and the phase should vary rapidly with $\frac{1}{\omega}$ and $\bar{\lambda}$. Thus we write the Ansatz as

$$\psi(x, t) = A(x, t) e^{i\varphi(x, t)}. \quad (2.3.7)$$

With the complex phase from the Ansatz we can define the wave vector field and angular frequency

$$\begin{aligned} k(x, t) &\equiv \nabla \varphi \\ \omega(x, t) &\equiv -\frac{\partial \varphi}{\partial t}. \end{aligned} \quad (2.3.8)$$

and we still want $\mathcal{L} \gg \frac{1}{k}$ and $\mathcal{T} \gg \frac{1}{\omega}$. The parameters A , k and ω may slowly vary such that the wave remains planar, $\varphi \approx k \cdot x - \omega t + \text{constant}$.

Remark. As keeping two parameters in the eye may become cumbersome, in the literature, as well as here, one introduces a bookkeeping parameter σ or ϵ for fixed length and time scale. Numerically, this has the value of unity but it helps keeping track of terms of different order in this parameters. As different sets of terms of different order in the parameter cannot cancel each other, we can use it to group these terms together and set them to 0 separately.

With this parameter σ we can rewrite the Ansatz (2.3.7) as

$$\psi = (A + \sigma B + \dots) e^{i\frac{\varphi}{\sigma}}. \quad (2.3.9)$$

2. Geometric optics

Using this Ansatz in the wave equation (2.3.3) we find

$$0 = (-\omega^2 + C^2 k^2) W \psi + i \left[-2 \left(\omega \frac{\partial A}{\partial t} + C^2 k_j A_{,j} \right) W - \frac{\partial(W\omega)}{\partial t} A - (WC^2 k_j)_{;j} A \right] e^{i\varphi} + \dots \quad (2.3.10)$$

where the first term scales as $\bar{\lambda}^{-2}$, the term in the bracket with $\bar{\lambda}^{-1}$ and everything we omitted with $\bar{\lambda}^0$.

We can now set each term to 0 separately and find a dispersion relation

$$\omega = \Omega(k, x, t) \equiv C(x, t) k. \quad (2.3.11)$$

Remark. As mentioned before, it is independent of W and coincides with the dispersion relation of a plane wave in a homogeneous medium.

From the second term we find a transport equation for the Amplitude A with group velocity $V_g = C \hat{k}$

$$\frac{dA}{dt} \equiv \left(\frac{\partial}{\partial t} + V_g \cdot \nabla \right) A = -\frac{1}{2W\omega} \left[\frac{\partial(W\omega)}{\partial t} + \nabla \cdot (WC^2 k) \right] A. \quad (2.3.12)$$

Remark. One can see, that the here used time derivative $\frac{d}{dt} = \frac{\partial}{\partial t} + V_g$ shares similarity with the derivative with respect to proper time along a world line in special relativity $\frac{d}{d\tau} = u^0 \frac{\partial}{\partial t} + u \cdot \nabla$.

As mentioned in previous chapters, the Amplitude A gets transported along world lines, or rays. These world lines are governed by Hamilton's equations of motion. In this regime, the dispersion relation describes the Hamiltonian and the wave vector the momentum. Thus

$$\frac{dx_j}{dt} = \left(\frac{\partial \Omega}{\partial k_j} \right)_{x,t} \equiv V_{gj} \quad (2.3.13)$$

$$\frac{dk_j}{dt} = - \left(\frac{\partial \Omega}{\partial x_j} \right)_{k,t} \quad (2.3.14)$$

$$\frac{d\omega}{dt} = \left(\frac{\partial \Omega}{\partial t} \right)_{x,k}. \quad (2.3.15)$$

Equation number one describes the group velocity. The second one shows, how the wave changes along a rays and for a given C we therefore find how the group velocity changes along the ray itself. The last equation tells us, how the frequency changes along the world line.

To deduce the second and third equation we first need the *eikonal equation*. This is obtained by inserting $\omega = -\frac{\partial \varphi}{\partial t}$ and $k = \nabla \varphi$ into the dispersion relation for an arbitrary

wave. We thus find

$$\frac{\partial \varphi}{\partial t} + \Omega(x, t, \nabla \varphi) = 0 . \quad (2.3.16)$$

Remark. This equation is formally the same as the Hamilton Jacobi equation in classical mechanics. Ω then describes the Hamiltonian and φ Hamilton's principal function.

Using this remark, we can take the same approach as one does in classical mechanics for deriving the second and third equation. From the gradient of the eikonal equation (2.3.16) we get

$$\frac{\partial^2 \varphi}{\partial t \partial x_j} + \frac{\partial \Omega}{\partial k_l} \frac{\partial^2 \varphi}{\partial x_l \partial x_j} + \frac{\partial \Omega}{\partial x_j} = 0 \quad (2.3.17)$$

and with the definitions of k and V we rewrite the equation to get $\frac{dk_j}{dt} = -\frac{\partial \Omega}{\partial x_j}$ which is exactly the second equation.

After the spatial derivatives, the only one left is the time derivative of the eikonal equation. From this derivative we find, that apart from the amplitude, the phase is also propagated along the rays

$$\frac{d\varphi}{dt} = \frac{\partial \varphi}{\partial t} + V_g \cdot \nabla \varphi = -\omega + V_g \dot{k} . \quad (2.3.18)$$

Remark. For dispersion less waves where $\omega = Ck$ and the group velocity is $V_g = C\hat{k}$, the phase is constant along each ray

$$\frac{d\varphi}{dt} = 0 .$$

2.3.1. Connection to quantum theory

In the previous chapters we already started to make connections to quantum theory which we will make more concise now. In quantum mechanics we now longer talk about continuous spectra or waves, instead, we have world lines or rays with specific, discretized energies. We call these the *quanta*. To get the momentum and energy we thus multiply the classical values with $\hbar$ and get

$$\begin{aligned} p &= \hbar k \\ \epsilon &= \hbar \omega . \end{aligned} \quad (2.3.19)$$

As we could relate the dispersion relation with the Hamiltonian in the classical case, we can do the same in the quantum mechanical case when we introduce $\hbar$ here as well. Thus we find

$$H(x, t, p) = \hbar \Omega(x, t, k = p/\hbar) . \quad (2.3.20)$$

The new equations of motion are then received trivially from the Hamiltonian.

We can now continue to examine, how the energy changes with properties of the medium. We therefore look back to the propagation law for the amplitude (2.3.12) and use the Ansatz $\psi = A \cos(\varphi)$ for the equations of the energy density (2.3.5) and energy flux

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(2.3.6). We then average over the wavelength and period with $\cos^2(\varphi) = \sin^2(\varphi) = \frac{1}{2}$ and thus get

$$\begin{aligned} U &= \frac{1}{2}WC^2k^2A^2 = \frac{1}{2}W\omega^2A^2 \\ F &= U(C\hat{k}) = UV_g . \end{aligned} \quad (2.3.21)$$

When we insert these into the conservation law (2.3.4) and use the propagation law (2.3.12) we finally get the differential equation governing the change of energy with time

$$\frac{\partial U}{\partial t} + \nabla \cdot F = U \frac{\partial \ln(C)}{\partial t} . \quad (2.3.22)$$

With the right side being 0 this would be the continuum equation again, but when it deviates from 0, the slow change in medium actively adds or removes to/from the energy, depending on the sign.

In quantum mechanics we find very handy notions of the number density and number flux defined as

$$n = \frac{U}{\hbar\omega} \quad (2.3.23)$$

$$S = \frac{F}{\hbar\omega} = nV_g \quad (2.3.24)$$

which we can combine with the differential equation for the energy (2.3.22) to see, how the number density changes with time

$$\frac{\partial n}{\partial t} + \nabla S = n \left[\frac{\partial \ln(C)}{\partial t} - \frac{d \ln(\omega)}{dt} \right] . \quad (2.3.25)$$

The third Hamilton equation (2.3.15) relates the change of frequency with time with the change of the dispersion relation with respect to time. Thus we find

$$\frac{d\omega}{dt} = \left(\frac{\partial \Omega}{\partial t} \right)_{x,k} = k \frac{\partial C}{\partial t} . \quad (2.3.26)$$

Inserting previous results we find $\frac{d \ln(\omega)}{dt} = \left(\frac{\partial \Omega}{\partial t} \right)_{x,k} = \left[\frac{\partial(Ck)}{\partial t} \right]_{x,k} = k \frac{\partial C}{\partial t}$ which comes in handy when we insert it into the differential equation for n (2.3.25) as this gives

$$\frac{\partial n}{\partial t} + \nabla \cdot S = 0 . \quad (2.3.27)$$

This is a very important result as it tells us, that the number of quanta is a conserved quantity. We can still enhance this result though, by using $S = nV_g$ and $\frac{d}{dt} = \frac{\partial}{\partial t} + V_g \cdot \nabla$ to rewrite the conservation law as

$$\frac{dn}{dt} + n \nabla \cdot V_g = 0 . \quad (2.3.28)$$

Remark. When we compare this result with the propagation law of the amplitude (2.3.12) we see, that it indeed describes the conservation law of quanta in a slowly varying field in terms of the amplitude. This result holds for any kind of wave.

2.4. Geometrical optics for general waves

Until now we only looked at non-dispersive waves. now we will generalize our waves to any kind of wave in a weakly inhomogeneous medium which may slowly vary with time. WE stay in the eikonal approximation and take the Ansatz

$$\psi = Ae^{i\varphi} . \quad (2.4.1)$$

Now, the Amplitude A may also change slowly with time while the phase φ may change rapidly. Depending on the type of A and therefore ψ this describes different kind of waves. For scalar ψ it may describe sound waves. Light may be described by ψ being a vector and for general tensors, the Ansatz describes gravitational waves.

As we are working in the eikonal approximation, we will again follow the approach with the two parameter expansion. When we insert the Ansatz into the wave equation we will thus get sets of terms with different orders in the bookkeeping parameter. The terms coming from the temporal and spatial derivative of the phase will constitute the leading order term. This term will take the form of the exponential scaled with a prefactor of $i\omega$ or ik . Apart from that, they should be equal to those leading order terms of the homogeneous plane wave which was the dispersion relation scaled by a prefactor multiplied with the wave itself. This makes calculations a bit easier as we can analyse the plane monochromatic wave in a homogeneous, time independent medium to get the dispersion relation and only after this let the medium change with time and location. All the terms where only one derivative acts on the phase exponential and the rest on the prefactor will constitute the subleading terms.

For the leading order terms we find, that the rays of general waves are governed by the Hamilton equations of the dispersion less wave

$$\frac{dx_j}{dt} = \left(\frac{\partial \Omega}{\partial k_j} \right)_{x,t} = V_{gj} \quad (2.4.2)$$

$$\frac{dk_j}{dt} = - \left(\frac{\partial \Omega}{\partial x_j} \right)_{k,t} \quad (2.4.3)$$

$$\frac{d\omega}{dt} = \left(\frac{\partial \Omega}{\partial t} \right)_{x,k} \quad (2.4.4)$$

the disperion relation, however, is now of a general form. These equation do not immediately provide a propagation law for the phase, but by combing the propagation laws for

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$\omega = -\frac{\partial\varphi}{\partial t}$ and $k_j = \frac{\partial\varphi}{\partial x_j}$ we find for the phase

$$\frac{d\varphi}{dt} = -\omega + V_g \cdot k . \quad (2.4.5)$$

Remark. It is important to note here, that the phase may not be constant along a ray of a general wave.

We can again make the connection to quantum theory and find the conservation laws

$$\begin{aligned} \frac{\partial n}{\partial t} + \nabla \cdot (nV_g) &= 0 \\ \frac{dn}{dt} + n \nabla \cdot V_g &= 0 \end{aligned} \quad (2.4.6)$$

if we have knowledge of the energy density U and the amplitude A and the relations to the number density $n = \frac{U}{\hbar\omega}$. These conservation laws show, that slow changes of the medium do not suffice to create or generate particles. Thus we find the propagation law for A

$$\frac{d(nCA)}{dt} = 0 \quad (2.4.7)$$

In the leading terms, we can replace one term of the form $ik_j A e^{i\varphi} = A(e^{i\varphi})_{,j}$ with $A_{;j} e^{i\varphi}$. This gives us the set of terms for subleading order

$$-2i\omega \frac{\partial A}{\partial t} - 2i\omega \frac{\partial \Omega}{\partial k_j} \frac{\partial A}{\partial x_j} = F \cdot A . \quad (2.4.8)$$

F here denotes proportionality terms. We can now use the group velocity and dispersion relation to get this into the form of a total time derivative on A along some ray

$$\frac{dA}{dt} \equiv \frac{\partial A}{\partial t} + V_g \cdot \nabla A = F \dot{A} \quad (2.4.9)$$

Example 1. To make the procedure more clear, we look at an explicit example. Spherical sound waves propagate radially outward through a homogeneous field from a spherical source similar to a radially oscillating ball. The dispersion relation is then given by

$$\Omega = Ck . \quad (2.4.10)$$

As we have spherical waves and the wave vector k is always perpendicular to the wave fronts, we immediately know that k must have the form of

$$k = A \cdot e_r \quad (2.4.11)$$

with a proportionality factor A . As we know that $\omega = \Omega(k) = Ck$ we find,

$$k = \frac{\omega}{C} e_r . \quad (2.4.12)$$

We can now use the first two Hamilton equations (2.4.2)

$$\begin{aligned}\frac{dx_j}{dt} &= \frac{\partial \Omega}{\partial k_j} \\ \frac{dk_j}{dt} &= -\frac{\partial \Omega}{\partial x_j}\end{aligned}\tag{2.4.13}$$

with $x_j = (r, \theta, \phi)$ and $k_j = (k_r, k_\theta, k_\phi)$. From the previous discussion we know that k only has a radial component, so we find

$$\begin{aligned}\frac{dr}{dt} &= \frac{\partial}{\partial k_r}(C \cdot k_r) = C \\ \frac{d\theta}{dt} &= 0 \\ \frac{d\phi}{dt} &= 0.\end{aligned}\tag{2.4.14}$$

Thus we can straightforwardly integrate these three differential equations and find

$$\begin{aligned}r &= Ct + c \\ \theta &= c \\ \phi &= c\end{aligned}\tag{2.4.15}$$

with c being the constant of integration. From the dispersion relation we saw that the wave is dispersion less. Thus, the phase must be conserved along the ray. With the wavefront given by Ct at $r(t)$, the phase must be a function of $Ct - r(t), \theta, \phi$. In radial coordinates k is given by

$$k = \frac{\partial \varphi}{\partial r} e_r + \frac{1}{r} \frac{\partial \varphi}{\partial \theta} e_\theta + \frac{1}{r \sin(\theta)} \frac{\partial \varphi}{\partial \phi} e_\phi.\tag{2.4.16}$$

If k is now nearly radial for completely spherical waves, we have

$$\left| \frac{\partial \varphi}{\partial r} \right| \gg \frac{\partial \varphi}{\partial \theta}, \frac{\partial \varphi}{\partial \phi}.\tag{2.4.17}$$

Thus, φ varies rapidly with $Ct - r$ but almost not with θ, ϕ . We can now look at the law of conservation of quanta in the form

$$\frac{dnC\mathcal{A}}{dt} = 0\tag{2.4.18}$$

where A is the cross sectional area of a bundle of rays around the ray and n is the number density. In our case, C factors out, as the medium is homogeneous, and therefore the propagation speed does not change. The density of quanta n is proportional to the square of the amplitude A

$$n \propto A^2\tag{2.4.19}$$

and the cross-sectional area $\mathcal{A}$ grows with r^2 because we are working with spherical waves

$$\mathcal{A} \propto r^2\tag{2.4.20}$$

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Thus we have

$$A^2 \mathcal{A} = \text{constant} \quad (2.4.21)$$

which corresponds to

$$A^2 r^2 = \text{constant} . \quad (2.4.22)$$

Taking the root we find that

$$A \cdot r = \text{constant} \quad (2.4.23)$$

from this results

$$\frac{drA}{dt} = 0 . \quad (2.4.24)$$

We can call the quantity $rA = \mathcal{B}$. Putting all together, we find that the pressure perturbation $\psi = \delta P$ of the wave has the form

$$\psi = \frac{\mathcal{B}(Ct - r, \theta, \phi)}{r} e^{i\varphi(Ct - r, \theta, \phi)} . \quad (2.4.25)$$

As discussed, φ varies rapidly with $Ct - r$ and slowly with θ and ϕ . $\mathcal{B}$ varies slowly with $Ct - r, \theta$ and ϕ .

2.5. Relation to the wave packets, limitations of the eikonal approximation and geometric optics

The Ansatz we looked at in the eikonal approximation $\psi = Ae^{i\varphi}$ can be used to describe many different forms of waves as long as the two length scale constraints are satisfied. The wave may be nearly planar but at the opposite extreme may also be very narrow and confined to a small region, as long as it is larger than its mean reduced wavelength. Evolution still stay governed by the equations deduced in the previous chapters.

One should not forget, however, that, as every approximation, the regime, where geometric optics provide useful results, has its borders as well. A very important property of wave packets, the spreading due to the dispersion, is not described at all. Thus, one has always to make sure, that the wave packet is either very large compared to its wavelength, or one only looks at short time of propagation. As soon as one considers diffraction, wave-wave coupling in a non-linear way, amplifications or rapid time variations are also not described by geometric optics, and one of the most fundamental properties of quantum field theory, generation and annihilation of particles needs enhanced models as well.

2.6. Fermat's principle

As long as the variations of the medium are independent of time, we can deduce the path of the rays directly from the variation principle and do not need the Hamilton equations of optics. Fermat stated, that the path, a particle takes from point a to point b extremized

the action

$$J = \int p \cdot dq , \quad (2.6.1)$$

with the generalized coordinates p and momentum q . For a time independent Hamiltonian, we can fix some initial location x_i and some final destination x_f . Thus, rays, that connect these two points should satisfy

$$\delta \int k \cdot dx = 0 . \quad (2.6.2)$$

As mentioned in previous chapters, all rays that deviate slightly will cancel out in the integral and only one will be left thus, for this ray holds $k = \nabla\varphi$. This is a very insightful result as it tells us, that the extremal value is equal to the phase difference of the wave between x_i and x_f . Thus we can identify the action with the phase difference along the path

$$\Delta\varphi = \int k \cdot dx . \quad (2.6.3)$$

This yields Fermat's principle, particles move along rays with extremal phase difference.

Remark. This result has a very intriguing connection to Feynman's path integral formalism. All paths for a particle have the same probability to be taken, such that we can construct the probability amplitudes $e^{i\Delta\varphi}$ for each path which we then should add up to find

$$\sum_{\text{paths}} e^{i\Delta\varphi} .$$

However, the contributions from deviating paths will again interfere destructively and therefore cancel out. Thus, only the neighbouring paths, that have the same value of phase difference $\Delta\varphi$ up to the first order in the path difference will remain. Only these paths from suitable rays or world lines for the particles, as only they extremize the action.

Example 2. We find a very simple example of Fermat's principle for a dispersion relation of the Form $\Omega = C(x)k$. The Hamiltonian stays time independent. In this case, k is parallel to dx for each trial path. Thus $k \cdot dx = |k|ds$ where s denotes the distance of the path. We can construct the value of k from the dispersion relation and find $|k| = \frac{\Omega}{C}$. C is then obtained from the Hamilton equation $\frac{dx^j}{dt} = \frac{\partial\Omega}{\partial k_j}$ which implies $\frac{ds}{dt} = C$. As the dispersion relation remains constant along the paths, Fermat's principle states, that the paths extremize time, thus, the rays extremize

$$\int dt = \int \frac{ds}{C(x)} = \int \frac{n(x)}{c} ds$$

between points x_i and x_f . For the sake of clarity, we have replaced $C(x)$ with the vacuum light speed c and the index of refraction $n(x)$.

As we find a lower border for the optical path between two points given by $n_{min}L$ where L is the distance between the two points we are guaranteed that there always exists one ray that connects these points, as long as there is no opaque object.

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We can now derive the Euler Lagrange equations

$$\frac{d}{ds} \left(n \frac{dx}{ds} \right) = \nabla n \quad (2.6.4)$$

or

$$\frac{d}{ds} \left(\frac{1}{C} \frac{dx}{ds} \right) = \nabla \left(\frac{1}{C} \right) \quad (2.6.5)$$

and we see that they are identical to the Hamilton equations. These lead us to *Snell's law of refraction*. With the start and endpoint of the ray or the starting point and starting direction, we can solve this equation and when $n = n(z)$ in Cartesian coordinates for the medium, the ELG can be projected perpendicular to e_z . Thus making $n \frac{dy}{ds}$ and $n \frac{dx}{ds}$ constant and we are left with

$$n \sin(\theta) = \text{constant} . \quad (2.6.6)$$

Thus the angle between the ray and the basis vector in z direction always remains constant, which is indeed a variant of Snell's law of refraction. In fact, it is also valid, when n is not continuous even though the approximation of geometric optics falls apart at discontinuities.

2.7. Polarization

So far we have not talked about polarization of waves. In the preceding chapters, we mostly looked at scalar waves but polarization is unique to vectorial and tensorial waves.

2.8. Polarization vector and its geometric optics propagation law

When travelling through a vacuum, the magnetic and electric field of an electromagnetic wave are always perpendicular to the direction of propagation. This generally holds for any isotropic dielectric medium and a dispersion free dispersion relation. Here, the group and phase velocities are also parallel to the direction of propagation. As soon as we allow the medium to not be isotropic any more or when we look at some plasma waves, this changes. Then, the magnetic field of the wave will direct itself along the background magnetic field which is generally at arbitrary angle to the direction of propagation.

For our study we will continue to focus on a simple case with an isotropic dielectric medium with dispersion free dispersion relation $\Omega = \frac{c}{n} k$. The magnetic field E may then oscillate linearly along a normalized polarization vector $\hat{f}$ perpendicular to the direction of propagation

$$\begin{aligned} E &= A e^{i\varphi} \hat{f} \\ \hat{f} \cdot \hat{k} &\equiv \hat{f} \cdot \nabla \varphi = 0 . \end{aligned} \quad (2.8.1)$$

here we again have introduced our Ansatz from the eikonal approximation into the electric field. We find, that that polarization vector also propagates along the rays. Instead of deriving the propagation law from the eikonal approximation and Maxwell's equations, we will deduce it from physical reasoning

1. As $\hat{f}$ is orthogonal to $\hat{k}$ for a plane wave, it must also be in the eikonal approximation.
2. As the medium cannot distinguish between a slow left hand or right-hand rotation when the ray is straight and the medium is isotropic, there will be no rotation at all and $\hat{f}$ will always point in the same direction, it will be kept parallel to itself during transportation.
3. When $\frac{d\hat{f}}{ds} \neq 0$, which means that the ray bends, $\hat{f}$ has to change as well to stay perpendicular to $\hat{k}$ and as the isotropic medium cannot provide any preferred direction, the direction of change for $\hat{f}$ must be $\hat{k}$. The magnitude of the change is determined by the requirements that $\hat{f} \cdot \hat{k} = 0$ and $\hat{k} \cdot \hat{k} = 1$

Thus, following these reasons, the propagation law yields

$$\frac{d\hat{f}}{ds} = -\hat{k} \left(\hat{f} \frac{d\hat{k}}{ds} \right). \quad (2.8.2)$$

This has the form of a parallel transport equation telling us, that the polarization vector indeed gets parallel transported along its ray.

2.8.1. Geometric phase

As the polarization gets parallel transported along its ray it is obvious, that when we look at a circular trajectory, there may be a deviation of the direction of the polarization vector from its initial direction after a full circle. This deviation depends on the geometry and such differences happening from the geometry of the medium are called *Berry's geometric phases*.

Intuitively speaking, we can look at a great circle around a sphere. This great circle may now be the trajectory of a particle or light. We can now choose any point along this great circle as our initial position and at this position we attach a vector tangent to the sphere. We can now start to transport this vector parallel along this great circle. We choose several other points along the great circle and at each of these points, the vector will show into a different direction while still being tangent to the sphere. After one rotation, we can compare the initial vector with the parallel transported vector and we will see that they still point into the same direction. This result stays true as long as the geometry of the background or the medium is trivial. AS soon as we introduce holes, for example, this changes. When the geometry of the background medium is not trivial any more, Berry's phase factor then corresponds to the holonomy of the ray the tangent vector is parallel transported along. [38]

2.9. Paraxial optics

The paraxial optics approximation is a very helpful tool when solving the geometric optics equation. In this approximation we can linearize this equation and use matrix methods to trace out the rays. This is possible as the paraxial approximation assumes, that a bundle of rays is almost parallel which means, that the angles between these rays are fairly small. We find this case when we observe light rays in space far away from their source star.

We start again with a time-independent, non-dispersive dispersion relation $\Omega = \frac{kc}{n(x)}$ for a dielectric medium or light lensed by a weak gravitational field. We further assume the existence of one special ray with a completely straight trajectory. This ray will be our *reference ray* or *optical axis*. The z coordinate of our coordinate system lies along this ray. In Cartesian components, the displacement of any other ray from this reference ray will be denoted by the two dimensional vector $x(z)$. As described, the norm of this displacement vector is very small compared to the length scale of the axis. We can now make a Taylor approximation for the refractive index

$$n(x, z) = n(0, z) + x_i n_{,i}(0, z) + \frac{1}{2} x_i x_j n_{,ij}(0, z) + \dots \quad (2.9.1)$$

which we can insert into the ray propagation equation (2.6.4) up to linear order to find the linearized form

$$\frac{d}{dz} \left(n(0, z) \frac{dx_i}{dz} \right) = n_{,i}(0, z) + x_j n_{,ij}(0, z) . \quad (2.9.2)$$

For the reference ray $x_i = 0$ this equation must be satisfied which means, that the refractive index must vanish. We thus find a linear, homogeneous, second order differential equation for the path of a nearby ray $x(z)$

$$\left(\frac{d}{dz} \right) \left(\frac{ndx_i}{dz} \right) x_j n_{,ij} . \quad (2.9.3)$$

This may be interpreted as the 2-dimensional motion of a particle in a quadratic potential well, when the z direction is associated with the time t .

Given the initial position and velocity this equation is solvable and the solution at any later point is linearly related to the starting values. The solution can then be put into a transfer matrix $J_{ab}(z, z')$ such that

$$V_a(z) = J_{ab}(z, z') \dot{V}_b(z') . \quad (2.9.4)$$

Remark. This transfer matrix is transitive. The transfer matrix between points x and z can be constructed from the transfer matrices from x to y and from y to z .

$$J_{ac}(z, z') = J_{ab}(z, z'') J_{bc}(z'', z) .$$

If we choose the refraction index to be asymmetrical like $n = n(\sqrt{x^2 + y^2}, z)$, the motion of the rays along the x and y direction is not coupled. Thus the equations of motion are identical to the ones along x and y and the transfer matrix becomes symmetrical with trace 0.

2.10. Tailored construction

The preceding chapters gave a rather general introduction into the topic of geometric optics. We will now use our general knowledge to construct a more concise approach tailored to our later calculations following *Dold* [7] and *Ralston* [29] [28].

We now look at the wave equation of the form

$$\square u = 0 . \quad (2.10.1)$$

For this equation we will take the Ansatz

$$(t, x) \rightarrow e^{ik\psi(t, x)} \sum_{j \geq 0} \frac{a_j(t, x)}{(ik)^j} , \quad (2.10.2)$$

This Ansatz is still very similar to the monochromatic plane waves we have looked at in the previous chapters. The coefficients a and ψ should be smooth functions in a given time interval. We do introduce another restriction, however. As an infinite sum can become rather cumbersome for calculations we truncate the sum at some arbitrary step $N \in \mathbb{N}$. Therefore, we can redefine the sum as

$$v_N := e^{ik\psi(t, x)} \sum_{j=0}^N \frac{a_j(t, x)}{(ik)^j} . \quad (2.10.3)$$

For the initial conditions, we choose a plane wave again

$$v_N(0, x) = a(x)e^{ik\varphi(x)} \quad (2.10.4)$$

where a and φ are both smooth functions. a may also be 0 while φ must strictly stay positive. Near the supremum of a we require $\nabla\varphi \neq 0$. Thus, we can assure that the error from the truncation of the sum in the wave equation stays small

$$\square v_N = O(k^{-\nu}) . \quad (2.10.5)$$

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Plugging the Ansatz into the wave equation and calculating the derivatives we find

$$\begin{aligned} \square v_n = e^{ik\psi} & \left(\square a_0 + \dots + \frac{\square a_N}{(ik)^N} \right) \\ & - 2ike^{ik\psi} \left[\partial_t \psi \left(a_0 + \dots + \frac{\partial_t a_N}{(ik)^N} \right) - \sum_{i=1}^n \partial_i \psi \left(\partial_i a_0 + \dots + \frac{\partial_i a_N}{(ik)^N} \right) \right] \\ & + ik \square \psi v_n + k^2 \left(|\partial_t \psi|^2 - |\nabla_x \psi|^2 \right) v_n . \end{aligned} \quad (2.10.6)$$

This is exactly the form from the two parameter expansion we have mentioned in previous chapters and with the later Ansatz we will essentially find a similar structure.

Looking at each order in k we find at k^2

$$e^{ik\psi} a_0 (|\partial_t \psi|^2 - |\nabla_x \psi|^2) \quad (2.10.7)$$

and in the subleading order k^1 we find the transport equation

$$\begin{aligned} ie^{ik\psi} a_0 \square \psi - ie^{ik\psi} (|\partial_t \psi|^2 - |\nabla_x \psi|^2) a_1 \\ - ie^{ik\psi} \left(2\partial_t \psi \frac{\partial a_0}{\partial t} - 2\nabla_x \psi \cdot \nabla_x a_0 \right) . \end{aligned} \quad (2.10.8)$$

This is, where we find a big difference with our later Ansatz. Instead of a transport equation we will find a Schrödinger type equation.

The other subleading orders for k^{1-j} with $j \geq 1$ can be written generally as

$$\begin{aligned} i^{1-j} e^{ik\psi} a_j \square \psi - i^{1-j} e^{ik\psi} a_{j+1} \left(|\partial_t \psi|^2 - |\nabla_x \psi|^2 \right) \\ 2i^{1-j} e^{ik\psi} \left(\partial_t \psi \partial_t a_1 - \sum_{i=1}^n \partial_i \psi \partial_i a_j \right) + i^{1-j} e^{ik\psi} \square a_0 . \end{aligned} \quad (2.10.9)$$

All of these subleading terms must give 0 separately since sets of terms of different orders can never cancel each other out. For the whole differential equation (2.10.1) to vanish, each order must vanish separately.

At leading order, $\varphi = \psi(0, x)$ must satisfy the eikonal equation

$$-\left| \frac{\partial \psi}{\partial t} \right|^2 + |\nabla_x \psi|^2 = 0 \quad (2.10.10)$$

Remark. This equation can be rewritten using the principal symbol of the wave equation. Thus we get

$$p_2 \left(t, x, \frac{\partial \psi}{\partial t}, \nabla_x \psi \right) = 0 . \quad (2.10.11)$$

This does not provide global solutions, just solutions localized in time. We need to introduce the Gaussian Beam approximation to weaken this condition such that it only

vanishes up to a certain order. Then we can guarantee global approximations.

At subleading order k^1 we find a transport equation

$$2 \frac{\partial \psi}{\partial t} \frac{\partial a_0}{\partial t} = 2 \nabla_x \psi \dot{\nabla}_x a_0 + a_0 \square \psi \quad (2.10.12)$$

for which we impose initial conditions since $\partial_t \varphi \neq 0$ for sufficiently small $|t|$ implied by (2.10.4)

$$a_0(0, x) = a(x) . \quad (2.10.13)$$

The next subleading order gives

$$2 \frac{\partial \psi}{\partial t} \frac{\partial a_j}{\partial t} = 2 \nabla_x \psi \cdot \nabla_x a_j - a_j \square \psi + \square a_{j-1} . \quad (2.10.14)$$

Equation (2.10.1) required

$$a_j(0, x) = 0 \quad (2.10.15)$$

thus, we find a unique solution for a_j at sufficiently small T .

Ultimately we find exactly what we intended

$$\square v_N = O(k^{-\nu}) . \quad (2.10.16)$$

We thus have shown, that the Ansatz of geometric optics is a suitable approximation for the solution of the wave equation. We will see a more detailed calculation later with our specialized Ansatz.

3. Gaussian beams

This introductory section is largely following the approach by *Goldsmith*[11]. We will start by looking at solutions in cylindrical coordinates and how to normalize them. Afterwards, it will also be done in Cartesian coordinates. Apart from looking at some properties like the concentration near the beam waist, the edge taper and average peak power density, we will go to the limit of Geometrical optics and higher order Gaussian beam mode solutions, again in cylindrical and Cartesian coordinates. Finally, we will look at the construction which is more refined for our later use case.

3.1. Introduction

So far we have studied the description of rays for any kind of wave. Although this was practical in some cases, we quickly find the borders of this approximation. Rays do not contain any information about the amplitude, phase or spatial extent of a wave which are all very important features. Apart from that, the plane waves provide an easy framework for calculation but they also lack rather important boundaries. Plane waves have infinite extent. Any wave, no matter of a light or particle wave, however, is spatially restricted and collimated. We already encountered a good addition to geometrical optics, the *paraxial approximation*. In this regime, we find spatially collimated waves which provide a far better description for real waves. We call such solutions *Gaussian beams*. We now gain a description for not only spatially collimated waves with a well-defined direction of propagation, but also allow transverse variations, which was not possible until now. The source of such a beam is now no longer an infinitesimal point but a finite extent region.

To construct the paraxial wave equation, let us take such a wave ψ , whose components can either describe the electric field E or magnetic field B of an electromagnetic wave, for example. For the sake of simplicity, we let it propagate in uniform medium. Such a wave fulfils the Helmholtz equation

$$(\nabla^2 + k^2)\psi = 0 . \quad (3.1.1)$$

Apart from the amplitude, our wave also consists of the typical phase factor $e^{i\omega t}$ with the angular frequency ω . With the non planar, complex valued function u we find

$$E(x, y, z) = u(x, y, z)e^{-ikz} \quad (3.1.2)$$

as a possible Ansatz for a wave propagating in z direction. We can plug this into our

3. Gaussian beams

wave equation (3.1.1) and find

$$\nabla^2 u - 2ik \frac{\partial u}{\partial z} = 0 . \quad (3.1.3)$$

Remark. The literature often refers to this as the *reduces wave equation*.

We can drop the differential with respect to z of the Laplace operator as the paraxial approximation assumes, that the variation of the amplitude along the direction of propagation, which we chose to be the z direction, is small over the distance of a wavelength. Apart from that, the axial variation should also be small compared to the variation perpendicular to this direction. We thus find the paraxial wave equation in Cartesian coordinates

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - 2ik \frac{\partial u}{\partial z} = 0 . \quad (3.1.4)$$

Solutions to this equation exactly form the *Gaussian beam* modes.

Remark. Although there is no rigorous cut-off until this approximation work, one usually considers it reasonable while the angular divergence stays below 0.5 radians to the z axis.

3.2. Solution in cylindrical coordinates

Gaussian beams provide us with very handy spherical symmetry, thus, it may be very beneficial, to look at solutions of the paraxial equation in cylindrical coordinates as well. We choose r as the distance perpendicular to the axis of propagation and φ to denote the angular coordinate. The paraxial equation can then be written as

$$\frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{1}{r} \frac{\partial^2 u}{\partial \varphi^2} - 2ik \frac{\partial u}{\partial z} = 0 . \quad (3.2.1)$$

In contrast to u depending on x, y and z in the Cartesian case, u is now a function of r and z . As we have spherical symmetry, the amplitude should not depend on the angular location given by φ . We can therefore already drop the differential with respect to this coordinate which gives

$$\frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} - 2ik \frac{\partial u}{\partial z} = 0 . \quad (3.2.2)$$

The simplest Ansatz provided by the literature [11] gives

$$u(r, z) = A(z) e^{-i \frac{kr^2}{2q(z)}} \quad (3.2.3)$$

with the complex amplitude A and a complex function q . With this ansatz we are starting to see where the name *Gaussian beams* comes from; it very much reminds us of a Gaussian distribution.

Inserting the Ansatz into the paraxial wave equation we find

$$-2ik \left(\frac{A}{q} + \frac{\partial A}{\partial z} \right) + \frac{k^2 r^2 A}{q^2} \left(\frac{\partial q}{\partial z} - 1 \right) = 0. \quad (3.2.4)$$

which we can separate into a part depending only on z and a part depending on z and r . Both of these parts must be satisfied individually and thus we find

$$\begin{aligned} \frac{\partial q}{\partial z} &= 1 \\ \frac{\partial A}{\partial z} &= -\frac{A}{q}. \end{aligned} \quad (3.2.5)$$

It is obvious, that the first equation is solved by a linear function and with defining a reference point $z_0 = 0$ we can write it as

$$q(z) = q(z_0) + (z - z_0) = q(0) + z. \quad (3.2.6)$$

Remark. q is frequently called the *complex beam - or Gaussian beam parameter*.

We can easily see, that q is again separable in its real and imaginary part, which we can use in the Ansatz (3.2.3) to separate the exponential

$$e^{-i \frac{kr^2}{2q}} = e^{\frac{-ikr^2}{2} \left(\frac{1}{q} \right)_r - \frac{kr^2}{2} \left(\frac{1}{q} \right)_i}. \quad (3.2.7)$$

we can analyse these two parts now and find, that the imaginary term has taken the form of a phase variation from a spherical wave front. With the curvature radius R of equiphase surfaces and a phase variation relative to the plane $z \cdot \phi(r)$ we can then write the delay in the phase for $r \ll R$ as

$$\phi(r) \approx \frac{\pi r^2}{\lambda R} = \frac{kr^2}{2R}. \quad (3.2.8)$$

Thus we see, that the radius of curvature depends on the position along the axis of propagation and we can identify the real part of $\frac{1}{q}$ with $\frac{1}{R}$.

When we look at the real term, it reminds us of a Gaussian variation depending on the distance from the axis of propagation. From the standard Gaussian form we know, that r_0 denotes the $\frac{1}{e}$ point relative to the on-axis value. Identifying this we find

$$\left(\frac{1}{q} \right)_i = \frac{2}{k\omega^2(z)} = \frac{\lambda}{\pi\omega^2} \quad (3.2.9)$$

This equation gives us a clear definition for the beam radius ω which again denotes the radial distance at which the field drops to a value of $\frac{1}{e}$ to its on-axis value. As q still depends on z , it is clear that the beam radius also depends on the position along the axis. We can thus write

$$\frac{1}{q} = \frac{1}{R} - \frac{i\lambda}{\pi\omega^2}. \quad (3.2.10)$$

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We can insert our results to our Ansatz and for $z = 0$ we just get $u(r, 0) = A(0)e^{\frac{-ikr^2}{2q(0)}}$. Using $\omega_0 = \left(\frac{\lambda q(0)}{i}\pi\right)^{\frac{1}{2}}$ we can simplify this further to be

$$u(r, 0) = u(0, 0)e^{-\frac{r^2}{\omega_0^2}}. \quad (3.2.11)$$

We therefore find a definition for the radius of curvature and the beam radius

$$R = z + \frac{1}{z} \left(\frac{\pi \omega_0^2}{\lambda} \right)^2 \quad (3.2.12)$$

$$\omega = \omega_0 \left[1 + \left(\frac{\lambda z}{\pi \omega_0^2} \right)^2 \right]^{\frac{1}{2}} \quad (3.2.13)$$

Remark. The term $\frac{\pi \omega_0^2}{\lambda}$ is called the *confocal distance*.

Looking at these equations, we see that exactly at the beam waist, we find infinite radius of curvature and the minimum of the beam radius.

Now we also have to look at the solution for the second equation of (3.2.5). This will give us a definition for the *Gaussian phase shift* ϕ_0 . To get to this result, we rewrite the equation as

$$\frac{dA}{A} = -\frac{dz}{q} \quad (3.2.14)$$

and we can use that $dz = dq$ to find

$$\frac{dA}{A} = -\frac{dq}{q} \quad (3.2.15)$$

. Inserting previous results we thus find

$$\frac{A(z)}{A(0)} = \frac{1 + i \frac{\lambda z}{\pi \omega_0^2}}{1 + \left(\frac{\lambda z}{\pi \omega_0^2} \right)^2} \quad (3.2.16)$$

which gives us the definition of a phasor

$$\tan(\phi_0) = \frac{\lambda z}{\pi \omega^2}. \quad (3.2.17)$$

This helps us simplifying the equation to

$$\frac{A(z)}{A(0)} = \frac{\omega_0}{\omega} e^{i\phi_0}. \quad (3.2.18)$$

with the Gaussian phase shift ϕ_0 .

With this, we finally find the *fundamental Gaussian beam mode*

$$u(r, z) = \frac{\omega_0}{\omega} e^{\frac{-r^2}{\omega^2} - \frac{i\pi r^2}{\lambda R} + j\phi_0} \quad (3.2.19)$$

and for the previously introduced electric field we get an additional factor of e^{-ikz}

$$E(r, z) = \frac{\omega_0}{\omega} e^{\frac{-r^2}{\omega^2} - ikz - \frac{i\pi r^2}{\lambda R} + j\phi_0} . \quad (3.2.20)$$

3.3. Normalization

We now have almost full knowledge about the behaviour of Gaussian beams in the paraxial limit, the only thing missing, is the normalization of the fundamental mode or the electric field. This is needed to find a meaningful relation to the total power transported by a propagating beam. We assume, that the electric and magnetic field share the same relation as in plane waves. Thus, the square integral of the electric field must give 1 to find a normalization $\int |E|^2 \cdot 2\pi r dr = 1$. At z_0 the integral results to $\frac{\pi\omega_0^2}{2}$ yielding the normalized electric field

$$E(r, z) = \left(\frac{2}{\pi\omega^2} \right)^{\frac{1}{2}} e^{-\frac{r^2}{\omega^2} - ikz - \frac{i\pi r^2}{\lambda R} + j\phi_0} \quad (3.3.1)$$

and therefore, with the equations of the beam radius and radius of curvature as well as the definition of the Gaussian phase shift,

$$R = z + \frac{1}{z} \left(\frac{\pi\omega_0^2}{\lambda} \right)^2 \quad (3.3.2)$$

$$\omega = \omega_0 \left[1 + \left(\frac{\lambda z}{\pi\omega_0^2} \right)^2 \right]^{\frac{1}{2}} \quad (3.3.3)$$

$$\tan(\phi_0) = \frac{\lambda z}{\pi\omega_0^2} , \quad (3.3.4)$$

we have complete knowledge of the behavior of Gaussian beams.

3.4. One dimensional fundamental Gaussian beam in Cartesian coordinates

Following the approach from the last chapter, we now concentrate at variations in one variable only. Thus the differential equation becomes

$$\frac{\partial^2 u}{\partial x^2} - 2ik \frac{\partial u}{\partial z} = 0 \quad (3.4.1)$$

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and we use the reduced Ansatz

$$u(x, z) = A_x(z) e^{-\frac{ikx^2}{2q(z)}} . \quad (3.4.2)$$

Following the same calculations as before, we find the conditions

$$\begin{aligned} \frac{\partial q_x}{\partial z} &= 1 \\ \frac{\partial A_x}{\partial z} &= -\frac{1}{2} \frac{A_x}{q_x} \end{aligned} \quad (3.4.3)$$

with the first condition being again solved by a linear equation identical to (3.2.5). Thus the result must be the same

$$q_x = \frac{i\pi\omega_{0x}^2}{\lambda} + z \quad (3.4.4)$$

and therefore

$$\frac{1}{q_x} = \frac{1}{R_x} - \frac{i\lambda}{\pi\omega_x^2} . \quad (3.4.5)$$

This provides the same solution as one gets with axial symmetry.

The second equation then yields

$$\frac{A_x(z)}{A(0)} = \left(\frac{q_x(0)}{q_x(z)} \right)^{\frac{1}{2}} . \quad (3.4.6)$$

We find a dependence on the square root of ω . The phase shift is also only half as large, as in the previous chapter. The normalized electric field then becomes

$$E(x, z) = \left(\frac{2}{\pi\omega_x^2} \right)^{\frac{1}{4}} e^{-\frac{x^2}{\omega_x^2} - ikz - \frac{i\pi x^2}{\lambda R_x} + \frac{1}{2}j\phi_{0x}} \quad (3.4.7)$$

3.5. Two-dimensional fundamental Gaussian beam mode in Cartesian coordinates

In the two dimensional case, we find the Amplitude constituted from a product of the two Amplitudes in each direction. Apart from that, the phase now also splits into a product of the phases in the different directions. Thus the Ansatz becomes

$$u(x, y, z) = A_x(z) A_y(z) e^{-\frac{ikx^2}{2q_x}} e^{-\frac{iky^2}{2q_y}} . \quad (3.5.1)$$

We can separate the solution and find the results

$$\begin{aligned} \frac{\partial q_{x/y}}{\partial z} &= 1 \\ \frac{\partial A_{x/y}}{\partial z} &= -\frac{1}{2} \frac{A_{x/y}}{q_{x/y}} . \end{aligned} \quad (3.5.2)$$

These are solved very similar as in the previous chapters and the electric field becomes

$$E(x, y, z) = \left(\frac{2}{\pi \omega_x \omega_y} \right)^{\frac{1}{2}} e^{-\frac{x^2}{\omega_x^2} - \frac{y^2}{\omega_y^2} - \frac{i\pi x^2}{\lambda R_x} - \frac{i\pi y^2}{\lambda R_y} + \frac{1}{2}j\phi_{0x} + \frac{1}{2}j\phi_{0y}} \quad (3.5.3)$$

as the field distribution separates into a product of the two dimensional parts. The other components give

$$\begin{aligned} w_{x/y} &= w_{0x/y} \left[1 + \left(\frac{\lambda z}{\pi \omega_{0x/y}^2} \right)^2 \right]^{\frac{1}{2}} \\ R_{x/y} &= z + \frac{1}{z} \left(\frac{\pi \omega_{0x/y}^2}{\lambda} \right)^2 \\ \phi_{x/y} &= \tan^{-1} \left(\frac{\lambda z}{\pi \omega_{0x/y}^2} \right)^2. \end{aligned} \quad (3.5.4)$$

Remark. As the equations separate this nicely, we can choose the reference points for the x and y direction separately and independently of each other. This would correspond to a relative phase shift.

3.6. Spatial extent

The field of a Gaussian beam is not uniformly spread. In fact, as the beam propagates, it broadens more and more. It has its maximum along the axis at $r = 0$ and we find the beam waist at $z = 0$. Moving away from the axis, the strength of the field distribution decreases as well as when we move along the axis. At a fixed point along the axis, the power density drops monotonically with r . When $\frac{r}{\omega_0} \leq \frac{1}{\sqrt{2}}$, the power density also drops monotonically with z . Ultimately, we find the maximum for fixed $r > \frac{\omega_0}{\sqrt{2}}$ at $z = \left(\frac{\pi \omega_0^2}{\lambda} \right) \left[2 \left(\frac{r}{\omega_0} \right)^2 - 1 \right]^{-1}$.

3.7. Fundamental mode Gaussian beam and edge taper

As we have seen in our analysis so far, Gaussian beams got their names from the appearance of a Gaussian distribution perpendicular to the direction of propagation. This becomes even more apparent, when we look at the ratio between the electric field density at some r and at $r = 0$

$$\frac{|E(r, z)|}{|E(0, z)|} = e^{-\left(\frac{r}{\omega}\right)^2} \quad (3.7.1)$$

as well as at the ratio of the power densities

$$\frac{P(r)}{P(0)} = e^{-2\left(\frac{r}{\omega}\right)^2}. \quad (3.7.2)$$

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r denotes the distance from the axis of propagation. So far we have always described the Gaussian beam mode by its electric field, it would be more natural, however, to use its field distribution. When we measure Gaussian beams, it is the power distribution, that we directly measure, thus, we want to characterize the fundamental mode now with the relative power level at some specified radius. This is called the *edge taper* T_e , the relative power at radius r_e

$$T_e = \frac{P(r_e)}{P(0)} . \quad (3.7.3)$$

Inserting the ratio between the power densities we find

$$T_e(r_e) = e^{-2\frac{r_e^2}{\omega^2}} . \quad (3.7.4)$$

The edge taper may vary through a very large dynamic range, thus, one frequently uses decibels to express it

$$T_e(dB) = -10 \log_{10}(T_e) . \quad (3.7.5)$$

The edge radius can be calculated from the edge taper

$$\frac{r_e}{\omega} = 0.3393 (T_e(dB))^{\frac{1}{2}} . \quad (3.7.6)$$

Remark. For as low as 3dB, the full width at half maximum is twice the radius, or 1.175ω . At 4ω we already have 34.7dB which already includes 99.7% of its power. This is sufficient to make diffraction effects but truncation very small.

We can express the edge taper in cylindrical coordinates as

$$F_e(r_e) = \int_{r=0}^{r=r_e} |E(r)|^2 \cdot 2\pi r dr = 1 - T_e(r_e) \quad (3.7.7)$$

which is useful to express the power contained within a circle of radius r_e centred around the beam axis.

A third approach to classify Gaussian beams would be, to use its radius of curvature. The equiphase planes appear as spherical surfaces with radius R and fixed z , we have quadratic variation of the phase perpendicular to the axis of the beam. The definition of the centre of the curvature follows from the radius of the curvature and it may vary with the distance from the beam waist.

3.8. Average and peak power density

Although normalization to a unit total power comes handy, at some point, one also wants to know the actual peak power density. In our laboratory system, we can spread the beam over a controlled region, thus reducing the power density. In such a way we can evaluate the dependency of the peak power density on the size of the beam.

The actual power density P_{act} is related to the total propagating power P_{tot} by

$$P_{act}(r) = P_{tot} \frac{2}{\pi \omega^2} e^{-2\left(\frac{r}{\omega}\right)^2}. \quad (3.8.1)$$

It is therefore natural, to relate the beam radius to the edge taper as

$$P_{max} = P_{act}(0) = \frac{T_e(db)}{4.343} \frac{P_{tot}}{\pi r_e^2}. \quad (3.8.2)$$

The second term of the right side defines the average power density

$$P_{av} = \frac{P_{tot}}{\pi r_e^2} \quad (3.8.3)$$

which can be related to the peak with

$$P_{max} = \frac{T_e(db)}{4.343} P_{av} = \frac{2r_e^2}{\omega^2} P_{av}. \quad (3.8.4)$$

Remark. As discussed before, at $r_e = 2\omega$ we find an edge taper of 34.7dB. Thus, the peak power gives $P_{max} = 8P_{av}$. If we take only half of r_e such that $r_e = \omega$ we already have an edge taper of only 8.69dB and therefore a peak power of $P_{max} = 2P_{av}$.

3.9. Confocal distance, near and far fields

We find a simple form of the variation of the Gaussian beam parameters by means of the *confocal distance* and *confocal parameter* defined as

$$z_c = \frac{\pi \omega_0^2}{\lambda}. \quad (3.9.1)$$

Remark. The confocal distance may also be referred to as the *Rayleigh range* in the literature.

In terms of the confocal distance we can rewrite the Gaussian beam parameters as

$$\begin{aligned} R &= z + \frac{z_c^2}{z} \\ \omega &= \omega_0 \left[1 + \left(\frac{z}{z_c} \right)^2 \right]^{\frac{1}{2}} \\ \phi_0 &= \tan^{-1} \left(\frac{z}{z_c} \right) \end{aligned} \quad (3.9.2)$$

Example 3. For a wavelength of 0.3cm and $\omega_0 = 1$ cm, we find a confocal distance of

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10.5cm.

The confocal distance has simplified these parameters a lot, leading to a very elegant description of Gaussian beams. In fact, these simple forms describe the whole behaviour of the Gaussian beam modes at all distances from the waist.

With the help of the confocal distance, we can split the beam into two distinct regions, the near field $z \ll z_c$ and the far field $z \gg z_c$. When we find $z = z_c$, ω has its minimum ω_0 and it is that place, where the field is most concentrated at. At this point, the radius of curvature becomes infinite, the phase front is completely planar and the phase shift $\phi_0 = 0$ at the waist by definition.

Moving away from the waist, the radius grows monotonically with hyperbolic variation of ω and z . The beam radius, however, remains essentially unchanged from its value at the waist $\omega \leq \sqrt{2}\omega_0$. With increasing distance, the radius of curvature decreases until we reach the confocal distance. At this point ω reaches a value of $\sqrt{2}\omega_0$. The radius of curvature becomes $2z_c$ and the phase shift reaches $\frac{\pi}{4}$. Going even farther. the beam radius grows significantly, as well as the radius of curvature. At some point, in the far field $z \gg z_c$, the growth becomes linear. The growth of the $\frac{1}{e}$ radius can be calculated from $\theta = \tan^{-1} \left(\frac{\omega}{z} \right)$ with the *asymptotic beam growth angle* θ_0 being defined as

$$\theta_0 = \lim_{z \gg z_c} \left[\tan^{-1} \left(\frac{\omega}{z} \right) \right] = \tan^{-1} \left(\frac{\lambda}{\pi\omega_0} \right). \quad (3.9.3)$$

Example 4. Let $\lambda = 0.3\text{cm}$, $\omega_0 = 1\text{cm}$. We find $\theta_0 \approx 0.1\text{radian}$.

Thus, showing one of the key assumptions of the paraxial approximation. The angle deviation from the axis must be very small, such that we can use the small angle approximation

$$\theta_0 \approx \frac{\lambda}{\pi\omega_0}. \quad (3.9.4)$$

Remark. In the far field, the electric field can be described as a function of the angle to the axis of propagation such that

$$\frac{E(\theta)}{E(0)} = e^{-\left(\frac{\theta}{\theta_0}\right)^2}. \quad (3.9.5)$$

Remark. For $R \rightarrow z$ in the far field $z \gg z_c$, equation (3.9.2) shows, that the radius of curvature increases linearly with the distance. The radius of curvature then becomes equal to the distance to the beam waist with an asymptotic phase shift of $\phi_0 = \frac{\pi}{2}$.

3.10. Geometrical optics limit of Gaussian beam propagation

We first introduced geometrical optics and generalized them to come to Gaussian beams, however, we can use our definitions to go back to geometrical optics as well, checking the compatibility of both theories. To get to rays, we simply have to let $\lambda \rightarrow 0$ again. Thus, diffraction effects vanish. This limit is non-trivial, however, as it also means, that the confocal distance reaches infinity $z_c \rightarrow \infty$ with fixed ω_0 . Apart from that, $\omega \rightarrow \omega_0$, $R \rightarrow \infty$ and $\theta_0 \rightarrow \theta$. This exactly means, that we get a collimated beam with no diffraction effects and our region of interest perfectly aligned in the near field of the beam waist. If we let the beam waist approach 0 with the wavelength as well, the confocal distance becomes finite. θ_0 will remain constant and $\omega \rightarrow \theta_0 \cdot z$ and $R \rightarrow z$. Thus we have a perfect ray again emerging from a point source showing, that geometrical optics is just an edge case of Gaussian beams.

3.11. Higher order Gaussian beam mode solutions of the paraxial wave equation

For not all real world applications are quasi-collimated solutions of the paraxial wave equation sufficient. In some cases, we need complex variations of the fields perpendicular to the direction of propagation. Such complex solutions constitute of other polynomials superimposed on the fundamental Gaussian beams and we call them *higher order Gaussian beam mode solutions*. We characterize them by the beam radius and radius of curvature, which both behave the same, as for the fundamental case while the phase shifts may differ. examples for cases, where we need these more complex solutions include radiating systems with high degree of axial symmetry for cylindrical coordinates, or off-axis mirrors or non-Gaussian distributions in a horn in Cartesian coordinates.

3.11.1. Cylindrical coordinates

While the full solution in cylindrical coordinates should also variations with the angle φ , the ansatz may not be purely Gaussian. It can still contain terms with radial dependence. From [11] we take the Ansatz

$$u(r, \varphi, z) = A(z)e^{-\frac{ikr^2}{2q(z)}} S(r)e^{im\varphi} . \quad (3.11.1)$$

$S(r)$ is some arbitrary function with radial dependence. m is some natural number. The paraxial wave equation reduces to a differential equation for S with solutions

$$S(r) = \left(\frac{\sqrt{2}r}{\omega} \right)^m L_{pm} \left(\frac{2r^2}{\omega^2} \right) \quad (3.11.2)$$

as long as q remains the same as it was in the fundamental Gaussian beam. The beam radius is again denoted by ω and L_{pm} stands for the Laguerre polynomial with radial

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index p and angular index q . We coll these solutions then the pm Gaussian beam mode and we get for our example electric field

$$E_{pm}(r, \varphi, z) = \left(\frac{2!}{\pi(p+m)!} \right)^{\frac{1}{2}} \frac{1}{\omega(z)} \left(\frac{\sqrt{2}r}{\omega(z)} \right)^m L_{pm} \left(\frac{2r^2}{\omega^2(z)} \right) \cdot \exp \left(-\frac{r^2}{\omega^2(z)} - ikz - \frac{i\pi r^2}{\lambda R(z)} - i(2p+m+1)\phi_0(z) \right) \cdot e^{im\varphi} \quad (3.11.3)$$

The main differences lie in the angular dependency and complex radial dependency. Very notable is the larger phase shift compared to the fundamental mode.

We want the field to be normalized to unit power fly and it should follow the orthogonality relationship

$$\iint r dr d\varphi E_{pm}(r, \varphi, z) E_{qn}^*(r, \varphi, z) = \delta_{pq} \delta_{mn} . \quad (3.11.4)$$

Higher order modes can be combines to real functions of φ by combining exponents into cos and sin functions, one has to be careful, though, as depending on the value of m one has to add an additional factor of 1 for $m = 0$ or $\sqrt{2}$ otherwise.

When we have radial symmetry, the beam is independent of φ which lets us take the subset where $m = 0$. Thus the electric field becomes

$$E_{p0}(r, z) = \left(\frac{2}{\pi\omega^2} \right)^{\frac{1}{2}} L_{p0} \left(\frac{2r^2}{\omega^2} \right) \exp \left(-c\frac{r^2}{\omega^2} - ikz - \frac{i\pi r^2}{\lambda R} + i(2p+1)\phi_0 \right) . \quad (3.11.5)$$

3.11.2. Cartesian coordinates

Higher order solutions in Cartesian coordinates are simply composed of one dimensional general solutions of the paraxial equation. Including the x subset, we get an additional function H depending on x changing our Ansatz to

$$u(x, z) = A(z) H \left(\frac{\sqrt{2}x}{\omega(z)} \right) e^{-\frac{ikx^2}{2q(z)}} . \quad (3.11.6)$$

H is not a random function, though, it defines the Hermite polynomial of order m . The exemplary electric field of order m then reads

$$E(x, z) = \left(\frac{2}{\pi} \right)^{\frac{1}{2}} \frac{1}{4} \left(\frac{1}{\omega_x 2^m m!} \right)^{\frac{1}{2}} H_m \left(\frac{\sqrt{2}x}{\omega_x} \right) \cdot \exp \left(-\frac{x^2}{\omega_x^2} - ikz - \frac{i\pi x^2}{\lambda R_x} + \frac{i(2m+1)\phi_{0x}}{2} \right) . \quad (3.11.7)$$

This solutions shares a lot of similarities with the fundamental mode. The main differences lie in the larger phase shifts. For E_0 we find the same equation as in the one dimensional fundamental mode.

For higher dimensions, like 2, we find just a product for each coordinate subspace, as mentioned before. The normalized electric field in two dimensions thus reads

$$E_{mn}(x, y, z) = \left(\frac{1}{\pi \omega_x \omega_y 2^{m+n-1} m! n!} \right)^{\frac{1}{2}} H_m \left(\frac{\sqrt{2}x}{\omega_x} \right) H_n \left(\frac{\sqrt{2}y}{\omega_y} \right) \cdot \exp \left(-\frac{x^2}{\omega_x^2} - \frac{y^2}{\omega_y^2} - ikz - \frac{i\pi x^2}{\lambda R_x} - \frac{i\pi y^2}{\lambda R_y} + \frac{i(2m+1)\phi_{0x}}{2} + \frac{i(2n+1)\phi_{0y}}{2} \right). \quad (3.11.8)$$

which fulfils the orthogonality relationship

$$\iint_{-\infty}^{\infty} E_{mn}(x, y, z) E_{pq}^*(x, y, z) dx dy = \delta_{mp} \delta_{nq}. \quad (3.11.9)$$

Remark. We find a special case, when the beams have equal waist radii in all directions for the same value of z . Then we find $\omega_x = \omega_y \equiv \omega$ and $R_x = R_y \equiv R$ and therefore

$$E_{mn}(x, y, z) = \left(\frac{1}{\pi \omega^2 2^{m+n-1} m! n!} \right)^{\frac{1}{2}} H_m \left(\frac{\sqrt{2}x}{\omega} \right) H_n \left(\frac{\sqrt{2}y}{\omega} \right) \cdot \exp \left(-\frac{x^2 + y^2}{\omega^2} - ikz - \frac{i\pi(x^2 + y^2)}{\lambda R} + i(m+n-1)\phi_0 \right). \quad (3.11.10)$$

If we further let $m = n = 0$ we find the fundamental beam mode with purely Gaussian distribution.

3.12. Size of Gaussian beams

As mentioned in previous chapters, measuring a beam mostly yields the power distribution. In our calculations, we calculated the field distribution, though. From the power distribution, however, it is easy to determine the beam radius at a particular point along the axis. For fundamental modes, the power inside a circle with radius r_0 increases smoothly with r_0 , this is not the case for higher order modes. In higher order modes, the power is not concentrated around the axis any more, it is concentrated away from the axis of propagation. The beam radius ω can now longer satisfactory describe the transverse extent. We therefore introduce the *spot size* of a Gaussian beam pm mode

$$\rho_{r-pm}^2 = 2 \iint I_{pm}(r, \varphi) r^2 dS = 2 \iint r^3 dr d\varphi |E_{pm}(r, \varphi)|^2. \quad (3.12.1)$$

Evaluating this integral using either an already normalized field distribution or normalizing it manually yields

$$\rho_{r-pm} = \omega(2p + m + 1)^{\frac{1}{2}}. \quad (3.12.2)$$

In this case, ρ is equal to the beam radius for the fundamental mode at $p = m = 0$.

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Remark. In 2 dimensional Cartesian coordinates we find analogously

$$\rho_{x-m}^2 = 2 \int |E_x(x)|^2 x^2 dx = \omega_x^2 \left(m + \frac{1}{2}\right)^{\frac{1}{2}}. \quad (3.12.3)$$

and for the n mode in y direction

$$\rho_{y-n} = \omega_y \left(n + \frac{1}{2}\right)^{\frac{1}{2}} \quad (3.12.4)$$

Analogously to the previous chapter, the beam sizes for multiple dimensions is just the sum of the beam sizes of the subdimensions such that

$$\rho_{xy-mn} = \omega(m + n + 1)^{\frac{1}{2}}. \quad (3.12.5)$$

which gives ω for $m = n = 0$.

Analysing these results, we find out, that the beam size grows with the square root of the mode number r . This again shows, that the power is concentrated at a larger distance from z at higher order modes.

3.13. Paraxial limit and improved solutions to the wave equations

At the end of the previous chapter we saw that geometrical optics has its boundaries until which it delivers satisfactory solutions. In the same way solutions to the paraxial wave equations have a limit. At some point, Gaussian beams can get so violently divergent, that the assumptions are no longer satisfied and the approximation breaks apart. When the divergence of a beam grows, at some point, the field gets so concentrated within a region of the order of a wavelength or even less. In this case, it is no longer suitable to assume, that variations only occur on large scales compared to the wavelength. At some point, the fields can no longer be completely and purely transverse when variations can reach such a small scale. The beam may now experience longitudinal or cross polarization. In this case, the variations in beam size no longer follow the Gaussian beam formulae as functions of the distance of the waist.

3.14. Alternative derivation of the Gaussian beam propagation formula

We will now have a quick overview on a different approach to deduce the propagation formula for our exemplary electric field. When we stay in the regime of small angles, as discussed in previous chapters and obliquity factors can be set to 1, we can use *Huygens*

Fresnel's diffraction integral. We then find

$$E(x', y', z') = \frac{i}{\lambda z'} e^{-(ikz')} \iint E_0(x, y, 0) e^{\frac{-ik(x'-x)^2 + (y'-y)^2}{2z'}} dx dy \quad (3.14.1)$$

for a planar phase distribution and with the amplitude illumination function E_0 . The primed indices denote the plane of observation while the unprimed indices denote the plane illuminated by the beam. When the beam is axially symmetric with a planar wave form such that $E_0 = e^{-\frac{(x^2+y^2)}{\omega_0^2}}$, the x and y integrals can be separated. This leads to simpler integration and we get essentially two expressions of the form

$$E_x(x', z') = \left(\frac{i}{\lambda z'} \right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\frac{x^2}{\omega_0^2} + \frac{ik(x'-x)^2}{2z'}} dx. \quad (3.14.2)$$

This can be integrated when we complete the square and use the identity

$$\int_{-\infty}^{\infty} e^{-ax^2+bx} dx = \left(\frac{\pi}{a} \right)^{\frac{1}{2}} e^{\frac{b^2}{4a}}. \quad (3.14.3)$$

Our electric field then reads for $a > 0$

$$E_x(x', z') = \left(\frac{\omega_0}{\omega} \right)^{\frac{1}{2}} e^{-\frac{x'^2}{\omega^2} - \frac{i\pi x'^2}{\lambda R} - \frac{i\phi_0}{2}}. \quad (3.14.4)$$

Ultimately we then find the parameters (3.3.2). This approach can be used for even higher order beams as well. The downside is the growing mathematical complexity.

3.15. Tailored construction

So far we have looked at a general approach to construct Gaussian beam modes. We have deduced their properties and their boundaries. We will now look at a more concise approach specific to our later usage where we will use our general knowledge to follow the description by *Dold* [7] and *Ralston* [29] [28].

We look at a differential operator $P(x, D)$ of the form (2.10.1) with principle value $p_m(x, \xi)$. We look at solutions u for this differential equation such that the solution becomes concentrated on the curve Γ when $k \rightarrow \infty$. The Gaussian beam Ansatz therefore takes the form

$$u(x, k) = e^{ik\psi(x)} \left(a_0(x) + \frac{a_1(x)}{k} + \dots + \frac{a_N(x)}{k^N} \right). \quad (3.15.1)$$

As in the previous section, we require (2.10.5). The phase function ψ should satisfy

- $\psi(x(s)) \in \mathbb{R}$

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- $\text{Im} \frac{\partial^2 \psi}{\partial x_i \partial x_j}(x(s))$ is positive definite on vectors orthogonal to $\dot{x}(s)$

such that the solution becomes concentrated on the curve Γ . We can clearly see the Gaussian curve form of our Ansatz which also ensures, that u decreases rapidly when deviating from the curve Γ .

When we now insert this Ansatz (3.15.1) into the wave equation we find

$$P(x, D)u = k^m p_m \left(x, \frac{\partial \psi(x)}{\partial x} \right) e^{ik\psi(x)} a_0(x) + O(k^{m-1}) . \quad (3.15.2)$$

We will now try to find ψ such that the principle symbol $p_m(x, \frac{\partial \psi(x)}{\partial x}) = 0$ vanishes. We only require, though, that it needs to vanish to high order on the curve, otherwise we may encounter solution which break down in finite time. Apart from that, every order must vanish separately, as no combination of lower orders can ever overtake some higher order such that the whole equation would vanish.

We start with order 0 at which we find

$$p_m(x(s), \xi(s)) = 0 \quad (3.15.3)$$

and for the next order

$$0 = \frac{\partial f}{\partial x_i} = \frac{\partial p_m}{\partial x_i} + \frac{\partial p_m}{\partial \xi_k} \frac{\partial^2 \psi}{\partial x_i \partial x_k} . \quad (3.15.4)$$

We can immediately say, that the imaginary part of this must be 0, as the principle symbol is real.

$$\frac{\partial p_m}{\partial \xi_k}(x(s), \xi(s)) \left(\text{Im} \frac{\partial^2 \psi}{\partial x_i \partial x_k}(x(s)) \right) = 0 . \quad (3.15.5)$$

This gives us a very nice intuitive insight. The derivative of the principle symbol with respect to ξ_k must always be parallel to $\dot{x}(s)$. Otherwise, there would always exist some s at which the imaginary part would not be positive definite in the orthogonal complement to $\dot{x}(s)$.

After reparametrisation we can write

$$\dot{x}(s) = \frac{\partial p_m}{\partial \xi}(x(s), \xi(s)) \quad (3.15.6)$$

which we can plug in into the equation for order 1 (3.15.4). This then gives

$$0 = \frac{\partial p_m}{\partial x_i} + \frac{dx_k}{ds} \frac{\partial^2 \psi}{\partial x_k \partial x_i} = \frac{\partial p_m}{\partial x_i} + \frac{dx_k}{ds} \frac{\partial \xi_i}{\partial x_k} \quad (3.15.7)$$

which we can solve for $\dot{\xi}$ and find

$$\dot{\xi}(s) = -\frac{\partial p_m}{\partial x}(x(s), \xi(s)) . \quad (3.15.8)$$

We now gained two important conditions that must be satisfied in order for us to be able

to construct a Gaussian beam along the curve Γ . The tuple $(x(s), \xi(s))$ must fulfil

$$\begin{aligned}\dot{x}(s) &= \frac{\partial p_m}{\partial \eta}(x(s), \eta(s)) \\ \dot{\eta}(s) &= -\frac{\partial p_m}{\partial x}(\dot{x}(s), \eta(s)) .\end{aligned}\tag{3.15.9}$$

Remark. Curves, that fulfil these two conditions are called *bicharacteristic curves* for a differential operator $P(x, D)$. The principle symbol will always remain constant along such curves and we can check for any curve

$$(x(s), \xi(s)) = \left(x(s), \frac{\partial \psi}{\partial x}(x(s)) \right)\tag{3.15.10}$$

if it is a bicharacteristic curve, by checking

$$p_m(x(0), \xi(0)) = 0 .\tag{3.15.11}$$

Remark. If a bicharacteristic curve also satisfies (3.15.3), we call them *null bicharacteristic curves*.

Thus we have seen, that in order to be able to construct a Gaussian beam along our curve, the pair $(x(s), \xi(s))$ must constitute a null bicharacteristic curve. From the properties of our differential operator we find another important property.

When we construct a polynomial

$$g(\xi_0) = p_m(x, \xi)\tag{3.15.12}$$

from the principle symbol of our differential operator, this polynomial cannot have multiple roots for $\xi_i \neq 0$, because we chose a strictly hyperbolic differential operator. As we also require $p_m(x, \xi) = 0$, it follows that

$$\frac{\partial p_m}{\partial \xi_0}(x, \xi) \neq 0\tag{3.15.13}$$

yielding

$$\dot{x} \neq 0 .\tag{3.15.14}$$

Thus, we can be sure, that $\dot{x}$ will never vanish for any s .

Another important observation is, that condition (3.15.3) is just a rewritten form of the compatibility condition

$$\dot{\xi}_i(s) = \frac{\partial^2 \psi}{\partial x_i \partial x_j} \dot{x}_j(s) .\tag{3.15.15}$$

We can now continue with the next order. At order 2 we find a non-linear ordinary differential equation. This must have a global solution, otherwise we would not be able

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to construct a Gaussian beam. We want

$$\begin{aligned}
0 &= \frac{\partial^2 f}{\partial x_j \partial x_i} \\
&= \frac{\partial^2 p_m}{\partial x_j \partial x_i} + \frac{\partial^2 p_m}{\partial \xi_k \partial x_i} \frac{\partial^2 \psi}{\partial x_j \partial x_k} + \frac{\partial^2 p_m}{\partial x_j \partial \xi_k} \frac{\partial^2 \psi}{\partial x_i \partial x_k} + \frac{\partial^2 p_m}{\partial \xi_l \partial \xi_k} \frac{\partial^2 \psi}{\partial x_i \partial x_k} \frac{\partial^2 \psi}{\partial x_j \partial x_l} + \frac{\partial p_m}{\partial \xi_k} \frac{\partial^3 \psi}{\partial x_j \partial x_k \partial x_i}
\end{aligned} \tag{3.15.16}$$

to hold along Γ . We can introduce matrices

$$\begin{aligned}
M(s)_{ij} &= \frac{\partial^2 \psi}{\partial x_i \partial x_j}(x(s)) \\
A(s)_{ij} &= \frac{\partial^2 p_m}{\partial x_i \partial x_j}(x(s), \xi(s)) \\
B(s)_{ij} &= \frac{\partial^2 p_m}{\partial \xi_i \partial x_j}(x(s), \xi(s)) \\
C(s)_{ij} &= \frac{\partial^2 p_m}{\partial \xi_i \partial \xi_j}(x(s), \xi(s))
\end{aligned} \tag{3.15.17}$$

thus we can rewrite the condition as

$$0 = A + MB + B^T M + MCM + \frac{dM}{ds} . \tag{3.15.18}$$

We already have good knowledge on how to fulfil this equation. We know the principle symbol of our differential operator and we also have information on our null bicharacteristic curve. Thus, the matrices $A(s)$, $B(s)$ and $C(s)$ are already fixed. The only thing left is to calculate $M(s)$ such that the equation is satisfied and we can construct ψ .

Remark. The equation has the form of a *Ricatti* equation for $M(s)$.

This remark guarantees, that we can indeed solve this equation globally. We must require

$$M(s)\dot{x}(s) = \dot{\xi}(s) , \tag{3.15.19}$$

though, as we want the solution to be symmetric. The imaginary part of $M(s)$ should also still remain positive definite in the orthogonal complement of $\dot{x}$. From these conditions we find 3 initial conditions for $M(0)$, thus the equation is solvable and to solve it, we construct the linear system

$$\begin{aligned}
\dot{Y} &= BY + CN \\
\dot{N} &= -AY + B^T N
\end{aligned} \tag{3.15.20}$$

It is not a coincidence, that the system is linear. This guarantees us, that there exists a unique solution $(Y(s), N(s))$. We can further assume $Y(s)$ to be invertible at some s_0 .

We can then calculate the derivative on NY^{-1}

$$\begin{aligned} \frac{d}{ds}(NY^{-1}) &= \dot{N}Y^{-1} - NY^{-1}\dot{Y}Y^{-1} \\ &= -A - B^T NY^{-1} - NY^{-1}B - NY^{-1}CNY^{-1}. \end{aligned} \quad (3.15.21)$$

showing us, that this is a valid solution around s_0 .

For Gaussian beams we can actually choose $Y(s)$ in a way that makes it invertible for all s which we will see in the following lemmas for a symmetric matrix $\mathcal{M}$ whose imaginary part is positive semidefinite on the orthogonal complement to $\dot{x}(s)$ and $\mathcal{M}\dot{x}(0) = \dot{\xi}(0)$. If we then choose (I, M) as the initial data, $Y(s)$ is invertible for all s and $M(s) = N(s)Y^{-1}(s)$ inherits the three derived properties from $\mathcal{M}$. Note that

$$M(0) = N(0)Y^{-1}(0) = \mathcal{M}.$$

The proofs for Lemmas 1 to 4 are found in [7].

Lemma 1. Let $(Y(s), N(s))$ be a solution to (3.15.20) with initial data $(Y(0), N(0)) = (I, \mathcal{M})$. Then it holds true that

$$(\dot{x}(s), \xi(s)) = (Y(s)\dot{x}(0), N(s)\dot{x}(0)) \quad (3.15.22)$$

Lemma 2. Let $(Y(s), N(s))$ be a solution to (3.15.20) with initial data $(Y(0), N(0)) = (I, \mathcal{M})$. Then $Y(s)$ is invertible for all s

Lemma 3. Let $(Y(s), N(s))$ be a solution to (3.15.20) with initial data $(Y(0), N(0)) = (I, \mathcal{M})$. Then $M(s) = N(s)Y^{-1}(s)$ is a symmetric matrix for all $s \in \mathbb{R}$.

Lemma 4. Let $M(s)$ be given as in the previous Lemma. Then for all s the matrix $M(s)$ is positive definite on the orthogonal complement of the tangent to the Curve Γ .

These lemmas guarantee, that as long as

$$Im \frac{\partial^2 \psi}{\partial x_i \partial x_j}(x(0)) \quad (3.15.23)$$

is positive definite on the orthogonal complement to $\dot{x}$, the principle value must vanish to second order on the curve. Thus we got another condition for ψ .

Stopping our calculations at order 2 would seem rather arbitrary. For higher orders, however, it turns out, that we always find linear ordinary differential equations. With a multi index α of length r , the equations $0 = \partial_x^\alpha f$ along Γ take the form

$$0 = \frac{\partial p_m}{\partial \xi_j} \frac{\partial}{\partial x_j} (\partial_x^\alpha \psi) + \sum_{|\beta|=r} c_{\alpha\beta} \partial_x^\beta \psi + d_\alpha. \quad (3.15.24)$$

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The coefficients $C_{\alpha\beta}, d_\alpha$ depend on the partial derivatives up to order $r - 1$ and as

$$\frac{\partial p_m}{\partial \xi} \cdot \frac{\partial(\partial_x^\alpha \psi)}{\partial x} = \frac{d}{ds}(\partial_x^\alpha \psi) \quad (3.15.25)$$

we can solve (3.15.24) as a linear system of ordinary differential equation on s . When we prescribe $\partial_x^\alpha \psi(x(0))$ for $|\alpha| = r$ we get the r th order derivatives of ψ on the whole curve and we can let the principle value vanish up to this order. This is only possible because of linearity. The partial derivatives of ψ must happen recursively and we need to be careful such that compatibility conditions like

$$\frac{\partial^3 \psi}{\partial x_i \partial x_j \partial x_k}(x(s)) \dot{x}_k(s) = \frac{d}{ds} \left(\frac{\partial^2 \psi}{\partial x_i \partial x_j}(x(s)) \right) \quad (3.15.26)$$

are satisfied. We can even be sure, that when we have chosen the partial derivative to be compatible at $x(0)$, they remain compatible for all s . Thus, as long as

$$\frac{\partial \psi}{\partial x}(x(s)) = \xi(s) \quad (3.15.27)$$

and

$$Im \frac{\partial^2 \psi}{\partial x_i \partial x_j}(x(0)) \quad (3.15.28)$$

is positive definite, we can be sure, that the principle value will vanish for arbitrary finite order on Γ . We thus have a valid construction of the phase ψ .

The other part of our Ansatz was the Taylor series of the coefficients $a_N(x)$ along the curve. The Ansatz makes it clear, that no tall powers of k will survive in the differential equation. In fact, the only ones, that we will find are $k^m, k^{m-1}, \dots, k^{-N+1}, k^{-N}$. Thus, we can simplify the equation to

$$P(x, D)u = \left(\sum_{s=-m}^N c_s(x) k^{-s} \right) e^{ik\psi(x)}. \quad (3.15.29)$$

From the previous parts we know

$$c_{-m}(x) = p_m \left(x, \frac{\partial \psi}{\partial x} \right) a_0(x). \quad (3.15.30)$$

This defines only one component, however. For the other coefficients, like $c_{-m+1}(x)$, we need to look at the terms of order $O(k^{m-1})$. From the differential operator we find such a term from the principle symbol of the $m - 1$ terms as

$$p_{m-1} \left(x, \frac{\partial \psi}{\partial x} \right) a_0(x) \quad (3.15.31)$$

and an additional coefficient is provided by

$$p_m \left(x, \frac{\partial \psi}{\partial x} \right) a_1(x). \quad (3.15.32)$$

All other terms will then arise from the terms of order k acting on $a_0(x)e^{ik\psi(x)}$. Similar to what we have seen in the previous chapter about geometrical optics, we need $k - 1$ derivatives acting on the phase exponential and the others acting on the products of a_0 with the terms obtained from previous derivatives of the exponential to get a term of order $K(k^{m-1})$. Generally, we find

$$c_{-m+1}(x) = La_0 + p_m \left(x, \frac{\partial \psi}{\partial x} \right) a_1 . \quad (3.15.33)$$

This can be rewritten with a function g_r depending on $\psi, a_0, \dots, a_{r-1}$ and their derivatives with $a_r = 0$ for $r > N$ as

$$c_{-m+r+1}(x) = La_r + p_m \left(x, \frac{\partial \psi}{\partial x} \right) a_{r+1} + g_r , \quad (3.15.34)$$

giving us a system of ordinary differential equations.

Equation (3.15.33) gives another very helpful insight. When we have a principle value vanishing to order R on our curve, we can choose the Taylor series up to order $R - 2$ in a way, that lets the coefficients $c_{-m+1}(x)$ vanish as well up to order $R - 2$. Generally, for the Taylor series for $a_{r-1}(x)$, the coefficients $c_{-m+r}(x)$ vanish up to order $R - 2r$.

The only thing left now for a successful construction of a Gaussian beam, is a k -independent function we multiply with u . This function is restricted to vanish outside a small neighbourhood $\mathcal{O}$ of Γ .

Following Lemma will ensure, that we have constructed an asymptotic solution to the partial differential equation. The proof is again found in *Dold* [7].

Lemma 5. Let $T > 0$ be given and let $c(x)$ be a function on $\mathcal{R}^{n+1}$ which vanishes to order $S - 1$ on Γ for some $S \geq 2$. Both the $\text{supp } c \cap \{|x_0| \leq T\}$ is compact and $\text{Im} \psi(x) \geq ad^2(x)$ on this set for some constant $a > 0$, where $d(x)$ denotes the distance from the point $x \in \mathcal{R}^{n+1}$ to Γ . Then there exists a constant C such that

$$\int_{|x_0| \leq T} \left| c(x) e^{ik\psi(x)} \right|^2 dx \leq C k^{-S - \frac{n}{2}} . \quad (3.15.35)$$

This Lemma is very important as it lets us at least estimate the Sobolev s-norm of our differential operator. We find

$$\int_{|x_0| \leq T} \left| c_{-m+r}(x) k^{m-r} e^{ik\psi(x)} \right|^2 dx \leq C k^{2(m-r)} k^{-(R+1-2r) - \frac{n}{2}} = C k^{2m - (R+1) - \frac{n}{2}} \quad (3.15.36)$$

as the coefficient $c_{-m+r}(x)$ vanishes to order $R - 2r$ on Γ . The neighbourhood is chosen in a way such that $\text{Im} \psi(x) \geq ad^2(x)$. Using $(w_1 + w_2 + \dots + w_l)^2 \leq 2(w_1^2 + w_2^2 + \dots + w_l^2)$

3. Gaussian beams

we finally arrive at

$$\begin{aligned}
||Pu||_0 &= \left(\int_{|x_0| \leq T} |Pu|^2 dx \right)^2 = \left(\int_{|x_0| \leq T} \left| \left(\sum_{j=-m}^N c_j(x) k^{-j} \right) e^{ik\psi(x)} \right|^2 dx \right)^{\frac{1}{2}} \\
&\leq \left(2 \sum_{j=-m}^N \int_{|x_0| \leq T} |x c_j(x) k^{-j} e^{ik\psi(x)}|^2 dx \right)^{\frac{1}{2}} \\
&\leq D k^{m - \frac{R+1}{2} - \frac{n}{4}} .
\end{aligned} \tag{3.15.37}$$

This concludes, that we have achieved what we intended at 2.10.5.

3.16. Tailored construction of the wave equation

We have now successfully constructed the Ansatz we want to use for our differential equation, however, we still do not have a valid differential equation. We just have a general discussion for a differential operator. For the sake of brevity, we will construct a 1 + 2 dimensional differential equation. Generalization to 1 + 3 dimensions is the straight forward.

The wave equation

$$\square u = -\frac{\partial^2 u}{\partial t^2} + \frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} = 0 \tag{3.16.1}$$

has principle value

$$p_2(x, \xi) = -\xi_0^2 + \xi_1^2 + \xi_2^2 . \tag{3.16.2}$$

This defines a strictly hyperbolic equation as long as $(\xi_1, \xi_2) \neq 0$. We thus find two distinct roots for the polynomial of the principle value. The Gaussian beam along its null characteristic curves is given by solutions of

$$\begin{aligned}
\dot{x}_0 &= -2\xi_0 \\
\dot{x}_i &= 2\xi_i
\end{aligned} \tag{3.16.3}$$

with $\dot{\xi} = 0$. We also have $p_2(x(s), \xi(s)) = 0$. From these, we can successfully deduce, that ξ_0, ξ_1, ξ_2 are constant along any given bicharacteristic curve. The solution therefore becomes

$$x(s) = (-2\xi_0 s, 2\xi_1 s, 2\xi_2 s) . \tag{3.16.4}$$

Example 5. An example for such a bicharacteristic curve is given by

$$(x(s), \xi(s)) = \left(s, 0, s, -\frac{1}{2}, 0, \frac{1}{2} \right) . \tag{3.16.5}$$

This is even a null bicharacteristic curve.

To construct the Gaussian beam with its projection $(s, 0, s)$ on Γ we use the Ansatz

$$u(x, k) = e^{ik\psi(x)} a_0(x) . \quad (3.16.6)$$

As described in the previous chapter, we start by defining the conditions on the phase ψ . As the bicharacteristic curve is null by definition, it suffices to check that

$$\frac{\partial \psi}{\partial x}(x(s)) = \xi(s) \quad (3.16.7)$$

which is equivalent to

$$\frac{\partial \psi}{\partial x}(s, 0, s) = \left(-\frac{1}{2}, 0, \frac{1}{2} \right) .$$

The matrix conditions of (3.15.18) simplify to

$$0 = MCM + \frac{dM}{ds} \quad (3.16.8)$$

and C takes the form

$$C = \begin{bmatrix} -2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix} . \quad (3.16.9)$$

We want to determine M given the differential equation

$$M(s)_{ij} = \frac{\partial^2 \psi}{\partial x_i \partial x_j}(x(s)) \quad (3.16.10)$$

for which we assume $M(0)$ to satisfy

$$M(0)\dot{x}(0) = \dot{\xi}(0) . \quad (3.16.11)$$

Or with values

$$M(0) \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} .$$

The orthogonal complement to $\dot{x}$ is spanned by $(0, 1, 0)$ and $(-1, 0, 1)$ and as $M(0)$ must be positive definite on this space, it can only be of the form

$$M(0) = \begin{bmatrix} bi & 0 & -bi \\ 0 & ai & 0 \\ -bi & 0 & bi \end{bmatrix} . \quad (3.16.12)$$

We assume the constants a and b to be positive. Thus we need to find a solution for the

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linear system

$$\begin{aligned}\dot{Y} &= CN \\ \dot{N} &= 0.\end{aligned}\tag{3.16.13}$$

We provide initial data $(Y(0), N(0)) = (I, M(0))$ from which we find from the second equation, that $N(s) = N(0) = M(0)$. We can use this in the first equation, to find $\dot{Y} = CM(0)$ which we can solve and get

$$Y(s) = Y(0) + sCM(0) = I + sCM(0).\tag{3.16.14}$$

Thus we finally find

$$M(s) = N(s)Y^{-1}(s) = M(0)(I + sCM(0))^{-1}.\tag{3.16.15}$$

From [7] we find a valid example for a phase factor, that satisfies the conditions (3.16.7) and (3.16.15) such that the principal value $p_2(x, \frac{\partial\psi(x)}{\partial x})$ vanishes to at least second order

$$\psi(x_0, x_1, x_2) = \frac{x_2 - x_0}{2} + \frac{a^2 x_0 x_1^2}{1 + 4a^2 x_0^2} + i \left[\left(\frac{a}{1 + 4a^2 x_0^2} \right) \frac{x_1^2}{2} + \frac{b(x_2 - x_0)^2}{2} \right].\tag{3.16.16}$$

Remark. This phase enables vanishing of the principle symbol even to order 3.

After the phase, we need to determine the Taylor series for the coefficients. We use $c_{-2+1}(x) = c_{-1}(x)$ and find a suitable function for $a_0(x)$. We further solve

$$\begin{aligned}\frac{\partial u}{\partial x_j} &= e^{ik\psi} \frac{\partial a_0}{\partial x_j} + \frac{\partial \psi}{\partial x_j} i k e^{ik\psi} a_0 \\ \frac{\partial^2 u}{\partial x_j^2} &= e^{ik\psi} \frac{\partial^2 a_0}{\partial x_j^2} + 2ik \frac{\partial \psi}{\partial x_j} \frac{\partial a_0}{\partial x_j} e^{ik\psi} + ik \frac{\partial^2 \psi}{\partial x_j^2} e^{ik\psi} a_0 - k^2 \left(\frac{\partial \psi}{\partial x_j} \right)^2 e^{ik\psi} a_0\end{aligned}\tag{3.16.17}$$

for $j = 0, 1, 2$. Collecting all terms into a sum, we finally get

$$c_{-1}(x) = \sum_{j=0}^2 \left(2i \frac{\partial \psi}{\partial x_j} \frac{\partial a_0}{\partial x_j} e^{ik\psi} + i \frac{\partial^2 \psi}{\partial x_j^2} e^{ik\psi} a_0 \right).\tag{3.16.18}$$

As we know, that

$$\begin{aligned}\frac{\partial \psi}{\partial x}(s, 0, s) &= \left(-\frac{1}{2}, 0, \frac{1}{2} \right) \\ \frac{da_0}{ds}(s, 0, s) &= \frac{\partial a_0}{\partial x_0}(s, 0, s) + \frac{\partial a_0}{\partial x_2}(s, 0, s)\end{aligned}\tag{3.16.19}$$

we can deduce, that $c_{-1}(x)$ vanishes on $(s, 0, s)$ if and only if

$$\frac{da_0}{ds} - (\square\psi)a_0 = 0 \quad (3.16.20)$$

is satisfied on Γ . To now solve for $a_0(x(s))$ we can use $\square\psi = -ia(1+2ais)^{-1}$ in (3.16.16). This allows us, to separate variables and with the initial condition $a_0(x(0)) = 1$ we find

$$a_0(x(s)) = (1 + 2ais)^{-\frac{1}{2}}. \quad (3.16.21)$$

The missing part now is, to fix a_0 not only on Γ but globally or at least in a sufficiently large neighbourhood of Γ . A good choice from [7] is

$$a_0(x_0, x_1, x_2) = (1 + 2aix_0)^{-\frac{1}{2}}. \quad (3.16.22)$$

With this, the coefficient $c_{-1}(x)$ will vanish up to first order.

To check, if the norm is satisfied, we use (3.15.37) and find

$$\|\square u(x, k)\|_0 = \left\| e^{ik\psi(x)} a_0(x) \right\|_0 \leq Dk^{2-\frac{3+1}{2}-\frac{2}{4}} = Dk^{-\frac{1}{2}} = O(k^{-\frac{1}{2}}). \quad (3.16.23)$$

Thus, concluding with a valid definition for the phase ψ , and the Taylor series for a such that we have an asymptotic solution which becomes concentrated on the curve $(s, 0, s)$ for $k \rightarrow \infty$.

We will now use the general principles and constructions to calculate the orders for our Ansatz in the next chapter.

4. Klein-Gordon equation and Ansatz

4.1. Introduction

In the preceding introductory chapters we got good insight into the general approach to calculate asymptotic solutions for specific Ansatzes for wave equations. We took general forms of differential operators and their properties with general forms of Gaussian waves and Gaussian wave packets to get insight into the steps needed to get a satisfactory solution.

We will now use our knowledge to find an asymptotic solution for a specific example. Instead of taking a general differential operator as it was used in the chapter about Gaussian beams 3 we will look at the massive Klein-Gordon equation

$$\left(\square - \frac{m^2}{\epsilon^2}\right)\phi = 0. \quad (4.1.1)$$

In this equation, m depicts the mass of a particle, $\square$ denotes the relativistic Wave operator

$$\square = g^{\mu\nu}\nabla_\mu\nabla_\nu$$

with the covariant derivatives ∇_μ . ϵ is a small expansion parameter which will be used in the two parameter expansion and ϕ denotes a complex scalar field. Comparing this to the construction in the introductory chapter 3.16 we already find a very important difference. The differential operator now has a potential term as well, and not only derivative terms. The principle value (3.16.2), however, only depends on the highest order, so it remains the same.

We now want to use a semi-classical wave packet describing the connection of a point in spacetime with a geodesic in terms of possible connecting geodesics. We get such an Ansatz as a relativistically generalized ansatz of the one considered in *Watson* [43]. The Ansatz takes the form

$$\phi(x, \gamma) = A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) e^{\frac{iS(x)}{\epsilon}}. \quad (4.1.2)$$

ϵ is again a small expansion parameter needed for a two parameter expansion being related to the wavelength. S is a real scalar function responsible for the phase and the complex amplitude is given by A^ϵ .

Remark. It is important to note, that by construction, the Ansatz ϕ is localized along a

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curve $\gamma^{\mu'}(\tau)$.

Even though the Ansatz depicts some semi-classical Gaussian wave packet, it introduces some non trivialities compared to the Gaussian beams introduces in the introductory chapter. In the non relativistic case, the phase was only dependent on a point in space. This is no longer meaningful in the regime of general relativity. To measure distances and define points in space we need to find geodesic on which we can measure distances. Therefore, the phase is also dependent on a function $u^{\mu'}$. This function denotes the tangent vector to the unique geodesic, that connects the curve γ at τ with the space time point x^μ , which, of course, must depend on the curve γ itself and the spacetime point. Thus, the derivations of the Ansatz get more involved, then what we have seen in the introductory chapters. In the end, however, when the differentiations are performed, we are still able to collect all the terms in their respective order in ϵ . Some terms, however, will initially appear in a different order. We will need two property of Snyge's world functions

$$\begin{aligned}\nabla_\beta v_{\alpha'}|_\gamma &= \epsilon^{-1/2} \nabla_\beta u_{\alpha'}|_\gamma = -\epsilon^{-1/2} [\sigma_{\alpha'\beta}] = \epsilon^{-1/2} g_{\alpha'\beta'}, \\ \nabla_\nu \nabla_\mu v_{\alpha'}|_\gamma &= \epsilon^{-1/2} \nabla_\nu \nabla_\mu u_{\alpha'}|_\gamma = -\epsilon^{-1/2} [\sigma_{\alpha'\mu\nu}] = 0.\end{aligned}\tag{4.1.3}$$

which can be calculated from the coincidence limits shown in *Poisson* [27]. These will help us, collect the mentioned terms in their true order.

Reaching the highest order, we will find the most interesting difference to the general discussion in the introductory chapters. While we have always found transport equations in the highest order of ϵ , we will now find a Schrödinger-like equation. We will bring this into a nice form after removing vanishing terms by defining a Hamilton function involving a matrix W , depending on the geometry of the space by the Riemann tensor. This will be contracted with vectors v , which result from the initial vector u by redefinition seen during the calculation, that are orthonormal to the direction of propagation. This will simplify the matrix, as it removes one dimension, which makes numerical integration in later chapters simpler.

We will now insert the Ansatz (4.1.2) into (4.1.1), with the resulting terms being required to vanish identically for each order of ϵ .

Letting the first derivative act on (4.1.2) we get

$$\begin{aligned} \nabla_\nu \phi(x, \gamma) &= \frac{i \nabla_\nu S(x)}{\epsilon} e^{\frac{iS(x)}{\epsilon}} A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) \\ &+ e^{\frac{iS(x)}{\epsilon}} \left[\frac{1}{\nabla_\nu} A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) + \frac{2}{\nabla_{\mu'}} A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) \cdot \nabla_\nu \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right] \end{aligned} \quad (4.1.4)$$

where we introduced the notation $\frac{1}{\nabla}$ and $\frac{2}{\nabla}$ for labelling the differentiation for the first or second argument of the Amplitude A , respectively. We can now let the second derivative act and find

$$\begin{aligned} \nabla_\gamma \nabla_\nu \phi &= \frac{i \nabla_\gamma \nabla_\nu S(x)}{\epsilon} e^{\frac{iS(x)}{\epsilon}} A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) \\ &- \frac{(\nabla_\gamma S(x)) (\nabla_\nu S(x))}{\epsilon^2} e^{\frac{iS(x)}{\epsilon}} A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) \\ &+ \frac{i \nabla_\nu S(x)}{\epsilon} e^{\frac{iS(x)}{\epsilon}} \left[\frac{1}{\nabla_\gamma} A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) + \frac{2}{\nabla_{\mu'}} A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) \nabla_\gamma \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right] \\ &+ \frac{i \nabla_\gamma S(x)}{\epsilon} e^{\frac{iS(x)}{\epsilon}} \left[\frac{1}{\nabla_\nu} A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) + \frac{2}{\nabla_{\mu'}} A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) \nabla_\nu \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right] \\ &+ e^{\frac{iS(x)}{\epsilon}} \left[\frac{1}{\nabla_\gamma} \frac{1}{\nabla_\nu} A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) + \frac{2}{\nabla_{\mu'}} \frac{1}{\nabla_\nu} A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) \left(\nabla_\gamma \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) \right. \\ &+ \frac{1}{\nabla_\gamma} \frac{2}{\nabla_{\mu'}} A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) \left(\nabla_\nu \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) + \frac{2}{\nabla_{\mu'}} A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) \left(\nabla_\gamma \nabla_\nu \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) \\ &\left. + \frac{2}{\nabla_{\mu'}} \frac{2}{\nabla_{\sigma'}} A^\epsilon \left(x, \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) \left(\nabla_\nu \frac{u^{\mu'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) \left(\nabla_\gamma \frac{u^{\sigma'}(x, \gamma)}{\epsilon^{\frac{1}{2}}} \right) \right]. \end{aligned} \quad (4.1.5)$$

For simplicity we will now introduce a parameter v such that we can evaluate the equation at $v = \frac{u}{\epsilon^{\frac{1}{2}}}$. Furthermore, we call $\nabla_\mu S(x) = k_\mu$ and we let the metric we get with the box operator act on the result. Finally, we get the result

$$\left(\square - \frac{m^2}{\epsilon^2} \right) \phi = Re e^{\frac{iS(x)}{\epsilon}} = 0 \quad (4.1.6)$$

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with

$$R = \left[-\epsilon^{-2} k^{\nu'} k_{\nu'} + i\epsilon^{-1} \left[2k_{\nu'} \overset{1}{\nabla}_{\nu} + \nabla_{\nu} k^{\nu} + 2k^{\nu} \nabla_{\nu} v^{\mu'} \overset{2}{\nabla}_{\mu'} \right] \right. \\ \left. + \overset{1}{\nabla}^{\nu} \overset{1}{\nabla}_{\nu} + 2 \left(\nabla^{\nu} v^{\mu'} \right) \overset{1}{\nabla}_{\nu} dv_{\mu'} + \left(\nabla^{\nu} \nabla_{\nu} v^{\mu'} \right) \overset{2}{\nabla}_{\mu'} + \left(\nabla^{\nu} v^{\mu'} \right) \left(\nabla_{\nu} v^{\sigma'} \right) \overset{2}{\nabla}_{\mu'} \overset{2}{\nabla}_{\sigma'} \right] A^{\epsilon}(x, v) \Big|_{v=\frac{u}{\sqrt{2\epsilon}}} \quad (4.1.7)$$

We can now expand A^{ϵ} as

$$A^{\epsilon} = A_0 + \epsilon^{\frac{1}{2}} A_{\frac{1}{2}} + \epsilon A_1 + O(\epsilon^{\frac{3}{2}}) \quad (4.1.8)$$

which gives a similar form to the two parameter expansion we saw in (2.10.6) and rewrite $A_{\epsilon} = a_{\epsilon}(v)b_0(x)$. We then order all the terms by their power in ϵ and get

$$R = \left\{ -\epsilon^{-2} (k^{\nu} k_{\nu} b_0)(x) a_0(v) - m^2 (a_0(v) b_0(x)) \right. \quad (4.1.9)$$

$$\left. - \epsilon^{-\frac{3}{2}} \left[\left(k^{\nu} k_{\nu} b_{\frac{1}{2}} \right)(x) a_{\frac{1}{2}}(v) - m^2 \left(a_{\frac{1}{2}}(v) b_{\frac{1}{2}}(x) \right) \right] \right\} \quad (4.1.10)$$

$$\left. - \epsilon^{-1} \left[\left(k^{\nu} k_{\nu} b_1 \right)(x) a_1(v) - i \left(2k^{\nu} \overset{1}{\nabla}_{\nu} b_0 + b_0 \nabla_{\nu} k^{\nu} + 2b_0 k^{\nu} \nabla_{\nu} v^{\mu'} \overset{2}{\nabla}_{\mu'} \right)(x) a_0(v) - m^2 (a_1(v) b_1(x)) \right] \right\} \quad (4.1.11)$$

$$\left. - \epsilon^{-\frac{1}{2}} \left[\left(k^{\nu} k_{\nu} b_{\frac{3}{2}} \right)(x) a_{\frac{3}{2}}(v) - i \left(2k^{\nu} \overset{1}{\nabla}_{\nu} b_{\frac{1}{2}} + b_{\frac{1}{2}} \nabla_{\nu} k^{\nu} + 2b_{\frac{1}{2}} k^{\nu} \nabla_{\nu} v^{\mu'} \overset{2}{\nabla}_{\mu'} \right)(x) a_{\frac{1}{2}}(v) - m^2 \left(a_{\frac{3}{2}}(v) b_{\frac{3}{2}}(x) \right) \right] \right\} \quad (4.1.12)$$

$$\left. - \epsilon^0 \left[\left(k^{\nu} k_{\nu} b_2 \right)(x) a_2(v) - i \left(2k^{\nu} \overset{1}{\nabla}_{\nu} b_1 + b_1 \nabla_{\nu} k^{\nu} + 2b_1 k^{\nu} \nabla_{\nu} v^{\mu'} \overset{2}{\nabla}_{\mu'} \right)(x) a_1(v) - m^2 (a_2(v) b_2(x)) \right] \right. \\ \left. + \epsilon^0 \left[\left[(\square b_0)(x) + 2 \left(\nabla_{\nu} v^{\mu'} \right) \left(\overset{1}{\nabla}_{\nu} b_0 \right) \overset{2}{\nabla}_{\mu'} + \left(\square v^{\mu'} \right) \overset{2}{\nabla}_{\mu'} + \left(\nabla_{\nu} v^{\mu'} \right) \left(\nabla_{\nu} v^{\sigma'} \right) \overset{2}{\nabla}_{\mu'} \overset{2}{\nabla}_{\sigma'} \right](x) a_0(v) \right. \right. \\ \left. \left. - m^2 (a_2(v) b_2(x)) \right] \right\} \quad (4.1.13)$$

$$\left. + O\left(\epsilon^{\frac{1}{2}}\right) \right\} \Big|_{v=\frac{u}{\sqrt{\epsilon}}} \quad (4.1.14)$$

We see that this result factorises into the form of $f(x)g(v)$ thus we can use the identity

$$f(x)g(v) \Big|_{v=\frac{u}{\sqrt{\epsilon}}} = f[\exp_{\gamma}(\sqrt{\epsilon}v)g(v)] \Big|_{v=\frac{u}{\sqrt{\epsilon}}} \quad (4.1.15)$$

and we can expand f to get

$$f[\exp_\gamma(\sqrt{\epsilon}v)] = f(\gamma) + \epsilon^{\frac{1}{2}} v^{\mu'} (\nabla_{\mu'} f)(\gamma) + \dots \quad (4.1.16)$$

After inserting these expansions we can start setting the terms for each order of ϵ to 0.

4.2. Order ϵ^{-2}

We now look at the term we find at order ϵ^{-2} given by (4.1.9). Here we are left with

$$(k^\nu k_\nu b_0)(\gamma) a_0(v) + m^2 (a_0(v) b_0(\gamma)) = 0. \quad (4.2.1)$$

which must be identically 0 such that, with all other orders also resulting to 0 identically, (4.1.6) is fulfilled. we can pull out a_0 and b_0 and as we are not interested in the trivial case where they are 0, respectively, we are left with

$$k^\nu k_\nu + m^2 = 0 \quad (4.2.2)$$

or

$$k^\nu k_\nu = -m^2. \quad (4.2.3)$$

4.3. Order $\epsilon^{-\frac{3}{2}}$

At this order we have the term from (4.1.10) as

$$(k^\nu k_\nu b_{\frac{1}{2}})(\gamma) a_{\frac{1}{2}}(v) + v^{\mu'} (\nabla'_{\mu'} (k^\nu k_\nu)) b_0(\gamma) a_0(v) + m^2 a_0(v) v^{\mu'} (\nabla'_{\mu'} b_0(\gamma)) + m^2 a_{\frac{1}{2}}(v) b_{\frac{1}{2}}(\gamma) = 0 \quad (4.3.1)$$

Using the result from (4.2) we are left with

$$v^{\mu'} (\nabla'_{\mu'} (k^\nu k_\nu b_0(\gamma))) a_0(v) + m^2 a_0(v) v^{\mu'} (\nabla'_{\mu'} b_0(\gamma)) = 0 \quad (4.3.2)$$

When we evaluate the derivative we see that the m^2 term gets cancelled and we are left with

$$v^{\mu'} [(\nabla'_{\mu'} k^\nu) k_\nu b_0(\gamma) + k^\nu (\nabla'_{\mu'} k_\nu) b_0(\gamma)] = 0 \quad (4.3.3)$$

We are not interested in the trivial case where v would just be the null vector or where $b_0 = 0$ thus we need

$$(\nabla'_{\mu'} k^\nu) k_\nu + k^\nu (\nabla'_{\mu'} k_\nu) = 0 \quad (4.3.4)$$

as k is just the gradient of a scalar function we can swap the indices and see that each term must be zero identically

$$(\nabla'_{\mu'} k^\nu) k_\nu = k^\nu (\nabla_\nu k_{\mu'}) = \dot{k}_{\nu'} = 0 \quad (4.3.5)$$

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From this we find that γ with $\dot{\gamma}^{\nu'} = k^{\nu'}$ must be a geodesic

$$\begin{aligned}
0 &= g^{\alpha'\beta'} \dot{k}_{\alpha'} = g^{\alpha'\beta'} \frac{dk_{\alpha'}}{d\tau} - g^{\alpha'\beta'} \Gamma_{\sigma'\alpha'}^{\delta'} k^{\sigma'} k_{\delta'} \\
&= g^{\alpha'\beta'} \frac{d(g_{\alpha'\sigma'} \dot{\gamma}^{\sigma'})}{d\tau} - g^{\alpha'\beta'} \Gamma_{\sigma'\alpha'}^{\delta'} k^{\sigma'} k_{\delta'} \\
&= \ddot{\gamma}^{\alpha'} + \dot{\gamma}^{\sigma'} g^{\alpha'\beta'} \dot{\gamma}^{\delta'} \partial_{\delta'} g_{\beta'\sigma'} - g^{\alpha'\beta'} \Gamma_{\sigma'\alpha'}^{\delta'} k^{\sigma'} k_{\delta'} \\
&= \ddot{\gamma}^{\alpha'} + \Gamma_{\sigma'\delta'}^{\alpha'} \dot{\gamma}^{\sigma'} \dot{\gamma}^{\delta'}
\end{aligned} \tag{4.3.6}$$

Since $\dot{\gamma}^{\nu'} = k^{\nu'}$ is a time-like vector and the wave packet amplitude depends on the direction of $u^{\nu'}$ orthogonal to $k^{\nu'}$ only, we can introduce a tetrad $\{k, e_A\}$ where $A \in \{1, 2, 3\}$ and e_A are space-like vectors orthogonal to k . Thus

$$e_A \cdot e_B = \delta_{AB} \tag{4.3.7}$$

With this choice we construct $u^{\mu'}$ and $v^{\nu'} \in \text{span}\{k, e_A\}$ and we can write the metric as

$$g_{\mu\nu} = P_{\mu\nu} - k_\mu k_\nu \tag{4.3.8}$$

with

$$P_{\mu\nu} = \delta_{AB} (e_\mu^A e_\nu^B) \tag{4.3.9}$$

4.4. Order ϵ^{-1}

For this order, we find the term given by (4.1.11). It turns out, however, that there still exist terms which appear in order 0, that should be at order -1 . We find these by using the two properties for Synge's world functions (4.1.3). Thus, we have

$$\begin{aligned}
&(k^\nu k_\nu b_1)(\gamma) a_1(v) + v^\alpha [\nabla_\alpha (k^\nu k_\nu b_{\frac{1}{2}})](\gamma) a_{\frac{1}{2}}(v) + \frac{1}{2} v^\alpha v^\beta (\nabla_\alpha \nabla_\beta k^\nu k_\nu b_0)(\gamma) a_0(v) \\
&- i \left(2k^\nu \nabla_\nu b_0 + b_0 \nabla_\nu k^\nu \right) (\gamma) a_0(v) - 2i \left(b_0 k^\nu \nabla_\nu v^\delta \right) (\gamma) \nabla_\delta a_0(v) \\
&- (b_0 g^{\mu\sigma})(\gamma) \nabla_\mu \nabla_\sigma a_0(v) \\
&- m^2 \frac{1}{2} a_0(v) v^{\mu'} v^{\nu'} (\nabla_{\mu'} \nabla_{\nu'} b_0)(\gamma) \\
&- m^2 a_{\frac{1}{2}}(v) v^{\mu'} (\nabla_{\mu'} b_{\frac{1}{2}})(\gamma) \\
&- m^2 a_1(v) b_1(\gamma) = 0
\end{aligned} \tag{4.4.1}$$

From previous results we see that the $a_1 b_1$ terms cancel, as well as the $a_{\frac{1}{2}} b_{\frac{1}{2}}$ after expanding the terms the same way as in the previous order. For the $a_0 b_0$ terms we calculate the

derivatives and we are left with

$$\begin{aligned}
& i(2k^\nu \nabla_\nu b_0 + b_0 \nabla_\nu k^\nu + 2b_0 k^\nu \nabla_\nu v^\delta)(\gamma) \overset{2}{\nabla}_\delta a_0(v) \\
& - (b_0 g^{\mu\sigma})(\gamma) \overset{2}{\nabla}_\mu \overset{2}{\nabla}_\sigma a_0(v) \\
& + v^\alpha v^\beta (\nabla_\alpha \nabla_\beta k_\nu) k^\nu b_0(\gamma) a_0(v) \\
& + v^\alpha v^\beta (\nabla_\beta k^\nu) (\nabla_\alpha k_\nu) b_0(\gamma) a_0(v) = 0
\end{aligned} \tag{4.4.2}$$

We can now define

$$(k^\nu \nabla_\nu v^{\mu'}) (\gamma) \overset{2}{\nabla}_{\mu'} a_0(v) = k^{\mu'} \overset{2}{\nabla}_{\mu'} a_0 = \dot{a}_0 \tag{4.4.3}$$

$$(k^\nu \overset{1}{\nabla}_\nu b_0)(\gamma) = \dot{b}_0 \tag{4.4.4}$$

Furthermore, using the expansion of $A_0(v, \tau)$ where the x dependence vanished because we are now on the geodesic, as $A_0(v, \tau) = a_0(v) b_0(\tau)$ we get

$$2i\dot{A}_0(v, \tau) = \left[-\frac{1}{2} g^{\nu'\sigma'} \overset{2}{\nabla}_{\nu'} \overset{2}{\nabla}_{\sigma'} + \frac{1}{2} v^\alpha v^\beta (\nabla_\alpha \nabla_\beta k_\nu) k^\nu + (\nabla_\beta k^\nu) (\nabla_\alpha k_\nu) + \nabla_\nu k^\nu \right] A_0(v, \tau) \tag{4.4.5}$$

This equation starts to look like a *Schrödinger* equation and thus we define

$$\mathcal{H} = -\frac{1}{2} g^{\nu'\sigma'}(\tau) \overset{2}{\nabla}_{\nu'} \overset{2}{\nabla}_{\sigma'} + \frac{1}{2} v^\alpha v^\beta W_{\alpha\beta} - \frac{i}{2} g^{\nu'\sigma'}(\tau) k_{\nu'\sigma'}(\tau) \tag{4.4.6}$$

and

$$\begin{aligned}
W_{\alpha\beta}(\tau) &= \frac{1}{2} \left[(\mathcal{R}_{\alpha\mu\beta}^\gamma k_\gamma + \nabla_\mu \nabla_\alpha k_\beta) k^\mu + g^{\mu\nu} k_{\alpha\mu} k_{\beta\nu} \right] \\
&= \frac{1}{2} \left[\dot{k}_{\alpha\beta} + g^{\mu\nu} k_{\alpha\mu} k_{\beta\nu} + \mathcal{R}_{\alpha\mu\beta}^\gamma k_\gamma k^\mu \right](\tau)
\end{aligned} \tag{4.4.7}$$

We further assume $k_{\mu\nu} = 0$ and we can separate the result into $a_0(v) b_0(\tau)$ again. As we want a to satisfy the Schrödinger equation, we see that b_0 must be identically 1, and that for all τ . Thus

$$i\dot{a}_0(v) = \frac{1}{2} \left[-g^{\nu'\sigma'}(\tau) \overset{2}{\nabla}_{\nu'} \overset{2}{\nabla}_{\sigma'} a_0(v) + v^\alpha v^\beta R_{\alpha\mu\beta}^\gamma k_\gamma k^\mu(\tau) a_0(v) \right] \tag{4.4.8}$$

or

$$i\dot{a}_0(v) = \frac{1}{2} \left[-g^{\nu'\sigma'}(\tau) \overset{2}{\nabla}_{\nu'} \overset{2}{\nabla}_{\sigma'} + v^\alpha v^\beta W_{\alpha\beta}(\tau) \right] a_0(v) \tag{4.4.9}$$

With the help of (4.3.8) we can rewrite this as

$$i\dot{a}_0(v) = \frac{1}{2} \left[-P^{\nu'\sigma'}(\tau) \overset{2}{\nabla}_{\nu'} \overset{2}{\nabla}_{\sigma'} + v^\alpha v^\beta W_{\alpha\beta}(\tau) \right] a_0(v) \tag{4.4.10}$$

We have reached the most interesting deviation from the calculations in the introductory chapters which followed calculations in a non-relativistic way. While we found a transport equation for the Amplitude in the non-relativistic case in flat spacetime in the

4. Klein-Gordon equation and Ansatz

introductory chapters, we now found a Schrödinger-like equation with our Ansatz involving influences from curved spacetime. Let us look at the result (4.4.9) more closely. We can differentiate it into two parts. The first part

$$-g^{\nu'\sigma'}(\tau)\nabla_{\nu'}^2\nabla_{\sigma'}^2 \quad (4.4.11)$$

in general denotes the Laplace operator. This describes the the spreading of the wave packet in transverse direction.

The second part

$$v^\alpha v^\beta W_{\alpha\beta}(\tau) \quad (4.4.12)$$

gives more interesting insights. Generally, one would describe this term as a potential, but it does not describe some "external" potential, like the electromagnetic potential, it directly relates the curvature of the spacetime, or the geodesic deviation to the movement of a particle described by this equation. Comparing this to general Schrödinger equations, we see, that our result (4.4.9) indeed describes the Schrödinger equation for a quantum wave packet in and external potential, but with the potential now being the whole space, the particle is moving in.

In the introductory chapters we promised, that this will also be a more general result, than the flat metric transport equations. This can be shown relatively easily. If the curvature of the space goes to zero, which would correspond to the flat Minkowski spacetime or the approximate spacetime far away from a black hole, the matrix W , which introduces the dependence to the curvature of the space with the Riemann tensor (4.4.7), gets essentially 0. In this case, the first part (4.4.11) of our differential equation (4.4.9) reduces to the generic Euclidean derivatives as well and we get the Amplitude transport along straight lines again. Thus we see, that this result includes all the information for the transport of the amplitude in flat spacetime but enlarges the space of information by influences of curved spacetime.

Compared to the differential equation from *Watson* [43], we also find some differences and get more insights to our case. The first difference can be seen in the first part of (4.4.9), the differential operators are contracted with a second derivative of Eigenenergies E . As this is obviously 1 in our case, we see, that our Eigenenergies have to be polynomials of order 2 restricted to a first derivative as a linear function with gradient 1.

Apart from that, we also have to identify our matrix W with the second derivative of some other matrix W' which was used in the paper by *Watson* [43] and the vectors y correspond to our vectors v which form an orthonormal system to the direction of propagation of the geodesic.

We see that this has the form of a non-dimensionalized time-dependent Schrödinger equation [43]. For this equation there already exists general solution by *Hagedorn* [14] and [13] as well as from *Faou* [9] as follows

$$a(v, t) = \frac{N}{[\det(A(t))]^{\frac{1}{2}}} \exp\left(i\frac{1}{2}v \cdot B(t)A^{-1}(t)v\right) \quad (4.4.13)$$

or in index notation

$$a(v^\mu, t) = \frac{N}{[\det(A(t))]^{\frac{1}{2}}} \exp \left(\frac{i}{2} g_{\alpha\beta} v^\beta B^\alpha_\delta A^\delta_\gamma v^\gamma \right) \quad (4.4.14)$$

with initial data

$$a_0(v) = \frac{N}{[\det A_0]^{\frac{1}{2}}} \exp \left(i \frac{1}{2} v \cdot B_0 A_0^{-1} v \right) \quad (4.4.15)$$

where $N \in \mathbb{C}$ is an arbitrary non-zero constant, and A_0, B_0 are $d \times d$ complex matrices which satisfy

$$A_0^T B_0 - B_0^T A_0 = 0 \quad (4.4.16)$$

$$\bar{A}_0^T B_0 - \bar{B}_0^T A_0 = 2iI \quad (4.4.17)$$

These conditions imply

1. B_0 and A_0 are invertible
2. $B_0 A_0^{-1}$ is complex symmetric: $(B_0 A_0^{-1})^T = B_0 A_0^{-1}$
3. The imaginary part of $B_0 A_0^{-1}$ is symmetric, positive definite and satisfies $Im B_0 A_0^{-1} = (A_0 \bar{A}_0^T)^{-1}$

Comparing the general solution (4.4.13) with our introductory chapters, we see that it forms a *Gaussian wavepacket*. We will now show that this is general solution is also a solution for our equation.

We start looking at the left side. Using Jacobi's formula for derivatives of determinants we find

$$\begin{aligned} i \frac{d}{dt} a(v, t) &= -i \frac{1}{2} \frac{N \cdot \det(A(t)) \cdot (A(t)^{-1})^\mu_\nu \frac{dA(t)^\nu_\mu}{dt}}{[\det(A(t))]^{\frac{3}{2}}} \exp \left(\frac{i}{2} g_{\alpha\beta} v^\beta B^\alpha_\delta (A^{-1})^\delta_\gamma v^\gamma \right) \\ &+ \frac{i}{2} \left[\frac{N}{[\det(A(t))]^{\frac{1}{2}}} v \left(\frac{dB(t)}{dt} A^{-1}(t) - B(t) A^{-1}(t) \frac{dA(t)}{dt} A^{-1} \right) v \right] \exp \left(\frac{i}{2} g_{\alpha\beta} v^\beta B^\alpha_\delta (A^{-1})^\delta_\gamma v^\gamma \right) \\ &= \frac{i}{2} \frac{N}{[\det(A(t))]^{-\frac{1}{2}}} \exp \left(\frac{i}{2} g_{\alpha\beta} v^\beta B^\alpha_\delta (A^{-1})^\delta_\gamma v^\gamma \right) \\ &\cdot \left[- (A(t)^{-1})^\mu_\nu \frac{dA(t)^\nu_\mu}{dt} \right. \\ &\left. + i \left[v_\alpha \left(\left(\frac{dB}{dt} \right)^\alpha_\delta (A^{-1})^\delta_\gamma + B^\alpha_\delta (A^{-1})^\delta_\rho \left(\frac{dA}{dt} \right)^\rho_\sigma (A^{-1})^\sigma_\gamma \right) v^\gamma \right] \right] \end{aligned} \quad (4.4.18)$$

4. Klein-Gordon equation and Ansatz

For the right side we find

$$\frac{1}{2} \left[-P^{\nu'\sigma'}(\tau) \overset{2}{\nabla}_{\mu'} \overset{2}{\nabla}_{\sigma'} + v^\alpha v^\beta W_{\alpha\beta}(\tau) \right] \frac{N}{[\det(A(t))^{\frac{1}{2}}]} \exp \left(\frac{i}{2} g_{\alpha\beta} v^\beta B^\alpha_\delta (A^{-1})^\delta{}_\gamma v^\gamma \right) \quad (4.4.19)$$

We let the first derivative with respect to v act and find

$$\overset{2}{\nabla}_\mu a(v, t) = \frac{N}{[\det(A(t))^{\frac{1}{2}}]} \frac{i}{2} \left[g_{\alpha\mu} B^\alpha_\delta (A^{-1})^\delta{}_\gamma v^\gamma + g_{\alpha\beta} v^\beta B^\alpha_\delta (A^{-1})^\delta{}_\mu \right] \exp \left(\frac{i}{2} g_{\alpha\beta} v^\beta B^\alpha_\delta (A^{-1})^\delta{}_\gamma v^\gamma \right) \quad (4.4.20)$$

The second derivative then gives

$$\begin{aligned} \overset{2}{\nabla}_\nu \overset{2}{\nabla}_\mu a(v, t) &= \frac{N}{[\det(A(t))^{\frac{1}{2}}]} \left[\frac{i}{2} \left(g_{\alpha\mu} B^\alpha_\delta (A^{-1})^\delta{}_\nu + g_{\alpha\nu} B^\alpha_\delta (A^{-1})^\delta{}_\beta \right) \right. \\ &\quad \left. - \frac{1}{4} \left(B_{\mu\delta} (A^{-1})^\delta{}_\gamma v^\gamma + v_\alpha B^\alpha_\delta (A^{-1})^\delta{}_\mu \right) \cdot \left(B_{\nu\delta} (A^{-1})^\delta{}_\gamma v^\gamma + v_\alpha B^\alpha_\delta (A^{-1})^\delta{}_\nu \right) \right] \\ &\quad \cdot \exp \left(\frac{i}{2} g_{\alpha\beta} v^\beta B^\alpha_\delta (A^{-1})^\delta{}_\gamma v^\gamma \right) \end{aligned} \quad (4.4.21)$$

Thus, the right side of (4.4.10) reads

$$\begin{aligned} &\frac{1}{2} \left[-P^{\nu'\sigma'} \left(-\frac{1}{4} \left(B_{\mu\delta} (A^{-1})^\delta{}_\gamma v^\gamma + v_\alpha B^\alpha_\delta (A^{-1})^\delta{}_\mu \right) \cdot \left(B_{\nu\delta} (A^{-1})^\delta{}_\gamma v^\gamma + v_\alpha B^\alpha_\delta (A^{-1})^\delta{}_\nu \right) \right. \right. \\ &\quad \left. \left. + i B_{\mu\delta} (A^{-1})^\delta{}_\gamma \right) \right. \\ &\quad \left. + v^\alpha v^\beta W_{\alpha\beta} \right] \cdot \frac{N}{[\det(A(t))^{\frac{1}{2}}]} \exp \left(\frac{i}{2} v B(t) A^{-1}(t) v \right) \end{aligned} \quad (4.4.22)$$

We see that the N term and the exponential cancel on both sides and we are left with

$$\begin{aligned} &\frac{i}{2} \cdot \left[- (A(t)^{-1})^\mu{}_\nu \frac{dA(t)^\nu{}_\mu}{dt} + i \left[v_\alpha \left(\left(\frac{dB}{dt} \right)^\alpha{}_\delta (A^{-1})^\delta{}_\gamma + B^\alpha_\delta (A^{-1})^\delta{}_\rho \left(\frac{dA}{dt} \right)^\rho{}_\sigma (A^{-1})^\sigma{}_\gamma \right) v^\gamma \right] \right] \\ &= \frac{1}{2} \left[-P^{\nu\mu} \left(-\frac{1}{4} \left(B_{\mu\delta} (A^{-1})^\delta{}_\gamma v^\gamma + v_\alpha B^\alpha_\delta (A^{-1})^\delta{}_\mu \right) \cdot \left(B_{\nu\delta} (A^{-1})^\delta{}_\gamma v^\gamma + v_\alpha B^\alpha_\delta (A^{-1})^\delta{}_\nu \right) \right. \right. \\ &\quad \left. \left. + i B_{\nu\delta} (A^{-1})^\delta{}_\mu \right) + v^\alpha v^\beta W_{\alpha\beta} \right] \end{aligned} \quad (4.4.23)$$

Cancelling the prefactor of $\frac{1}{2}$ and collecting all the terms of order v^0 and v^2 respectively

we get two equations

$$-i(A(t)^{-1})^\mu{}_\nu \frac{dA(t)^\nu{}_\mu}{dt} = -iP^{\nu\mu} B_{\nu\delta} (A^{-1})^\delta{}_\mu \quad (4.4.24)$$

and

$$\begin{aligned} & - \left[v_\alpha \left(\left(\frac{dB}{dt} \right)^\alpha{}_\delta (A^{-1})^\delta{}_\gamma \right. \right. \\ & \left. \left. + B^\alpha{}_\delta (A^{-1})^\delta{}_\rho \left(\frac{dA}{dt} \right)^\rho{}_\sigma (A^{-1})^\sigma{}_\gamma \right) v^\gamma \right] = P^{\nu\mu} \left(\frac{1}{4} \left(B_{\mu\delta} A^\delta{}_\gamma v^\gamma + v_\alpha B^\alpha{}_\delta (A^{-1})^\delta{}_\mu \right) \right. \\ & \quad \cdot \left(B_{\nu\delta} (A^{-1})^\delta{}_\gamma v^\gamma + v_\alpha B^\alpha{}_\delta (A^{-1})^\delta{}_\nu \right) \\ & \quad \left. + i B_{\nu\delta} (A^{-1})^\delta{}_\mu \right) \\ & \quad + v^\alpha v^\beta W_{\alpha\beta} \end{aligned} \quad (4.4.25)$$

We can now continue looking at the results of each equation separately, which will ultimately yield a set of two differential equations for the matrices A and B .

4.4.1. Order v^0

We rewrite the first equation (4.4.24) in index notation and find

$$-i(A(t)^{-1})^\mu{}_\nu \frac{dA(t)^\nu{}_\mu}{dt} = -iP^{\nu'\sigma'} g_{\nu'\delta'} B(t)^{\delta'}{}_\mu (A^{-1}(t))^\mu{}_{\sigma'} \quad (4.4.26)$$

We bring both on the left side, eliminate the $-i$ sign and pull out $(A^{-1})^\mu{}_\nu$ so we find

$$(A(t)^{-1})^\mu{}_{\sigma'} \left[\frac{dA(t)^{\sigma'}{}_\mu}{dt} - P^{\nu'\sigma'} g_{\nu'\delta'} B(t)^{\delta'}{}_\mu \right] = 0 \quad (4.4.27)$$

As A is invertible, we know that the kernel $\ker(A) = \{0\}$ must be trivial. Thus,

$$\frac{dA(t)^{\sigma'}{}_\mu}{dt} - P^{\nu'\sigma'} g_{\nu'\delta'} B(t)^{\delta'}{}_\mu = 0 \quad (4.4.28)$$

and therefore

$$\frac{dA(t)^{\sigma'}{}_\mu}{dt} = P^{\nu'\sigma'} g_{\nu'\delta'} B(t)^{\delta'}{}_\mu \quad (4.4.29)$$

Contracting the metric and the projector we finally land at

$$\frac{dA(t)^{\sigma'}{}_\mu}{dt} = B(t)^{\sigma'}{}_\mu \quad (4.4.30)$$

4.4.2. Order v^2

The second equation, (4.4.25), comes from all terms of order v^2 . We write them in index notation and find

$$\begin{aligned} & - \left[v_\alpha \left(\left(\frac{dB}{dt} \right)^\alpha{}_\delta (A^{-1})^\delta{}_\gamma + B^\alpha{}_\delta (A^{-1})^\delta{}_\rho \left(\frac{dA}{dt} \right)^\rho{}_\sigma (A^{-1})^\sigma{}_\gamma \right) v^\gamma \right] \\ & = P^{\mu\nu} \frac{1}{4} \left(B_{\mu\delta} (A^{-1})^\delta{}_\gamma v^\gamma + v_\alpha B^\alpha{}_\delta (A^{-1})^\delta{}_\mu \right) \cdot \left(B_{\nu\delta} (A^{-1})^\delta{}_\gamma v^\gamma + v_\alpha B^\alpha{}_\delta (A^{-1})^\delta{}_\nu \right) + v^\alpha v^\beta W_{\alpha\beta} \end{aligned} \quad (4.4.31)$$

multiplying the right side out we find

$$\begin{aligned} & - \left[v_\alpha \left(\left(\frac{dB}{dt} \right)^\alpha{}_\delta (A^{-1})^\delta{}_\gamma \right. \right. \\ & \left. \left. + B^\alpha{}_\delta (A^{-1})^\delta{}_\rho B^\rho{}_\sigma (A^{-1})^\sigma{}_\gamma \right) v^\gamma \right] = \frac{1}{4} P^{\mu\nu} \left[B_{\mu\delta} A^\delta{}_\gamma v^\gamma B_{\nu\delta} (A^{-1})^\delta{}_\gamma v^\gamma \right. \\ & \quad + B_{\mu\delta} (A^{-1})^\delta{}_\gamma v^\gamma v_\alpha B^\alpha{}_\delta (A^{-1})^\delta{}_\nu \\ & \quad + v_\alpha B^\alpha{}_\delta (A^{-1})^\delta{}_\mu B_{\nu\delta} (A^{-1})^\delta{}_\gamma v^\gamma \\ & \quad \left. + v_\alpha B^\alpha{}_\delta (A^{-1})^\delta{}_\mu v_\alpha B^\alpha{}_\delta (A^{-1})^\delta{}_\nu \right] \\ & \quad + v^\alpha v^\beta W_{\alpha\beta} \end{aligned} \quad (4.4.32)$$

As the matrix $B^\alpha{}_\delta (A^{-1})^\delta{}_\nu$ must be symmetric, the terms on the right side are all equal and we can cancel them with the left side, such that we are left with

$$-v_\alpha \left(\frac{dB}{dt} \right)^\alpha{}_\delta (A^{-1})^\delta{}_\gamma v^\gamma = v^\alpha v^\beta W_{\alpha\beta} \quad (4.4.33)$$

Multiplying with $A^\gamma{}_\delta$ from the right and renaming indices leaves us with the condition

$$\left(\frac{dB}{dt} \right)^\alpha{}_\beta = -W_{\alpha\delta} A^\delta{}_\beta \quad (4.4.34)$$

5. Simulation and Results

5.1. Simulation

After our calculations we now have a new set of differential equations for our Ansatz (4.4.13) for the matrices A and B . The set is given by (4.4.30) and (4.4.34). We now want to numerically integrate this to get insight in the behaviour of the wave's amplitude while the particle is moving around a Schwarzschild black hole.

To achieve this, we choose Wolfram Mathematica as our framework. We set up the Schwarzschild metric with Black hole mass $M = 1$ and Schwarzschild radius $r_s = 2M$. As geodesic motion in the Schwarzschild metric is always planar, we define $\theta = \frac{\pi}{2}$. For the case of purely orbital motion with constant radius r we can solve the geodesic equation for the position vector X_o analytically and find with

$$V = 1 - \frac{2M}{r} , \quad (5.1.1)$$

$$X_o = \left(V^{-1} \cdot E \cdot \tau, r, \frac{\pi}{2}, \sqrt{\frac{M}{r^3}} \cdot \tau \right) \quad (5.1.2)$$

and for purely radial motion with constant φ we find the velocity vector $\dot{X}_r$ analytically from the geodesic equation and find

$$\dot{X}_r = \left(V^{-1} \cdot E, \pm \sqrt{E - V}, 0, 0 \right) \quad (5.1.3)$$

where $+$ denotes radial inwards motion and $-$ radial outwards motion. The position vector is then calculated numerically at each step using

$$\frac{\partial r}{\partial \tau} = \pm \sqrt{E - V} .$$

For the other case of movement in r and φ solving the geodesic equation happens numerically as well.

Together with the Christoffel symbols and the Riemann tensor we can then setup the matrix W following the definition (4.4.7) which ultimately lets us set up the final set of differential equations for each case, radial inwards, radial outwards, orbital at 3 different radii and general motion. As the Ansatz tells us that W is multiplied with two copies of v which are orthogonal to the direction of propagation by definition, we also set up an orthonormal frame at each point consisting of the velocity vector and three vectors

orthonormal to the velocity. W is then transformed into this basis before solving the differential equations for each step.

5.2. Results

Each case is integrated from $\tau = 0$ to $\tau_{\max} = 1000$ and we then choose 3 different points along the geodesic to calculate the level sets for the components of the vectors v we find in the Ansatz (4.4.13) which gives us a good insight into the dynamics of the waves amplitude along its voyage around the black hole. For all cases the initial conditions on the matrices are given by

$$A = \frac{1}{\sigma} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (5.2.1)$$

$$B = \frac{1}{\sigma} \cdot i \cdot \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (5.2.2)$$

with σ being a prefactor to control the size of the initial wave packet. For all following calculations it is chosen to be $\sigma = 1000$.

For all cases, the initial state was therefore a sphere and the initial position in each plot is marked with an orange point.

The code that was used for numerical calculations including one example of the logic that was used to create the plots can be seen in Appendix A.

5.3. Radial inwards movement

For radial inwards movement we choose the initial conditions

$$r = 10r_s . \quad (5.3.1)$$

The first plot of 5.3.1 shows the 3D evolution of the sphere with the colour of the ellipsoid corresponding to the point along the geodesic in the second and third plot. We can clearly see that while the particle is moving inwards, it experiences stronger and stronger gravitational forces from the black hole which leads to deformation in preferred regions which deform the sphere into an ellipsoid. The second row of 5.3.1 shows the 2 dimensional outlines for the three planes through 0 in detail where we can see the elongation along a preferred axis.

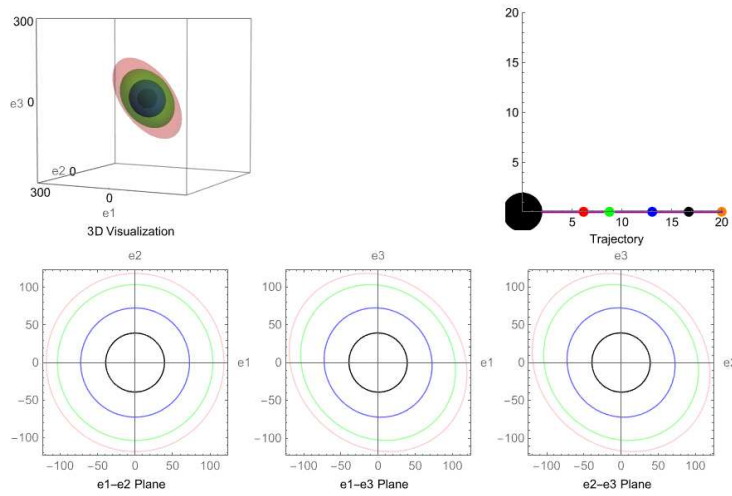


Figure 5.3.1.: Evolution for radial inwards movement. Top left: 3D visualisation of Enveloping shells. Top right: Trajectory of the particle with points corresponding to the shell of equal colour at timestep 0 (orange), 10 (black), 20 (blue), 30 (green) and 35 (red). Bottom row displays the 2D projections on the planes going through the centre with shell colour corresponding to the appropriate point on the trajectory.

5.4. Radial outwards movement

The initial conditions are the same as for radial inwards movement.

We see again deformation of the initial sphere into an ellipsoid in 5.4.1 but as we would expect, the deformation is not as significant. Indeed, for an outwards moving particle the gravitational forces get weaker with r^2 . We can even see that the difference in the deformation for each step get less and less which goes hand in hand with the approximation that we find flat Minkowski Coordinates far away from the black hole. Though not away far enough, smaller differences between shells imply that the curvature of the coordinates decreases.

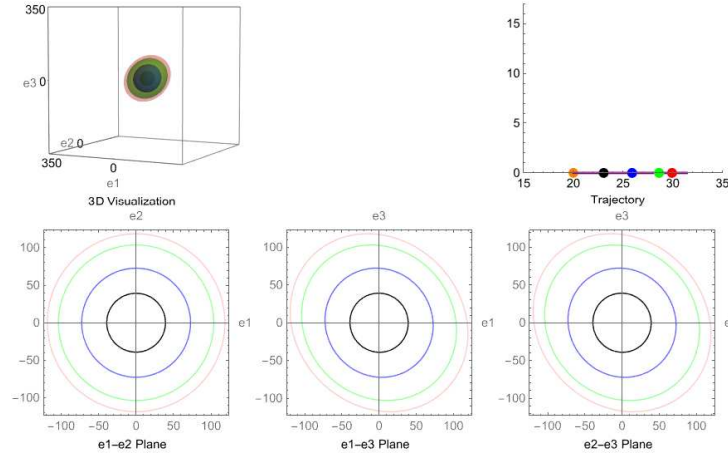


Figure 5.4.1.: Evolution for radial outwards movement. Top left: 3D visualisation of Enveloping shells. Top right: Trajectory of the particle with points corresponding to the shell of equal colour at timestep 0 (orange), 10 (black), 20 (blue), 30 (green) and 35 (red). Bottom row displays the 2D projections on the planes going through the centre with shell colour corresponding to the appropriate point on the trajectory.

5.5. Orbital movement at $10 r_s$

For the first and nearest orbital case at constant radius the radius is chosen to be $r = 10r_s$, just outside the border where orbits get unstable at $r \approx 6r_s$. In this nearest case, we find the strongest deformation of the initial sphere as seen in 5.5.1. Here, as in all other orbital cases we have to choose the evaluation points very near at the start as soon, one reaches the limit of our approximation.

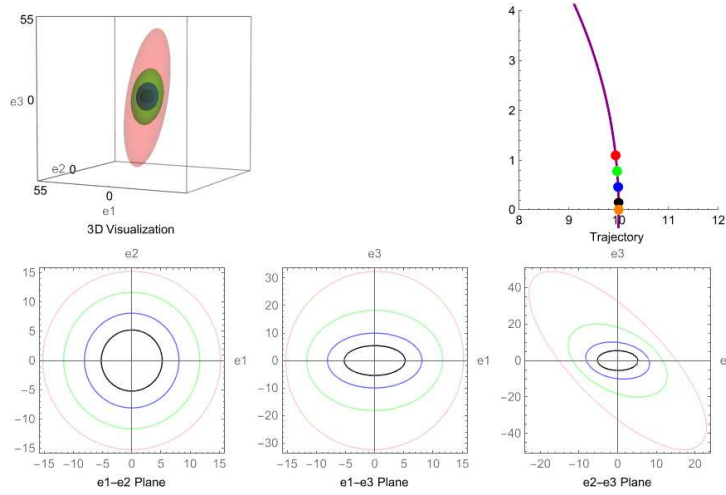


Figure 5.5.1.: Evolution for orbital movement at $10r_s$. Top left: 3D visualisation of Enveloping shells. Top right: Trajectory of the particle with points corresponding to the shell of equal colour at timestep 0 (orange), 0.5 (black), 1.5 (blue), 2.5 (green) and 3.5 (red). Bottom row displays the 2D projections on the planes going through the centre with shell colour corresponding to the appropriate point on the trajectory.

5.6. Orbital movement at $15r_s$

We are now a bit more far away from the black hole, but still, as seen in 5.6.1 the tidal forces of the black hole provide significant impact onto the amplitude of the wave. Even though the deformation does not happen as quickly as in the case for $r = 10r_s$ we soon hit the point where our approximation breaks apart.

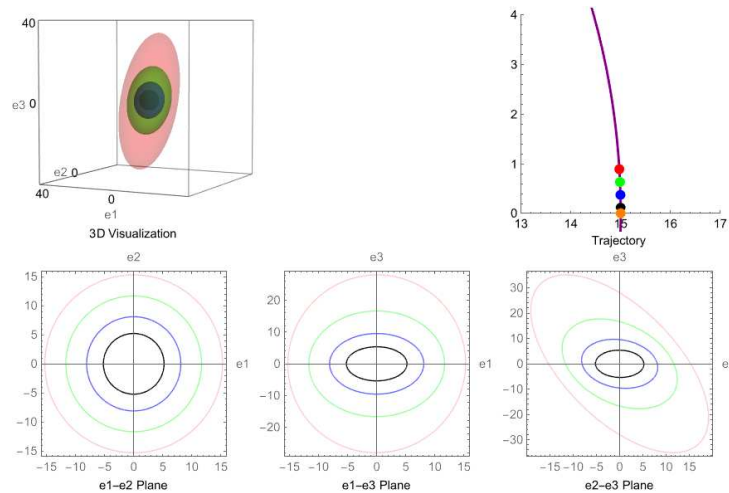


Figure 5.6.1.: Evolution for orbital movement at $15r_s$. Top left: 3D visualisation of Enveloping shells. Top right: Trajectory of the particle with points corresponding to the shell of equal colour at timestep 0 (orange), 0.5 (black), 1.5 (blue), 2.5 (green) and 3.5 (red). Bottom row displays the 2D projections on the planes going through the centre with shell colour corresponding to the appropriate point on the trajectory.

5.7. Orbital movement at $20r_s$

At a radius of $r = 20r_s$ we look at the farthest orbit. In 5.7.1 we can clearly see that the deformation does not happen as quickly as in the other cases which is as expected. With distance from the black hole the gravitational forces decrease as well, though even here we quickly get into the situation where our approximation breaks apart.

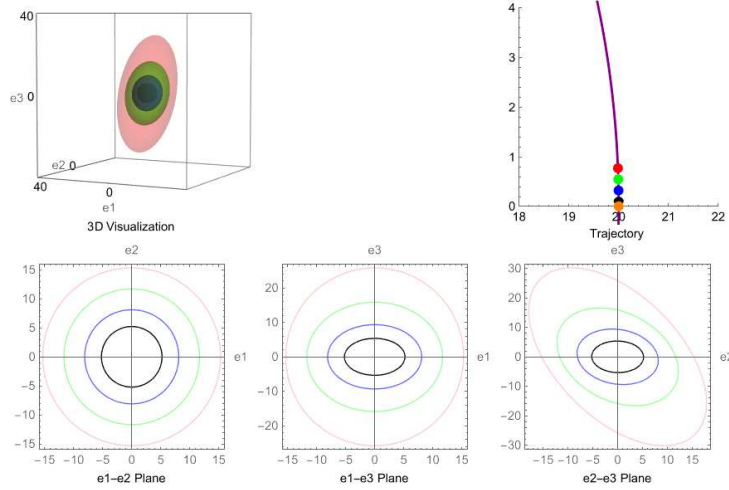


Figure 5.7.1.: Evolution for orbital movement at $20r_s$. Top left: 3D visualisation of Enveloping shells. Top right: Trajectory of the particle with points corresponding to the shell of equal colour at timestep 0 (orange), 0.5 (black), 1.5 (blue), 2.5 (green) and 3.5 (red). Bottom row displays the 2D projections on the planes going through the centre with shell colour corresponding to the appropriate point on the trajectory.

5.8. General movement

For the case of general movement, we choose initial conditions

$$\tau = 0 \tag{5.8.1}$$

$$r = 5r_s \tag{5.8.2}$$

$$\theta = \frac{\pi}{2} \tag{5.8.3}$$

$$\varphi = \tag{5.8.4}$$

with initial momenta

$$p_r = -0.5 \tag{5.8.5}$$

$$p_\theta = 0 \tag{5.8.6}$$

$$p_\varphi = 5 \tag{5.8.7}$$

so we clearly have movement in the r and φ direction. Following the trajectory in 5.8.1 and comparing with the appropriate ellipsoid we see that at the beginning, where we do not have strong gravitational influence yet, the sphere mostly stays a sphere but with decreasing radius the gravitational impacts get stronger which leads to stronger deformations of the initial sphere. However, the simulation breaks apart soon, with the beam getting narrower in the center until it breaks into two pieces and opening up on the outsides. Due to different overlapping it was needed to change the colour scheme for visibility.

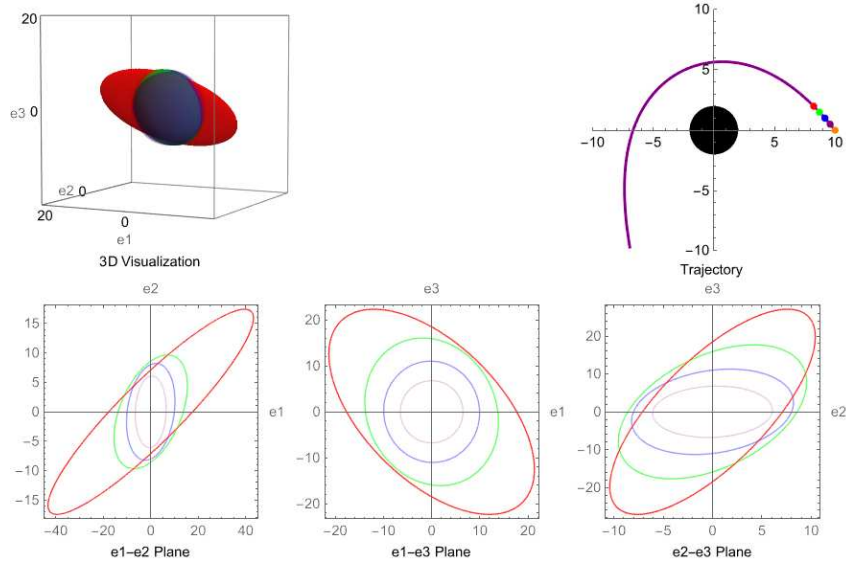


Figure 5.8.1.: Evolution for general movement. Top left: 3D visualisation of Enveloping shells. Top right: Trajectory of the particle with points corresponding to the shell of equal colour at timestep 0 (orange), 1 (purple), 2 (blue), 3 (green) and 4 (red). Bottom row displays the 2D projections on the planes going through the centre with shell colour corresponding to the appropriate point on the trajectory.

6. Conclusion and outlook

We started our calculations by introducing and refreshing our knowledge about *geometric optics*. Here we also had a closer look at the *two parameter expansion* which was the basis for being able to use our Ansatz in the Klein-Gordon equation. We then built a bridge to Gaussian beams which form our Ansatz and introduced some preliminary concepts to get a deeper understanding in the calculations we were about to perform.

After the preliminaries were introduced, we stated the Klein-Gordon equation and our special Ansatz. We quickly came into very involved calculations from which we got great insight into the components and their behaviour which compose the Ansatz. At the highest order we found a Schrödinger-like equation for which an Ansatz already existed in the literature. We introduced this Ansatz and after plugging it into the Schrödinger like equation we found a system of two coupled differential equations. This marked a good spot to continue calculations numerically. Using Wolfram Mathematica as the framework for numeric calculations we set up different cases for particle motion around some black hole. Setting up the position vector for purely orbital movement with constant r was possible analytically. For purely radial movement with constant φ it was possible to set up the velocity vector analytically with the position being calculated numerically during integration. The velocity and position vectors for general movement was done numerically only. Along the geodesic we could then choose different points with explicit values for the matrices A and B for which we calculated the level sets for the components of the vector v from the Ansatz (4.4.13). The evolution of these level sets gave us great insight into the behaviour of the system at different times and positions around the black hole while it also met our expectations for this evolution. There is more research required for the numerical calculations, especially for orbital evolution as the solutions break up too fast, to define specific reasons for this. It is too early for some kind of caustics. We expect, that there must be some stability problem in the numerical calculation or Mathematica not having enough resources.

From this view it would be very insightful to continue our calculations with more sophisticated Ansatzes in the form of superpositions of multiple Gaussian waves which tend to have much better behaviour for more complicated trajectories with stronger gravitational impacts. With the right higher order Gaussian beam mode it then may also be possible to compare the phases of the particle in orbital motion with from the start with the phase after one full orbit to find the Berry phase difference. Apart from that, it would be beneficial to also look at the case for null geodesics and get insight in how the amplitudes change in that case since for the null case, the basis orthogonal to the wave vector becomes more complicated as well.

A. Mathematica Code for numerical integration

```

1 ClearAll["Global`*"]
2 $Assumptions =
3   Element[x0[\[Tau]], Reals] && Element[x1[\[Tau]], Reals] &&
4   Element[x2[\[Tau]], Reals] && Element[x3[\[Tau]], Reals] &&
5   Element[p0[\[Tau]], Reals] && Element[p1[\[Tau]], Reals] &&
6   Element[p2[\[Tau]], Reals] && Element[p3[\[Tau]], Reals] &&
7   Element[s, Reals] && x1[\[Tau]] > 2 M && Element[a, Reals] &&
8   0 < x2[\[Tau]] < \[Pi];
9
10 X = {x0[\[Tau]], x1[\[Tau]], x2[\[Tau]], x3[\[Tau]]};
11 P = {p0[\[Tau]], p1[\[Tau]], p2[\[Tau]], p3[\[Tau]]} /. p2[\[Tau]] -> 0;
12 p = {p1[\[Tau]], p2[\[Tau]], p3[\[Tau]]} /. p2[\[Tau]] -> 0;
13
14 A = Table[Subscript[a, i, j][\[Tau]], {i, 3}, {j, 3}];
15 B = Table[Subscript[b, i, j][\[Tau]], {i, 3}, {j, 3}];
16
17 M = 1;
18 particleMass = 1;
19 rs = 2 M;
20 Energy = 1;
21 J = Sqrt[M*radius^2/(radius - 3 M)];
22 EnergyOrbital = Sqrt[J^2*((1 - 2 M/radius)^2)/(M*radius)];
23 V = 1 - 2 M/x1[\[Tau]];
24
25 xDotRadialIn = {Energy/(1 - 2 M/x1[\[Tau]]), -Sqrt[Energy^2 - (1 - 2 M/x1[\[Tau]]^2)], 0, 0};
26 xDotRadialOut = {Energy/(1 - 2 M/x1[\[Tau]]), Sqrt[Energy^2 - (1 - 2 M/x1[\[Tau]]^2)], 0, 0};
27 xOrbital = {V^-1*Energy*\[Tau], radius, Pi/2, Sqrt[M/radius^3]*\[Tau]};
28 xOrbitalFunc[radius_, \[Tau]_] := {radius, Pi/2, Sqrt[M/radius^3]*\[Tau]}
29 xDotOrbital = Evaluate[D[xOrbital, \[Tau]]];
30
31 g = {{-(1 - 2 M/r[\[Tau]]), 0, 0, 0}, {0, 1/(1 - 2 M/r[\[Tau]]), 0, 0}, {0, 0, r[\[Tau]]^2, 0}, {0, 0, 0, r[\[Tau]]^2 Sin[\[Theta][\[Tau]]^2]}} /. r -> x1 /. \[Theta][\[Tau]] -> Pi/2 /. \[Phi] -> x3;
32 ig = Inverse[g] // Simplify;
33 igFunc[x1[\[Tau]_, x2[\[Tau]_] := Simplify[Inverse[g] /. {x1[\[Tau]] -> x1[\[Tau], x2[\[Tau]] -> x2[\[Tau]}];
34 Detg = Det[g] // Simplify;
35 DetgFunc[x1[\[Tau]_, x2[\[Tau]_] := Simplify[Det[g] /. {x1[\[Tau]] -> x1[\[Tau], x2[\[Tau]] -> x2[\[Tau]}];
36

```

```

37 \[CapitalGamma] = 1/2 Parallelize[Table[(Sum[(ig[[i]][[m]]*(D[g[[m]][[j]], X[[k]]] + D[g[[m]][[k]], X[[j]]] - D[g[[j]][[k]], X[[m]]])) /. {x2\[Tau] -> Pi/2} // Simplify), {i,1,4},{j,1,4},{k,1,4}]]];
38 christoffel = \[CapitalGamma];
39 christoffel1 = Simplify[Table[Sum[(1/2) ig[[\[Mu], \[Sigma]]] (D[g[[\[Sigma], \[Nu]]], {x0,x1,x2,x3}[[\[Rho]]]] + D[g[[\[Sigma], \[Rho]]], {x0,x1,x2,x3}[[\[Nu]]]) - D[g[[\[Nu], \[Rho]]], {x0,x1,x2,x3}[[\[Sigma]]]]) /. {x2\[Tau] -> Pi/2}, {\[Sigma],1,4}, {\[Mu],1,4}, {\[Nu],1,4}, {\[Rho],1,4}]]];
40
41 Riem = Table[(D[\[CapitalGamma][[i]][[1]][[j]], X[[k]]] - D[\[CapitalGamma][[i]][[k]][[j]], X[[1]]] + Sum[(\[CapitalGamma][[i]][[k]][[m]] \[CapitalGamma][[m]][[1]][[j]] - \[CapitalGamma][[i]][[1]][[m]] \[CapitalGamma][[m]][[k]][[j]])], {m,1,4}]) // Simplify, {i,1,4},{j,1,4},{k,1,4},{1,1,4} // Parallelize;
42 R = Table[(Sum[(g[[i1]][[i]] (Riem[[i1]][[j]][[k]][[1]])), {i1,1,4}]) // Simplify, {i,1,4},{j,1,4},{k,1,4},{1,1,4} // Parallelize;
43
44 Pu = Table[(Sum[(ig[[\[Mu]]][\[Alpha]] P[[\[Alpha]]]) /. x2\[Tau] -> Pi/2 // Simplify), {\[Mu],1,4} // Parallelize;
45
46 pt0 = Sqrt[-(Sum[ig[[i]][[j]] P[[i]] P[[j]], {i,2,4},{j,2,4} + 1)/ig[[1,1]]];
47
48 Xdot = Parallelize[Table[(Pu[[i]]) /. {p0\[Tau] -> pt0, p2\[Tau] -> 0, x2\[Tau] -> Pi/2}, {i,1,4}]]];
49 pdot = Parallelize[Table[(-1/2) * Sum[D[ig[[b]][[c]], X[[a]]] * P[[b]]*P[[c]], {b,1,4},{c,1,4}] /. {p0\[Tau] -> pt0, x2\[Tau] -> Pi/2}, {a,2,4}]]];
50 W = Parallelize[Table[Sum[Riem[[mu, alpha, beta, nu]] * P[[mu]]*P[[beta]], {alpha,1,4},{beta,1,4}, {mu,1,4},{nu,1,4}]] /. {p0\[Tau] -> pt0, p2\[Tau] -> 0, x2\[Tau] -> Pi/2};
51
52 sqrtAbsDetg = Simplify[Sqrt[Abs[Detg]]];
53
54 LeviCivitaSymbol4D[i_, j_, k_, l_] := Signature[{i,j,k,l}];
55 LeviCivitaTensorDown[i_, j_, k_, l_] := sqrtAbsDetg * LeviCivitaSymbol4D[i,j,k,l];
56 LeviCivitaTensorUpDown[mu_, nu_, rho_, sigma_] := Sum[ig[[mu+1, alpha+1]] LeviCivitaTensorDown[alpha, nu, rho, sigma], {alpha,0,3}];
57
58 e0 = Xdot;
59 e1 = {0,0,1,0};
60 e2Try = {0,0,1,1};
61 orthogonalizeThirdVector[v1_,v2_,v3_,metric_] := Module[{inner,proj1,proj2,v3perp,v3norm},inner[u_,v_] := u.metric.v;proj1=Simplify[(inner[v3,v1]/inner[v1,v1]) v1];proj2=Simplify[(inner[v3,v2]/inner[v2,v2]) v2];v3perp=Simplify[v3-proj1-proj2];v3norm=Simplify[v3perp/Sqrt[Abs[inner[v3perp,v3perp]]]];v3norm];
62 e2 = orthogonalizeThirdVector[e0,e1,e2Try,g];
63 e3 = Simplify[Table[Sum[LeviCivitaTensorUpDown[\[Mu],\[Nu],\[Alpha],\[Beta]] * e0[[\[Nu]+1]] * e1[[\[Alpha]+1]] * e2[[\[Beta]+1]], {\[Nu],0,3},{\[Alpha],0,3},{\[Beta],0,3}], {\[Mu],0,3}]]];
64
65 e0norm = Simplify[e0/Sqrt[Abs[e0.g.e0]]];
66 e1norm = Simplify[e1/Sqrt[Abs[e1.g.e1]]];
67 e2norm = Simplify[e2/Sqrt[Abs[e2.g.e2]]];

```

```

68 e3norm = Simplify[e3/Sqrt[Abs[e3.g.e3]]];
69 eVector = {e0norm,e1norm,e2norm,e3norm};
70 Wtrans = Simplify[Table[Flatten[eVector[[i]]].W.eVector[[c]],{i,2,4},{c,2,4}]];
71
72 (* Analytic radial vectors and transforms *)
73 e0AnaIn = xDotRadialIn;
74 e0AnaOut = xDotRadialOut;
75 e1AnaRad = {0,0,1,0};
76 e2AnaRad = {0,0,0,1};
77 e3AnaIn = Simplify[Table[Sum[LeviCivitaTensorUpDown[\[Mu],\[Nu],\[Alpha],\[Beta
    ]]*e0AnaIn[[\[Nu]+1]]*e1AnaRad[[\[Alpha]+1]]*e2AnaRad[[\[Beta]+1]],{\[Nu
    ],0,3},{\[Alpha],0,3},{\[Beta],0,3},{\[Mu],0,3}]];
78 e3AnaOut = Simplify[Table[Sum[LeviCivitaTensorUpDown[\[Mu],\[Nu],\[Alpha],\[Beta
    ]]*e0AnaOut[[\[Nu]+1]]*e1AnaRad[[\[Alpha]+1]]*e2AnaRad[[\[Beta]+1]],{\[Nu
    ],0,3},{\[Alpha],0,3},{\[Beta],0,3},{\[Mu],0,3}]];
79
80 e0normAnaIn = Simplify[e0AnaIn/Sqrt[Abs[e0AnaIn.g.e0AnaIn]]];
81 e0normAnaOut = Simplify[e0AnaOut/Sqrt[Abs[e0AnaOut.g.e0AnaOut]]];
82 e1normAnaRad = Simplify[e1AnaRad/Sqrt[Abs[e1AnaRad.g.e1AnaRad]]];
83 e2normAnaRad = Simplify[e2AnaRad/Sqrt[Abs[e2AnaRad.g.e2AnaRad]]];
84 e3normAnaIn = Simplify[e3AnaIn/Sqrt[Abs[e3AnaIn.g.e3AnaIn]]];
85 e3normAnaOut = Simplify[e3AnaOut/Sqrt[Abs[e3AnaOut.g.e3AnaOut]]];
86 eVectorAnaIn = {e0normAnaIn,e1normAnaRad,e2normAnaRad,e3normAnaIn};
87 eVectorAnaOut = {e0normAnaOut,e1normAnaRad,e2normAnaRad,e3normAnaOut};
88 WtransAnaIn = Simplify[Table[Flatten[eVectorAnaIn[[i]]].W.eVectorAnaIn[[c]],{i
    ,2,4},{c,2,4}]] /. {p1[\[Tau]]->particleMass*xDotRadialIn[[2]], p3[\[Tau]]->
    particleMass*xDotRadialIn[[4]]};
89 WtransAnaOut = Simplify[Table[Flatten[eVectorAnaOut[[i]]].W.eVectorAnaOut[[c]],{i
    ,2,4},{c,2,4}]] /. {p1[\[Tau]]->particleMass*xDotRadialOut[[2]], p3[\[Tau]
    ]->particleMass*xDotRadialOut[[4]]};
90
91 (* Equations of Motion *)
92 EOM = {D[X,\[Tau]]==Xdot, D[p,\[Tau]]==pdot, D[A,\[Tau]]==B, D[B,\[Tau]]==
    Wtrans.A};
93 EOMAnaIn = {D[X[[2]],\[Tau]]==xDotRadialIn[[2]], D[A,\[Tau]]==B, D[B,\[Tau]]==
    WtransAnaIn.A};
94
95 (* Initial conditions *)
96 \[Tau]0=0; \[Tau]max=1000;
97 smallConstant=1000;
98 x1i1=10*rs;
99 x0i3=0; x1i3=5*rs; x2i3=\[Pi]/2; x3i3=0;
100 p1i3=-0.5; p2i3=0; p3i3=5;
101 Ainit=1/smallConstant*IdentityMatrix[3];
102 Binit=1/smallConstant*I*IdentityMatrix[3];
103
104 id1 = (X[[2]]/. \[Tau]->\[Tau]0)==x1i1 && (A/. \[Tau]->\[Tau]0)==Ainit && (B/.
    \[Tau]->\[Tau]0)==Binit;
105 id3 = (X/. \[Tau]->\[Tau]0)=={x0i3,x1i3,x2i3,x3i3} && (p/. \[Tau]->\[Tau]0)=={
    p1i3,p2i3,p3i3} && (A/. \[Tau]->\[Tau]0)==Ainit && (B/. \[Tau]->\[Tau]0)==
    Binit;
106
107 \[Tau]int0 = \[Tau]max;

```

```

108 horizon0 = WhenEvent[x1[\[Tau]] <= 1.01*(M+Sqrt[M^2]), {"StopIntegration", \[Tau]
    int0=\[Tau]};
109 Aclean = A/.f_[\[Tau]]:>f; Bclean = B/.f_[\[Tau]]:>f;
110
111 solAnaIn = NDSolve[EOMAnaIn && id1 && horizon0, Flatten[{x1[\[Tau]], Flatten[A],
    Flatten[B]}], {\[Tau], \[Tau]0, \[Tau]max}];
112 sol2 = NDSolve[EOM && id3 && horizon0, Flatten[{x0[\[Tau]], x1[\[Tau]], x2[\[Tau]
    ]], x3[\[Tau]], p1[\[Tau]], p2[\[Tau]], p3[\[Tau]], Flatten[A], Flatten[B]}], {\[
    Tau], \[Tau]0, \[Tau]max}];
113
114 AvalAnaIn[\[Tau]val_] := Evaluate[A/.solAnaIn/. \[Tau]->\[Tau]val];
115 BvalAnaIn[\[Tau]val_] := Evaluate[B/.solAnaIn/. \[Tau]->\[Tau]val];
116 XvalAnaIn[tval_] := Evaluate[X/.solAnaIn/. \[Tau]->tval];
117
118 Anum1 = Ainit;
119 detANum1 = Det[Anum1];
120 Bnum1 = Binit;
121 BAinv1 = Bnum1 . Inverse[Anum1];
122
123 (* Radial inwards computation *)
124 computeBAinvFinalAnaIn[evalPointAnaIn_] :=
125 Module[{AnumFinalAnaIn, BnumFinalAnaIn, detANumFinalAnaIn, BAinvFinalAnaIn},
126   AnumFinalAnaIn = First[AvalAnaIn[evalPointAnaIn]];
127   BnumFinalAnaIn = First[BvalAnaIn[evalPointAnaIn]];
128   detANumFinalAnaIn = Det[AnumFinalAnaIn];
129   BAinvFinalAnaIn = BnumFinalAnaIn . Inverse[AnumFinalAnaIn];
130   {detANumFinalAnaIn, BAinvFinalAnaIn}]
131
132 a[v1_, v2_, v3_, det_, BA_] := 1/Sqrt[det] * Exp[I*1/2 * {v1, v2, v3}.BA.{v1, v2
    , v3}];
133
134 range = 20 rs;
135 \[Tau]plot0 = Min[\[Tau]int0, \[Tau]max];
136 \[Tau]plot1 = Min[\[Tau]int0, \[Tau]max];
137 \[Tau]plot2 = Min[\[Tau]int0, \[Tau]max];
138
139 BH = Graphics[{Black, Disk[{0, 0}, M + Sqrt[M^2]]}];
140 diskRadius = 0.5;
141 plot1AnaInBorder = 300;
142
143 evalPoints = {10, 20, 30, 35};
144 colors = {Black, Blue, Green, Red};
145 opacities = {1.0, 0.6, 0.4, 0.2};
146
147 sourceAnaIn = Graphics[{Orange,
148   Disk[{Evaluate[(XvalAnaIn[0][[1]][[2]] Sin[Pi/2] Cos[0]) /. solAnaIn][[1]],
149     Evaluate[(XvalAnaIn[0][[1]][[2]] Sin[Pi/2] Sin[0]) /. solAnaIn][[1]]},
150     0.5]}];
151
152 trajectoryAnaIn = ParametricPlot[
153   {Evaluate[(x1[\[Tau]] Sin[Pi/2] Cos[0]) /. solAnaIn][[1]],
154     Evaluate[(x1[\[Tau]] Sin[Pi/2] Sin[0]) /. solAnaIn][[1]]},
155   {\[Tau], \[Tau]0, \[Tau]plot0},

```

```

155 PlotStyle -> {Thick, Purple},
156 PlotPoints -> 3000,
157 PlotRange -> {{-20, 20}, {-20, 20}}
158 ];
159
160 plotPointsAnaIn = Table[
161   Module[{r, pos},
162     r = (XvalAnaIn[evalPoints[[i]]][[1]][[2]] /. solAnaIn)[[1]];
163     pos = {r Sin[Pi/2] Cos[0], r Sin[Pi/2] Sin[0]};
164     Graphics[{Directive[colors[[i]]], Disk[pos, diskRadius]}]
165   ],
166   {i, Length[evalPoints]}
167 ];
168
169 plotsAnaIn = Table[
170   Module[{detA, bAInv, color, opacity},
171     {detA, bAInv} = computeBAinvFinalAnaIn[evalPoints[[i]]];
172     color = colors[[i]]; opacity = opacities[[i]];
173     ContourPlot3D[
174       Abs[a[v1, v2, v3, detA, bAInv]],
175       {v1, -plot1AnaInBorder, plot1AnaInBorder},
176       {v2, -plot1AnaInBorder, plot1AnaInBorder},
177       {v3, -plot1AnaInBorder, plot1AnaInBorder},
178       Contours -> {0.5},
179       ContourStyle -> Directive[color, Opacity[opacity]],
180       Mesh -> None,
181       ViewPoint -> {-3, -2, 0.5},
182       ViewVertical -> {0, 0, 1},
183       AxesLabel -> {"e1", "e2", "e3"},
184       AxesEdge -> {{1, -1}, {-1, -1}, {-1, 1}}
185     ]
186   ],
187   {i, Length[evalPoints]}
188 ];
189
190 plots2DAnaInxyAbs = Table[
191   Module[{detA, bAInv, color, opacity},
192     {detA, bAInv} = computeBAinvFinalAnaOut[evalPoints[[i]]];
193     color = colors[[i]]; opacity = opacities[[i]];
194     ContourPlot[
195       Abs[a[v1, v2, 0, detA, bAInv]],
196       {v1, -plot1AnaInBorder, plot1AnaInBorder},
197       {v2, -plot1AnaInBorder, plot1AnaInBorder},
198       Contours -> {0.5},
199       ContourStyle -> Directive[color, Opacity[opacity]],
200       Mesh -> None,
201       AxesLabel -> {"e1", "e2"},
202       PlotRange -> All,
203       ContourShading -> None,
204       PlotPoints -> 100
205     ]
206   ],
207   {i, Length[evalPoints]}

```

```

208 ];
209
210 plots2DAAnaInxzAbs = Table[
211   Module[{detA, bAInv, color, opacity},
212     {detA, bAInv} = computeBAinvFinalAnaOut[evalPoints[[i]]];
213     color = colors[[i]]; opacity = opacities[[i]];
214     ContourPlot[
215       Abs[a[v1, 0, v3, detA, bAInv]],
216       {v1, -plot1AnaInBorder, plot1AnaInBorder},
217       {v3, -plot1AnaInBorder, plot1AnaInBorder},
218       Contours -> {0.5},
219       ContourStyle -> Directive[color, Opacity[opacity]],
220       Mesh -> None,
221       AxesLabel -> {"e1", "e3"},
222       PlotRange -> All,
223       ContourShading -> None,
224       PlotPoints -> 100
225     ]
226   ],
227   {i, Length[evalPoints]}
228 ];
229
230 plots2DAAnaInyzAbs = Table[
231   Module[{detA, bAInv, color, opacity},
232     {detA, bAInv} = computeBAinvFinalAnaOut[evalPoints[[i]]];
233     color = colors[[i]]; opacity = opacities[[i]];
234     ContourPlot[
235       Abs[a[0, v2, v3, detA, bAInv]],
236       {v2, -plot1AnaInBorder, plot1AnaInBorder},
237       {v3, -plot1AnaInBorder, plot1AnaInBorder},
238       Contours -> {0.5},
239       ContourStyle -> Directive[color, Opacity[opacity]],
240       Mesh -> None,
241       AxesLabel -> {"e2", "e3"},
242       PlotRange -> All,
243       ContourShading -> None,
244       PlotPoints -> 100
245     ]
246   ],
247   {i, Length[evalPoints]}
248 ];

```

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